Dynamic simulation of flow controller for the production of Cyclohexanone

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ABSTRACT

Cyclohexanone has many industrial uses, in general as an industrial chemical intermediate product. The consumption of cyclohexanone is mostly for the nylon industry, to produce caprolactam. A large portion of the world's caprolactam production is from cyclohexanone. In this paper, the dynamic simulation of flow controlling for the production of cyclohexanone has been studied. The UNISIM software R460 is used for the simulation processes. Dynamic simulation of a plant is established and the dynamic analysis focuses on the time-changing behaviour of the system. Proportional integral controllers and proportional integral derivative controllers are used for the flow controlling of the system. Also evaluation of the performance of these two controllers has been carried out.

Key terms used:

Dynamic simulation,
Cyclohexanone,
UNISIM,
Proportional integral controllers,
Proportional integral derivative controllers.

ABBREVIATION

PSRV – Peng- Robinson-Stryjek-Vera, VLV-Valve, PV- Process Variable, OP- Controller Output, SP- Set-Point, PI- Proportional-Integral, PID- Proportional-Integral-Derivative, FIC-Flow Indicator and Controller, PFR- Plug Flow Reactor.

1.INTRODUCTION

The major aim of an industry is to produce products with maximum quality and at low cost. Apart from product quality, energy and cost efficiency, the most important thing is safety. The major concern is occupational and environmental safety [1]. In the design stage, all parameters should be considered itself. At these conditions plant, automation and simulation become more important and are considered as the most recognized and effective way to achieve the production goals in the industry [6]. Process simulation is a method, which can represent different types of operations such as chemical, biological, physical and other unit operations in an industry. The modelling and simulation can be done using design software [3]. The software can calculate the mathematical models of the reactions using available information on the physical and chemical properties of components [17]. A chemical industry mainly the petrochemical industry has series of unit operations. This operation can represent through a process flow diagram. In simulation software, these unit operations can connect as per the flow diagram to model the process industry. The modelling and simulation of the cyclohexanone production plant can be done with the assistance of UNISIM design software. The software helps to represent the real process in a better way [4,5]. Cyclohexanone is an organic compound produced from the oxidation of cyclohexane. Cyclohexane is formed by the reaction of hydrogen and benzene. For the production of Nylon 6,6 and Nylon 6 cyclohexanone is consumed in large. It is also used as a leveling agent for dyeing and matting, as well as a degreaser for polishing metal, wood coloring, and painting [3,9]. Developing a dynamic simulation will help to increase the maximum production with minimal cost. This paper deals with the dynamic simulation of flow controlling for the production of cyclohexanone.

2. MATERIALS AND METHODS

2.1 PROCESS DESCRIPTION

Dynamic simulation is done only after steady-state simulation. Simulation of the process is carried out by using UNISIM software R460. A thermodynamic model was selected as the preliminary step of the simulation. Different types of thermodynamic packages are available with the UNISIM model [2]. We will obtain a wide variety of physical property calculations from each package for different compounds at a particular temperature range. The PRSV model is the property package used for cyclohexanone production. This model is a two-fold modification of the Peng- Robinson equation of state [15, 16]. The data required for the dynamic simulation are taken from steady-state simulation. First of all, to study the process for the production of cyclohexanone, the process is divided into different steps. The first step is the drying process where the raw material benzene is stored in water at 320 C. Benzene is heat exchanged from 320 C to 760 C [11]. This feed is fed to the separator to separate water and benzene and to get 0.68 mole fraction benzene and 0.32 mole fraction of water. In the separator, undissolved water is separated and drained to the sewer system. The top products are heat exchanged and are transferred to the plug flow reactor. The second step is hydrogenation of benzene, for which the plug flow reactors are connected in series and the benzene reacts with hydrogen to form cyclohexane [13]. This cyclohexane product containing undissolved water content can be removed by using a separator. In the third step, the top product leaving from the separator is mixed with the externally supplied oxygen. Cyclohexane-oxygen mix gets reacted in the series connected plug flow reactor to release the final product cyclohexanone. The steady state simulation model built in UNISIM Design R460 is modified when converted into the dynamic simulation. A dynamic simulation is a powerful tool that is adopted by various industries for modelling and simulating a process. The transient system should be controlled in such a way that it should not affect the product quality and also should incorporate the safety aspects. Dynamic simulation is an extension of steady-state simulation and it will account for several things that will affect the process [12].

