

## **Design and Control of Acrylic Acid Production Process**

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### **Abstract**

*This paper presents the design and control of acrylic acid production process using Aspen Plus and Aspen Dynamics. The design and control of acrylic acid production process has been studied. A plant-wide control structure is developed and demonstrated to provide effective control for large disturbances. Propylene reacts with oxygen and produces acrylic acid and water. Plant-wide operability and control of the entire acrylic acid production plant with controllers is explained. The results indicate that the proposed process gives good dynamic performance (a settling time of less than 3 h).*

**Keywords:** Aspen plus, Aspen Dynamics, dynamic performance, plant-wide operability

### **INTRODUCTION:**

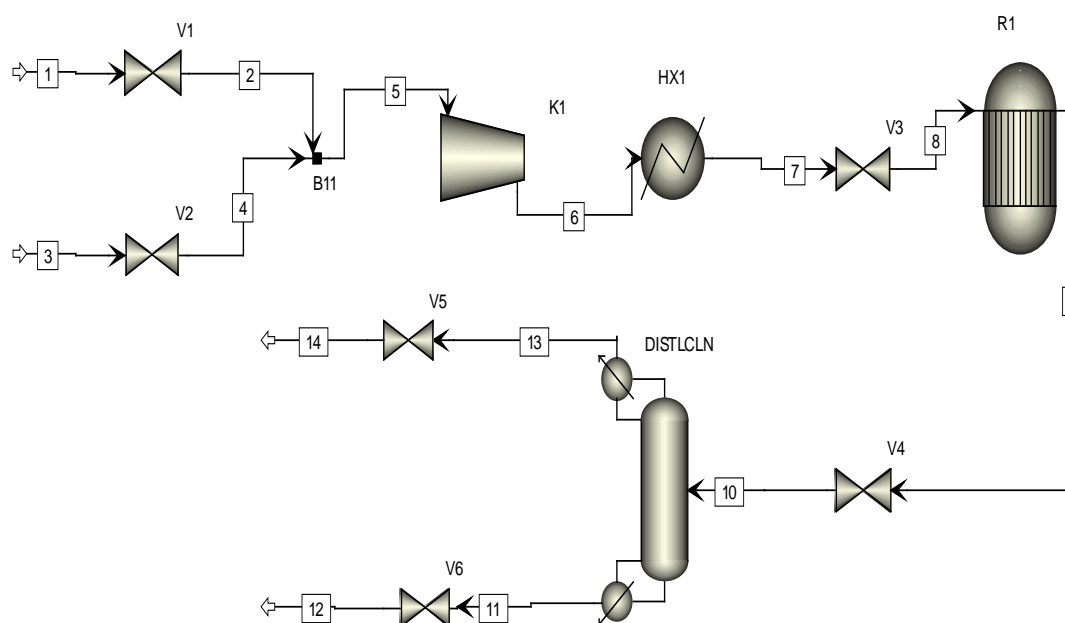
Process design involves the development of an effective flow sheet to transform raw materials into products in a profitable, safe, environmentally friendly, and controllable plant [1–4]. Acrylic acid is one of the primary materials used as a starting material in various commercial processes [4–6]. Because of its wide applications (in plastics, paper manufacture and coating, exterior house paints, treatment of sewage, printing inks, interior wall paints, industrial primers, textile sizing, leather impregnation and finishing, lubricating and fuel oil additives, pharmaceutical binders, etc.), this paper studies the process to convert propylene into acrylic acid. A Gibbs reactor is used to react propylene with oxygen to produce acrylic acid and a distillation column is used to separate the products from the reactor. Process plants are integration of several unit operations and the disturbances cannot be avoided; so it is necessary to control the process plant from various disturbances [5–13]. The above-mentioned problems motivated the present study to propose acrylic acid production process with plant-wide control structure to meet safe and efficient plant operation. The developed plant-wide control structure efficiency is tested with feedback relay tests with different conditions.

