SIMULATION BASED HEURISTICS METHODOLOGY FOR PLANT-WIDE CONTROL OF INDUSTRIAL PROCESSES

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Abstract: An integrated framework of simulation and heuristics is proposed. The main emphasis 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. This framework is successfully applied to Hydrodealkylation of toluene (HDA) process. An analysis of the results shows that the proposed framework builds synergies between the powers of simulation and heuristics thereby resulting in a practical PWC methodology to develop a viable control system.

Keywords: Plantwide, Integrated Plant Control, Simulators, Heuristics.

1. INTRODUCTION

In the past, unit-based control system design methodology has been widely used to design PWC control systems. However, recent stringent environmental regulations, safety concerns and economic considerations, demand design engineers to make chemical processes highly integrated with material and/or energy recycles. Several researchers (e.g., Luyben et al., 1998) studied the effect of these recycles on the overall dynamics and concluded that these 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, because of the highly integrated nature of recent plants, unit-based methodology seems to be scarcely equipped to design the control system for such complex plants. This necessitates development of better methodologies which can deal with the highly integrated processes in a more efficient way. This leads to the concept of PWC which demands *Plant-Wide* perspective while designing PWC systems.

Designing control systems for the integrated processes is challenging because of the large combinatorial search space available. For example, Price and Georgakis (1993) observed 70 alternative control strategies for a simple hypothetical reactor-separator process with a single recycle. In view of this large combinatorial search space, the ultimate solution may be counter intuitive or can even be unconventional. Motivated by these unique complex characteristics of PWC problem, several researchers have addressed them over the last two decades and proposed many methodologies (Ponton and Laing, 1993; Price and Georgakis, 1993; Luyben et al., 1998; McAvoy, 1999; Stephanopoulos, 2000; Dimian et al., 2001; Skogestad, 2004; etc.). Some PWC methodologies are not attractive in terms of their applicability to highly integrated industrial processes. For example, application of some mathematical based methodologies to integrated processes seems to be highly tedious. After a critical review of various methodologies, heuristic-based methodologies seem 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 (i.e., process simulators) like HYSYS that are becoming increasingly popular and can give *'virtual hands-on experience'* to novices. In addition, heuristics cannot always be totally relied upon as the solution can sometimes be unconventional. Motivated by these, we developed a simulation based heuristic methodology that can handle PWC problems effectively and realistically. In this paper, the proposed methodology and its successful application to the HDA process are described.

2. SIMULATION OF HDA PROCESS

HDA process (Fig. 1) is a typical petrochemical process, extensively used by Douglas (1988) to develop a conceptual design procedure. Designing control system for such a process is really a challenging task because of the high level of interaction (due to material and energy recycles) and three highly nonlinear (due to high purity specifications) multi-component distillation columns. Steady-state simulation model of HDA process is prepared using HYSYS.PLANT that provides an integrated steady-state and dynamic simulation capability. In this integrated simulation environment, the dynamic model shares the same physical property packages and flow-sheet 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. So, while moving from steady state to the dynamic mode, a systematic procedure (including plumbing, pressure-flow specifications, equipment sizing etc.) need to be followed.