2.2 DYNAMIC SIMULATION

The selected controller parameters are studied using disturbance to the system and how the device responds to that. The disturbance may be executed by either changing the initial output level (OP), which is known as load disturbance or via the set point (SP), which is referred to as set-point disturbance. The change can be either negative or positive relative to the steady-state value [7].

3.RESULTS AND DISCUSSION

The parameter required for the dynamic simulation are taken after completing the steady state simulation. The flow controlling is controlled by using two types of controllers, PI and PID controllers.

3.1 SET-POINT CHANGE PROBLEM

3.1.1 SEPARATOR

In this problem, the excess flow of benzene-water mixture to the separator is controlled and the flow rate is maintained at an optimum value. The molar flow rate of the feed to the separator is 43.05 kmol/h. A flow controller (figure 1) is given to regulate the plant inlet flow. The FIC -100 controls the position of the valve VLV-100 at the actuator desired. The flow through the valve is taken as a process variable (PV) and actuator desired position of the valve is taken as OP. The controller tuning parameters are decided on with the aid of the use of the auto-tuning phase using best tuning controllers [10]. Two instances are taken into consideration right here: The primary case represents (figure 2), the PID flow control unit using gain constant Kc= 0.835, derivative time constant Td= 4.14X10-3 min. and integral time constant Ti= 1.86X10-2 min. Figure 3, shows the second case, which represents the PI flow control using gain constant = 0.596, integral time constant Ti= 0.002 min.

Figure 1 Dynamic simulation flow diagram for separator.

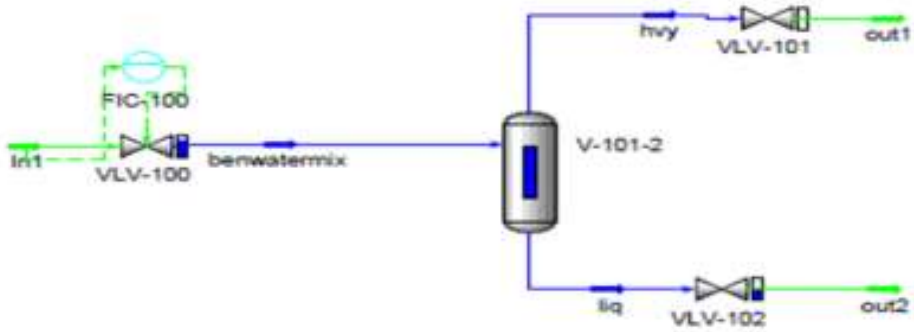


Figure 2: Dynamic response of PID controller FIC-100.

