A design method for the integration of heat and control in a process of toluene hydrodealkylation

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Abstract. The integration of heat and process control, strategies for designing a process that consumes minimum energy and improves controllability has been received an increasing interest by process engineers. The techniques of heat integration to improve efficiency of energy consumption normally consume necessary degree of freedom and raise difficulties in control design. This study aims to develop a method that compromise between heat recovery of a heat exchanger network and control performance of a process by balancing the duties of utility streams. A process without heat recovery should transfer all required energy (Q-Total) using utilities. This study suggested to leave a part of Q-Total as utility streams (Q-Utility) to serve as manipulated variables of a control system. This method can be described in a four-step procedure. In the first step, the Q-Utility of a process is determined. The pinch technology is applied to develop a heat exchanger network for heat recovery in the second step. The streams which relates to the Q-Utility should not be included in the pinch analysis. In the third step, a control system is properly designed by using the Q-Utility streams as manipulated variables. In the fourth step, some disturbances are introduced to the system in the form of pulse inputs to test the controllability and resiliency of the control system. This method was applied successfully to an industrial scale case study which was hydrodealkylation of toluene process. The control system was considered with three levels of Q-Utility which were 5\%, 10\% and 100\% of Q-Total. The dynamic performance results revealed that when disturbances occurred, the process with 100\%-Utility was very stable at its designed parameters. However, the alternative with 100\%-Utility is not a good option because of its economic waste. Either 5\% case or 10\% case involved its own benefits and drawbacks. If a plant is well equipped with a good emergency response system and fast troubleshooting, then the 5\% case should be chosen. It means the utility percentage for control design can be decreased and economic benefits of heat recovery can be increased. If the 10\% case is chosen, the controllability can be improved but it should be compensated by increasing the utility cost.

1. Introduction
Heat integration and process control are significant parts of an industrial process. Heat integration methods aim to optimize the cost of a process unit by balancing between the equipment cost and heat recovery. However, the strict application of heat integration consume all control degrees of freedom, lead to process structures that are difficult to operate and control. Process control also plays an significant role to ensure the feasibility of a process. The recent studies seem to focus on individual
issues, either heat integration or process control. The integration of heat and process control, strategies for designing a process that consumes minimum energy and improves controllability has been received an increasing interest by process engineers. A method to solve the conflicts between heat integration and process control can assist process engineers to overcome difficulties in designing a process. Moreover, it enables to consider the trade-off between the cost saving of heat recovery and controllability of a process.

Design a heat exchanger network is a common method to obtain the heat integration. A chemical process consists many streams that need to heat up or cool down by using utilities. Instead of using utilities, streams in a process can exchange heat with each other to reduce required quantities of utilities, resulting in reducing operating cost. Several techniques have been proposed to design a heat exchanger network (HEN). Some of them are based on thermodynamic insights, such as Pinch Analysis [1-3], and others are based on mathematical programming [4-6].

Control design of a process with a HEN seems to be a challenge. Although heat integration is motivated by economic benefits, the network configuration impacts the process behavior by increasing interactions among streams. Moreover, the heat integration also can decrease the degree of freedom of a process by reducing the number of utility streams which may be used as manipulators of a control system. In many cases, the integration made the process difficult to control and operate [7]. Therefore, considerations of flexibility and controllability are significant in a HEN design, but they are usually neglected, especially the controllability, during the design phase. Therefore, when designing a HEN, it is significant to have a control strategy that can improve reasonable dynamic performance of a process.

The work of Marselle et al. [8] was a pioneer in operability considerations of HENs. It was proposed a manual combination of a series of optimal designs under different worst-case scenarios [9]. Kotjabasakis and Linhoff [10] studied the flexibility of HENs by introducing the sensitivity tables for the design of HENs, but the authors did not provide any information about the controllability of different configurations. Westphalen et al. [11] also present a new controllability index for HEN to choose the best control scheme that does not depend on control strategy or manipulated variables. Westphalen et al. claim that this tool can enable process engineers to combine process control issues at an early stage of the conceptual design. Mathisen et al. [7, 12-14] studied different controllability measures, proposed to take controllability into consideration by adding control related constraints to the problem formulation. They concluded that the control of all vital design targets can be fulfilled by either adding the utility streams, or by placing bypasses. Yang et al. [15] introduced a modelling approach to quantify disturbance propagation in heat exchanger networks at steady-state level. The model can be used to quickly estimate the maximum deviation of process outputs when they experience the worst combination of various types of disturbances. However, this modelling approach does not include terms representing feasibility and controllability. Continue with the work of Yang et al., Yan et al. [16] extended the model including both disturbance propagation and control. The model is embedded into an iterative design procedure for optimally selecting bypasses that includes their locations and nominal fractions, with the minimum penalty on capital cost. Lersbamrungsuk et al. [17] proposed a systematic procedure to find a control structure for heat exchanger networks with optimal operation ensuring all controlled temperature are kept at their targets and the utility cost is minimized.