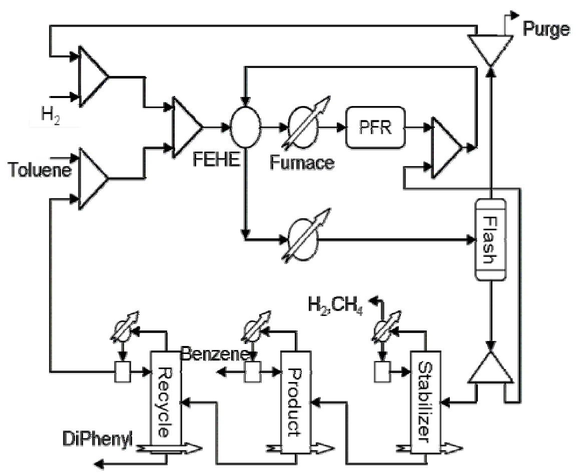

Figure 1: HDA Process Flowsheet

3. INTEGRATED FRAMEWORK OF SIMULATION AND HEURISTICS

The dynamic simulation model without a proper control system often makes no sense. Hence, a control system must be placed. But, it is often difficult to proceed further, particularly in the context of PWC. For example, if there is any problem while running the dynamic model, 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 exactly where heuristics can aid us to proceed further via a step by step systematic procedure. The pioneering work in this direction is by Luyben et al. (1998) who proposed a 9-step heuristic procedure. They have sub-divided the big task of designing the overall PWC system into smaller tasks. However, in set production rate and material inventory steps, the decision is ad-hoc which would impede the usage of this methodology by novices. Though they have given some generic description, specific guidelines are not apparent from this discussion. So, we adopted the guidelines from Price and Georgakis (1993) to facilitate the decision making and the improved heuristic methodology is given (Table 1). Furthermore, Luyben et al. (1998) propose to keep the flow in the recycle loop constant to avoid snowball effect. However, this may result in unbalanced control systems (Yu, 1999) and the closed-loop system can even become unstable at times (Balasubramanian et al., 2003). Moreover, fixing the flow in the recycle loop does not really eliminate the snowball effect from the process, but transfers it to the some other part of the process (Yu, 1999). So, it is proposed to analyze the integration effects towards the end with the aid of rigorous nonlinear simulation models and taking necessary corrective action accordingly (step 7 in Table 1).

An important feature of the proposed integrated framework of simulation and heuristics is the way we utilize the simulation tools for PWC system design with the aid of heuristics is totally different from how these tools have been utilized traditionally. Unlike any other methodology (which have used the simulation tools only at the end to validate/evaluate the control system), the proposed method uses the simulation tools at each and every step (Fig. 2). The proposed framework has two advantages. Firstly, simulation tools can be effectively utilized with the aid of heuristics. Secondly, they provide invaluable support to the heuristics at every stage of the proposed methodology for PWC system design. These are illustrated in the application of the proposed methodology to HDA process (Section 4).

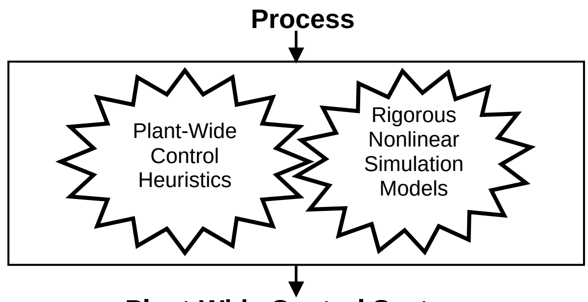

Figure 2: Proposed Integrated Framework of Heuristics and Simulation for PWC System Design

Table 1: Improved Heuristic Methodology

	Things that need to be dealt with
1	1.1. Define Plant-Wide Control Objectives 1.2. Determine Control Degrees of Freedom
2	2.1. Identify and Analyze Plant-Wide 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 & 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 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 the Presence of Snow Ball Effect and Analyze its Severity ➢ Is there a need to fix composition in the recycle loop to achieve a balanced control structure? ➢ Or, is it necessary to fix a flow at a strategic position in the recycle loop?
8	**Improve dynamic controllability, if possible.**

4. APPLICATION OF PROPOSED METHODOLOGY TO HDA PROCESS

Because of space limitations, only a brief description of all steps in the application of the proposed methodology to the HDA process is given. This part of the study would reveal features of the proposed integrated framework of simulation and heuristics in the context of PWC. Step number in the following refers to that in Table 1.

Step 1.1: Control objectives (production specifications and process constraints) are taken from Douglas (1988). Coming to the stability related objectives, steady-state perturbation analysis showed that the process is open-loop unstable because of the presence of plug flow reactor with feed effluent heat exchanger. It is also observed that the process can be stabilized by fixing the reactor inlet temperature.

