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Comparative Analysis Between PI Conventional and Cascade Control in Heater-PFR-Series

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Abstract

The goals of this work are to compare and analyze the use of PI conventional and Cascade control configuration in heater-plug-flow-reactor-series (Heater-PFR-series) to produce benzene through the reaction of hydrodealkylation of toluene (HDA). The two control configurations were rigorously examined in UniSim dynamic simulation environment. The PI control parameters were tuned by using "autotuner" mode of UniSim. As shown in dynamic simulation study, the two control configurations with its tuning parameters gave the fast and stable responses. This study revealed that the Cascade control acted very well and its responses were better and faster than those in PI-conventional.

Keywords: *cascade control; dynamic simulation; PFR; PI conventional; UniSim*

INTRODUCTION

The process of heater-reactor-series is frequently met in the chemical process industries, such as isomerization process to convert normal butane into isobutane, hydrodealkylation (HDA) of toluene to produce benzene, and vinyl acetate process (Luyben et al., 1999). However, the reactor (outlet or inlet) temperature really affects the reactor performance and the produced products. The reactor temperature that is out of range can cause the problems, for example the reactor temperature should not be higher than upper limit to avoid the formation of by-product or damage to the catalyst. And vice versa, the reactor temperature that is less than lower limit can reduce the rate of reaction, so that the main-product will decrease. When the disturbance enters the reactor, it has to propagate through the reactor and make the reactor outlet temperature deviate from its desired value before feedback controller takes corrective action. Therefore, for a heater-reactor-series process, it is important to study the control strategies, with implementation of feedback conventional and cascade strategies, in order to achieve the desired operating conditions, and the fast and stable responses.

There have been many contributions to the design of cascade control. To name but a few, far back to year of 1988, Yu (1988) has proposed a design procedure based on the parallel cascade control structure for disturbance-rejection. Yu (1988) stated that the proposed approach offered a simple and effective alternative for disturbance-rejection. Urrea-Garcıa et al. (2015) has proposed the control structure which allows the controller to adapt to temperature error variations along the tubular reactor. They explored the application of a variable control structure for tubular reactors, based on multiple temperature measurements. Ahmed et al. (2013) has utilized cascade control strategy to control the temperature inside a jacketed exothermic continuous stirred tank reactor (CSTR).

Along with the growth of chemical process industries, the use of computational tools such as Matlab, Scilab, Hysys, UniSim is therefore very important to carry out dynamic simulation and explore its dynamic behavior. Several studies (Hermawan and Haryono 2012, Hermawan and Puspitasari 2018, and Hermawan et al. 2016) have used Scilab to carry out steady state and dynamic simulation in a 10 L mixing tank. Hermawan (2005) has used Hysys to carry out both steady state and dynamic simulations in HDA process with energy integration schemes. Wongsri and Hermawan (2005) also utilized Hysys to examine the proposed control structure in a complex HDA plant. Wongsri and Hermawan (2005) has proposed heat pathway heuristics (HPH) in conjunction with the plantwide control procedure given by Luyben et al. (1997) to model heat pathway management systems and the control configuration of a complex energy-integrated HDA plant. Recently, Hermawan (2020) has comprehensively explained the use of UniSim in steady state mode.

The goal of this work is to device control configurations in heater-plug-flow-reactor-series (Heater-PFR-Series) to produce benzene through the reaction of hydrodealkylation of toluene (HDA). Proportional-Integral (PI) conventional and Cascade control configurations will be used and compared for controlling the reactor outlet/inlet temperature. UniSim simulator from Honeywell is utilized to carry out both the steady state and dynamic simulations

MATERIAL AND METHOD

This work will be carried out through literature study and process simulation using UniSim simulator. The process of hydrodealkilation of toluene (HDA) to produce benzene at high reactor temperature is chosen as a case study. In order to achieve the desired goals, this work is carried out through the following stages:

Steady State Simulation

First, a steady-state model of Heater-PFR-Series is built in UniSim, using equipment design information, mainly taken from Hermawan (2005) and Luyben et al. (1999). The Peng-Robinson model is chosen in this simulation for the calculation of the physical properties because of its reliability in predicting the properties of most hydrocarbon-based fluids over a wide range of operating conditions (Wongsri and Hermawan, 2005).

