

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/231372144>

Plantwide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics

ARTICLE *in* INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · SEPTEMBER 2005

Impact Factor: 2.59 · DOI: 10.1021/ie048951z

CITATIONS

41

READS

122

3 AUTHORS, INCLUDING:



Murthy Konda

Lawrence Berkeley National Laboratory

25 PUBLICATIONS 159 CITATIONS

SEE PROFILE



Gade Pandu Rangaiah

National University of Singapore

240 PUBLICATIONS 2,381 CITATIONS

SEE PROFILE

Plantwide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics

N. V. S. N. Murthy Konda, G. P. Rangaiah,* and P. R. Krishnaswamy

Department of Chemical and Biomolecular Engineering, National University of Singapore, 10, Kent Ridge Crescent, Singapore 119260

The novel plantwide control (PWC) methodologies are becoming increasingly important as chemical processes are becoming more and more integrated with recycles for reasons of safety, environmental considerations, and economics. Hence, in the present work, an integrated framework of simulation and heuristics is proposed. The main emphasis here is on vertical integration of simulation and heuristics which exploits the inherent interlink between them. By adopting this framework, simulators can be more efficiently utilized and they also offer invaluable support to the decisions taken by heuristics. The proposed framework is then successfully applied to an industrially relevant case study: the hydrodealkylation of toluene (HDA) process. An analysis of results shows that the proposed framework builds synergies between the powers of both the simulation and the heuristics, thereby resulting in a practical PWC methodology that leads to a viable control system.

1. Introduction

1.1. Plantwide Control. In the past, unit-based control system design methodology (Umeda et al.¹) has been widely used to design control systems for complete plants. However, the recent stringent environmental regulations, safety concerns, and economic considerations demand the design engineers to make the chemical processes highly integrated with material and energy recycles. Several researchers^{2–15} studied the effect of these recycles on the overall dynamics and concluded that recycles need special attention while designing PWC systems as they change the dynamics of the plant in a way which may not always be apparent from the dynamics of the individual unit operations. Hence, the unit-based methodology seems to be scarcely equipped to design the control system for such complex plants. For example, Downs¹⁶ reported a control strategy for a scrubber-distillation column with a liquid recycle which did not work from an overall point of view, though the control of individual unit operations was satisfactory. Luyben¹⁷ also demonstrated how control decisions vary based on perception, i.e., whether the unit is considered as a single unit operation or an integral part of the plant. Thus, there is a need for better methodologies which can deal with the highly integrated processes in a more efficient way. This leads to the concept of PWC which demands *plantwide* perspective while designing PWC systems.

Designing control systems for highly integrated processes is challenging because of the large combinatorial search space available. For example, Price and Georgakis¹⁸ observed 70 alternative control strategies for a simple hypothetical reactor-separator process with a single recycle. Keeping in view of this large combinatorial search space, the ultimate solution may not be so intuitively obvious. So many researchers have addressed PWC problem over the last 2 decades and came up with various methodologies. After a critical review of various methodologies, the heuristic-based methodologies are

found to be easier not only to understand but also to implement. However, novices often face difficulties while adopting some of these heuristics which need experience and basic process understanding for their effective usage. This problem can be best addressed by using simulation tools such as HYSYS, which are becoming increasingly popular and can give “virtual hands-on experience” to novices. Moreover, heuristics cannot always be totally relied upon as the solution can sometimes be unconventional. In addition, heuristics can sometimes be contradictory and leave the designer in a dilemma.¹⁹ Motivated by these, we integrated simulation tools and heuristics to develop a simulation-based heuristic methodology which can handle the PWC problem effectively and realistically.

1.2. Chemical Process Simulators. Although simulation tools have seen widespread usage in process control related applications in the past, most of these studies are based on steady-state simulation and a few of them are based on dynamic simulation of individual unit operations with little emphasis on PWC.²⁰ It is only around early 1990s that the advent of computer technology permitted the development of commercial plantwide dynamic simulators. Since then, the field of dynamic simulation is rapidly growing and, today, several commercial dynamic simulators, such as Hysys Dynamics, which can effectively model large-scale processes, are available. However, even with the present day advances, using dynamic simulators, especially for complex applications such as PWC system design, is not easy. It is just not enough to know the simulators per se. It demands more than that along with the application of solid engineering principles and significant amount of time. These issues are much more pronounced especially in the context of PWC. So integrating the PWC heuristics with the dynamic simulation capabilities, as discussed in this paper, greatly facilitates the PWC system design and increases use of dynamic simulation.

Some design heuristics and simulation techniques have already evolved as integrated tools and some of the process design studies are being carried out using

* Corresponding author. Tel.: (65) 68742187. Fax: (65) 67791936. E-mail: chegpr@nus.edu.sg.

simulators along with the aid of heuristics, which proved to be very beneficial. For example, a designer can save time if the design heuristic, keep the operating reflux ratio at 1.2 times the minimum reflux ratio, is known. Else, the designer would have to explore a larger search space to find the optimal solution. Applying this heuristic certainly makes the designer's task easier while simulating and optimizing distillation columns.

Most of the single unit operation control studies can also be done fairly easily by using dynamic simulation tools. But the complexities associated with dynamic simulation tools precluded the application of these tools especially to PWC problems. Thus, rigorous nonlinear simulation was used in a few studies only to evaluate/validate the control systems once they are developed. However, the recent technological advances made the simulation technology mature enough to handle even the complex problems within a reasonable amount of time.²¹ Moreover, Moore's law states that the computing speed doubles every 18 months which in turn nurtures progress in the simulation technology. Hence, simulators are therefore likely to gain widespread use throughout the process industries and in academia. With the promise of these improvements in the simulation technology, the PWC community can benefit by addressing PWC problems with the aid of the simulation tools.

The rest of the paper is organized as follows: the next section presents an integrated framework of simulation and heuristics for PWC of industrial processes. the third section includes the details of HDA process and its steady-state modeling using HYSYS. Application of the proposed methodology to HDA process and the resulting control systems' performance evaluation are presented in the fourth section. Finally, conclusions are given in the fifth section.

2. Integrated Framework of Simulation and Heuristics

The objective of this section is to develop a unified PWC methodology which is amenable to study practical concerns in a flexible way which in turn would lead to the best-practical solution (control system). After a careful review of PWC methodologies, heuristic-based methodologies are found to be intuitively attractive because they are easier to understand and implement. Heuristic-based methodologies just need the basic understanding of the process along with some experience. So we have chosen to develop a heuristic-based methodology. Mathematical tools such as RGA are also used, wherever necessary, to reap more benefits. Pioneering work in this direction is by Luyben et al.²² who proposed a 9-step heuristic procedure. This procedure will be referred as Luyben's methodology hereafter. While this methodology does not have any serious limitations, it does have some shortcomings. For example, Luyben et al.²² subdivided the big task of designing the overall PWC system into smaller tasks. However, in each step (especially set production rate and material inventory steps) the decision is ad hoc, which would impede the usage of this methodology. As throughput manipulator dictates the overall control system structure and thereby performance, the production rate must be set carefully. To make the situation worse, production rate is a typical kind of variable for which one can find many alternatives. Moreover, overall material inventory control is obviously a plantwide concern as it must be a self-consistent structure.¹⁸ Though a general discussion is

given in Luyben et al.,²² specific guidelines are not apparent from this discussion. Systematic guidelines at this stage are essential. So we adopted the guidelines from Price and Georgakis¹⁸ to facilitate the selection of manipulators for throughput and inventory regulation.

One of the heuristics in Luyben's methodology is to fix a flow in the recycle loop to avoid snowball effect, which is popularly known as Luyben's rule. It gives an impression that the flow in the recycle loop has to be controlled whenever there is a recycle. But this need not always necessarily be true. For example, the proposed integrated framework develops a viable control system (discussed in section 4) which does not require any flow control in the recycle loop. Similar observation was made by Bildea et al.¹² and Dimian.²³ The former formulated a mathematical criterion based on which one can judge when the conventional control structure can perform better than the control structure developed by applying Luyben's rule. Dimian²³ presented some cases wherein the conventional control structure can perform better than the control structure developed by applying Luyben's rule. Balasubramanian et al.²⁴ showed that fixing a flow in the recycle loop can result in instabilities especially when there are delays which are often the case in reality. Moreover, snowball effect cannot really be eliminated from the process by fixing a flow in the recycle loop but it is only transferred from one location to another.²⁵ So better alternatives to avoid snowball effect rather than fixing flow in the recycle loop are needed.

