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# Application of Dynamic Simulation in Design of Isopropyl Benzene Plant

Yi Guo, Weisheng Yang*

Department of Development and Design, Sinopec Shanghai Research Institute of Petrochemical Technology, No 1658, North Pudong Road, 201208, Shanghai, China
yangws.sshy@sinopec.com

Dynamic simulation is a powerful tool for chemical process optimizing design, which gives an intuitionistic sight for engineer to understand chemical process and analyzing process design. In this work, a dynamic simulation model for the full flow isopropyl benzene plant is presented. The dynamic model is based on detailed configuration of equipment data from a 300,000 t/a isopropyl benzene plant. It was discovered that the benzene column has the problem of pressure fluctuation. The cause of this fluctuation was analysed and the solutions to solve problem were presented by using dynamic model. Emergency condition, and partial power failure, both were considered for isopropyl benzene column design. The dynamic relieving rate was calculated, and the results compared with that calculated from conventional method. In order to avoiding the relieving rate, high integrated protective system (HIPPS) was applied to the dynamic model. The results shown that (1) The reason of benzene column pressure fluctuation is that the solubility of propane in condensate is sensitive to process parameters. A pressure control scheme with tuned PID parameters was proved in good performance; (2) The relieving rate of isopropyl benzene column calculated from dynamic model decrease 65% compared with that of conventional method; (3) The relieving rate of isopropyl benzene column was cut to zero by using HIPPS.

## 1. Introduction

The chemical industry is a transnational, multiscale section that could elevate social economic development and the quality of life of the people, and featured with energy-intensive processes. There are some environmental and safety problems during chemical plant start-up, regular run and emergency condition. In current China, environmental regulations are getting more stringent. The administration pays attention to greenhouse gas reduction. As new chemical process development becomes more and more common, chemical engineers are confronting more unexpected process problems. Dynamic simulation developed from steady state simulation could describe chemical plant’s dynamic behaviour. This advantage of dynamic simulation could help process engineers in checking chemical plant’s flexible operation (Saracevic et al., 2017) and .identifying application model limits (Manenti et al., 2009).

Isopropyl benzene is a bulky petrochemical intermediate for manufacturing phenol, acetone and α-methyl styrene. In the industrial process, isopropyl benzene is produced by the alkylation of benzene with propylene, and the main by-product of the alkylation is poly-isopropyl benzene (Foureman, 1999). In early 1945, SPA method for producing isopropyl benzene from propylene were introduced, and benzene reaction were under the presence of acid catalyst. However, this method does not comprise transalkylation unit running under relative high molar ratio of benzene to propylene, the yield of isopropyl benzene of the process is less than 95 %. From the 1990s, companies including Dow, Sinopec, CD Tech, Mobil-Badger, UOP etc. successively disclosed the fixed bed process by using microporous zeolite as catalysts, which is capable of transalkylation feature. In the state of the art, benzene and propylene first react in an alkylation reactor, producing isopropyl benzene and poly-isopropyl benzene; and after being separated in a distillation system, the poly-isopropyl benzene mixes with benzene and the mixture is fed into a reactor filled with fixed catalyst bed for transalkylation (Shahid M et al., 2016).

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There are only few studies have been focused on dynamic behaviour of the isopropyl benzene plant. Luyben (2010) researched the effect of design optimization variables of alkylation reactor to plant wide energy costs, capital investment, and developed a control structure to handle large disturbances in production rate. Gera et al. (2013) studied an isopropyl benzene process control scheme for a large throughput range by dynamic simulation, they optimized a 12 steady state operating degree of freedom process for maximum hourly profit. Norouzi et al. (2014) developed a mathematical model to intensify an industrial-scale production process of isopropyl benzene, which obtained higher profitability and reduce the energy requirements of the process.
In all the above mentioned previous work, there are no full flow model of isopropyl benzene plant containing liquid phase alkylation and transalkylation reactor have been established, and still lack of analysing design flaws for the process and investigate the dynamic characteristic of emergency relieving of column with HIPPS. The purpose of this paper is to establish the full framwork of dynamic model, optimize the isopropyl benzene process control scheme and research the effect of HIPPS in a column under emergency condition.