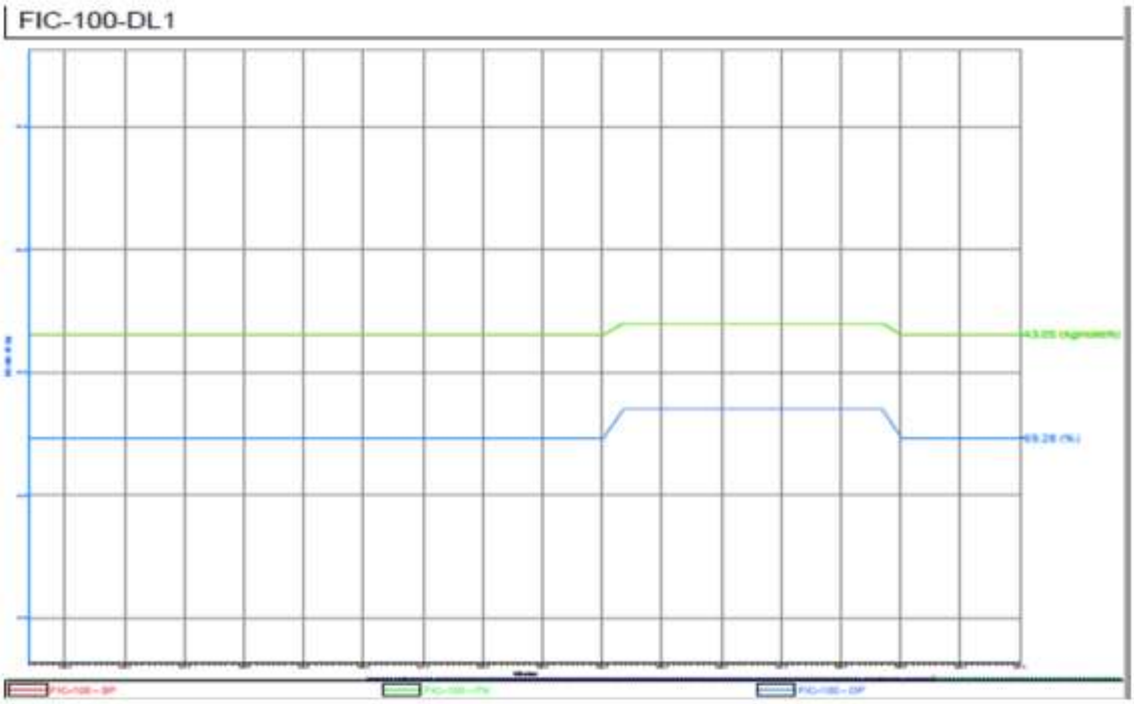
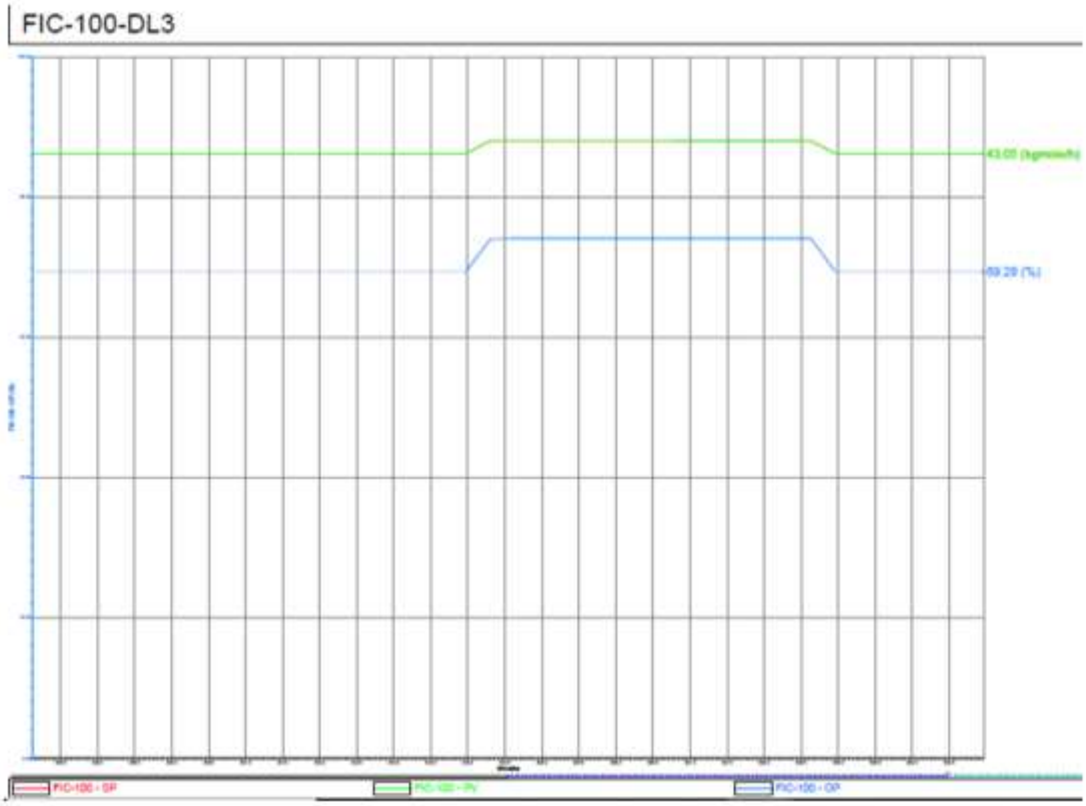
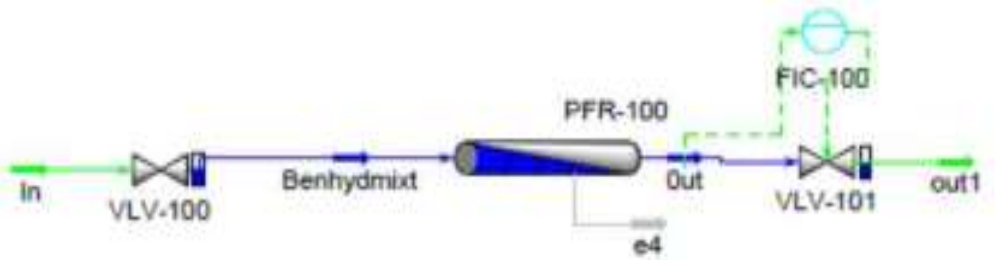