Though Luyben's methodology²² yields viable control structures, some of them are "unbalanced" which is not desirable. [If there is any disturbance affecting the process, flow rates of all streams in the process will have to vary according to material balances. But fixing a flow in the recycle loop forces the control system to act on the system to reach a forced steady state in which one or more units need to take more rigorous action than others. This kind of control structures is called unbalanced control structure.²⁵] In addition to this, Luyben's methodology may yield so-called "self-inconsistent" structures (self-consistency is discussed in Appendix A). Though these structures may be workable control strategies, extensive simulation studies by Price and Georgakis¹⁸ have shown that they are inferior to self-consistent structures in terms of performance. There are other issues (especially in complex integrated processes) that are not intuitive. As these issues can be best addressed by dynamic simulation, dynamic simulation and heuristics are integrated to find a practical solution. In every level/stage, nonlinear steady-state and dynamic models of the plant are used to take the decision or to support the decision suggested by heuristics. A few reported studies on PWC are based on steady-state models. One of the major downsides of these methodologies is that the steady-state feasibility of the process does not guarantee the plantwide controllability. In addition, steady-state analysis might not be adequate for control studies all the time.²⁶ So dynamic simulation should be more emphasized, especially in the context of PWC.

The improved heuristic methodology consists of eight levels (Table 1). Various steps involved along with the role of simulation models in each step of the methodology are discussed below.

Level 1. Define Plantwide Control Objectives. PWC objectives should be formulated from the opera-

Table 1. Improved Heuristic Methodology

level	things that need to be dealt with
1	1.1. define plantwide control objectives 1.2. determine control degrees of freedom
2	2.1. identify and analyze plantwide disturbances 2.2. set performance and tuning criteria
3	product specifications 3.1. production rate manipulator selection identify primary process path implicit/internal manipulators explicit/external manipulators fixed feed flow control on-demand control 3.2. product quality manipulator selection
4	“must-controlled” variables 4.1. selection of manipulators for more severe controlled variables process constraints (equipment and operating constraints, safety concerns, environmental regulations) especially those associated with reactor 4.2. selection of manipulators for less severe controlled variables material inventory: levels for liquid and pressures for gases levels in primary process path: make sure the control will be self-consistent levels in side chains: make sure that the control structure will direct the disturbances away from the primary process path pressures in the process
5	control of unit operations
6	check component material balances
7	effects due to integration (i.e., due to recycles) identify presence of snowball effect and analyze its severity analyze the need to fix composition in the recycle loop to arrive at a balanced control structure or is it necessary to fix a flow at a strategic position in the recycle loop?
8	enhance control system performance, if possible

tional requirements of the plant. These control objectives typically include product quality, production rate, stable operation of the plant, process and equipment constraints, safety concerns, and environmental regulations. Many a times, there can be disagreement between the plantwide objectives and unit operations objectives. For example, the best local control decisions (in the context of single units) may have long-range effects throughout the plant.²⁷ In this case, the plantwide objectives should be given priority as ultimately the plant as a whole should operate properly. Considerable attention needs to be paid while defining the PWC objectives as the control system decisions are dictated more by the underlying operating objectives than the control performance.¹⁶

Role of Simulation Models. All the objectives, except the stability-related objectives, can be set by process requirements. Coming to the objectives related to the process stability, the question at this stage is whether the process is operating at stable steady state or not. This can be answered by the steady-state simulation models. For example, in the case of feed effluent heat exchanger with a plug flow reactor, the steady-state simulation model with and without energy recycle can be perturbed to see whether it is converging to the same values in both the cases. If so, one can conclude that the process is operating at stable operating conditions; otherwise, the process is operating at unstable steady state. Dynamic simulation models can also be used to check whether the process is stable or not (i.e., by checking the process variables' responses are bounded or not). The dynamic stability is guaranteed later in Level 4.

Determine Control Degrees of Freedom. Luyben et al.²² proposed to count the number of control valves to find the control degrees of freedom (DOF) of the process. This is true but not a practical solution at this stage because, many a times, it is the job of the control

engineer to place the control valves in the process flow diagram which needs the knowledge of control DOF of the process. That means the control DOF is a priori information that needs to be known before the placement of control valves. Accordingly, control valves can be placed in strategic locations in the plant. Else, it may so happen that more or less control valves may be placed if the engineer is not familiar with the plumbing rules. These kinds of problems occur more frequently if the process is highly integrated, and the impact would be very severe.

Traditionally, control DOF is obtained by subtracting the sum of number of equations and externally defined variables from the number of variables.^{28,29} This procedure is impractical for highly integrated plants and prone to error²⁸ (p 238). Ponton³⁰ proposed a method for control DOF by counting the number of streams and subtracting the number of extra phases (i.e., if there is more than one phase present in that unit). However, simple examples can easily be constructed where this method fails. For example, control DOF for a heater/cooler remains the same irrespective of the number of phases involved in the unit. Larrson³¹ also observed some cases wherein Ponton's³⁰ method fails. So a simpler and accurate procedure to calculate the control DOF will be more useful. However, developing such a procedure is beyond the scope of this paper and is discussed in a separate paper.³² For the time being, it is assumed that the information about control DOF is available (e.g., by counting the number of valves in the process).

Level 2. Unlike many works, a full PWC system design problem including the parametric decisions (tuning parameters) is addressed here. Hence, the following issues are mandatory.

Identify and Analyze Plantwide Disturbances. It is important to have a notion about the nature of disturbances expected along with their sources and

magnitude and also how they propagate through the plant as they have considerable impact on the selection of control structure^{18,33,34} and controller tuning. For example, Price and Georgakis¹⁸ observed different control structures performing differently for different disturbances.

Role of Simulation Models. Expected disturbances can be tried out on the steady-state simulation model to observe how the effect of the disturbances is propagating throughout the plant. While trying out various disturbances on the steady-state simulation model, one must make sure that the specifications given are appropriate. For example, keeping a flow specification on one stream and observing the variation in that flow with several disturbances does not make sense. This analysis would be useful later while tuning the controllers. For example, anticipated disturbances can have more severe effects at some sections of the plant and hence the controllers in these sections should be tuned more conservatively to make all the sections of the plant equally robust.

Set Performance and Tuning Criteria. This step should be considered before any structural/parametric decisions as performance criteria have considerable impact on structural/parametric decisions. For example, Price et al.³⁵ showed that control structure may differ with the performance criteria chosen. Setting a unanimous performance criterion for the overall plant control system is a challenging task as there can be many loops of different dynamics. For example, one would prefer quick settling for fast-responding loops like levels and will go for P-only controllers where offset is not very important. On the other hand, one would prefer zero offset for slow-responding loops like composition. To make the situation worse, it is not only the kind of loop but also the location of the loop dictates the performance criteria. For example, in the case of level control, one cannot always go for averaging control; one will have to go for less conservative tuning if the level is in a distillation column and the performance criteria would also depend on the control structure selected. Control structure for distillation bottoms composition and reboiler level is a good example wherein the performance criteria change with the control structure considered; if the column base level is controlled by reboiler heat input and bottoms composition is controlled by bottoms flow, then the level control should be tightly tuned since it is nested inside the composition loop which otherwise would have been tuned conservatively.³⁶

Performance criteria such as integral error can be considered but analysis would be much more difficult. Hence, in the preliminary stages, settling time is usually considered as the performance criterion (while making sure that all the process objectives and constraints are satisfied) for highly complicated processes with dozens of control loops involved. Integral error can be chosen as the performance criterion for more rigorous studies in later stages. As the improved heuristic methodology is integrated with dynamic simulation, the controller needs to be tuned once the structural decision regarding that particular loop is taken.

Role of Simulation Models. Simulation tools are very useful for tuning. Often, preliminary tuning of flow, level, and pressure loops is a trivial task and can be done fairly easily based on standard guidelines.³⁶ But composition and temperature loops need careful tuning. Making use of built-in tools in dynamic simulators is

effective; for example, autotuning (closed loop relay-feedback technique) can be used to estimate good initial controller settings. One of the advantages of autotuning is that it can also be used for open-loop unstable systems if there exists a stable limit cycle.²⁵

Level 3. Structural decisions regarding product specifications should be taken even before considering the process stability, which is the basic criterion of any control system. This is inevitable as the chemical process industry is becoming more product-centered than process-centered.

Production Rate Manipulator Selection. This involves identifying the primary process path (from main raw material to main product). Many primary process paths may exist when there are several raw materials and products. Each primary process path may be considered to develop alternatives if the best one cannot be found at this stage. After identification of the primary process path, internal/implicit variables on this path are preferred as throughput manipulators (TPMs) over external/explicit variables (fixed-feed or on-demand) as the former are found to be dynamically more effective.¹⁸ The former are usually associated with the reactor operating conditions. Between fixed-feed or on-demand options, the former is preferred over the latter as it is shown to be superior in terms of performance.^{18,37}

Role of Simulation Models. The dynamic simulation model cannot be made use of to take the decision about throughput manipulator at this stage as the overall control strategy is not yet in place. But, as a good starting point, one can make use of a steady-state simulation model to choose the primary process path. Some processes may have multiple inputs and outputs with several reactions taking place in the reactor; in which case this procedure will be of great use. For example, for processes involving dominant side reactions, the most intuitive TPM (e.g., limiting reactant flow rate) may not be the best. After selecting the primary process path, the TPM can be selected along this line by using a steady-state simulation model. Obviously, the one with maximum steady-state gain will be the preliminary choice as the TPM.