The previous studies seems to overcome the problem of controlling a heat exchanger networks by using bypass fractions. Actually, a process with no heat integration is very easy to control because utility streams is free to become manipulated variables. After the heat integration, such as pinch analysis and HEN design, it is not enough utility streams for coupling to process streams in control design. Therefore, it makes the control design of a process with a HEN become very complex. The bypass fractions can increase number of streams which can be used as manipulators in a control system. However, a drawback of using the bypass solution is the difficulty in determining the correct placements of a bypass such as location and nominal values in order to reject disturbances. Therefore, the bypass solution are also relatively ineffective in handling disturbances. To overcome the drawback, instead of using all utility energy in the pinch analysis, this study aimed to leave a part of utility energy for the control design.
2. Method of design
A process without heat recovery should transfer all required energy (Q-Total) using utilities. This study suggested to separate the Q-Total into two parts. The first part (Q-Utility) is used to develop a control system, therefore, the energy of this part should come from utility streams. The second part is used to develop a HEN for heat integration. This study suggested to consider two cases which are Q-Utility=5%Q-Total and Q-Utility =10%Q-Total. The separation of transferred energy is described in figure 1.

![Figure 1. Decomposition of transferred energy for hot and cool streams](image)

The method is described in a four-step procedure. In the first step, the Q-Total and Q-Utility are proposed. In the second step, the pinch technology is applied to the second part of energy. The energy of the second part of hot streams is recovered by properly matching hot and cold streams using pinch technology. The remaining heat loads are left for utility system. The utility streams, which are placed at the terminal of a heating/cooling stream, are responsible for maintenance of target outlet temperatures when the process is exposed to a certain extent of disturbances. In the third step, a control system was properly designed by using utility streams as manipulated variables. The control system is designed based on the work of Konda et al. [18]. In the fourth step, some common disturbances are introduced to the system in the form of pulse inputs to test the controllability and disturbance resiliency of the system.

3. A case study: design a process of toluene hydrodealkylation (HDA)

3.1. Process description
This method was applied to design a process of toluene hydrodealkylation (HDA). The HDA is a highly integrated and nonlinear petrochemical process. The presence of heat-integrated adiabatic plug flow reactor with exothermic reactions and multicomponent, high-purity distillation columns and high level of interaction makes it really a challenging process for control system design. There are two main reactions occurring in the HDA process.

\[
\begin{align*}
C_6H_5 - CH_3 + H_2 & \rightarrow C_6H_4 + CH_4 & (1) \\
2C_6H_5 \leftrightarrow C_6H_4 - C_6H_6 + H_2 & & (2)
\end{align*}
\]

The base case model was simulated in steady-state using Aspen Hysys® software. Thermodynamic and kinetic data of the reactions (1) and (2) are taken from the work of Emets [19]. To prevent coking and hydrocracking, the reactor temperature must not exceed 1300°F (721°C) and the ratio between
hydrogen and toluene in the feed stream should be at least five [20,21]. The base case model is shown in figure 2 and process parameters are presented in table 1.

![Base case model of HDA Process](image)

**Figure 2.** Base case model of HDA Process

**Table 1.** Main process parameters

| Sub-system | Process Parameters |
|------------|--------------------|
| Reactors   | Molar flow of each toluene feed: 83.33 kmole/h  
Molar flow of fresh hydrogen: 262.8 kmole/h  
Reactor PFR1: P=3427 kPa, T=621°C, V=28 m³, Conversion: 88.37%  
Reactor PFR2: P=3407 kPa, T=610°C, V=120 m³, Conversion: 96.75%  
Reactor PFR3: P=3387 kPa, T=621°C, V=110 m³, Conversion: 82.97%  |
| Separator  | Flash Chamber: P=3347 kPa, T=40°C, V=25 m³  |
| Stabilizer | Benzene molar flow in vapor overhead stream: 0.5 kmole/h  
Reboiler Pressure: 857.8 kPa  |
| Benzene Column | Benzene mole fraction: 0.995 in distillate stream, 1 ppm in bottom stream  |
| Pressure: Condenser 140 kPa and Reboiler 173 kPa |