The feed stream with conditions as shown in Table 1 is heated in Heater until the target temperature of 1150 °F. Then, the heated stream from Heater is flowed to the plug-flow-reactor (PFR) for doing the two vapor-phase reactions:

$$\underset{\text{Toluene}}{C_7H_8} + \underset{\text{Hydrogen}}{H_2} \rightarrow \underset{\text{Benzene}}{C_6H_6} + \underset{\text{Methane}}{CH_4} \quad (1)$$

$$\underset{\text{Benzene}}{2C_6H_6} \leftrightarrow \underset{\text{Biphenyl}}{C_1\ H_1} + \underset{\text{Hydrogen}}{H_2} \quad (2)$$

Benzene is a main-product, while Methane and Biphenyl are by-products.

Table 1. Feed conditions.

Stream Name	feed
Temperature [F]	1100
Pressure [psia]	556
Molar Flow [lbmol/hr]	5000
Component mole fraction:	
Hydrogen	0.4169
Methane	0.4922
Benzene	0.0080
Toluene	0.0829
Biphenyl	0.0000

The two kinetic expressions are modeled with standard Arhenius kinetic expression available in UniSim. The two-reaction rates (R_1 and R_2) are given in Luyben (2002) and functions of partial pressures as follows:

$$R_1 = \left(3{,}686\text{x}10^6\, e^{\frac{-9}{R}}\right) P_T P_H^{0,5} \quad (3)$$

$$R_2 = \left(9\text{x}10^4 e^{\frac{-9}{R}}\right) P_B^2 - \left(2{,}553\text{x}10^5 e^{\frac{-9}{R}}\right) P_D P_H \quad (4)$$

where the reaction base is partial pressure (psia), vapor phase, R_1 and R_2 have units of lbmole/ft^3/minute. P_T, P_H, and P_D are partial pressure of Toluene, Hydrogen, and Biphenyl, respectively (in psia). Activation energi (E) is in Btu/lbmole and the temperature is in Rankin.

For further dynamic simulation, we need some informations about equipment's specification. The spesifications of PFR, and Heater are listed in Table 2, and 3, respectively. PFR has pressure drop of 17 psig and is operated adiabatically. Heater has volume of 300 cuft and pressure drop of 5 psig.

Table 2. PFR specification and operating condition.

Temperature (F)	1150
Pressure (psia)	521
Diameter (in)	9.53
Length (ft)	57
Pressure drop (psi)	17
Process	adiabatic

Table 3. Heater's specification

Model	Supplied duty
Pressure drop (psig)	5
Volume (ft^3)	300

Table 4. Control valve's specification

Valve	Stream	Press. Drop (psi)	Cv (USGPM)	Size (in)
V1	feed	30	471.2	10
V2	rout	30	514.8	10

The plumbing system, specifically control valve, need to be inserted in UniSim flowsheet before switching to dynamics (Luyben, 2002). We choose Masoneilan Valve with type of DP Globe, V-Port, and *quick opening*. The valve coefficient (Cv) can be obtained by using "size valve" menu available in UniSim. The control valve's specifications are listed in Table 4.

Design of Control Configuration

The feedback control (FBC) with Proportional-Integral-Conventional (PI-Conventional) and Cascade control model would be applied to Heater-PFR-Series. In general, there are three controllers in Heater-PFR-Series, they are Flow Controller (FC), Temperature Controller (TC), and Pressure Controller (PC), for maintaining the feed flowrate, the reactor outlet/inlet temperature, and the reactor outlet pressure, constant at its set-point, respectively.

In PI-Conventional, controller TC is used to keep the reactor outlet temperature (T_{rout}) constant at its set-point, and lets the reactor inlet temperature (T_{rin}) changes as the input disturbance changes. Therefore, controller TC will react only the process has been upset (Smith and Corripio, 1997).

In order to overcome the disadvantage of PI-Conventional, a secondary measurement and a secondary feedback controller should be employed. These secondary instruments are used to measure and control T_{rin}, so that it recognizes the upset condition sooner. This approach is called Cascade control (Seborg et al., 2011). In Cascade control configuration, there is one manipulated variable, i.e. heater duty (q_{fur}) and two measurements, i.e. reactor outlet temperature (T_{rout}) and reactor inlet temperature (T_{rin}).