Product Quality Manipulator Selection. In this step, one selects the manipulated variable for product quality. Other composition loops, if any, will be dealt with after the material inventory loops (levels) are taken care of as the latter respond faster and so better handles need to be reserved for levels. In addition, as most of the levels are integrating (non-self-regulating), level loops need to be given priority over composition loops as stability concerns are associated with levels. Hence, other composition loops will be dealt in level 5 (control of unit operations).

Role of Simulation Models. This stage deals with product purity, which is often a local decision; i.e., manipulator for product quality can be found in/around the unit with which the product stream is associated.⁵ Though the product quality is a local decision, it has to be considered before other plantwide decisions (such as material inventory and component balances) because of its ultimate importance. The unit producing the product stream can be separately simulated for selecting the best manipulator for product quality. Other structural decisions that are taken for simulating the unit need not be the best from the overall plant point of view and so these decisions need not be carried forward to the next levels except the product quality manipulator.

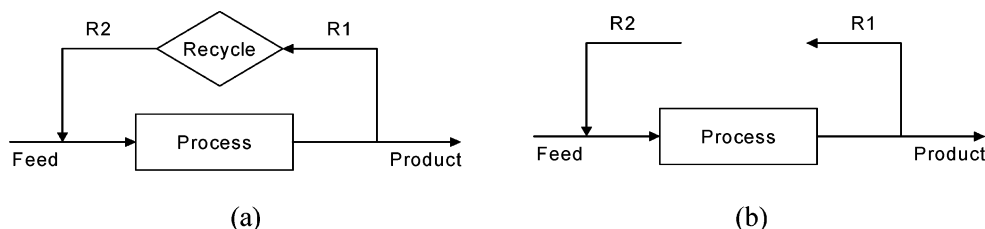


Figure 1. Schematic showing (a) process with recycle and (b) process without recycle obtained by removing the recycle block (i.e., tearing the recycle loop).

Level 4. Selection of Manipulators for More Severe Controlled Variables. Process constraints such as equipment and operating constraints, safety concerns, and process stability issues will be dealt with in this stage as they have severe operability implications.

Role of Simulation Models. Dynamic simulation model can be made use of to choose the best manipulators for meeting severe process constraints. Good initial estimates for the tuning parameters can also be obtained using in-built tools of the simulator such as autotuning.

Selection of Manipulators for Less Severe Controlled Variables. Levels need to be taken care of while ensuring that the levels in the primary process path are self-consistent (Appendix A). Other levels that are in the side chains should be controlled in such a way that the control will direct the disturbances away from the primary process path. Last, pressures (often self-regulating in nature) need to be controlled.

Role of Simulation Models. Level loops are placed so that they will form a self-consistent structure. Process knowledge from simulation must also be used while taking the decision based on heuristics. Decisions supported by simulation must be chosen in the case of any conflict because heuristics need not always be true. Finally, pressure loops can be placed with the aid of dynamic simulation models. In highly integrated processes, with long gas-processing lines, it is often difficult to decide whether to control the pressure at a particular location or not. For example, in the Tennessee Eastman (TE) process, it is often adequate to control the pressure of the vapor in an entire section of the process by using a manipulator at a single location and allowing the remaining vapor inventories to float, if the pressure drops in the gas loop are small. Dynamic simulation model would be of great use while taking this decision.

Level 5. Control of Unit Operations. *Control of individual unit operations* is considered prior to *checking component material balances*. By doing so, some of the component inventory loops will be implicitly taken care of in this stage, thereby making the analysis in the next stage (checking component inventory) easier.

Role of Simulation Models. At this level, all the individual unit operations can be simulated. This step mainly deals with the composition loops (or temperature loops) as all other loops (levels and pressures) have already been taken care of in the earlier stages. While placing the control loops on individual unit operations, one must ensure that the plantwide objectives are not violated. Finally, these can be tuned using the built-in tools of simulators.

Level 6. Check Component Material Balances. Component inventory control can be assured in the case of single-unit operations, but from a plantwide perspective, component inventory may not always be self-regulating as it usually involves reaction and separation

sections with recycles. This characteristic feature urges coordination of various control strategies over different sections in the plant to ensure that the rate of accumulation of each component in the overall process is zero. In addition, designing the control systems for highly integrated processes is really challenging because of recycles. To develop efficient control systems, the designer needs to understand the severity of the recycles. To do so, it is proposed to compare the plant behavior with and without recycle loop (as illustrated in Figure 1) in Level 7. Hence, in the present step, analysis is carried out without recycle loop and effect of recycles is considered in the next level. This approach is essential for isolating the problems that may arise due to component inventory regulation and recycles, thereby making the overall problem more easily tractable.

Role of Simulation Models. In simulation, flow rates of all components at various locations can be accessed. Using these along with reaction stoichiometry to account for generation and consumption of components via reactions, accumulation tables can be prepared to check whether the rate of accumulation is going to be zero while the plant without recycle loops is in operation (i.e., while the simulation is running). If there is any accumulation, process topology must be analyzed carefully to ensure that some component inventory loops are not forgotten. In some complex processes, it is difficult to ensure that all the inventory loops are in place. So one can make use of simulation to ensure that all the inventory loops are placed according to the process requirements.

Level 7. Effects due to Integration. This step needs to be analyzed only after all the above issues (in the previous steps) have been taken care of. Luyben et al.²² considered this step in the earlier stages. Their reasoning is that the plantwide decisions need to be given higher priority and therefore need to be satisfied in the earlier stages. But the hierarchy should ideally be based on how severe the integration effects are from a plantwide perspective. One can argue that if found to be very severe based on the steady-state analysis, this step can be done earlier and Luyben's rule can be applied. However, in this case, the probability of arriving at unbalanced structures and self-inconsistent structures would be higher, which is not desirable. Besides, from our tests with simulators, it is observed that there is an inherent interlink between component inventory regulation and introduction of recycles. It would thus be easier and more appropriate to analyze them in consecutive steps. Hence, it is better to analyze the integration effects at the end and take appropriate action. There are no solid guidelines at this stage except making use of rigorous simulation models to design a workable control strategy. It would give the control engineer flexibility to choose the better one which

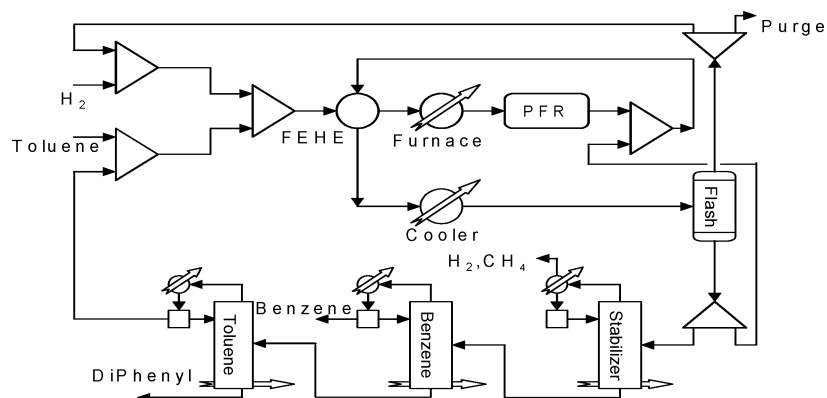


Figure 2. HDA process flow sheet to produce benzene from toluene.

otherwise would have been eliminated by applying some heuristics. Note that Luyben's rule is not rejected here but considered as one of the potential alternatives based on necessity, rather than as a rule.

Role of Simulation Models. To understand the severity of the recycle dynamics, the process with and without the recycles should be simulated for anticipated disturbances. Typically, the process with the recycles exhibits slower (or even unstable) dynamics. If not, the recycle dynamics can be concluded as not severe. In the case of slower or unstable dynamics, the control structure has to be altered either by including additional control loops or by revising the control decisions that have been taken in the earlier stages. Decision making at this stage is going to be process-specific and hence cannot be generalized. One can try out the two suggestions in the improved heuristic methodology (Table 1). These guidelines need not necessarily result in a control system with satisfactory performance and stability requirements. In such a case, rigorous simulation can be used to troubleshoot the process. Needless to say, the decisions in the earlier stages need to be revised, if a workable control strategy cannot be generated at this stage. Finally, one can simulate and evaluate the performance of alternative control structures, if any, to find the best.

Level 8. Enhance Control System Performance, If Possible. The designer can look into possible modifications to further enhance the performance of the control system. For example, one can look into reconfiguring the loops or re-structuring the control system. One can even analyze the necessity and feasibility of implementing advanced control strategies.

The proposed integrated framework is clearly more detailed on how to go about the PWC problem and can be applied to any industrial process. The framework is logically developed and has several new features as indicated below:

(1) Heuristics-based methodology is improved with more specific and useful guidelines wherever necessary.

(2) The sequence in Luyben's heuristics-based methodology is altered to facilitate the use of rigorous nonlinear simulation models and also to make the PWC problem more tractable. For example, severity of the recycle dynamics is systematically analyzed, to take necessary corrective action, toward the end (i.e., in the 7th stage).