3.2. *Step 1 - Calculation of the duties of utility streams*

The duties of all utility streams in the base case (100%-Utility) were calculated. In the base case, there is no heat integration and all utility streams are used as manipulators in control design. The duty of a utility stream in this case is call Q-Total or 100%-Utility. The 5%-Utility and 10%-Utility are two cases in which the utility duties used as manipulators are 5% and 10% of Q-Total. The remaining duties should be recovered by a heat exchanger network which are designed using pinch technology in the third step. The duties of all streams are shown in table 2.
Table 2. Heat stream decomposition results

| Heat stream                                      | Total heat load (MW) | Utility duty as manipulator (MW) |
|--------------------------------------------------|----------------------|----------------------------------|
|                                                  | 5%-Utility       | 10%-Utility         | 100%-Utility (Base case) |
| Feed stream to PFR1 (Q1)                        | 7.2               | 0.36                | 0.72                   | 7.2             |
| Feed stream to PFR2 (Q2)                        | 1.36              | 0.068               | 0.136                 | 1.36            |
| Feed stream to PFR3 (Q3)                        | 2.54              | 0.127               | 0.254                 | 2.54            |
| Feed stream to Reboiler of Stabilizer column    | 1.93              | 0.0965              | 0.193                 | 1.93            |
| Feed stream to Reboiler of Benzene column       | 5.25              | 0.2625              | 0.525                 | 5.25            |
| Effluent stream from PFR3                       | 16.12             | 0.806               | 0.1612                | 16.12           |
| Feed stream to Condenser of Benzene column      | 6.21              | 0.3105              | 0.621                 | 6.21            |

3.3. Step 2 – Pinch analysis for heat integration

After the calculation of Q-Utility in all cases, the pinch technology was performed to design heat exchanger networks for 5%-Utility and 10%-Utility cases. Aspen Energy Analyzer was used to design an optimal heat exchanger network for each case. The resulting heat exchanger networks of 5%-Utility case and 10%-Utility case are shown in figures 3 and 4.

During pinch analysis, the additional utility streams may be required. Indeed, the heat loads hot streams and cool streams may not well match together. There may be some streams that require additional utilities to compensate the different energies between hot streams and cool streams. Therefore, it should have a small difference between the actual Q-Utility percentage and the pre-defined 5%-Utility or 10%-Utility. The actual utility percentages of Q-utility are shown in table 3. It can be seen that the actual utility percentages of the cases of 5%-Utility or 10%-Utility were 6.3% and 11.4% respectively.

Table 3. Actual utility duty in dynamic simulation after pinch analysis

| Heat stream                                      | Total heat load (MW) | Utility duty as manipulator (MW) |
|--------------------------------------------------|----------------------|----------------------------------|
|                                                  | 5%-Utility       | 10%-Utility         |
| Feed stream to PFR1                              | 7.2               | 0.3481               | 0.7404               |
| Feed stream to PFR2                              | 1.36              | 0.3272               | 0.4313               |
| Feed stream to PFR3                              | 2.54              | 0.0085               | 0.0757               |
| Feed stream to Reboiler of Benzene column        | 5.25              | 0.3463               | 0.6162               |
| Total                                            | 16.35             | 1.03                 | 1.86                 |
| Actual utility duty percentage (%)               | 6.3               | 11.4                 |

3.4. Step 3 - Control design for the HDA process

After the heat exchanger network was added in the process, the control system was designed based on the guidance from the work of Konda et al. [18]. Actually, the heat integration of step 2 and control design in step 3 can be done in parallel because the utility streams were separated from the heat integration. The flowsheets of 5%-Utility and 10%-Utility cases with control systems are shown in figure 5 and 6 respectively. In general, the control system of all cases are the same. For the purpose of surveying controllability and disturbance resiliency, both the control structure and controller parameters were kept the same in all cases.
Figure 3. Heat exchanger network design for 5%-Utility case

Figure 4. Heat exchanger network design for 10%-Utility case
Figure 5. Process flowsheet of 5%-Utility case with control system

Figure 6. Process flowsheet of 10%-Utility case with control system
3.5. Step 4 – Dynamic performance of the process with HEN

Performances and resiliency of the control system were verified by introducing disturbances to the system in the form of pulse inputs. Durations of the disturbances were varied from 30 to 60 minutes. Process variables should be fluctuated because of the disturbance. After the disturbances were ended, the system is expected to settle to the setpoints. The time to reach the set point with an error of less than 5% is called the settling time [22]. The disturbances which were introduced in this study were the feed flowrate disturbance of ±10%, the feed composition disturbances, the feed temperature disturbance of ±10°C. The summary of all disturbances is represented in Table 4.