Dynamic Simulation

First of all, before switching to dynamics, the equpments' size and the plumbing must be specified. The Unisim Dynamic Assistant can be used to know the lack of required data or information in dynamic simulation. Dynamic Assistant will give some suggestions or considerations so that dynamic simulation can be carried out well.

Another important thing to support dynamic simulation is the value of feedback control parameters, such as proportional gain (K_c), integral time constant (τ_I), and derivative time constant (τ_D). The value of these parameters greatly affects the stability of the control system. The Proportional-Integral (PI) controller would be used in Heater-PFR-Series. Therefore, the only two parameters, i.e. K_c and τ_I, need to be tuned properly. The PI control parameters are tuned by using "autotuner" mode of UniSim, and its results are directly used in dynamic simulation.

In order to examine the two control configurations and evaluate the resulted PI controller parameters, the closed loop dynamic simulation should be carried out. In addition, the closed loop dynamic simulation is also aimed to examine the robustness of the two control configurations to a change in input disturbance. In this work, the feed flowrate (f_{feed}) and feed temperature (T_{feed}) are selected as the disturbance variables (DV). The two disturbances are made based on step fuction.

RESULTS AND DISCUSSION

Steady State Simulation Results

UniSim flowsheet of Heater-PFR-Series is shown in Figure 1. For heating of feed stream 5000 lbmole/hour from 1100 ºF to 1150 ºF, the heater duty (q_{fur}) is 4.05 MMBtu/hour.

After heating process, the feed stream enters PFR to carry out the two reactions. The conversion of the first and second reaction are X_1=69.60% and X_2=24.22%, respectively. Since the first reaction is exothermic (heat of reaction -18000 Btu/lbmole), and the second is slightly edothermic (heat of reaction 3500 Btu/lbmole), the reactor outlet temperature rises to 1222 ºF.

These steady state simulation results of PFR are compared with those in Hermawan (2005) and Luyben (2002). The HYSYS simulator was used in both Hermawan (2005) and Luyben (2002). These results are the same as those given by Hermawan (2005) and Luyben (2002). The steady state simulation results of Heater-PFR can be viewed in UniSim workbook as shown in Figure 2.

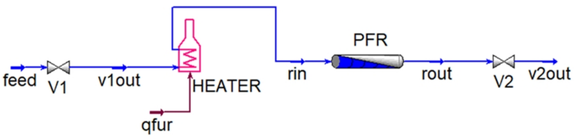

Figure 1. UniSim flowsheet of Heater-PFR-series.

Name	feed	rout	v1out	v2out	rin
Vapour Fraction	1,0000	1,0000	1,0000	1,0000	1,0000
Temperature [F]	1100	1222	1100	1222	1150
Pressure [psia]	556,0	504,0	526,0	474,0	521,0
Molar Flow [lbmole/hr]	5000	5000	5000	5000	5000
Mass Flow [lb/hr]	8,500e+004	8,500e+004	8,500e+004	8,500e+004	8,500e+004
Heat Flow [MMBtu/hr]	-3,132	0,9235	-3,132	0,9235	0,9235
Master Comp Mole Frac (Hydrogen)	0,416900	0,360172	0,416900	0,360172	0,416900
Master Comp Mole Frac (Methane)	0,492200	0,549897	0,492200	0,549897	0,492200
Master Comp Mole Frac (Benzene)	0,008000	0,063760	0,008000	0,063760	0,008000
Master Comp Mole Frac (Toluene)	0,082900	0,025203	0,082900	0,025203	0,082900
Master Comp Mole Frac (BiPhenyl)	0,000000	0,000969	0,000000	0,000969	0,000000

Figure 2. Workbook of Heater-PFR-Series.

