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Implementation of Dynamic Simulation to Study the Deviation Consequences Along a Complex Process

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The dynamic simulation of a chemical process is carried out to quantify the potential consequences that may arise in response to a deviation propagation. For this purpose, a case study is based on the industrial alkylation of benzene by propene to cumene with the production of a by-product (diisopropylbenzene). It consists of a packed bed reactor and a train of three distillation columns (C-1 to C-3). The presence of a recycle stream from the second distillation column to the reactor feed should be noted. This study examines various scenarios that describe the dynamic response of the alkylation process to a temperature reduction of the reboiler steam in one of the distillation columns. Then, the behaviour of the reactor and the separation unit is analysed to determine the consequences. The computational results show that the effects associated with a temperature reduction of 20 °C of the steam in C-1 can propagate through all the units of the chemical process. This result is due to an increased concentration of light hydrocarbons in downstream equipment. Therefore, a permanent overpressure and a vent release are observed at the top of C-2. On the contrary, C-3 only has a temporary pressure increase that is not high enough to open the safety valve of this column.

The objective of this study is to examine the influence of the characteristics of the process safety valve installed at the top of C-2 on the deviation propagation consequences. The results show how these effects are determined not only by the operating conditions of the equipment but also by the vent relief specifications. This study demonstrates in particular that dynamic simulations can be recognized as an important tool for safer industrial operations due to their capability of studying the process deviation propagation.

1. Introduction

The Process Hazard Analysis (PHA) is an important tool to identify and evaluate the potential hazards in an industrial facility and ensure process safety (Kang and Guo, 2016). The PHA methodologies allow assessing the risk levels of a scenario through the implementation of quantitative and semi-quantitative approaches. The HAZOP analysis is one of the most applied PHA methodologies in the industry. However, it is determined by the expertise of the analyst group and requires long hours of teamwork (Rossing et al., 2010). Hereby, the development of dynamic simulation-based quantitative methods is necessary to reduce the uncertainty of risk analyses through a deviation reasoning work (Salm et al., 2017; Tian et al., 2015).

The dynamic simulation-based risk methods can be performed by analysing the consequences and the dynamic response of a chemical process during the propagation of a previously defined deviation. This analysis describes the behaviour of a chemical process when an unwanted event occurs (Baldissone et al., 2017). For this purpose, a case study must be developed by considering the main characteristics of the process units such as equipment sizes, control structures, and relief devices. These specifications determine the dynamic response of the system to the propagation of a deviation occurred in one of its units. Thereafter, the simulation results allow establishing the magnitude of the deviations from normal operating conditions. Subsequently, the scenarios that may lead to serious accidents and the required safety barriers can be identified (Eizenberg et al., 2006; Luyben, 2012).

In this paper, the influence of the vent characteristics on the dynamic response of a chemical process to a deviation propagation is discussed. For this purpose, a case study evaluates a set of scenarios in which the specifications are modified in one of the relief devices.

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2. Case study

The analysis discussed in this paper is based on the industrial benzene alkylation with propene (Figure 1) in which 85.6 kton/y of cumene are produced with an efficiency of 95 %. The facility comprises a Packed Bed Reactor (PBR), four intermediate heat exchangers (E-1 to E-4), two pumps (P-1 and P-2) and three distillation columns with total condensers (C-1 to C-3). In this chemical process, two makeup streams are mixed with a recycle stream and fed to PBR in order to obtain a benzene/propene molar ratio equal to 7:1 and a flowrate of 807.1 kmol/h in the Reactor Feed (RF). The main products of the alkylation process are cumene and diisopropylbenzene (by product). Subsequently, the Reactor Outlet (RO) is fed to a distillation train in which the excess reagents and the products are separated according to the sequence proposed by Dimian and Bildea (2008).