## PROCESS STUDIED

The process flow sheet is shown in Figure 1. The process developed is to produce acrylic acid (97% pure) using propylene and oxygen as raw materials. The Aspen NRTL physical property model is used in all units of the process.

### Compression and Reactor Preheating

Propylene and oxygen mixture feed at 298.15 K and 1 atm pressure is compressed in a compressor (K1) to 10 atm. The compressor consumes 5714.65 kW of electric energy. Compressed Propylene and oxygen gaseous mixture is preheated to 573.14 K in a heat exchanger (HX1).



**Fig. 1: Process Flow Sheet for Production of Acrylic Acid.**

### Control Valves (V1, V2, V3, V4, V5, and V6)

Control valves are used to control the flow rates of propylene feed, oxygen feed, inlet and outlet flows of reactor, and distillation column tops and bottoms. The types of valves used are adiabatic flash with specified outlet pressure.

### Reactor (RGIBBS)

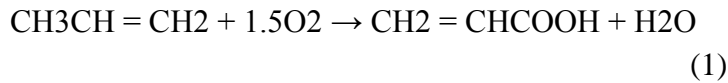
The Gibbs reactor is specified as tubular reactor with length 1 m and diameter 1 m, operating at 573.14 K which is the favorable condition for the reaction to take place in the reactor. The heat duty of the reactor is -65707.8 kW. Reactor effluent is at 573.14 K.

### Distillation Column (DISTLMN)

Outlet stream from the reactor contains propylene, oxygen, acrylic acid and water and it is the feed for separation in the distillation column. The numbers of trays in the column are 10. Condenser is partial vapor. Reboiler is kettle type. Reflux ratio is 2. Feed stream enters above the stage 5 of the column. Heat duty of the condenser is -15400 kW and the temperature is 389.83 K. Reboiler temperature is 506.32 K and heat duty is 10762.3 kW.

## REACTION KINETICS

The production of acrylic acid involves the oxidation of propylene in a high-temperature gas phase reactor.



The reaction is irreversible. The reactor should be operated at high pressure, which would raise the concentration of acrylic acid and drive the reaction toward the products from the Le Chatelier's principle; raising the pressure should drive the reaction toward the products since there are two moles of product generated from 2.5 mol of reactants.

Kinetics for the above reaction:

$$E_o = 15,000 \text{ cal/mol}$$

$$K_o = 159000 \text{ kmol/m}^3/\text{h}$$

Second reaction is



Kinetics for the above reaction:

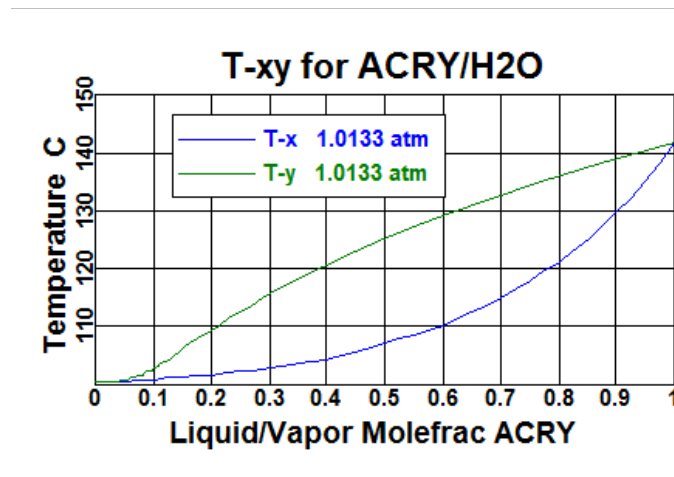
$$E_o = 20,000 \text{ cal/mol}$$

$$K_o = 883000 \text{ kmol/m}^3/\text{h}$$

All reaction rates have units of kmol/m<sup>3</sup>/h. Concentration units are molarity. From the above two reactions, the activation energy of the undesirable reaction is larger than that of the desirable reaction. As the second reaction selectivity is less compared to the first reaction, so it is not considered in the present problem.