Step 1.2: Control degrees of freedom is found to be 23.

Step 2.1: Most anticipated load disturbances (toluene feed flow rate/composition variations) and set-point disturbances are considered. Steady state simulation model is used to analyze their propagation through the entire process. For example, 5% variation in the toluene feed flow rate is observed to cause large variations in the down-stream flow rates (10% variation in the flow rate of the stream entering the stabilizer and ~20% variation in the liquid recycle stream flow rate). This analysis gives an idea on how conservative the tuning should be in different parts of the plant.

Step 2.2: Setting up unique performance criteria for the overall plant control system is not a trivial task as there can be dozens of loops with different dynamics. So, to simplify the analysis in the preliminary stages, settling time is chosen as the performance criterion. Inbuilt tools of the simulator (Hysys) are then used to find good initial values for controller parameters.

Step 3.1: Through steady-state sensitivity analysis, toluene feed flow rate is observed to be the best throughput manipulator (TPM). Conversion (implicit manipulator) can not be chosen as TPM as it is observed (from extensive Plant-Wide optimization studies) that conversion should be maintained at an optimal value.

Step 3.2: Dynamic simulation of the product column showed that the reflux is the best manipulator for product composition.

Steps 4.1 and 4.2: Simulation models (both steady state and dynamic) are made use of wherever necessary to choose the manipulators for the 'Must-Controlled' variables.

Step 5: Every unit operation is simulated separately in the dynamic-mode and observed to be giving satisfactory performance.

Step 6: The analysis in this step is carried out without the liquid recycle loop. (The gas recycle is observed to be having less impact on the overall dynamics of the plant when compared to the effect of liquid recycle and hence the focus in this section is mainly on liquid recycle.) The rationale is to isolate problems that will arise by component inventory regulation and recycles so that they can be easily tractable in consecutive steps. The component inventory tables/plots for various components in the process without liquid recycle have been prepared and analyzed for anticipated disturbances. It is observed that component inventories have been regulated. Based on this, one should not conclude that a proper control system has been designed. It should be analyzed with liquid recycle with expected disturbances.

Step 7: After the first 6 steps, the proposed methodology resulted in a viable control system. Further analysis on the effect of liquid recycle on the overall plant dynamics helped to arrive at a more efficient control system. This is a key issue in developing a PWC system, and is discussed in detail below

Problem Identification: At this stage, the liquid recycle loop is closed and the dynamic simulation is run. The process is observed to be reaching steady-state. One must analyze its performance in the presence of disturbances. When the expected load disturbances (5% and 25% variation in the Toluene feed flow rate) are given, three main inefficient features of the control system are observed:

1. The control system is able to settle the process at some steady state by attenuating the effect of disturbances. However, the new steady-state conversion (~80%) is far away from the near-optimal steady-state conversion of ~70% (Fig. 3), which results in loss of economical performance.

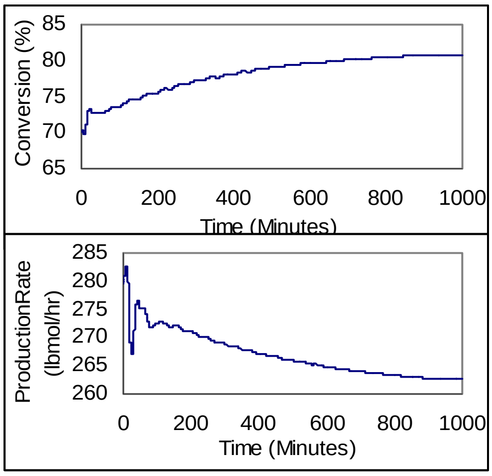

Figure 3: Conversion (top) and Production Rate (bottom) Transients for the Process (with Liquid Recycle and before installing Conversion Controller) for 5% Variation in the Toluene Feed Flow Rate

2. Though the control system is able to attenuate the disturbance, it is taking too long (~1000 min) to reach the new steady-state (Fig 3). This poor performance is because of conversion, which is a typical kind of process variable, particularly for HDA process. Conversion 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 other controllers in the process to reach steady state. Hence it is advisable to fix the conversion for good overall performance of the control system.
3. For the worst-case disturbance (25% variation in the toluene feed flow rate), some liquid level control loops are hitting the equipment/valve constraints. Fig. 4 shows that actuator saturation occurs in the recycle column condenser level. This is not at all desirable from the safety point of view.