Table 4. Performances of the control systems with HEN

| Disturbance type                  | Max. tested duration to retain the resiliency of cases |
|-----------------------------------|-------------------------------------------------------|
| +10% toluene feed flowrate        | 45 minutes Stable Stable Base case                     |
| -10% toluene feed flowrate        | 25 minutes Stable Stable Base case                     |
| -5% of hydrogen feed composition  | Stable Stable Stable Stable                           |
| +10°C toluene feed temperature    | Stable Stable Stable Stable                           |
| -10°C toluene feed temperature    | Stable Stable Stable Stable                           |

Table 4 shows the control performance results with different disturbances. The “stable” in table 4 means the system resiliency was retained very well with the respective disturbance whose duration varied in the whole range of 30-60 minutes. It can be seen that the base case and the 10%-Utility case can tolerate all common disturbances within the whole range. It was dynamically successful in resettling its controlled variables to set points with zero offset and bringing the system back to the steady state in a reasonable amount of time. In the 5%-Utility case, with the hydrogen feed composition disturbance and the toluene feed temperature disturbances, the resiliency of the system was also very good within the range. However, the 5%-Utility case cannot withstand the disturbances of 10% increase and decrease of the toluene feed flowrate if the disturbance durations are longer than 45 and 25 minutes respectively.

Figure 7 shows the performance of the 5%-Utility case under the decrease of hydrogen feed composition of 5% during 30 minutes. It can be seen that when the disturbance occurred, the system did not deviate far from the set point, and when the disturbance was gone, the system recovered within a reasonable time. Therefore, it can be concluded that the 5%-Utility case is very stable with the disturbance.

Table 5. Cost estimation

| Case        | Capital cost ($10^3$/year) | Operating cost ($10^3$/year) | Total cost ($10^3$/year) |
|-------------|-----------------------------|-------------------------------|---------------------------|
| 5%-Utility  | 993.7                       | 387.8                         | 707.9                     |
| 10%-Utility | 1085.4                      | 418.5                         | 768.1                     |
| Base case   | 2714.7                      | 2162.1                        | 3036.5                    |

It can be predictable that the total cost of the base case was much higher than 5% and 10%-Utility cases. Although the controllability and disturbance resiliency of the base case was better than that of 5% and 10%-Utility cases, it is not worthy for spending four times of the total cost. The dynamic analysis reveals that the controllability and disturbance resiliency of 10%-Utility case was not much worse than the base case. Therefore, the base case should not be considered as an option. Comparing to the 10%-Utility case, the 5%-Utility case had the lowest total costs. The control system of the 5%-Utility case can be tolerable with hydrogen composition and toluene feed temperature disturbances within the duration of 30-60 minutes. However, with the toluene feed flowrate disturbances, the performances of the 5%-Utility case were worse than the 10%-Utility case. However, to exchange such benefits, the 10%-Utility design had to trade-off an increase of total cost of 60.2 $/year which accounts for the increase of 8.5% compared to the 5%-Utility design.
Figure 7. The performances of the 5%-Utility case: (a) Hydrogen feed composition disturbance during 30 minutes, (b) the fluctuation of toluene feed flowrate, (c) the fluctuation of benzene production rate, (d) the fluctuation of benzene product quality.

4. Conclusions and recommendations

In this study, an integration of design and control of a heat exchanger network was presented. The four-step method was successfully applied to an industrial case study which is a HDA process. A control system for this HDA process with heat exchanger network was proposed. The dynamic behaviors of the system was investigated to assure reliability of the control system design. The proposed design method is a promising tool to overcome the disadvantages of pinch technology. Moreover, it enables to design and control a heat exchange network simultaneously because the second and the third steps of the proposed method can be done in parallel.

The proposed method can clarify the trade-off between economic cost and dynamic behaviors of a heat exchanger network. In the HDA process, the dynamic analysis reveals that the behaviors of the 10%-Utility case were as good as the base case. Therefore, the base case should not be chosen because it was a dominated alternative. While the 5%-Utility case should be the best option for a plant that is confident in disturbance troubleshooting. As an example, the maximum response time for the decrease of toluene feed flowrate of 10% was 25 minutes. If plants do not ensure the response time to the disturbance, the 10%-Utility design should be a good option.