## PHASE EQUILIBRIUM

NRTL physical properties are used in Aspen simulations. Figures 2–5 give T-xy diagrams for several binary pairs. They are acrylic acid/water, propylene/oxygen, acrylic acid/oxygen and acrylic acid/propylene. The boiling points of the four components involved in the process are quite different, so the separations are very easy. The normal boiling point of acrylic acid is 314.15 K, water 373.15 K, propylene 225.55 K, and oxygen 90.15 K. The separation is easy, so the resulting distillation column does not require a large number of trays. The T-xy curves are fairly fat, so the required number of trays and the reflux ratio (RR) in the distillation column are low.



*Fig. 2: T-xy Plot for Acrylic Acid and Water.*

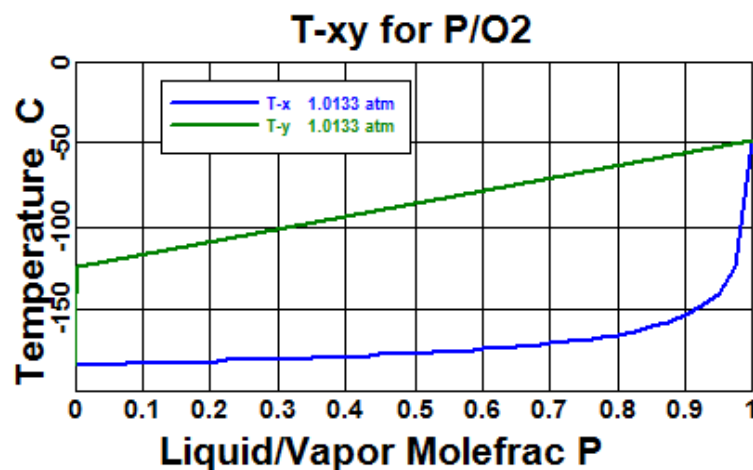


Fig. 3: T-xy Plot for Propylene and Oxygen.

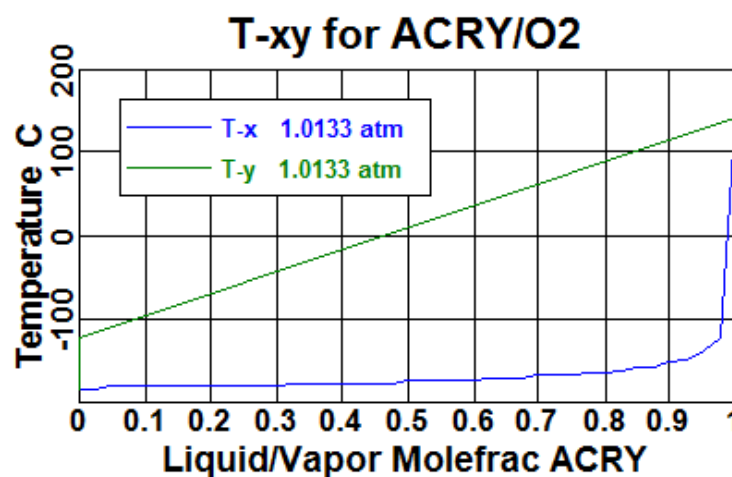


Fig. 4: T-xy Plot for Acrylic Acid and Oxygen.