## 2. Methodology

### 2.1 DYNSIM

Process simulation software DYNSIM version 5.2.1 was used herein. It is a dynamic version of PRO/II, and has the same components database, thermodynamic model, unit equipment like PRO/II. All these features making the software perform dynamic calculations and solve time-dependent case reliable.
To build a dynamic model, detailed parameters of process unit, like equipment, controller PID and valve etc. are required. Table 1 lists the typical parameters needed by different unit equipments.

*Table 1: Required parameters for different equipments in dynamic simulation*

| Equipment type | Reactor | Heat Exchanger | Column | Compressor |
|---|---|---|---|---|
| Structural parameters needed for model | Reaction kinetics, Catalyst parameters etc. | Area, Heat transfer coefficient for shell side and tube side, process flow referenced, Process CV etc. | Diameter, Actual tray number, Tray efficiency, Weir length, Outer weir height, Flow path number, Downcomer area etc. | Performance curve |

These unit equipment models coupled with rigorous thermodynamic, control models and electrical models enable the dynamic simulation to simulate all kind of process plant including process control system, safety control system and electrical distribution system etc. Figure 1 shows the characteristic structure of DYNSIM.

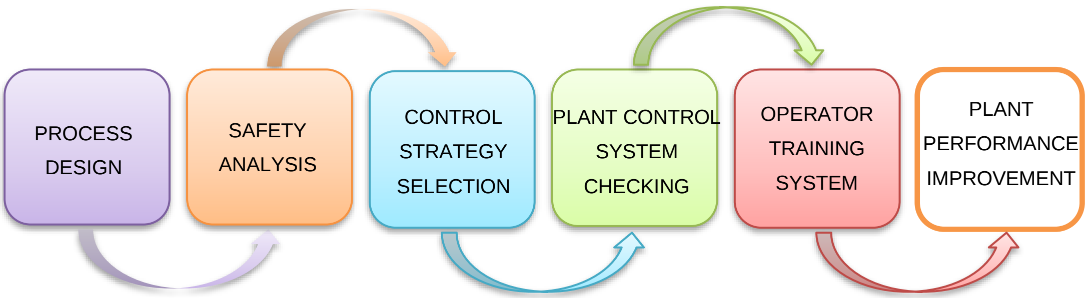
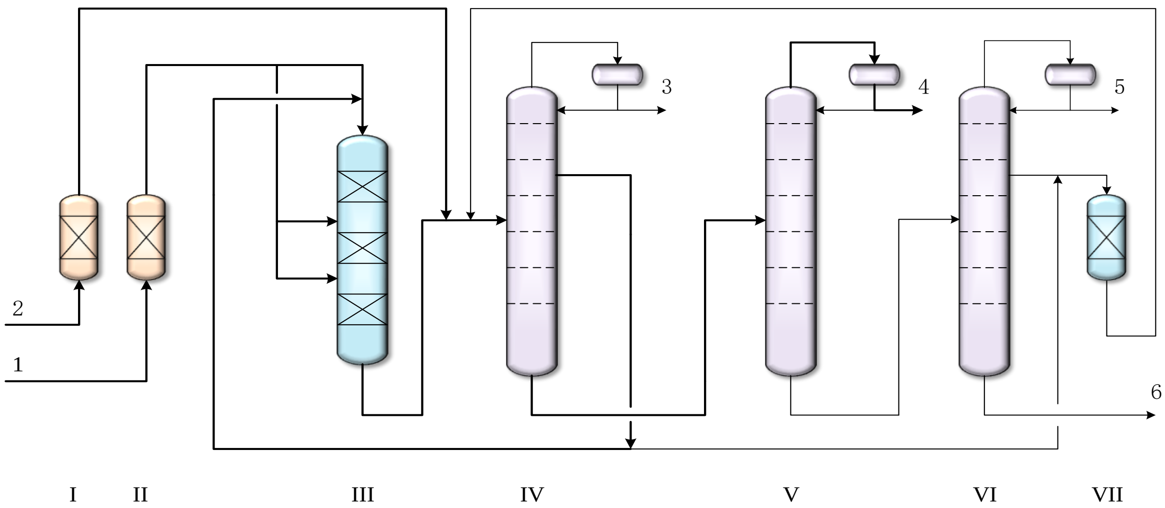