(3) Several studies in the past used dynamic simulation to validate and evaluate alternative control system designs after they are developed. On the other hand, the proposed framework integrates heuristics and simulation models at each stage of the procedure (and not

simply at the end) to achieve greater insight. This has several benefits.

(a) The rigorous simulation models are very useful in gauging and screening any of the heuristics, thereby resulting in more efficient control system(s).

(b) The proposed framework is likely to reduce the number of alternative control systems (by screening unattractive alternatives at each stage) that need to be evaluated at the end, thereby making the overall task easier.

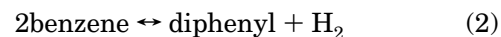
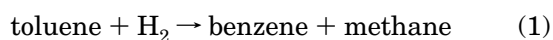
(c) The integrated framework will be very useful to novices as simulation models offer virtual hands-on experience.

(d) The framework will increase applications of dynamic simulation of process plants, which is often not possible without a basic regulatory control system.

3. Simulation of HDA Process

The most widely utilized test beds for the PWC studies are TE plant³⁸ and the classical reactor-separator-recycle section. These have been proved to be beneficial for the PWC community to better understand the PWC problems. However, there is a need to study additional processes which are of practical importance (i.e., typical industrial processes with real components and many standard unit operations) and complex enough (with material and energy recycles) to be representative in its essential features as PWC applications. So we have chosen the HDA process which is a highly integrated and nonlinear petrochemical process. The presence of heat-integrated adiabatic plug flow reactor (PFR) with exothermic reactions and three multicomponent, high-purity distillation columns and high level of interaction (because of the presence of material and energy recycles) makes it really a challenging process for control system design. Reported studies on the HDA process are by Luyben et al.²² and Qiu et al.³⁹

3.1. HDA Process Description. In the HDA process, fresh toluene (pure) and hydrogen (95% hydrogen and 5% methane) are mixed with recycled toluene and hydrogen (Figure 2). This reactant mixture is preheated in a feed-effluent heat exchanger (FEHE) using the reactor effluent stream and then to the reaction temperature in a furnace before being fed to the adiabatic PFR. Two main reactions taking place inside this reactor are



The reactor effluent is quenched with a portion of the recycle separator liquid to prevent coking, and further cooled in the FEHE and cooler before being fed to the vapor–liquid separator. A portion of unconverted hydrogen and methane overhead vapor from the separator is purged (to avoid accumulation of methane within the process) while the remainder is compressed and recycled to the reactor. The liquid from the separator is processed in the separation section consisting of three distillation columns. The stabilizer column removes hydrogen and methane as the overhead product, and benzene is the desired product from the benzene column top. Finally, in the recycle column, toluene is separated from diphenyl, as the distillate, and recycled back.

3.2. Steady-State Modeling. The success of any steady-state simulation model largely depends on the selection of a suitable thermodynamic package.^{40–42} In this study, improved Peng–Robinson (PR) equation of state is selected for property estimation as it is very reliable for predicting the properties of hydrocarbon-based components over a wide range of conditions and is generally recommended for oil, gas, and petrochemical applications. With use of the default templates in Hysys, the steady-state simulation model of the HDA process has been developed according to the flow-sheet topology (Figure 2) and the process information from Douglas.⁴³ Though Douglas⁴³ considered 75% as the optimal conversion, recent studies by Phimister et al.⁴⁴ showed that the optimal conversion is 70% and hence the base case HDA process flowsheet is developed based on 70% conversion. This variation is not unexpected and can be qualitatively explained based on the variation in the feedstock and utility prices since 1988.

Distillation columns are modeled by rigorous tray-by-tray calculations. Preliminary estimates of the number of trays and feed tray location have been calculated using the shortcut methods. Rigorous modeling is extremely important, especially while designing the equipment such as distillation columns which have a great impact on control studies. For example, Douglas⁴³ assumed constant vapor flow rate in the stabilizer for sizing, which is satisfactory for preliminary design. The steady-state simulation of the stabilizer shows that there is significant variation in vapor flow rate from top to bottom. Hence, the assumption of constant vapor flow rate in the stabilizer is not valid and inappropriate for control studies.

3.3. Moving from Steady-State to Dynamic Simulation. Hysys provides an integrated steady-state and dynamic simulation capability. In this integrated simulation environment, the dynamic model shares the same physical property packages and flowsheet topology as the steady-state model. Thus, it is easy to switch from steady state to dynamic mode. However, there are several differences in both these environments in terms of specifications given and solution methodology. One major difference is the pressure drop in distillation columns; a constant value has to be specified for this in steady-state mode whereas it will be calculated in dynamic mode based on the given tray data. So, while moving to the dynamic mode, a systematic procedure of many steps, namely, plumbing, pressure-flow (P–F) specifications, and equipment sizing, needs to be followed. (These aspects are not covered here because of space limitations.)

In principle, we can then switch over to dynamic mode. However, without a proper control system the

dynamic simulation makes no sense. Hence, a control system must be placed. But it is often difficult to proceed further. For example, if there is any problem while simulating, it is difficult to identify whether the problem is due to convergence of iterations or inefficiency of the control system. So proper guidelines are necessary at this stage to resolve this problem. This is where heuristics can aid us to proceed further via a step-by-step systematic procedure. Both the steady-state and dynamic simulation models are made use of to integrate simulation with the proposed improved heuristic methodology to design the PWC system for the HDA process in the following section.

4. Application of Proposed Methodology to HDA Process

The dynamic simulation model of the HDA process consists of 959 nonlinear, highly coupled algebraic and differential equations. This part of the study would also reveal the capability of dynamic simulation in the context of PWC.

Step 1.1: Plantwide Control Objectives

(1) Production rate: 280 lb mol of benzene/h (9.92 tonnes/h)

(2) Product quality: benzene purity $\geq 99.97\%$

(3) Process stability: the feed effluent heat exchanger with plug flow reactor has been simulated and perturbed with and without heat integration, and the results reveal that the process with heat integration is operating at unstable steady state. It has also been observed that maintaining the reactor inlet temperature at a constant value stabilizes the process.

(4) Process constraints:⁴³

(a) The temperature at the reactor inlet should be around 1150 °F. This is an optimization decision to have better reaction rates.

(b) The ratio of hydrogen to aromatics (i.e., benzene, toluene, and biphenyl) has to be at least 5 at the inlet. This is basically to provide a thermal sink, thereby avoiding coking that takes place at higher temperatures. Also, excess hydrogen encourages the primary reaction and discourages the secondary reaction.⁴⁵

(c) The temperature at the reactor outlet should not exceed 1300 °F to avoid coking.

(d) The outlet stream from the reactor must be quenched to 1150 °F to prevent thermal decomposition of products and to avoid fouling in FEHE.

Step 1.2: Control Degrees of Freedom

Available control DOF is found to be 23.²²

Step 2.1: Identify and Analyze the Plantwide Disturbances

The important plantwide disturbances in the HDA process are $\pm 25\%$ variation in toluene feed rate, -2.5% variation in hydrogen feed purity, and $\pm 5\%$ variation in the set-point of flash drum level. From the steady-state simulation model, it is observed that 5% (25%) variation in the toluene feed flow rate produced a large variation, up to 20% (85%), in the flows of separation section. This information will be useful while taking tuning decisions in the next step.

Step 2.2: Set Performance and Tuning Criteria

Settling time is chosen as the performance criterion for the preliminary studies. The analysis in the previous step showed that small variations in the toluene feed flow rate produced larger variations in the flows of separation section. So separation section controllers

must be more conservatively tuned compared to those in other parts of the plant.

Step 3.1: Production Rate Manipulator Selection

From steady-state simulation, the steady-state gain of toluene to benzene is found to be much larger than that of hydrogen to benzene. So the primary process path can be selected as toluene to benzene (Figure 2). As reactor conversion is an optimization decision, reactor conditions (internal throughput manipulators) like temperature, etc., cannot be used as TPMs. So the next best alternative, i.e., fixed-feed flow of toluene, is considered as the TPM. Jorgensen and Jorgensen⁴⁶ reported that the hydrogen feed stream is the better TPM than the toluene feed stream. Their contention is that the toluene as TPM fails to account for the side reaction and increasing the hydrogen concentration limits the extent of side reaction, leading to better selectivity and higher production rate. At first sight, Jorgensen and Jorgensen's⁴⁶ argument seems to be all right. However, it fails to take into consideration the extent of reactions. From the steady-state simulation, it can be seen that the extent of side reaction is negligible when compared to that of the main reaction. In this regard, toluene would still be a better TPM because of its larger gain.

Step 3.2: Product Quality Manipulator Selection

Based on RGA analysis (Svrcek et al.⁴⁷) of the benzene column, it is found that both the reflux flow and the distillate flow are equally good for controlling the composition of benzene in the product stream. Hence, the conventional structure wherein reflux is the manipulator for product quality is selected.