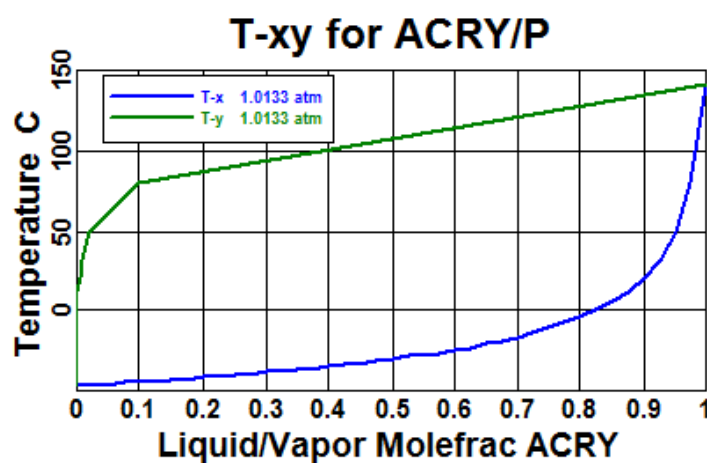


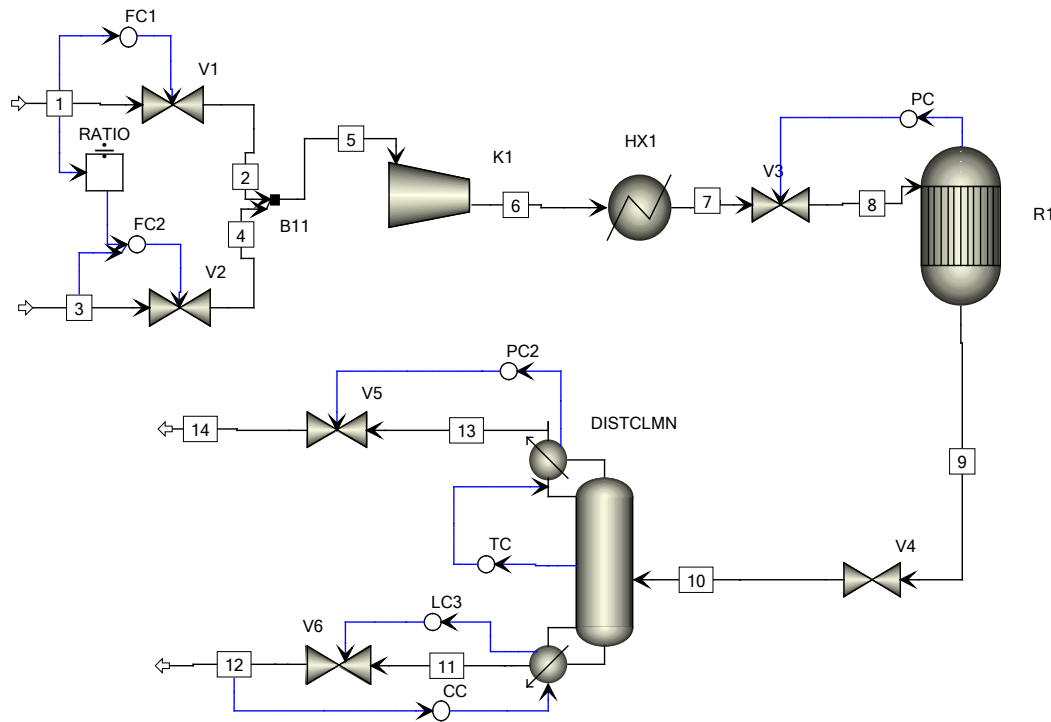
Fig. 5: T-xy Plot for Acrylic Acid and Propylene.

## EFFECT OF DESIGN VARIABLES

From sensitivity analysis, it is observed that increasing the pressure increased the production of acrylic acid and optimum temperature for the production of acrylic acid is identified as 573.14 K. The above observations can also be justified by using Lechatelier's principle. High pressure in the reactor favors the production of acrylic acid because of the increase in reactant partial pressures. High pressures drive the reaction from left to the right.

## PROCESS DYNAMICS AND CONTROL

For dynamic simulation, the size of the reflux drum and column base in the distillation column is sized to provide 0.19625 m<sup>3</sup> of liquid holdup. From the steady state design, the size of the reactor is 0.785 m<sup>3</sup> and the distillation column is 21.85 m<sup>3</sup>. Systematic plant-wide control structure development presented below is based on the heuristic procedure proposed and has been successfully applied to many industrial processes.