Figure 3 Dynamic response of PI controller FIC-100.



3.1.2 PLUG FLOW REACTOR- 100

Figure 1 Dynamic simulation flow diagram for plug flow reactor-100.



The flow controller controls the product flow rate. Here the product is cyclohexane at a rate of 99 kgmol/h. The first order transfer function with a time constant of some seconds is consistent, which means that first order fuction may be lag the response of the actuator position changes to the desired actuator position [14]. The controller tuning parameters are decided on using auto tuning. Two cases are considered here: In the first case, the PID controller is used for controlling the flow of the stream. The PID flow control unit is having gain constant Kc= 0.149, integral time constant Ti= 2.13X10-2 min. and derivative time constant Td= 4.74X10-3 min. The dynamic response of the controller that controls the flow rate is shown in figure 5. The second case indicates the PI flow control of gain constant Kc= 0.123, integral time constant Ti= 4.03X10-

Figure 2 Dynamic response of PID controlled FIC-100 for PFR-100

3 min.

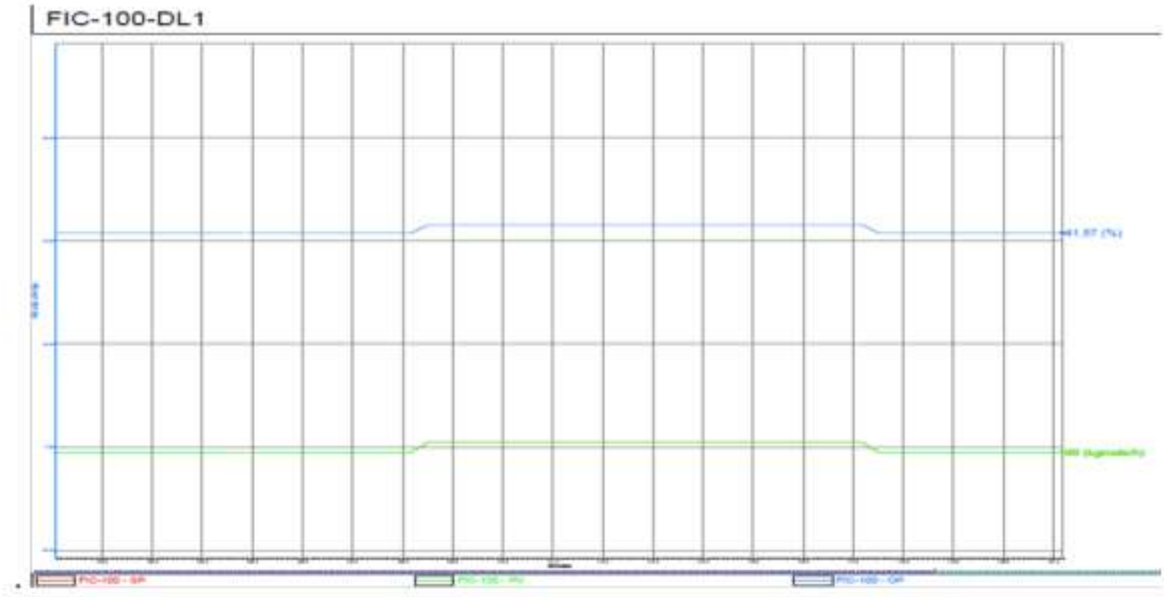
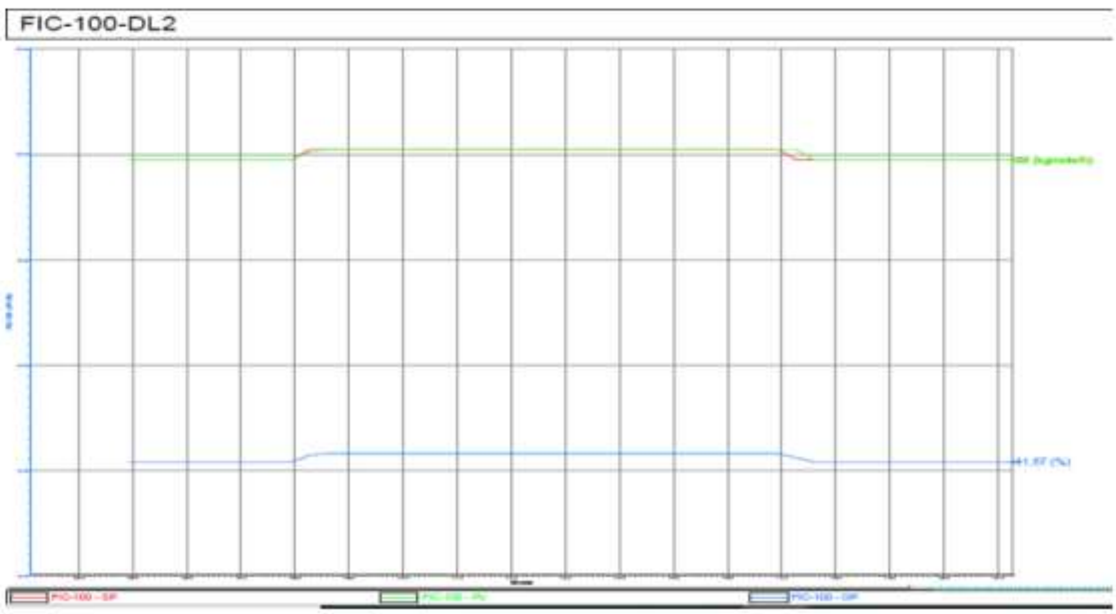


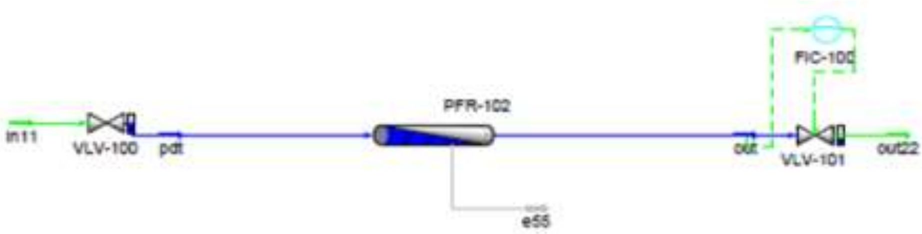
Figure 3 Dynamic response of PI controlled FIC-100 for PFR-100.