Root Cause Analysis: It is suspected that liquid recycle is the root cause because everything else has been taken care of systematically in the earlier steps. To confirm this, dynamic simulation is run by tearing the recycle stream for the same disturbance (5% variation in the toluene feed flow rate). Now the process is able to handle the disturbance and converges quickly to the new steady-state which is not far away from the optimal steady-state (Fig. 5). Hence, it can be concluded that the recycle is creating additional problems which need to be taken care of.

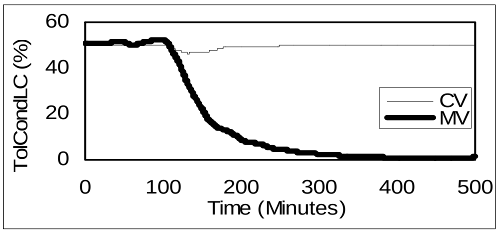

Figure 4: Recycle Column Condenser Level Transient for the Process (with Liquid Recycle and before installing Conversion Controller) for 25% Variation in Toluene Feed Flow Rate

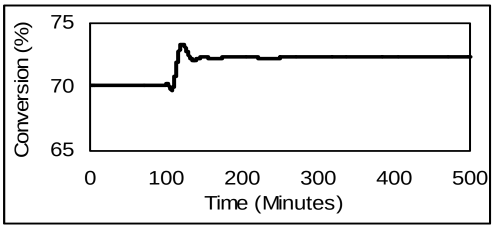

Figure 5: Conversion Transient for the Process (without Liquid Recycle and before installing Conversion Controller) for 5% Variation in Toluene Feed Flow Rate

Identifying the Solution: Luyben's rule (fixing a flow in the recycle loop) is not preferred for this case as the steady-state simulation showed that a small variation (5%) in the toluene feed stream causes ~20% in the recycle flow. That is the recycle effects are not very severe which is expected as the process is operating at high conversion (~70%). Further, Luyben's rule does not guarantee a balanced control system (Yu, 1999), and so some other alternative is needed to solve the problem.

Based on the analysis given in the *Problem Identification* section above, controlling the conversion (or reactor outlet toluene concentration) is one promising alternative. This is implemented and tested for disturbances. It is observed that the presence of conversion controller can overcome all the above mentioned three problems.

1. Fig. 6 shows that conversion is controlled at the near-optimal value (~70%) despite the disturbance to maintain economical performance.
2. As the conversion settles very fast (Fig. 6), the other process variables also settle down quickly as shown by the production rate profile in Fig. 6; it just took around 300 minutes to reach steady-state.
3. Even in the case of worst-case disturbance, the control system is able to handle without hitting the equipment constraints for the recycle column

condenser level. This happens as the conversion controller makes the control structure a balanced one by distributing the effect of load disturbance among different points in the plant, namely, reaction and separation sections.

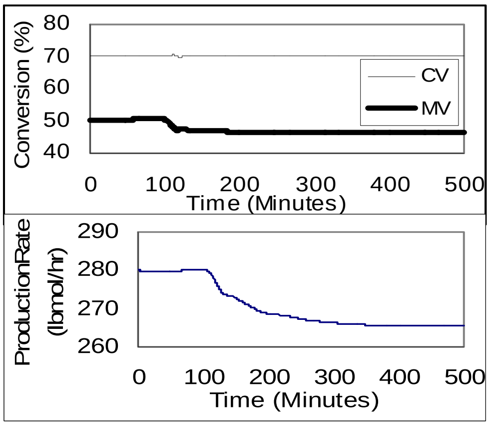

Figure 6: Conversion (top) and Production Rate (bottom) Transient for the Process (with Liquid recycle and Conversion Controller) for 5% Variation in the Toluene Feed Flow Rate

Based on the above analysis, it is necessary to have conversion controller. Except Ng and Stephanopoulos (1996), no one else has suggested conversion controller for HDA process. However, they did not give any simulation results and reasoning for it.