Step 4.1: Selection of Manipulators for More Severe Controlled Variables

The reactor inlet temperature is controlled by furnace duty and the PFR with FEHE is observed to be stable in the dynamic mode. Here the decision is quite straightforward. But in certain cases (e.g., if we consider bypass to FEHE) dynamic simulation can be used to take the decision. The initial estimates for the tuning parameters are calculated using the autotuning tool in Hysys Dynamics. The second process constraint is on the hydrogen-to-aromatics ratio at the reactor inlet. So hydrogen feed is selected to maintain the ratio of hydrogen to aromatics into the reactor. In this case, it turns out to be a quite straightforward decision. It is implemented as a ratio control using a spreadsheet available in Hysys Dynamics. In the control strategy of Luyben et al.,²² there is no explicit control of hydrogen-to-aromatics ratio. However, it is advisable to handle the process constraints explicitly as in our case. The hydrogen-to-toluene ratio has been considered in the previous studies whereas the actual process constraint is on the ratio of hydrogen to aromatics.⁴⁸ This constraint is very important as there can be coking if the hydrogen-to-aromatics ratio is less than five and the process will not be economically attractive if the ratio is more than five. So it is most advisable to have explicit control over this process constraint.

The third process constraint is to maintain the outlet temperature of the reactor within 1300 °F. From the steady-state simulation model, it can be seen that reactor outlet temperature (1220.1 °F) is well below 1300 °F. So this is an inactive process constraint (even in the presence of worst-case disturbance) and an

explicit control action is not needed. The last process constraint is to quench the reactor effluent stream to 1150 °F. From the process knowledge, the most intuitive manipulator is the quench stream from the flash drum.

Step 4.2: Selection of Manipulators for Less Severe Controlled Variables

Levels in the primary process path are controlled in the direction of flow (as fixed feed flow is the TPM) to have self-consistent structure (Appendix A and Figure 3). But there is one unavoidable exception to this; the toluene column condenser level should not be controlled by distillate stream as it back-propagates the disturbances to primary process path. But the other immediate alternative, reflux flow as the manipulator, is very inadequate as the reflux ratio is very small ($L/D = 0.05$). This compelled us to violate the heuristic. Levels that are in side paths are controlled in such a way that the disturbances are directed away from the primary process path. Again, there is an exception here; according to this guideline, the toluene column reboiler level must be controlled by bottoms flow. Fonyo⁴⁹ also considered bottoms flow as the manipulator for toluene column reboiler level which appears to be quite obvious. But dynamic simulations showed that the reboiler duty affects the reboiler level more than the bottoms flows and hence is a better manipulated variable for reboiler level control in the toluene column. This can be intuitively explained based on the fact that the reboil (boil-up) ratio is very high (~ 24) and bottoms flow rate (i.e., biphenyl) is very small (as the selectivity losses toward biphenyl for base case HDA process are considerably low). These two examples show that the heuristics cannot always be relied upon. The heuristics simplify the overall task but they need to be applied with a good dose of engineering judgment and process-specific knowledge.

Finally, operating pressures of three distillation columns, and flash drum pressure, are controlled appropriately. One interesting issue is the decision regarding pressure control in the gas line. When the process, like in the HDA process, has a very long gas line with many unit operations, it is difficult to decide the number of points at which the pressure needs to be controlled and their strategic locations. In this case, dynamic simulation can be used. For the HDA process, dynamic simulation showed that controlling the pressure in the flash drum would ensure the pressure control in the total gas line. Reactor pressure does not require any explicit control action.

Step 5: Control of Individual Unit Operations

In this step, all unit operations are analyzed and control loops are placed wherever necessary. Dual composition control for all three distillation columns is considered as it is relatively more optimal than the single end composition control and also offers better control from the plantwide perspective. For example, for the recycle column as an individual unit operation, single end composition control should be sufficient as the main objective is not to lose toluene from the bottom stream. However, from a plantwide perspective minimizing the disturbance propagation through the recycle stream is also as important as minimizing the toluene loss which results in dual-composition control. Hence, plantwide perception is given due importance and dual-composition control is chosen for the recycle column.

Flash drum inlet temperature has to be controlled which can be achieved by the duty of the cooler before

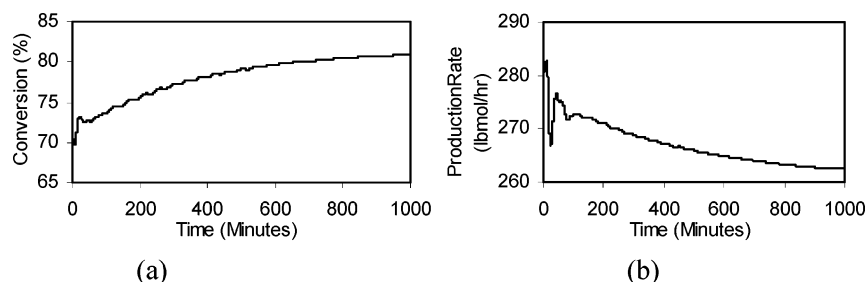


Figure 4. (a) Conversion and (b) production rate transients for the process (with recycles and before installing conversion controller) for 5% variation in toluene feed flow rate.

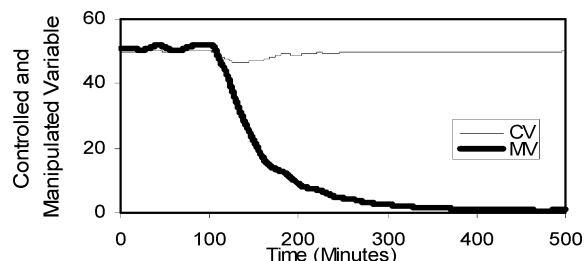


Figure 5. Recycle column condenser level response to 25% increase in toluene feed flow rate in the process with recycles and before installing conversion controller.

flow rate manipulation which in turn affects the gas recycle flow rate to control purge composition.

Effect of Liquid Recycle on Overall Plant Dynamics. Problem Identification. Both the gas and liquid recycles are closed and the closed-loop dynamic simulation is run for 5% and 25% variation in the toluene feed flow rate. Though the closed-loop system is stable, three main inefficient features of the control system in handling the disturbances are observed.

(1) The control system is able to settle the process at some steady state but, as can be seen from Figure 4a, the conversion at the new steady state ($\sim 80\%$) is totally different from the optimal conversion ($\sim 70\%$).

(2) Although the control system is able to attenuate the 5% load disturbance, it is taking too long (around 1000 min) to reach the new steady state (Figure 4). Qualitative analysis to this poor performance can be given: conversion is a typical kind of process variable, particularly for the HDA process, which affects almost all other process variables because of the highly integrated nature of the process. So unless the conversion settles, it is not possible for any other controller in the process to settle down. Hence, it is advisable to keep the conversion constant for better performance of the control system.

(3) For the worst-case disturbance of 25% variation in toluene feed flow rate, some liquid level control loops, especially those in the recycle loop, are hitting the equipment/valve constraints; Figure 5 shows actuator saturation in the control loop for level in the recycle column condenser, which is not desirable. It is advisable to operate a valve between 10 and 80% of the valve stroke across the expected range of operation.⁵²

Root Cause Analysis. It is suspected that the liquid recycle is the root cause because everything else has been taken care of systematically in the earlier stages. To confirm this, the process without liquid recycle is simulated for the same disturbance (5% variation in the toluene feed flow rate). Now the process is able to handle the disturbance and quickly reaches new steady state, which is not far away from the optimal steady state (unlike the process with liquid recycle). Hence, it can

be concluded that the liquid recycle is creating additional problems which need to be taken care of.

Identifying the Solution. Based on the analysis given in the *Problem Identification* section above, controlling the conversion (or reactor outlet toluene concentration) is one of the promising alternatives.

Choice of Manipulator for Conversion Controller. There can be basically three potential manipulators: (1) reactor inlet composition, (2) pressure, and (3) temperature. However, there are additional constraints (both economical and operational) on inlet composition (i.e., ratio of hydrogen and aromatics) and cannot be considered as a manipulator for conversion. Of the remaining two alternatives, temperature is found to be more dominating. Hence, reactor inlet temperature is selected as the manipulator (which in turn was manipulated by furnace duty).

The closed loop simulation, carried out (for expected disturbances) with conversion controller, is found to overcome all the above-mentioned problems: (1) Figure 6a shows that the conversion has been controlled at the optimal value ($\sim 70\%$) despite the presence of the disturbance. (2) As the conversion settles very fast (Figure 6a), other process variables also settle down quickly; Figure 6b shows that production rate just took around 200 min to reach steady state. (3) The control system is able to handle the worst-case disturbance without hitting the equipment constraints; Figure 7 shows the response of the toluene column condenser level controller. Thus, the conversion controller provides a balanced control structure by distributing the effect of load disturbance at different points in the plant, say, reaction and separation sections. Hence, it is essential to have the conversion controller. Except Ng and Stephanopoulos⁵³ and Douglas,⁵⁴ nobody else has made use of conversion controller for the HDA process. However, they did not give any simulation results for the use of conversion controller.