3.1.3 PLUG FLOW REACTOR- 102

The final product of this project is cyclohexanone, and it is produced from the plug flow reactor at optimum temperature-pressure conditions. So it is important to control the flow rate of the product leaving from the reactor.

Figure 4 Dynamic simulation flow diagram for plug flow reactor-102.



In the dynamic simulation of PFR-102, cyclohexanone flows at a rate of 86 kmol/hr and autotuning has been carried out for selecting the controller tuning parameters (figure 7). Consider some cases here: The first case shows (figure 8) the PID flow control unit using gain constant Kc= 0.118, integral time constant Ti= 2.15X10-2 min. and derivative time constant Td= 4.77X10-3 min. Figure 9 indicates the performance of the flow controller of PI. We introduced a small positive set change to the system and the disturbance was analysed. The PI flow control of gain constant Kc= 0.120, integral time constant Ti= 4.05X10-3 min.

Figure 5 Dynamic response of PID controlled FIC-100 for PFR-102.

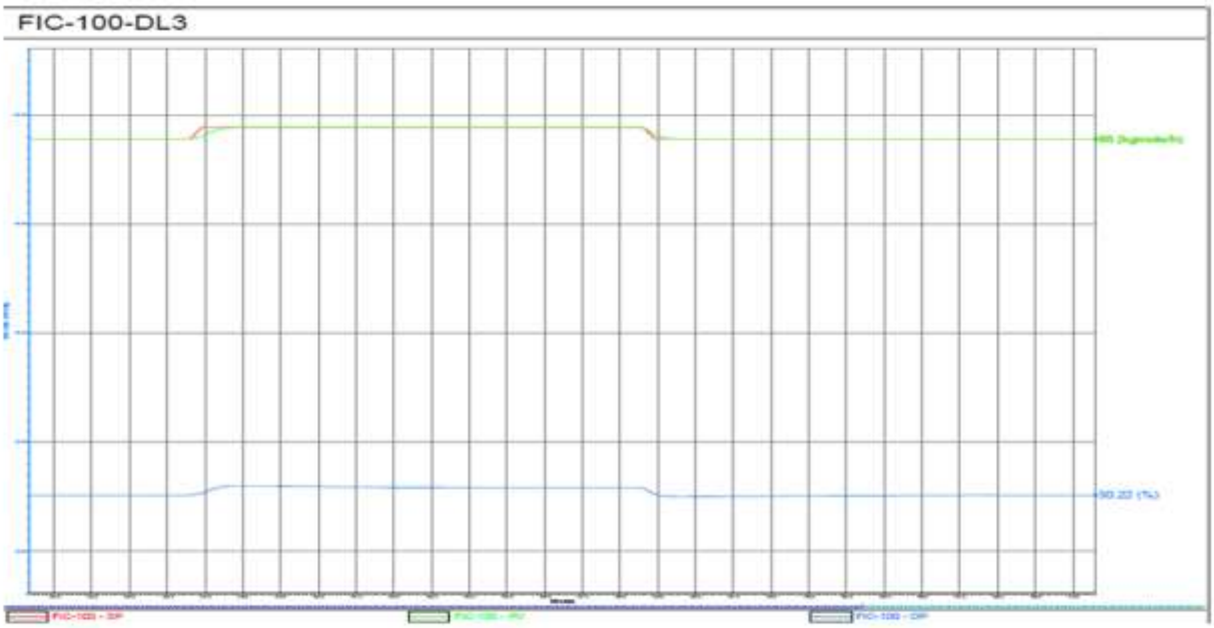
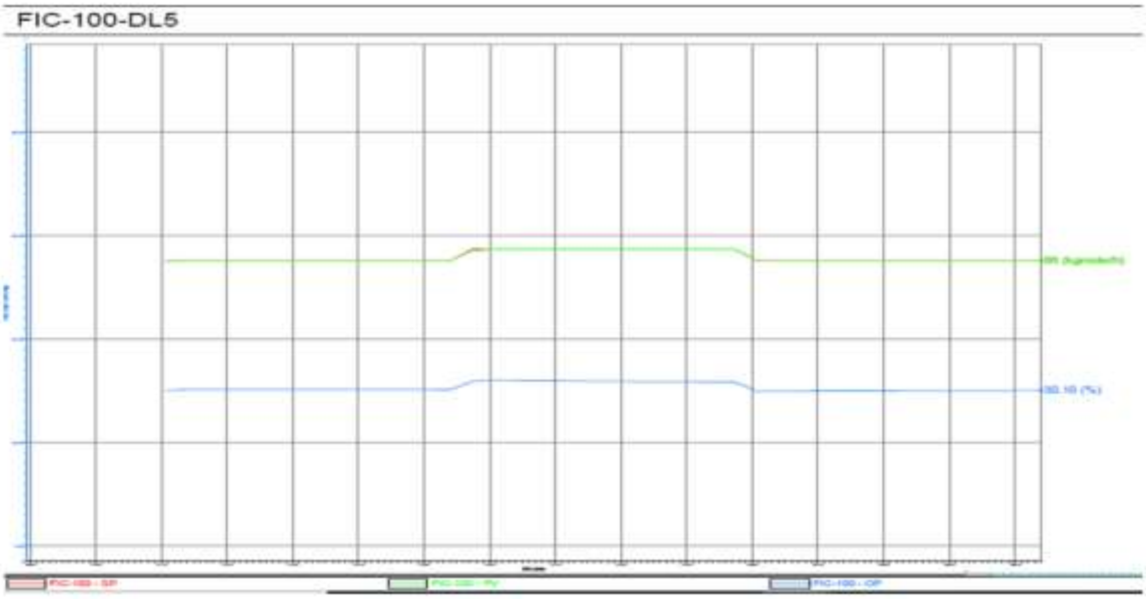