The Control Configurations

The PI conventional control configuration of Heater-PFR-series is shown in Figure 3. This configuration has the following loops:

1. Feed stream is flow controlled by controller FC1. The output (OP) target of FC1 is valve V1.
2. The reactor outlet temperature (T_{rout}) is controlled by controller TC1, and its OP target is heater duty (q_{fur}). Direct Q model is selected to control T_{rout} by manipulating a heat removal rate (q_{fur}). Range of q_{fur} is in between 0 and 8 MMBtu/hr.
3. The reactor outlet pressure is controlled by controller PC1. The OP signal changes the position of valve V2, which manipulates the reactor outlet flowrate (rout flowrate).

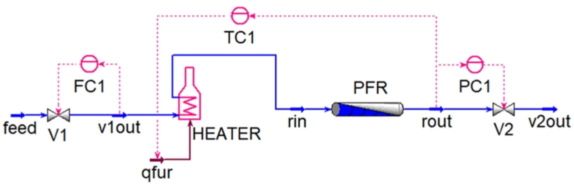

Figure 3. The PI Conventional Control Configuration of Heater-PFR-Series.

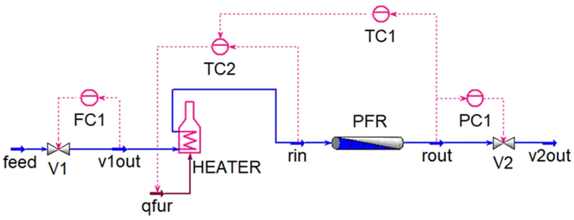

Figure 4. The Cascade Control Configuration of Heater-PFR-Series.

Figure 4 shows the cascade control configuration of Heater-PFR-series. The cascade loop is similar with PI conventional loop, except in the reactor outlet temperature controller TC1. A secondary measurement and a secondary feedback temperature controller (TC2) are employed to measure and control the reactor inlet temperature (T_{rin}), so that it recognizes the upset condition sooner. The controller TC2 can be achieved by using a remote set-point, that is the secondary controller TC2 receives set-point signal from controller TC1.

Controller Acting and Tuning Results

Another important thing for dynamic simulation is selection of controller action. There are two types of controller actions, they are reverse and direct. The flow controller (FC1) would be reverse acting since an increase in flow should result in moving the valve V1 toward the closed position (increasing PV decreases OP). The reactor outlet/inlet temperature controllers (TC1/TC2) would also be reverse acting, increasing the reactor outlet/inlet temperature (PV) decreases the heater duty (OP). Unlike FC1, TC1, and TC2, the reactor outlet pressure controller (PC1) would be direct acting since an increase in pressure should result in moving the valve V2 toward the open position (increasing PV increases OP). The actions of controllers are shown in Table 5 and 6.

Table 5. Controller's parameters in PI-Conventional

Controller	Action	Kc	τ_I (minute)	Set-point
FC1	Reverse	0.102	4.12E-3	5000 lbmole/hr
TC1	Reverse	0.639	1.68	1221 ºF
PC1	Direct	4.08	3.11E-2	504 psia

The controller parameters, i.e. proportional gain (K_c), and integral time constant (τ_I), must be tuned well before carry out dynamic simulations. The values of K_c and τ_I resulted by "autotuner" mode of UniSim are listed in Table 5, and Table 6, for PI-Conventional, and Cascade, respectively. These results are then directly used in dynamic simulation. Other than that, the ranges of sensor/transmitter should also be determined, and the ranges are listed in Table 7.

Table 6. Controller's parameters in Cascade

Controller	Action	Kc	τ_I (minute)	Set-point
FC1	Reverse	0.102	4.12E-3	5000 lbmole/hr
TC1	Reverse	0.132	1.83	1221 ºF
TC2	Reverse	1.74	8.27E-2	***Remote set-point***
PC1	Direct	4.08	3.11E-2	504 psia

Table 7. Range of CV (PV)

Controller	Range	Unit
FC1	3000 - 7000	lbmole/hr
TC1	900 - 1400	ºF
TC2	900 - 1400	ºF
PC1	404 - 604	psia

Dynamic Simulation Results

In order to examine the two control configurations and to evaluate the resulted controller parameters, two disturbance system are made and discussed as follows:

Dynamic Responses to Set-point Changes in Controller FC1

Set-pont changes in controller FC1 as shown in Figure 5 can be made as follows:

- At time equal 10 minutes, the set-point of feed flow controller FC1 is changed from 5000 lbmole/hour to 6000 lbmole/hour.
- At time equal 60 minutes, the set-point of FC1 is changed from 6000 lbmole/hour to 4000 lbmole/hour.
- At time equal 120 minutes, the set-point of FC1 is changed from 4000 lbmole/hour to 5000 lbmole/hour.