**Fig. 6: Plant-Wide Control Structure for Acrylic Acid Production Process.**

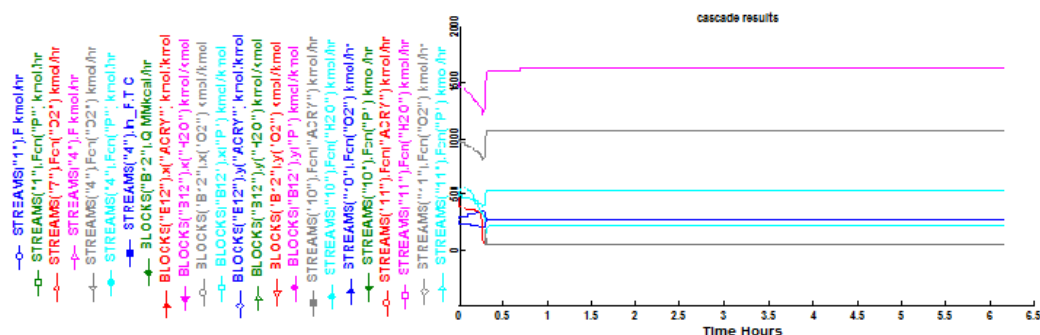
### Control Structure

Figure 6 shows the plant-wide control structure developed for this process. Before performing the dynamic simulations on the developed control structure using Aspen Dynamics, conventional PID controllers are used in all loops. All level loops are proportional with  $K_C = 1$ . Flow controllers that manipulate the flow to the compressor are a gain of 1 and an integral time of 20 min. The temperature and composition controllers are tuned by using relay feedback tests to obtain ultimate gains and periods, and then applying Tyreus-Luyben tuning rules.

The following are the loops used in the control structure with their controlled and manipulated variables and the results are shown as cascade results in Figure 7.

1. The propylene gas flow is controlled by manipulating the pressure.
2. The oxygen gas flow is controlled by manipulating the pressure.
3. A ratio controller is used to adjust the flow ratios of propylene to oxygen
4. A pressure controller(PC) is used to control reactor pressure by manipulating the heat duty of the reactor (reactor pressure disturbance comes to steady state at 2.97 h).
5. A composition controller (CC) manipulates the reboiler heat input.
6. Base liquid level in the column is controlled by manipulating bottoms' flowrate. This is the acrylic acid product stream leaving the process.
7. Reflux-drum pressure is controlled by manipulating distillate flow rate. This is the water and excess oxygen product stream leaving the process.
8. Column pressure is controlled by manipulating condenser heat removal (cooling water). Condenser heat duty is  $-15400$  kW, stage 1 temperature  $389.83$  K, reboiler temperature  $506.32$  K.
9. The temperature in stage 8 is controlled by manipulating reboiler heat input (low-temperature steam).

The throughput is set by the propylene and oxygen gases into the process, and inventory loops are in the direction of flow.



**Fig. 7: Cascade Plot for Process Variables of the Process.**

### Selecting Temperature/Composition Control Tray Location

Identification of the tray to be controlled in distillation is important. Several methods are available to locate this tray. The simple and effective approach is to select a tray for which significant changes in temperature are present. Figure 8 shows a large change in the temperature profile in the higher part of the column. Stage 8 is selected, which has a temperature of  $463.15$  K. Figure 9 shows the column composition profile.

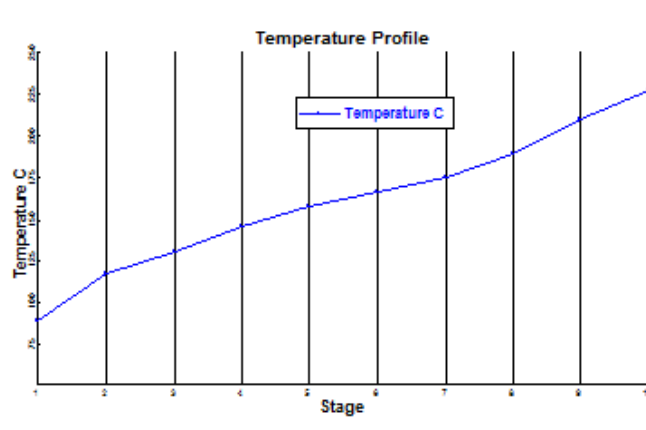


Fig. 8: Temperature Profile for Distillation Column.