Figure 6 Dynamic response of PI controlled FIC-100 for PFR-102.



3.2 COMPARISON STUDY BETWEEN PI AND PID CONTROLLERS

Depending upon the controller tuning parameters, many of the systems have oscillatory responses, hence the selection of the best controller tuning parameters is very important. Commonly PI controllers are used in the majority of chemical process plants. A study of PI and PID controllers is carried out when it is generated in the dynamic system [8]. Tuning parameters can be selected based on auto-tune variation systems.

Parameter	Stability	Accuracy	Speed of response
Increasing Kc	deteriorates	improves	Increases
Increasing Ti	deteriorates	improves	Decreases
Increasing Td	improves	No impact	Increases

Table 3 Response comparison of PI and PID

The study inferred that the PID controller is better than PI controllers because there is no steady-state error when there is decrease in rising time, overshoot and settling time. This is due to the presence of derivative control action.

4.CONCLUSION

The paper presented the process description of the cyclohexanone production and dynamic simulation of the flow control. Dynamic simulation is done by using the software UNISIM R460. The Dynamic simulation of flow controller for the plant has been studied with the installation of different controllers. The controller parameters are selected in both modes (i.e., PI as well as the PID) and their results are compared. The flow rate of cyclohexanone is 86 kmol/hr, the values of gain constant and integral time constant obtained by using PI controllers are 0.120 and 4.02X10-3 min. respectively, whereas in PID the values of gain constant, integral time constant and derivative time constant are respectively 0.118, 2.15X10-2 min and 4.77X10-3 min. When disturbance occurs in the system, these two controllers take an action to maintain the flow rate. The performance of the PI and PID controllers are analyzed from the dynamic response diagram. From the results, we concluded that the PID controller is better than the PI controller. The selected controller parameters are controlled reasonably, but the PID controller has less speed when compared to that of the PI controller.