*Figure 1: Characteristic Structure of DYNSIM*

### 2.2 Simulation of the Isopropyl Benzene Plant

The capacity of investigated isopropyl benzene plant is 300,000 t/y. Figure 2 shows schematic process flowsheet of Isopropyl benzene plant. The plant is comprised of four parts, which are (1) raw material pre-treat system, consisted of I, II; (2) propylene and benzene alkylation reaction system, consisted of III; (3) transalkylation of benzene and poly-isopropyl benzene reaction system, consisted of VII; (4) fractionation system, consisted of IV, V, VI. In this process, benzene and propylene are raw material and isopropyl benzene is main product. Considering the components of isopropyl benzene plant are aromatics, propylene and tiny amount of water, Soave-Redlich-Kwong (SRK) method was used in the process simulation.




1 - Propylene, 2 - Benzene, 3 - Oil Water, 4 - Isopropyl Benzene, 5 - Oil Water, 6 – Light Tar
I – Fresh Benzene Pretreater, II – Propylene Pretreater, III – Alkylation Reactor, IV – Benzene Column, V - Isopropyl Benzene Column, VI – Poly-isopropyl Benzene Column, VII – Transalkylation Reactor

*Figure 2: Schematic Draw of Isopropyl Benzene Plant*

The main methods of building dynamic simulation are as follows:

- Since the Raw material pretreater remove trace impurities, it simplified to a pressure node without components change. The liquid reaction kinetics in alkylation and transalkylation reactor are regressed by pilot data.
- Material flow rate between unit equipment are solved by pressure balance equation. Reverse flow are considered in all equipment except check valve. Tray efficiency of distillation model is verified by steady state model and plant actual running data. The tray parameters influencing tray holdup and column pressure drop are adjusted according to actual column tray parameters.
- DYNSIM could calculate shell side and tube side dynamic heat transfer coefficient (HTC) respectively by associating the side HTC to a reference flow in that side according to Eq(1). Heat exchanger software HTRI was used to obtain data of HTCs and related reference flows. The parameter of $h_{exp}$ in Eq(1) was regressed by these data.

$$h = h_{ref}\left(w/w_{ref}\right)^{h_{exp}} \quad (1)$$

- Control strategy, PID parameters are the same with design data.

In the basic design stage, the dynamic model is a preliminary version which conducted by licensor normally. Some detailed parameters are estimated. This model does not fully represent the real plant features through the engineering corporation complete the detailed design, the missing parameters are determined and provided. Then the dynamic simulation model supplemented with these parameters gets improved enough to describe the real plant.

## 3. Results and discussion

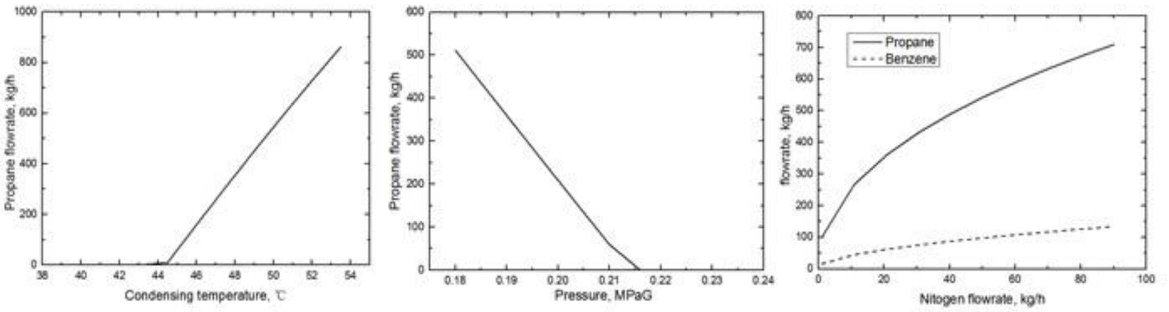
### 3.1 Start-up, running, and shutdown

The start-up, shutdown process are inevitable abnormal operations to chemical plant. For the first time commercial applying technology, it is important to use dynamic simulation for testing start-up and shutdown operations.