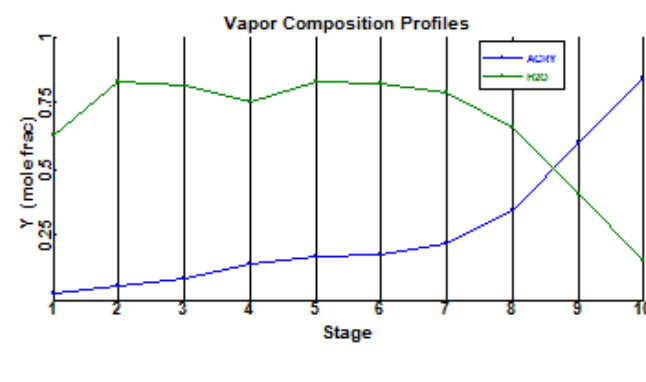


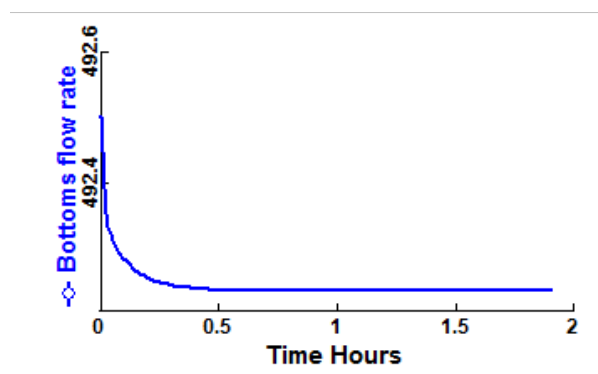
Fig. 9: Composition Profile for Distillation Column.

### Dynamic Performance Results

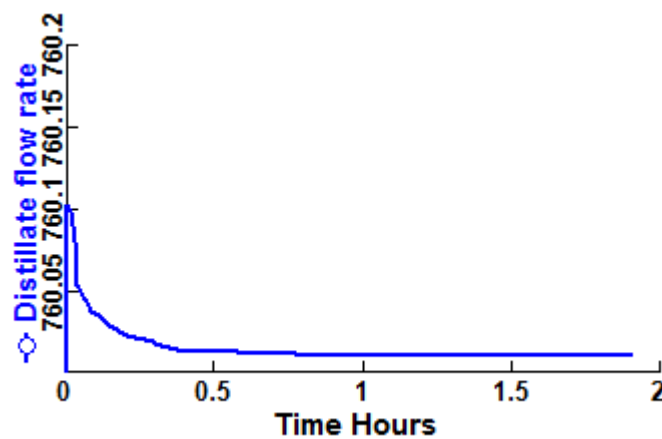
To test the ability of the proposed plant, disturbances are made. These disturbances include propylene and oxygen gas flow rates and compositions of compressor feed.

### Throughput Disturbances

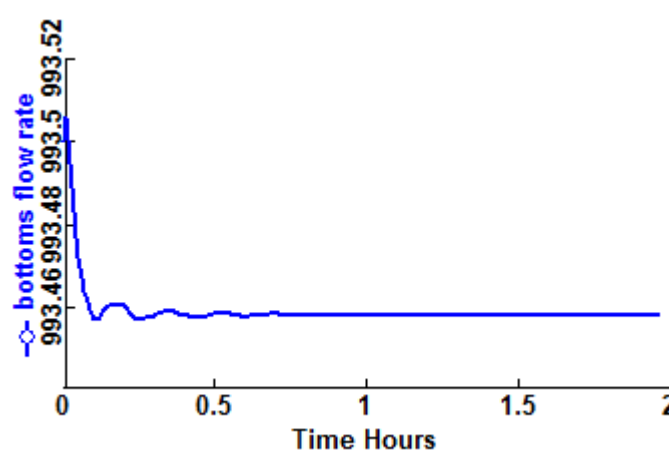
Figures 10 and 11 give the results for dynamic response of the process proposed and the time taken for steady state is less than 1 h. After that a 20% change in the set points of reactant gases are made and the responses of the plot are shown in Figures 12 and 13. They indicated that for a 20% increase in flow rates of propylene and oxygen, distillate and bottoms flow rates increased. A stage-8 temperature is controlled by manipulating the reboiler heat input and the corresponding temperature, pressure profiles of the column are shown in Figures 14 and 15.