5.REFERENCES

1. A. A. Gaile, G. D. Zalishchevskii, N. N. Gafur, L. V. Semenov, O. M. Varshavskii, N. P. Fedyanin & L. L. Koldobskaya. (2014). Removal of Aromatic Hydrocarbons from Reforming Naphtha. Combined Extraction — Extractive–Azeotropic Distillation Process. Chemistry and Technology of Fuels and Oils. 40 (1), p215-221.
2. Ali Al-Matar. (2015). Selecting Fluid Packages (Thermodynamic Model) for HYSYS/ Aspen Plus/ ChemCAD Process Simulators. Aspen HYSYS. 1 (1), P1.
3. Adolfo Henríquez, Victoria Melin, Nataly Moreno, Héctor D. Mansilla & David Contreras. (2019). Optimization of Cyclohexanol and Cyclohexanone Yield in the Photocatalytic Oxo functionalization of Cyclohexane over Degussa P-25 under Visible Light. Solar Chemicals Production and Environmental Remediation with Semiconductor/Carbon Photocatalysts. 24 (12), p1.
4. Amine Mounaam, Yasser Harmen, Younes Chhiti, Ahmed Souissi, Mohamed Salouhi, Khalid Benjelloun, Mohamed Elkhouakhi & Laurent Deshayes. (2020). Dynamic behavior analysis of tubular heat exchanger: Experimental and theoretical study. International Conference on Renewable Energies for Developing Countries (REDEC). 1 (1), p1.

5. Angel Martin & Fidel A. Mato. (2008). Hint: An educational software for heat exchanger network design with the pinch method. Education for Chemical Engineers. 3 (1), p6-14.
6. C. Patrascioiu & M. Jamali. (2018). Crude Distillation Process Simulation Using Unisim Design Simulator. International Journal of Chemical and Molecular Engineering. 12 (7), p1.
7. Chao Seader & Grayson. (2013). Property Package Descriptions. Available: http://www.razifar.com/cariboost_files/Property_20Package_20Descriptions.pdf. Last accessed 22nd Aug 2020.
8. Chinju P T & Syama S. (2020). Process simulation and optimization of cyclohexane manufacturing plant using unisim and hint. Journal of Chemical Engineering & Process Technology. 1 (1), p1.
9. Emmanuel A. Dada & Luke Achenie. (2012). Production of cyclohexane from hydrogenation of benzene using micro reactor technology. Computer Aided Chemical Engineering. 31 (1), p240-244.
10. Greg Dolph. (2000). The use of dynamic simulation to develop control strategies for emergencies. Computers & Chemical Engineering. 24 (2-7), p1181-1186.
11. Hall S, S. Ahmad & Robin Smith. (1990). Capital cost targets for heat exchanger networks comprising mixed materials of construction, pressure ratings and equipment types. Computers & Chemical Engineering. 1 (1), p1.
12. Hon Loong Lam, Jirı Jaromır Klemes, Zdravko Kravanja & Petar Sabev Varbanov. (2011). Software tools overview: process integration, modelling and optimisation for energy saving and pollution reduction. Asia-Pacific Journal of Chemical Engineering. 21 (5), p48-7.
13. J. P. G. Kehoe & J. B. Butt. (1972). Kinetics of benzene hydrogenation by supported nickel at low temperature. Journal of Applied Chemistry and Biotechnology. 22 (1), p23-30.
14. Marsh K., Satyro M. A. (1994). Integration of Databases and their Impact on Process Simulation and Design. Conference, Lake Tahoe. 1 (1), p1-14.
15. M. G. Balaton, LNagy & F. Szeifert. (2013). Operator training simulator process model implementation of a batch processing unit in a packaged simulation software. Computers & Chemical Engineering. 48 (1), p335-344.
16. Rhodes C. L. (1996). The Process Simulation Revolution: Thermophysical Property Needs and Concerns. J.Chem.Eng.Data. 41 (5), p947-950.
17. Zamora J. M & Ignacio E.Grossmann. (1997). A comprehensive global optimization approach for the synthesis of heat exchanger networks with no stream splits. Computers & Chemical Engineering. 21 (1), pS65-S70