In the start-up operation, the dynamic model was running to 100 % design loading according to start-up procedure. When the dynamic model reaches steady state, the simulation results were compared to steady state model's results. Then the plant operating capacities was varied among the designed operation range to check if there are any bottlenecks for producing qualifying products.

It is found that the top pressure of benzene column fluctuates all the time and hard to reach steady state. For benzene column, the reactor effluents from alkylation and transalkylation, fresh benzene are inlet. Non-aromatics, trace water and a certain amount of benzene are distilled from top of the column as condensate. Propane is purge gas. Dry benzene is side draw as reactor inlet. The column is heated by 4.1 MPaG steam.

Because the amount purge gas is little, it has to choose split range control scheme for the top pressure. Low pressure nitrogen is make-up and non-condensable gas is purge gas. The top pressure controller is given a set of PID parameters. At steady state adjusted by manual, the purge gas of benzene column is 37 kg/h, but propane dissolved in the reflux is 3,625 kg/h, moreover, the reflux drum contains 1,020 kg propane.
In order to determine the reason of benzene column fluctuating, the solubility of non-condensable gas in condensate was calculated. It is inconvenient to perform case study by dynamic simulation so this calculation was done by steady state simulation. The column purge gas flowrate with variation impacts of top pressure, condensing temperature and make-up nitrogen flowrate are shown in Figure 3.




a b c

a – The purged flowrate change with condensing temperature, b - The purged flowrate change with top pressure, c - The purged flowrate change with nitrogen make-up flowrate

*Figure3: Process variation's impact on solubility of propane in condensate*

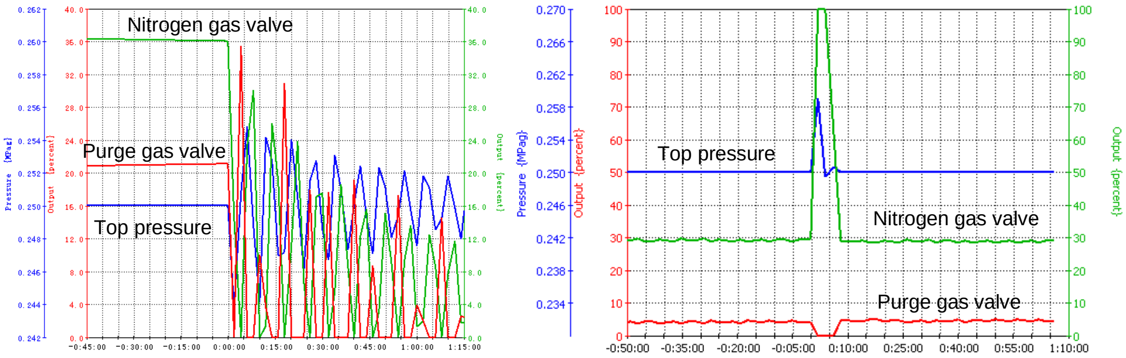
It is shown that at operating pressure if the condensing temperature rises 2 ℃, the flowrate of purged propane will change 118 %. That is because of the solubility of propane decreases while temperature rising. Similarly, when condensing temperature is 45 ℃, top pressure decreases 1 kPa, the flowrate of purged gas rises 25 %. In Figure 3c, when the make-up nitrogen flowrate increases 1kg/h, the flowrate of purged propane rises 1.4 %. That is because the partial pressure of propane in reflux drum as condenser decrease due to the nitrogen flowrate increase. If these process parameters fluctuating together, the flowrate of purged gas will greatly change which leads to the column's top pressure unstable.
Proportion, Integral, Derivative are the main parameters of PID controller. For a closed loop control system, the PID parameters are key points for its performance. Typically, the PID parameters were determined using experience. To pressure control loop, the time constant varies directly as the volume of system, the larger the volume, the bigger the proportion. The integral time is usually tens of seconds to a few minutes. PID parameter tuning is performed in two ways, one is theoretical method, the other is engineering method. The theoretical method is generally used for scientific research. The engineering method is an approximate method but widely used in practical operation. The engineering method is that the PID parameters are changed directly when the control variable is running and observe the transition of control variable. For the investigated plant, the initial PID parameters are given by experience and then change it on the running dynamic simulation to see the trend of control variable Table 2 lists the two set of PID parameters.