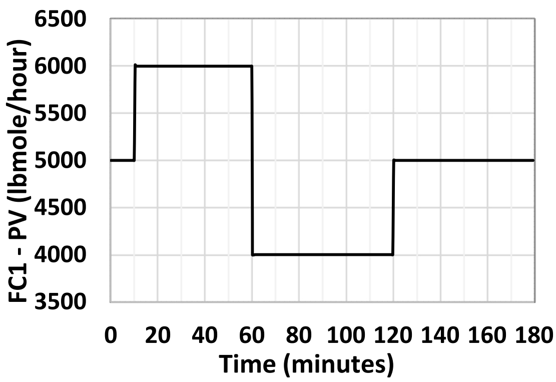

Figure 5. Set-point Changes in Controller FC1

Dynamic responses of control system in Heater-PFR-Series to set-point changes in controller FC1 are shown in Figure 6 to 11. The reactor outlet pressure P_{rout} (Figure 6) decreases (and increases) as feed flowrate increases (and decreases), but controller

PC1 can return the pressure P_{rout} to its set point of 504 psia quickly.

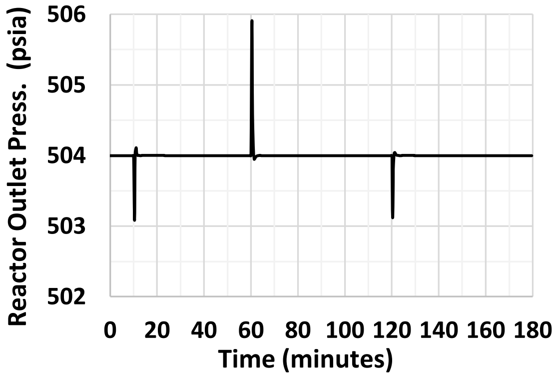

Figure 6. Dynamic Response of Reactor Outlet Pressure to Set-point Changes in Controller FC1.

Figure 7 and 8 show dynamic response of the reactor outlet and inlet temperature (T_{rout} and T_{rin}), respectively, to set-point changes in controller FC1. In general, first the temperatures T_{rout} and T_{rin} drop as the feed flowrate increases, and then their values can be returned to their set-points by increasing heater duty (q_{fur}) from to 4.05 to 5.40 MMBtu/hour as shown in Figure 9. As can be seen in Figures 10 and 11, the conversions of the firt and second reactions (X_1 and X_2) decrease as the reactor temperature decreases. When the feed flowrate decreases from 6000 to 4000 lbmole/hour at time equals 60 minutes (Figure 5), the temperatures T_{rout} and T_{rin} (Figures 7 and 8), and the conversions X_1 and X_2 (Figures 10 and 11) increase quickly, and their values can be returned to their set-points by decreasing the heater duty (Figure 9).

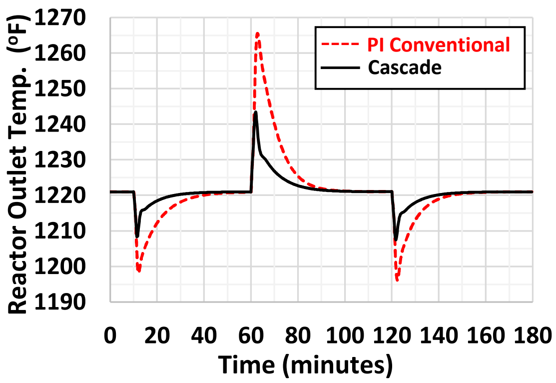

Figure 7. Dynamic Response of Reactor Outlet Temperature to Set-point Changes in Controller FC1.