Justification for Conversion Controller: It can be easily justified from simulation results that introduction of liquid recycle loop necessitates the use of conversion controller because it has been observed (Fig. 7) that the introduction of conversion controller does not make a big difference if there is no liquid recycle. In both cases (with and without conversion controller) the process reached the steady-state in comparable time. So there is no question of conversion controller for the process without liquid recycle.

However, for the process with liquid recycle, conversion controller is observed to be giving superior performance. This conversion controller is required as the introduction of recycle is causing additional problems. But the question now is: why does liquid recycle create additional problems? It can be explained it terms of the regulatory nature of component inventories. Fig. 8 shows that there is an inherent interlink between the inventory of toluene (toluene is the only component that is being recycled in this case study) and the introduction of the recycle.

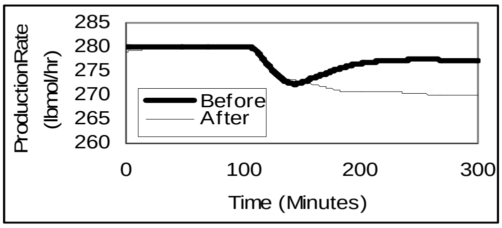

Figure 7: Production Rate Transient for the Process without Liquid Recycle (Before & After Installing Conversion Controller) for 5% Variation in the Toluene Feed Flow Rate

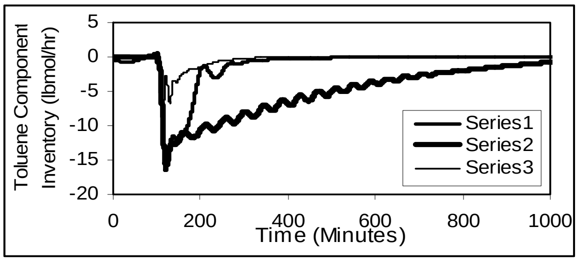

Figure 8: Toluene Inventory Transient in the Process for 5% Variation in the Toluene Feed Flow Rate. **Series 1**: without liquid recycle before installing the conversion controller. **Series 2**: with liquid recycle before installing the conversion controller. **Series 3**: with liquid recycle after installing conversion controller.

Without liquid recycle (Series1), the control system is able to control the inventory of the recycling component within 350 minutes (Fig. 8). However, it takes more than 1000 minutes for the same control system to regulate the recycling component inventory in the presence of recycle (Series2). So, additional control loop (conversion controller) is placed to regulate the recycling component inventory as quickly as possible thereby improving the overall performance of the control system (Series3). It can be understood that the faster a control system can regulate the component inventories the better is going to be its performance.

From Table 2, it can be concluded that there exists an interrelationship between the recycling component inventory, introduction of the liquid recycle and performance of the control system. That is why it is better to study the '*check component balances*' and '*effects due to integration*' in consecutive steps. The resulting control system is shown in Fig. 9. For the sake of clarity some of the controllers are placed in the sub-flowsheet environment of distillation columns which can't be seen in figure 9. Finally, the efficiency of the control system is evaluated for various expected disturbances and set-point changes, and satisfactory performance is observed.