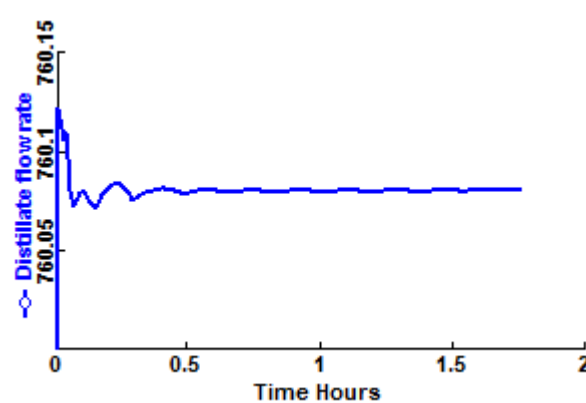
*Fig. 10: Response of Process for Process Conditions.*



*Fig. 11: Response of Process for Process Conditions.*



*Fig. 12: Response of Bottoms for 20% Increase in Feed Flow Rate.*



*Fig. 13: Response of Distillate Rate for 20% Increase in Feed Flow Rate.*

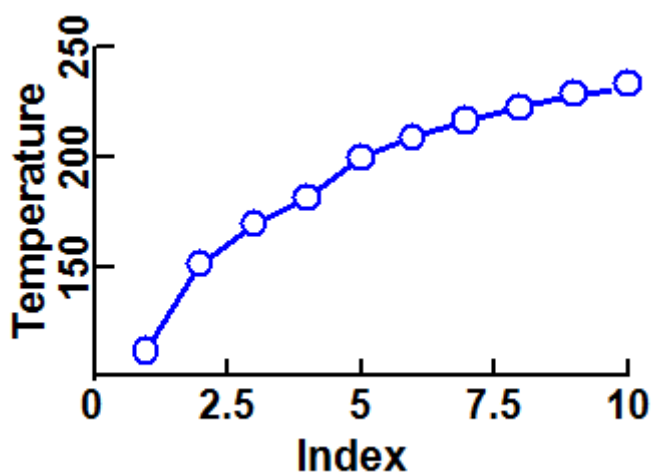


Fig. 14: Temperature Profile for Distillation Column.

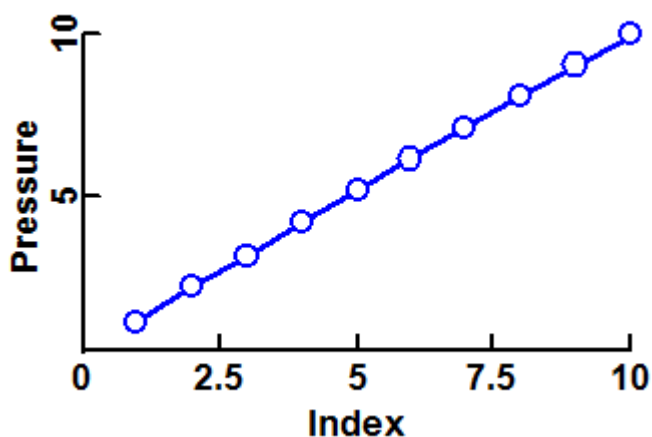


Fig. 15: Pressure Profile for Distillation Column.

#### Reactant Concentrations in the Feed

Propylene-to-oxygen ratio is adjusted by ratio controller. When there is a disturbance in propylene feed rate, the controller automatically adjusts the flow rate of oxygen 1.5 times of the propylene feed rate.

#### CONCLUSIONS

The design and control of acrylic acid production process has been studied. A plant-wide control structure is developed and demonstrated to provide effective control for large disturbances.

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