The comparison of dynamic responses between PI Conventional and Cascade are represented by the dashed and solid line, respectively (Figures 7 to 11). The dynamic responses of Cascade are faster than PI Conventional. But PI Conventional produces a bigger overshoot than Cascade. The conversion X_2 resulted by PI Conventional is bigger than that resulted by Cascade (Figure 11). This implies that PI conventional produces more by-product (Biphenyl) than Cascade. Cascade can improve the response of PI Conventional by measuring temperature T_{rin} and taking control action before its effect has been felt by the reacting mixture in PFR. This agree with those in Stephanopoulos (1984), and Smith and Corripio (1997).

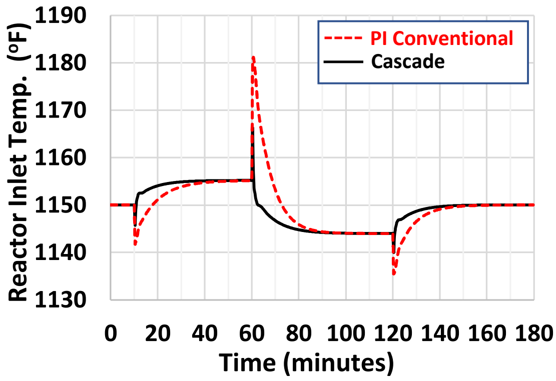

Figure 8. Dynamic Response of Reactor Intlet Temperature to Set-point Changes in Controller FC1.

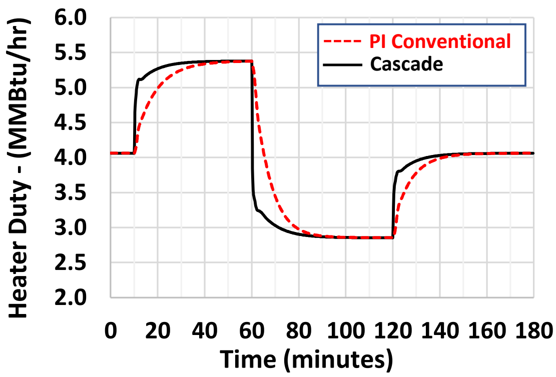

Figure 9. Dynamic Response of Heater Duty to Set-point Changes in Controller FC1.

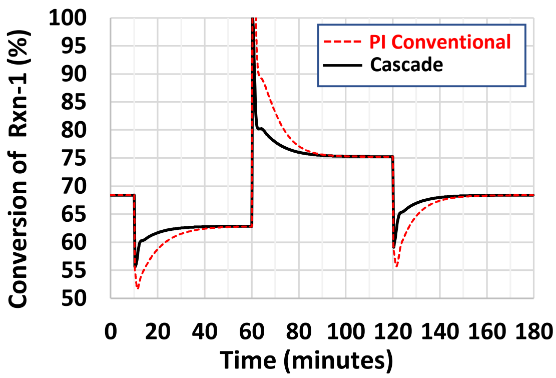

Figure 10. Dynamic Response of Conversion of Reaction-1 to Set-point Changes in Controller FC1.

Dynamic Responses to Disturbance Changes in Feed Temperature

Disturbance changes in the feed temperature as shown in Figure 12 can be made as follows:

- At time equal 10 minutes, the feed temperature is changed from 1100 °F to 1110 °F.
- At time equal 60 minutes, the feed temperature is changed from 1110 °F to 1090 °F.
- At time equal 120 minutes, the feed temperature is changed from 1090 °F to 1100 °F.

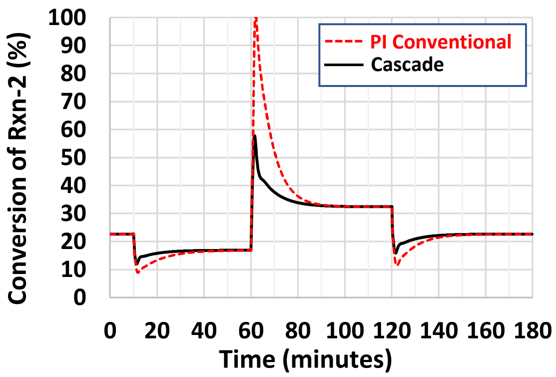

Figure 11. Dynamic Response of Conversion of Reaction-2 to Set-point Changes in Controller FC1.