Table 2: Effect of Liquid Recycle on Control System Performance

Performance Measure	Without Liquid Recycle		With Liquid Recycle	
	Without CC	*With CC*	*Without CC*	*With CC*
Conversion *(Measure of Economic Performance)*	72% (√)	70% (√)	80% (×)	70% (√)
Settling Time *(Measure of Dynamic Performance)*	100 (√)	100 (√)	1000 (×)	300 (√)
Equipment Constraints *(Measure of Safe Operation)*	√	√	×	√

5. CONCLUSIONS

An integrated framework of simulation and heuristics for PWC system design of industrial processes is proposed and successfully applied to HDA process. It also includes an improved heuristic methodology for PWC system design. Results show that a viable control system can be generated by the proposed framework which retains the powers of both heuristics and simulation. The gist of the present work is that the control system design (especially for complex processes) can't be accomplished just by heuristics and/or quantitative techniques without the aid of rigorous nonlinear simulation tools. It seems like common sense but it is worth repeating at this stage, especially in the context of PWC as researchers in the past have not given enough attention to the *Plant-Wide* simulators in PWC system design.

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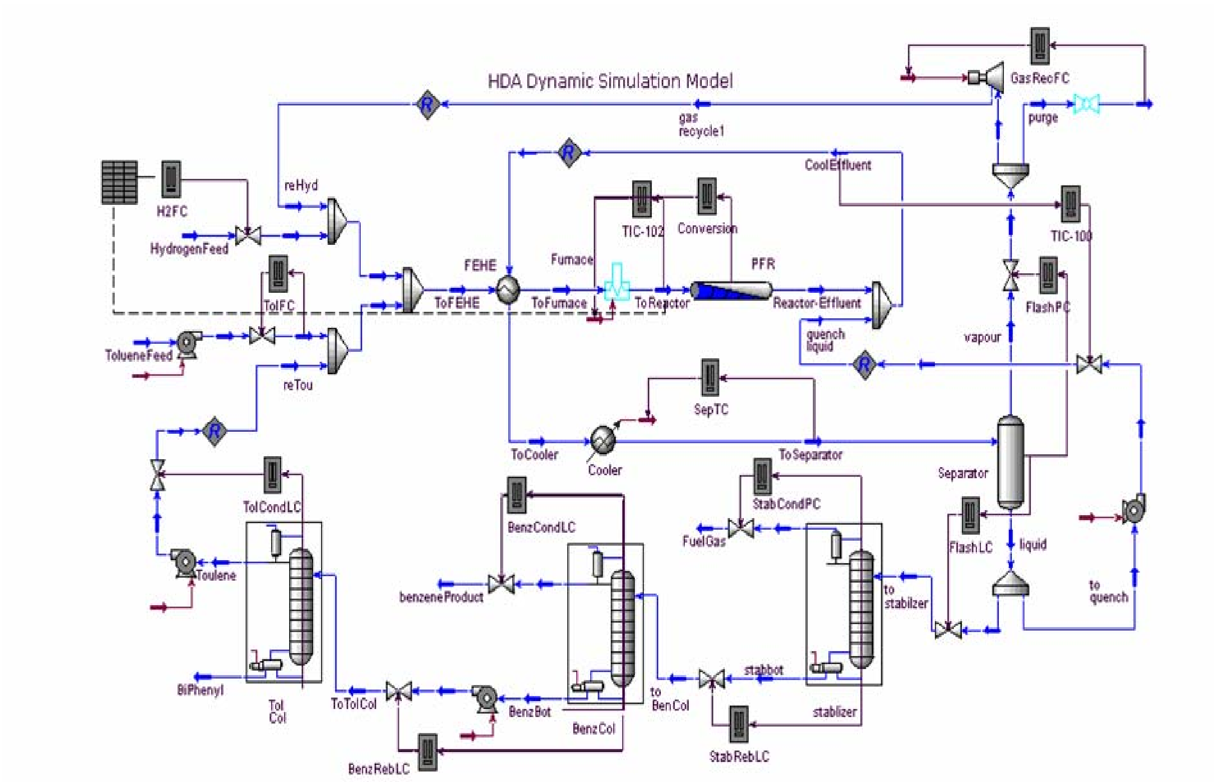

Figure 9: Dynamic Simulation Model of HDA Process