*Table 2: Control scheme with different PID parameters*

| Control scheme | Conventional parameters | Tuned parameters |
|---|---|---|
| Proportion | 1.51 | 9.89 |
| Integral time, min | 0.33 | 1.05 |
| Derivative | 2.1 | 2.1 |
| Control variable | Top pressure | Top pressure |
| Adjust variable | Make-up nitrogen and non-condensable gas | Make-up nitrogen and non-condensable gas |

Figure 4 is the top pressure curve with different PID parameters. At the beginning of test, the top pressure controller of benzene column was set in manual mode to adjust to steady state manually. What follows is that the top pressure controller was switch to auto mode, and then give the top pressure some disturbance, when the top pressure deviate from design point about 20 %~30 % withdraw the disturbance.

Figure 4a shows that the control scheme with experience PID parameters tended to converge the top pressure. But after 1.25 h, the top pressure still can't reach to steady state. On the contrary, in Figure 4b, the top pressure goes to steady state with tuned PID parameters within 10 min.




a b

a - top pressure controller with conventional PID parameters, b – top pressure controller with tuned PID parameters.

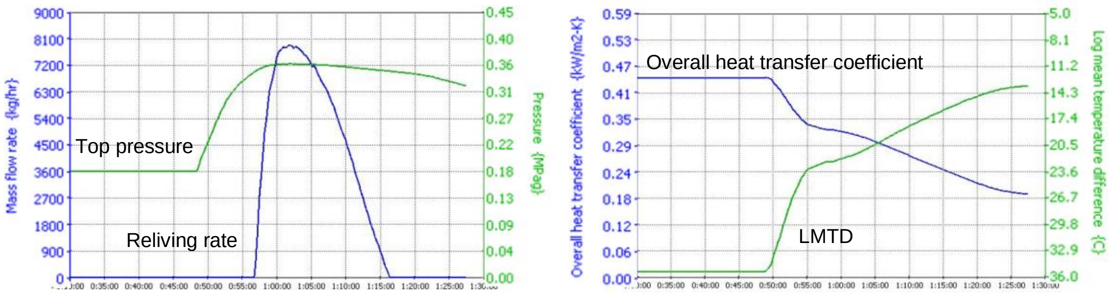
*Figure 4: Top pressure with different control scheme*

The tuned PID parameters were setup in an actual plant and proved to have a good effect.

### 3.2 Analysis of discharge under emergency condition

In actual production process, system overpressure occurs in conditions like personnel disoperation, equipment failure, utilities suspending etc. The overpressure could lead to safety accident like pipeline and equipment burst, injuries. Reliving analysis and discharge rate under emergency conditions are difficulties for engineering design. It is becoming a common sense that dynamic simulation could give an accurate analysis of relieving. In emergency condition, it is inevitable that some waste process fluid that contains hazardous material has to be discharged. It is of great beneficial to avoid relieving conditions.

Partial power failure is one of the severe emergency conditions that the pressure sources are still working while the outlet conveying equipment are failure. In order to simulate the partial power failure condition, the offline equipment of isopropyl benzene column system are set to reflux pump, cooled water supply pump, inlet pump, bottom pump. In the same time heat source, 4.1 MPaG steam is still working. The relieving rate and variation of other process parameters are shown in Figure 5.