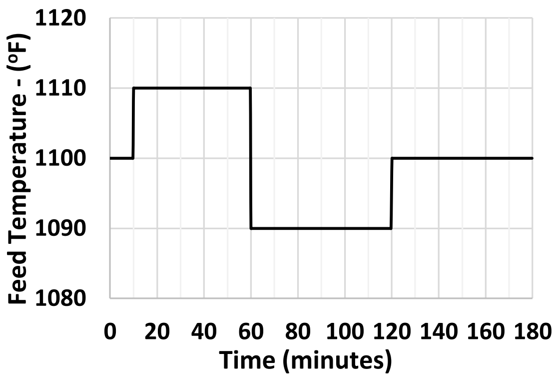

Figure 12. Disturbance Changes in Feed Temperature.

Figures 13 to 18 show dynamic responses of control system in Heater-PFR-Series to disturbance changes in the feed temperature. Dynamic response of the reactor outlet pressure P_{rout} (Figure 13) is very fast. Controller PC1 can maintain P_{rout} at its set point of 504 psia well.

Dynamic responses of the reactor outlet and inlet temperature (T_{rout} and T_{rin}) to disturbance changes in the feed temperature are shown in Figure 14 and 15, respectively. In general, first the temperatures T_{rout} and T_{rin} increase as the feed temperature increases, and then their values can be returned to their set-points by decreasing heater duty (q_{fur}) from to 4.05 to 3.25 MMBtu/hour as shown in Figure 16. The conversions of the firt and second reactions (X_1 and X_2) increase as the reactor temperature increases. When the feed temperature decreases from 1110 to 1090 °F at time equals 60 minutes (Figure 12), the temperatures T_{rout} and T_{rin} (Figures 14 and 15), and the conversions X_1 and X_2 (Figures 17 and 18) decrease quickly. However, the temperature controller can return values of the process variables to their set-points by increasing the heater duty (Figure 16).

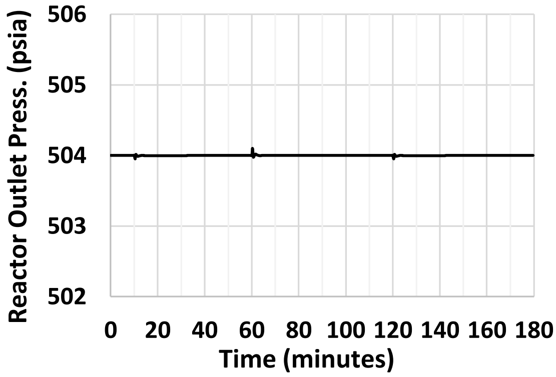

Figure 13. Dynamic Response of Reactor Outlet Pressure to Disturbance Changes in Feed Temperature.

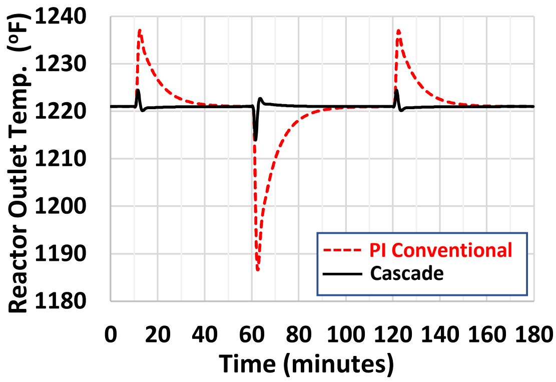

Figure 14. Dynamic Response of Reactor Outlet Temperature to Disturbance Changes in Feed Temperature.

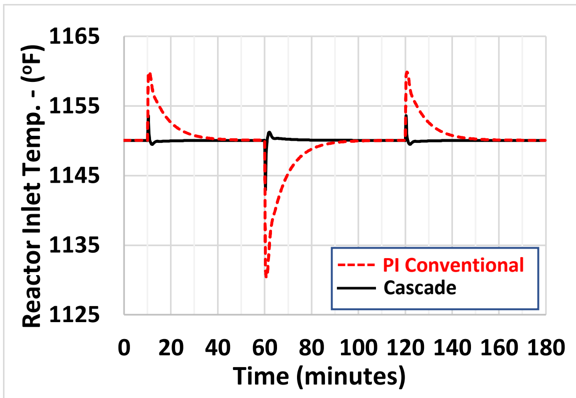

Figure 15. Dynamic Response of Reactor Inlet Temperature to Disturbance Changes in Feed Temperature.