- Column C-1 (12 bar): Non-reacted propene and propane are recovered in the distillate (D1).
- Column C-2 (3 bar): Non-reacted benzene is recovered in the distillate (D2). This stream is recycled to the reactor feed.
- Column C-3 (1 bar): Cumene is recovered in the distillate (D3) whereas the by-product is recovered at the bottoms (B3).

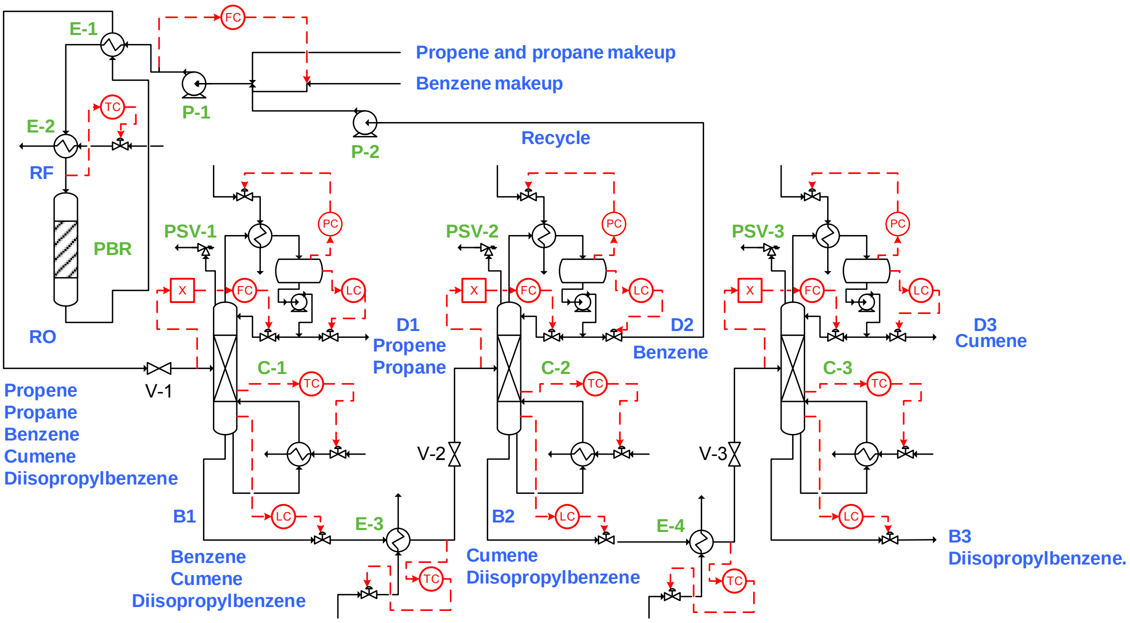

Figure 1: Process flow diagram of the benzene alkylation production

A set of scenarios is simulated in ASPEN PLUS DYNAMICS™ 9.0 in order to evaluate the variations in the operating conditions of an industrial unit after cooling the steam used in the reboiler of C-1. Kister (1990) established that the reduction of the heating efficiency in a column can induce an overpressure in downstream equipment. This fact is due to a significant decrease of the vapor flowrate of the column that generates its dumping condition. This abnormal operation results in an increase of the flowrate and the light compounds fraction of the feed stream of the downstream column. In accordance with this statement, the cooling of the steam of C-1 generates an overpressure in C-2 and downstream equipment due to the variations in their feeds. Moreover, the recycle of the distillate of C-2 to the reactor enhances the propagation of this deviation since the upstream equipment is also affected. The difficulty of the definition of safety systems is due in particular to numerous interactions among the chemical process units. This aspect is analysed in this study through the variation of the specifications of the relief valve of the column C-2 (PSV-2) and the description of the dynamic response of the chemical process to the temperature deviation occurred in the C-1 steam.