Justification for the Introduction of Conversion Controller. It is observed (from Table 2) that introduction of the conversion controller does not make much difference when there is no liquid recycle. So there is no question of conversion controller for the process without liquid recycle. However, for the process with recycle, the conversion controller gives superior performance (Figure 8). Hence, the conversion controller is required as introduction of liquid recycle is causing the control system to take longer time to regulate the component inventories because of the recycle dynamics. From Figure 8, it can be observed that the conversion controller here resembles the "recycle compensator" used by Scali and Ferrari⁵⁵ as it is trying to suppress the recycle effects and bring the control system performance closer to that can be achieved in the absence of recycle. Further justification for the conversion controller can be given

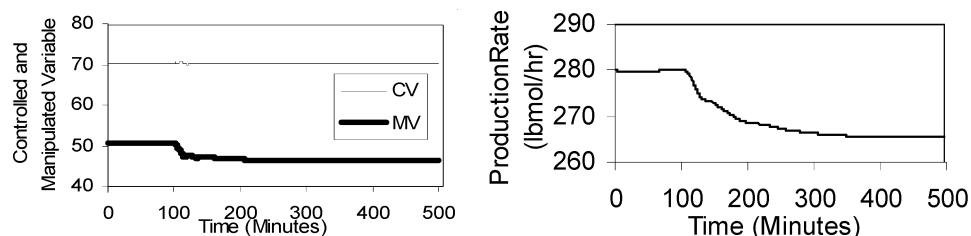


Figure 6. (a) Conversion and (b) production rate transients for the process with liquid recycle after installing conversion controller for 5% variation in the toluene feed flow rate.

Table 2. Effect of Recycle on Component Inventory Regulation and Control System Performance^a

	without liquid recycle		with liquid recycle	
	without conversion controller	with conversion controller	without conversion controller	with conversion controller
conversion (measure of economic performance)	72% (✓)	70% (✓)	80% (×)	70% (✓)
settling time (measure of dynamic performance)	200 (✓)	100 (✓)	1000 (×)	200 (✓)
equipment constraints (measure of safe operation)	✓	✓	×	✓

^a Note: ×, not desirable, and ✓, good/acceptable.

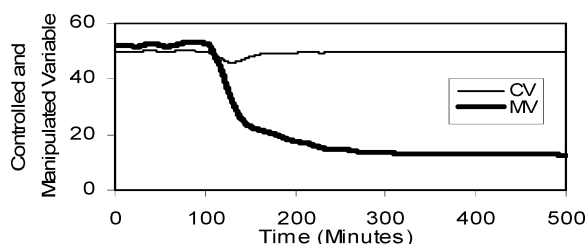


Figure 7. Recycle column condenser level response to 25% variation in toluene feed flow rate for the process with liquid recycle and conversion controller.

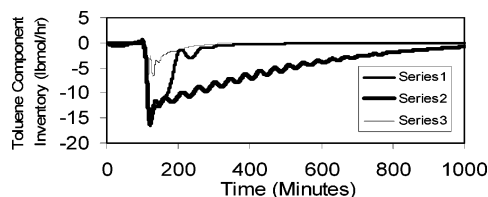


Figure 8. Toluene inventory transient for 5% variation in toluene feed flow rate. Series 1, without recycle and before installing conversion controller; Series 2, with recycle and before installing conversion controller; and Series 3, with recycle and after installing conversion controller.

based on the steady-state implications. From the steady-state simulation model, the snowball effect is found to be more severe (85% variation in the recycle flow rate for 25% variation in the feed flow rate) in the case of constant temperature controller than that (25% variation in the recycle flow rate for 25% variation in the feed flow rate) in the case of constant conversion controller. Dynamic simulations also confirmed this observation. Hence, the presence of conversion controller makes the overall control system superior to that of Ponton and Laing.⁵⁰

Control system performance under different situations, with and without recycle, and with and without conversion controller, is summarized in Table 2, which indicates an inter-relationship among the recycle component (toluene) inventory, introduction of the recycle and performance of the control system. Hence, it is appropriate and easier to study the “check component balances” and “effects due to integration” in consecutive

Table 3. Values of Set Point (SP), Process Variable (PV), and Controller Output (OP) of All Controllers after 100 min of Simulation Time

no.	controller	set point	process variable	controller output
1	Flash LC	50.00	51.87	68.71
2	StabRebLC	50.00	50.09	50.18
3	StabCondLC	50.00	50.81	45.96
4	StabCondPC	9.826	9.824	51.26
5	BenzCondLC	50.00	49.82	49.63
6	BenzRebLC	50.00	49.88	49.76
7	BenzCondPC	2.246	2.247	50.10
8	TolCondLC	50.00	49.02	48.04
9	TolRebLC	50.00	50.17	50.87
10	TolCondPC	2.177	2.169	49.41
11	FlashPC	31.98	31.98	49.35
12	TolFC	290.0	290.0	51.55
13	H2CC	5.000	5.000	51.08
14	PurgeCC	0.6013	0.6013	52.15
15	BiPhenylCC	0.9999	1.0000	52.89
16	StabCC	112.2	112.2	49.75
17	BenzCC	130.5	130.5	50.33
18	conversion	70.12	70.12	50.54
19	MCC (MethaneCC)	0.9129	0.9129	49.24
20	BCC (BenzeneCC)	0.9999	0.9999	50.39
21	TCC (TolueneCC)	0.9999	0.9999	53.73
22	ReacEffTC	621.1	621.1	50.70
23	SepTC	37.78	37.78	50.00

steps. Also, the summary in Table 2 emphasizes the importance and usefulness of dynamic simulation in order to design efficient control systems.

Evaluation of the Control System. The control system designed for the HDA process has 23 control loops (Figure 3). The complete plant with this control system but without any disturbance is simulated for 100 min. The set point, process variable, and controller output of all the control loops are reported in Table 3, which shows that all the process variables are maintained close to their set points. In the absence of the disturbances, we usually expect the controller output near 50% valve opening as they are designed for 50% opening at steady-state base case conditions. However, this is not so for some loops in Table 3 because pressures at different nodes in the dynamic mode are calculated by pressure-flow solver whereas they are specified in steady-state mode. This leads to some pressure varia-

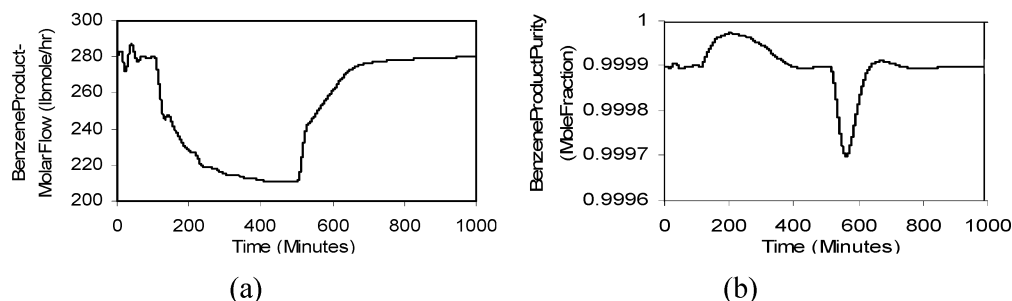


Figure 9. (a) Production rate and (b) product quality transients due to load disturbances in toluene feed flow rate.

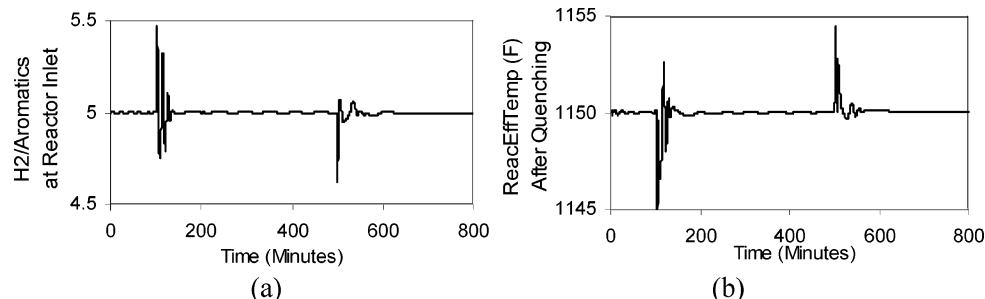


Figure 10. (a) Hydrogen to aromatics ratio and (b) reactor effluent temperature after quenching transients due to load disturbances in toluene feed flow rate.

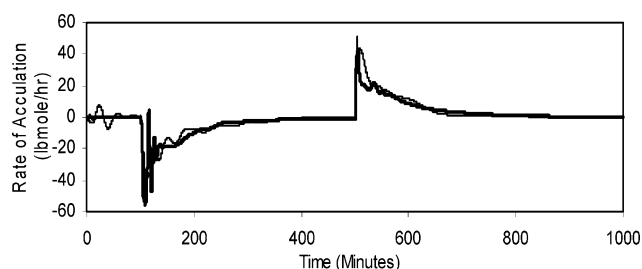


Figure 11. Rate of accumulation of toluene (thick line) and benzene (thin line) during load disturbances in toluene feed flow rate.

tions within the process in the dynamic mode when compared to the steady-state mode. So there is small offset from 50% in some of the valve openings as they depend on the neighboring pressures also. The level

controller in the flash drum (No. 1, FlashLC controller in Table 3) has settled at 68.71% opening because of liquid choking (flashing) inside the valve.