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References

[1] Linnhoff and E. Hindmarsh, "The pinch design method for heat exchanger networks," Chemical Engineering Science, vol. 38, no. 5, pp. 745-763, 1983.

[2] U. V. Shenoy, Heat Exchanger Network Synthesis: Process Optimization by Energy and Resource Analysis. Oxford, United Kingdom: Elsevier Science & Technology, 1995.

[3] C. Kemp, Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy, Second ed. Elsevier, 2006.

[4] J. Cerda, A. W. Westerberg, D. Mason, and B. Linnhoff, "Minimum utility usage in heat exchanger network synthesis A transportation problem," Chemical Engineering Science, vol. 38, no. 3, pp. 373-387, 1983.

[5] C. A. Floudas, A. R. Ciric, and I. E. Grossmann, "Automatic Synthesis of Heat Exchanger Networks," American Institute of Chemical Engineers Journal, vol. 32, no. 2, pp. 276-290, 1986.

[6] V. Briones and A. C. Kokossis, "Hypertargets: A conceptual programming approach for the optimisation of industrial heat exchanger networks—I. Grassroots design and network complexity," Chemical Engineering Science, vol. 54, no. 4, pp. 519-539, 1999.

[7] K. W. Mathisen, "Integrated Design and Control of Heat Exchanger Networks," 1994.

[8] D. F. Marselle, M. Morari, and D. F. Rudd, "Design of resilient processing plants—II Design and control of energy management systems," Chemical Engineering Science, vol. 37, no. 2, pp. 259-270, 1982.

[9] M. Escobar, J. O. Trierweiler, and I. E. Grossman, "Simultaneous Synthesis of Heat Exchanger Networks with Operability Considerations: Flexibility and Controllability," Computers & Chemical Engineering, vol. 55, pp. 158-180, 2013.

[10] E. Kotjabasakis and B. Linnhoff, "Sensitivity Tables for the Design of Flexible Processes (1)—How Much Contingency in HENs is Cost-Effective?," Chemical Engineering Research and Design, pp. 197-211, 1986.

[11] D. L. Westphalen, B. R. Young, and W. Y. Svrcek, "Strategies For The Operation and Control Of Heat Exchanger Networks," 2003.

[12] K. W. Mathisen, S. Skogestad, and E. Wolff, "Controllability of Heat Exchanger Network," presented at the AIChE Annual Meeting, Los Angeles, 1991.

[13] K. W. Mathisen, S. Skogestad, and T. Gundersen, "Optimal Bypass Placement in Heat Exchanger Networks," presented at the AIChE Spring National Meeting, New Orleans, 1992.

[14] K. W. Mathisen, S. Skogestad, and E. Wolff, "A Bypass Selection for Control of Heat Exchanger Networks," presented at the First European Symposium on Computer Aided Process Engineering – ESCAPE 1, Denmark, 1992.

[15] Y. H. Yang, J. P. Gong, and Y. L. Huang, "A Simplified System Model for Rapid Evaluation of Disturbance Propagation through a Heat Exchanger Network," Industrial & Engineering Chemistry Research, vol. 35, no. 12, pp. 4550-4558, 1996.

[16] Q. Z. Yan, Y. H. Yang, and Y. L. Huang, "Cost Effective Bypass Design of Highly Controllable Heat Exchanger Networks," American Institute of Chemical Engineers, vol. 47, no. 10, pp. 2253-2276, 2001.

[17] V. Lersbamrungsuk, S. Skogestad, and T. Srinophakun, "A Simple Strategy for Operation of Heat Exchanger Networks," presented at the International Conference on Modeling in Chemical and Biological Engineering Sciences, 2006.

[18] N. V. S. N. M. Konda, G. P. Rangaiah, and D. K. H. Lim, "Optimal Process Design and Effective Plantwide Control of Industrial Processes by a Simulation-Based Heuristic Approach," Industrial & Engineering Chemistry Research, vol. 45, no. 17, pp. 5955-5970, 2006.

[19] S. V. Emets, "An Examination Of Modified Hierarchical Design Structure For Chemical Processes," Master Of Science, Texas Tech University, 2003.

[20] R. Smith, Chemical Process: Design and Integration. 2005.

[21] R. Smith, Chemical Process Design. Singapore: McGraw-Hill, 1995.

[22] P. Alberto, P. Sala, and A. Sala, Multi Variable Control Systems. London, UK: Springer, 2004.