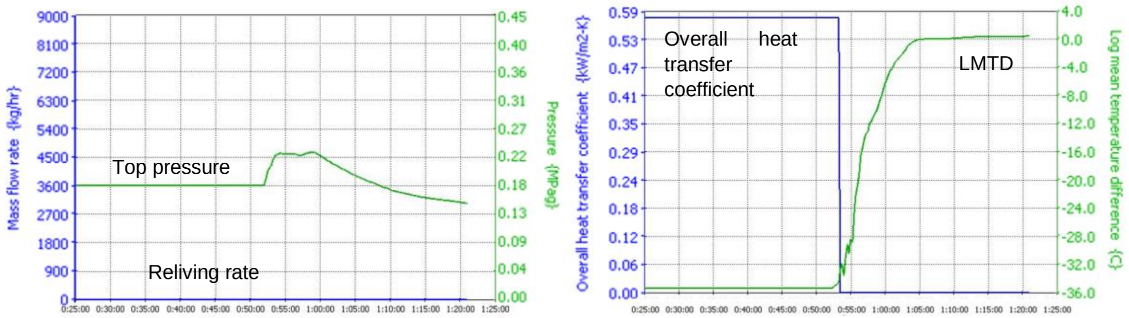

a b

a – Top pressure and relieving rate of isopropyl benzene column; b – total heat transfer coefficient and temperature difference of reboiler;

*Figure 5: Relieving rate and variation of parameters of isopropyl benzene column under emergency condition*

It is shown in Figure 5a that the relieving rate was about 7.8 t/ h. The accumulate pressure was 0.36 MPaG which was 1.06 times of design pressure of isopropyl benzene column. This means that the size of relief valve was selected properly. On the other hand, it will be 22.3 t/h of relieving rate given by conventional method which normally select the vapor flow from top stage as relieving rate. In figure 5b, the heat transfer process of reboiler shown that as the emergency condition come up, the heat transfer coefficient decreasing because of the rising of bottom temperature and pressure makes the cold flow of reboiler decreasing.

HIPPS is applied to prevent over-pressurisation of a plant or pipeline by shutting off the source of the high pressure. The HIPPS will shut off the source of the high pressure before the design pressure of the system is exceed. A HIPPS was setup in the isopropyl benzene column system. If emergency condition appears, the top pressure goes to the set point, HIPPS will active and shut off valve on the steam pipe. The dynamic behavior of the isopropyl benzene column with HIPPS in emergency condition was shown in Figure 6. The top pressure set point of HIPPS is 0.23 MPaG as an example.




a b

a – Top pressure and relieving rate of isopropyl benzene column; b – total heat transfer coefficient and temperature difference of reboiler

*Figure 6: Process parameters of isopropyl benzene column with HIPPS under emergency condition*

The emergency condition was appeared at 52 min., the top pressure went up from 0.18 MPaG to 0.23 MPaG in 2 min. At that time the HIPPS was active and shut off steam. It can be seen in Figure 6b that the total heat transfer coefficient plunged to zero because of interrupting of heat source. Then the top pressure of isopropyl benzene column moved down. Throughout the process, there was no relieving happened. The HIPPS effectively avoid relieving situation.

## 4. Conclusions

This paper gives detailed information about using dynamic simulation method to improve process design on the isopropyl benzene plant. Dynamic simulation could find out problems that wouldn't be appeared in conventional design method or steady state simulation. The benzene column top pressure fluctuation problems were found out, and the top pressure control scheme with a set of tuned PID parameters has been proved in good performances by dynamic model. The dynamic relieving rate of isopropyl benzene column in emergency condition based on actual equipment detail parameters was shown. High-integrity pressure protection system (HIPPS) was used for avoiding relieving. The model of isopropyl benzene column with HIPPS gives a reliable process results based on the mechanical dynamic model.

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