Figures 14 to 18 also show the comparison of dynamic responses between PI Conventional and Cascade. The dashed line in Figures 14 to 18 represents PI Conventional responses, while the solid line represents Cascade responses. Again, the dynamic reponses of Cascade are faster than PI Conventional, and the PI Conventional produces a bigger avershoot than Cascade. The conversion X_1 resulted by PI Conventional is smaller than that resulted by Cascade. This implies that PI Conventional produces less main-product (Benzene) than Cascade.

As explained in Seborg et al. (2011), a disadvantage of PI Conventional is that corrective action for disturbances does not begin until after the controlled variable deviates from the set point. Therefore, in order to overcome this problem, a secondary measurement point and secondary temperature feedback controller should be employed in the PFR. This approach is known as cascade control.

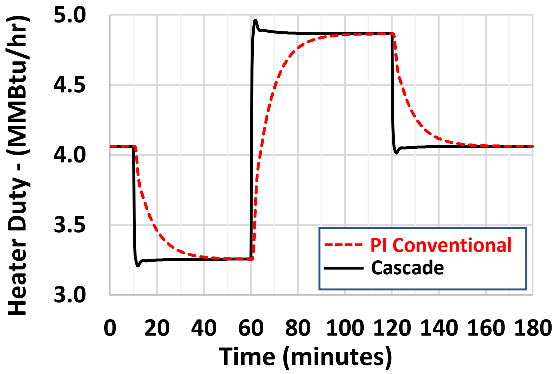

Figure 16. Dynamic Response of Heater Duty to Disturbance Changes in Feed Temperature.

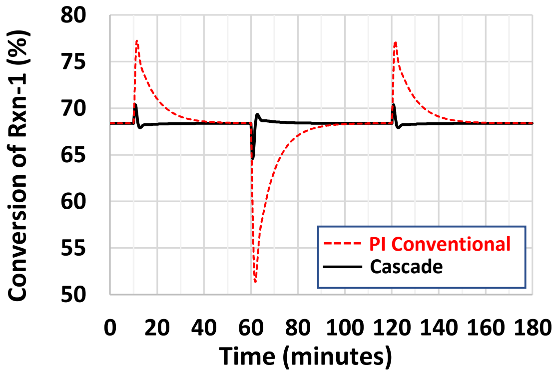

Figure 17. Dynamic Response of Conversion of Reaction-1 to Disturbance Changes in Feed Temperature.

CONCLUSION

Study on the hydrodealkylation (HDA) process to produce benzene, tuning of PI parameters, dynamic simulation and control in Heater-PFR-series have been successfully done through the closed loop simulation using UniSim simulator. Two control configurations of PI-conventional and Cascade control have been applied to Heater-PFR-Series. The closed loop dynamic behaviors of the two control configurations have also been explored and compared.

According to our dynamic simulation results, the resulted controller gains (K_c) and integral time constants (τ_I) were able to produce the fast and stable responses to both of set-point changes in flow controller and disturbance changes in feed temperature. The most robust control is obtained when a Cascade control is employed.

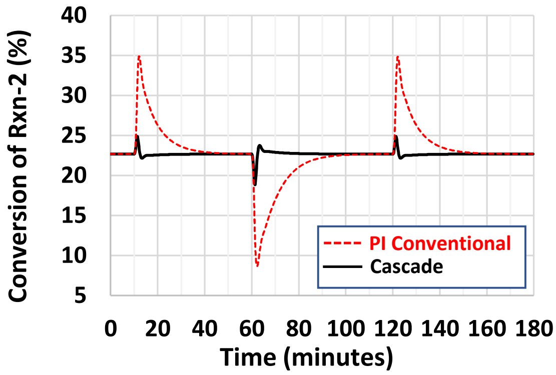

Figure 18. Dynamic Response of Conversion of Reaction-2 to Disturbance Changes in Feed Temperature.

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