Various disturbances (load and set-point variations) are now introduced, and the transient responses of some important process variables are given in Figures 9–13 to show the effectiveness of the control system. It can be seen that the control system is able to attenuate the disturbances in reasonable settling time, which varies depending on the nature of the loop (Figures 9–13).

Feed Flow Rate Disturbance. At 100 min, -25% variation in the feed toluene supply rate is introduced as the disturbance and later removed at 500 min. In both the cases, the control system is able to attenuate the disturbances (Figures 9–11). The transient in the first 100 min is due to switching from steady state to dynamic mode.

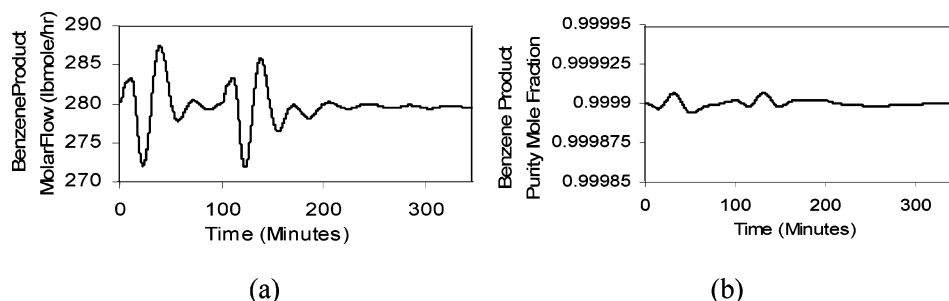


Figure 12. (a) Production rate and (b) product quality variation due to feed composition disturbance.

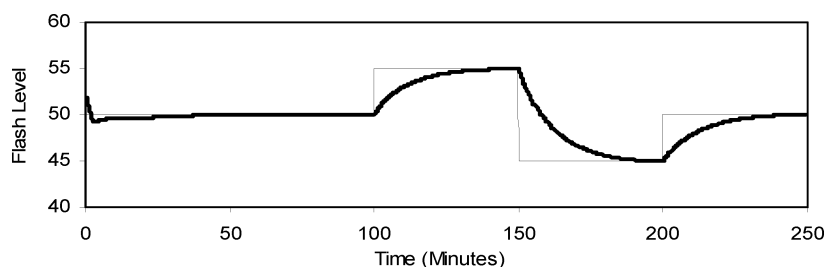


Figure 13. Set-point tracking performance of flash level controller.

Feed Composition as Disturbance. Transient responses for production rate and product quality due to hydrogen feed composition change from 0.95 to 0.925 at 100 min are given in Figure 12. Other process variables also settled within reasonable times. The variation in production rate and quality (Figure 12) is not significant because the ratio between hydrogen and aromatics is controlled at the reactor inlet. So though the feed quality changes, there is not much change in the production rate and quality.

Servo Tracking. The set-point of flash level control (FlashLC controller) is changed from 50% to 55% at 100 min, from 55% to 45% at 150 min, and from 45 to 50% at 200 min. In all these cases, the controller is able to track the set-point quickly (Figure 13). The set-point change in the flash level control is an important plantwide disturbance as it affects all the process variables in the separation section which in turn affects the process variables in the reaction section. In addition to the good servo tracking response all other process variables are also observed to be maintained at the desired set-points.

The use of rigorous nonlinear simulation is inevitable, whatever may be the methodology. Some previous studies employed it for validation purposes at the end and some other studies have not validated the resulting control system design via rigorous nonlinear simulation. This may lead to unworkable control systems. For example, Vasbinder et al.⁵⁶ observed that the PWC systems developed by Stephanopoulos⁵¹ and Fisher et al.⁵⁷ are infeasible. The proposed framework has the unique advantage of making the simulation an integral part of the control system design. This takes care of validation along with the development of a control system, which were done sequentially in all the previous methodologies.

5. Conclusions

An improved heuristic methodology is proposed by addressing the limitations associated with the 9-step heuristic procedure of Luyben et al.²² For example, more specific and yet generic guidelines are included which will facilitate the decision making for throughput and inventory control. They will also aid the novices to understand the potential alternatives at each stage and choose the better one based on the process knowledge and requirements. The improved heuristic procedure is integrated with simulation as the heuristics cannot always be relied on for PWC decisions. The proposed integrated framework is successfully applied to the HDA process. Results show that a viable control system can be generated by the proposed framework which synergizes the powers of both heuristics and simulation. The gist of the present work is that the control system design (especially for complex processes) cannot be accomplished just by heuristics without the aid of rigorous nonlinear simulation tools. It seems like common sense but it is worth repeating, especially in the context of PWC as researchers have not so far given enough attention to process simulators. Interested readers are welcome to contact the corresponding author for the Hysys Dynamics model of the HDA process.

Acknowledgment

Authors gratefully acknowledge the technical assistance from Hyprotech/Aspentech support center. The

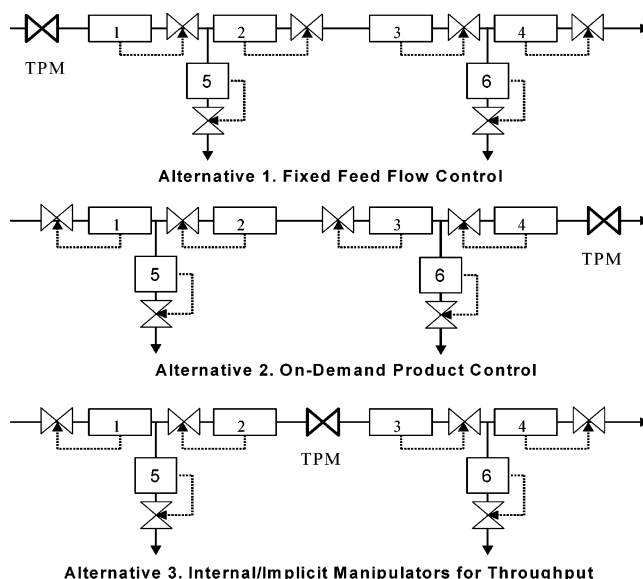


Figure 14. Alternative configurations for throughput manipulator. Blocks 1–6 represent units with inventory.

first author would like to thank the National University of Singapore for financial support to pursue graduate studies.

Appendix A: Self-consistency for Inventory Control

Price and Georgakis¹⁸ defined three self-consistent inventory control structures based on throughput manipulator (TPM) decision. If the flow control on the feed is selected as the TPM (alternative 1), the inventory should be controlled in the direction of flow. On the other hand, if TPM is the flow control over the product stream (alternative 2), the inventory should be controlled in the direction opposite to flow. If the TPM is other than these two choices, the inventory should be controlled as shown in alternative 3 where the TPM is an internal/implicit variable such as reactor temperature. The inventory in the side chains should be controlled in such a way that the disturbance propagation is away from the primary process path (Figure 14). Price and Georgakis¹⁸ proved that these self-inconsistent structures are superior to self-inconsistent structures in terms of performance as they have better disturbance attenuation capability. Hence, the concept of self-consistency is very useful in the design and analysis of PWC systems.

Literature Cited

- (1) Umeda, T.; Kuriyama, T.; Ichidawa, A. *A Logical Structure for Process Control System Synthesis*. Proceedings of IFAC Congress, Helsinki, 1978.
- (2) Denn, M. M.; Lavie, R. Dynamics of Plants with Recycle. *Chem. Eng. J.* **1982**, *24*, 55–59.
- (3) Kapoor, N.; McAvoy, T. J.; Marlin, T. E. Effect of Recycle Structure on Distillation Tower Time Constants. *AIChE J.* **1986**, *32*, 411–418.
- (4) Papadourakis, A.; Doherty, M. F.; Douglas, J. M. Relative Gain Array for Units in Plants with Recycle. *Ind. Eng. Chem. Res.* **1987**, *26*, 1259–1262.
- (5) Luyben, W. L. Dynamics and Control of Recycle Systems. 1. Simple Open-loop and Closed-Loop Systems. *Ind. Eng. Chem. Res.* **1993**, *32*, 466–475.
- (6) Luyben, W. L. Snowball Effects in Reactor/Separator Processes with Recycle. *Ind. Eng. Chem. Res.* **1994**, *33*, 299–305.

- (7) Morud, J.; Skogestad, S. Effects of Recycle on Dynamics and Control of Chemical Processing Plants. *Comput. Chem. Eng.* **1994**, 18, S529–S534.
- (8) Morud, J.; Skogestad, S. Dynamic Behavior of Integrated Plants. *J. Process Control*. **1996**, 6 (2/3), 145–156.
- (9) Hugo, A. J.; Taylor, P. A.; Wright, J. D. Approximate Dynamic Models for Recycle Systems. *Ind. Eng. Chem. Res.* **1996**, 35, 485–487.
- (10) Wu, K. L.; Yu, C. C. Reactor/Separator Processes with Recycle-1. Candidate Control Structure for Operability. *Comput. Chem. Eng.* **1996**, 20, 1291–1316.
- (11) Wu, K. L.; Yu, C. C. Operability for Processes with Recycles: Interaction between Design and Operation with Application to the Tennessee Eastman Challenge Process. *Ind. Eng. Chem. Res.* **1997**, 36, 2239–2251.
- (12) Bildea, C. S.; Dimian, A. C.; Iedema, P. D. Nonlinear Behavior of Reactor-Separator-Recycle Systems. *Comput. Chem. Eng.* **2000**, 24, 209–215.
- (13) Chodavarapu, S. K.; Zheng, A. Control System Design for Recycle Systems. *J. Process Control* **2001**, 11, 459–468.
- (14) Bildea, C. S.; Dimian, A. C. Fixing Flow Rates in Recycle Systems: Luyben's Rule Revisited. *Ind. Eng. Chem. Res.* **2003**, 42, 4578–4585.
- (15) Cheng, Y. C.; Yu, C. C. Effects of Process Design on Recycle Dynamics and its Implication to Control Structure Selection. *Ind. Eng. Chem. Res.* **2003**, 42, 4348–4365.
- (16) Downs, J. J. Distillation Control in a Plantwide Control Environment. In *Practical Distillation Control*; Luyben, W. L., Ed.; Van Nostrand Reinhold: New York, 1992; pp 413–439.
- (17) Luyben, W. L. Control of Outlet Temperature in Adiabatic Tubular Reactors. *Ind. Eng. Chem. Res.* **2000**, 39, 1271–1278.
- (18) Price, R. M.; Georgakis, C. Plantwide Regulatory Control Design Procedure Using Tiered Framework. *Ind. Eng. Chem. Res.* **1993**, 32, 2693–2705.
- (19) Douglas, J. M. A Hierarchical Decision Procedure for Process Synthesis. *AIChE J.* **1985**, 31, 353–362.
- (20) Tyreus, B. D. Object Oriented Simulation. In *Practical Distillation Control*; Luyben, W. L., Ed.; Van Nostrand Reinhold: New York, 1992; pp 72–85.
- (21) Sowa, C. J. Make the Move to Dynamic Simulation. *Chem. Eng. Prog.* **1997**, 44–47.
- (22) Luyben, W. L.; Tyreus, B. D.; Luyben, M. L. *Plantwide Process Control*; McGraw-Hill: New York, 1998.
- (23) Dimian, A. C. *Integrated Design and Simulation of Chemical Processes*; Elsevier: Boston, 2003.
- (24) Balasubramanian, P.; Kosuri, M. R.; Pushapavanam, S.; Kienle, A. Effect of Delay on the Stability of a Coupled Reactor-Separator System. *Ind. Eng. Chem. Res.* **2003**, 42, 3758–3764.
- (25) Yu, C. C. *Autotuning of PID Controllers: Relay Feedback Approach*; Springer: New York, 1999.
- (26) Skogestad, S.; Jacobsen, E. W.; Morari, M. Inadequacy of Steady-State Analysis for Feedback Control: Distillate-Bottom Control of Distillation Columns. *Ind. Eng. Chem. Res.* **1990**, 29, 2339–2346.
- (27) Stephanopoulos, G.; Ng, C. Perspectives on the Synthesis of Plant-Wide Control Structures. *J. Process Control* **2000**, 10, 97–111.
- (28) Seborg, E.; Edgar, T. F.; Mellichamp, D. A. *Process Dynamics and Control*; John Wiley & Sons: New York, 2004.
- (29) Seider, W. D.; Seader, J. D.; Lewin, D. R. *Product and Process Design Principles: Synthesis, Analysis and Evaluation*; John Wiley & Sons: New York, 2004.
- (30) Ponton, J. W. Degrees of Freedom Analysis in Process Control. *Chem. Eng. Sci.* **1994**, 49, 2089–2095.
- (31) Larsson, T. Studies on Plantwide Control. Dr. Ing. Thesis, Department of Chemical Engineering, Norwegian University of Science and Technology, 2000.
- (32) Konda, N. V. S. N. M.; Rangaiah, G. P.; Krishnaswamy, P. R. A Simple and Effective Procedure for Control Degrees of Freedom. *Chem. Eng. Sci.*, in press.
- (33) Moore, C. F. Selection of Controlled and Manipulated Variables. In *Practical Distillation Control*; Luyben, W. L., Ed.; Van Nostrand Reinhold: New York, 1992; pp 413–439.
- (34) Marlin, T. E. *Process Control: Designing Processes and Control Systems for Dynamic Performance*; McGraw-Hill: Singapore, 1995.
- (35) Price, R. M.; Lyman, P. R.; Georgakis, C. Throughput Manipulation in Plantwide Control Structures. *Ind. Eng. Chem. Res.* **1994**, 33, 1197–1207.
- (36) Luyben, W. L. *Plantwide Dynamic Simulators in Chemical Processing and Control*; Marcel Dekker: New York, 2002.
- (37) Luyben, W. L. Inherent Dynamic Problems with On-Demand Control Structures. *Ind. Eng. Chem. Res.* **1999**, 38, 2315–2329.
- (38) Downs, J. J.; Vogel, E. F. A Plant-Wide Industrial Process Control Problem. *Comput. Chem. Eng.* **1993**, 17 (3), 245–255.
- (39) Qiu, Q. F.; Rangaiah, G. P.; Krishnaswamy, P. R. Application of a Plant-Wide Control Design to the HDA Process. *Comput. Chem. Eng.* **2003**, 27, 73–94.
- (40) Carlson, E. C. Don't Gamble with Physical Properties for Simulations. *Chem. Eng. Prog.* **1996**, 37–46.
- (41) Horwitz, B. A.; Nocera, A. J. Are You "Scotomatized" by Your Simulation Software? *Chem. Eng. Prog.* **1996**, 68–71.
- (42) Benyahia, F. Flowsheeting Packages: Reliable or Fictitious Process Models? *Trans. IChemE* **2000**, 78 (Part A), 840–844.
- (43) Douglas, J. M. *Conceptual Design of Chemical Processes*; McGraw-Hill: New York, 1988.
- (44) Phimister, J. R.; Fraga, E. S.; Ponton, J. W. The Synthesis of Multistep Process Plant Configurations. *Comput. Chem. Eng.* **1999**, 23, 315–326.
- (45) Smith, R. *Chemical Process Design*; McGraw-Hill: Singapore, 1995.
- (46) Jorgensen, J. B.; Jorgensen, S. B. Towards Automatic Decentralized Control Structure Selection. *Comput. Chem. Eng.* **2000**, 24, 841–846.
- (47) Svrcek, W. Y.; Mahoney, D. P.; Young, B. R. *A Real-Time Approach to Process Control*; John Wiley & Sons: New York, 2000.
- (48) McKetta, J. J., Ed. *Encyclopedia of Chemical Processing and Design*; Marcel Dekker: New York, 1977; pp 183–235.
- (49) Fonyo, Z. Design Modifications and Proper Plantwide Control. *Comput. Chem. Eng.* **1994**, 18, S483–S492.
- (50) Ponton, J. W.; Laing, D. M. A Hierarchical Approach to the Design of Process Control Systems. *Trans. IChemE* **1993**, 17, 181–188.
- (51) Stephanopoulos, G. *Chemical Process Control: An Introduction to Theory and Practice*; Prentice Hall: New Delhi, 1984.
- (52) Bishop, T.; Chapeaux, M.; Jaffer, L.; Nair, K.; Patel, S. Ease Control Valve Selection. *Chem. Eng. Prog.* **2002**, November, 52–56.
- (53) Ng, C. S.; Stephanopoulos, G. Synthesis of Control Systems for Chemical Plants. *Comput. Chem. Eng.* **1996**, 20, S999–S1004.
- (54) Douglas, J. M. Process Operability and Control of Preliminary Designs. In *Chemical Process Control – II*; Seborg, D. E., Edgar, T. F., Eds; Proceedings of Engineering Foundation Conference, Sea Island, GA, 1981; pp 497–524.
- (55) Scali, C.; Ferrari, F. Performance of Control Systems based on Recycle compensators in Integrated Plants. *J. Process Control* **1999**, 9, 425–437.
- (56) Vasbinder, E. M.; Hoo, K. A.; Mann, U. Synthesis of Plantwide Control Structures Using a Decision-Based Methodology. In *The Integration of Process Design and Control*; Seferlis, P., Georgiadis, M. C., Eds; Elsevier: New York, 2004; pp 375–400.
- (57) Fisher, W. R.; Doherty, M. F.; Douglas, J. M. The Interface between Design and Control. 3. Selecting a Set of Controlled Variables. *Ind. Eng. Chem. Res.* **1988**, 27, 611–615.

Received for review October 29, 2004

Revised manuscript received August 8, 2005

Accepted August 19, 2005

IE048951Z