3. Pressure safety valves

The technical specifications of the pressure safety valves determine the vent flowrate when an overpressure is generated in a distillation column. Initially, these valves are defined with a linear dependency between the opening percentage and the vent flowrate (Figure 2b). Then, the nozzle diameters are calculated according to the DIERS sizing method and adjusted according to API 520 standard (American Petroleum Institute, 1993). This standard assigns a letter from D to T to the orifice size of each relief valve.

In this study, the steam temperature deviation induces an abnormal feed of propane and propane to the column C-2. Therefore, an excessive vapor rate is expected in this equipment due to its operation at a lower pressure (3 bar). This aspect is critical for this dynamic analysis. Indeed, the highest nominal distillate flowrate (615 kmol/h) is associated with C-2 due to the separation of non-reacted benzene. In fact, an excessive feed of light hydrocarbons to this tower leads to the opening of PSV-2 as well as an undesired benzene feed to C-3. For this reason, the sizing specifications of the relief valve of C-2 determine the main characteristics of the temperature deviation propagation.

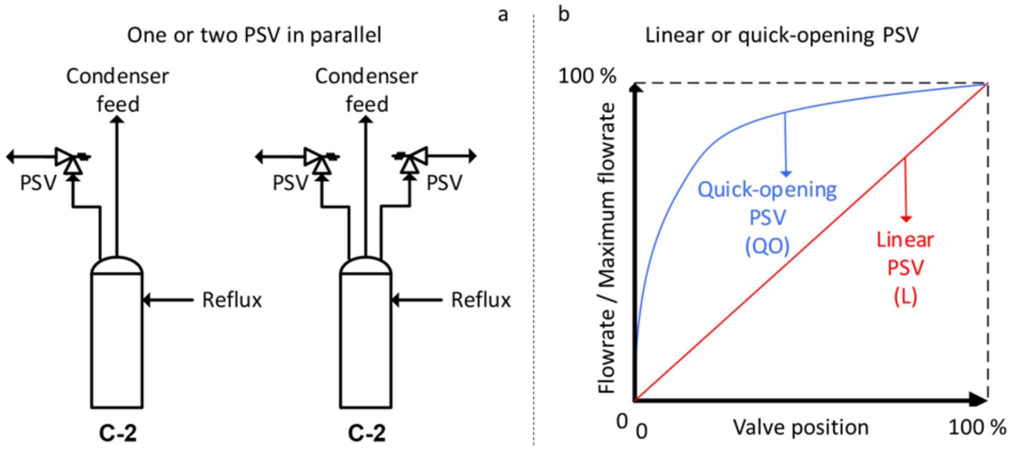

Figure 2: PSV-2 configurations

The influence of PSV-2 characteristics is studied through the simulation of a temperature deviation at the reboiler of C-1 with various process safety valves configurations. These options are listed in Table 1 and described in Figure 2. The simulation scenario number 1 represents the specifications established according the standard rules. The additional configurations are chosen according to two criteria: increase vent area and type of opening profile.

Table 1: Configurations of PSV-2 in the simulation scenarios

Simulation scenario	Reference	PSV-2 configuration	Nozzle diameter (m)	Total vent area (m^2)
1	L(T)	One linear opening valve (size reference T)	0.146	0.017
2	QO(R)	One quick-opening valve (size reference R)	0.115	0.010
3	QO(T)	One quick-opening valve (size reference T)	0.146	0.017
4	L(R) & L(R)	Two linear opening valves (size reference R)	0.115 & 0.115	0.020
5	L(T) & L(T)	Two linear opening valves (size reference T)	0.146 & 0.146	0.034
6	QO(R) & QO(R)	Two quick-opening valves (size reference R)	0.115 & 0.115	0.020
7	QO(T) & L(R)	One quick-opening valve (size reference T) & one linear opening valve (size reference R)	0.146 & 0.115	0.027
8	QO(T) & L(T)	One quick-opening valve (size reference T) & one linear opening valve (size reference T)	0.146 & 0.146	0.034

4. Simulation results

For each scenario, six hours of normal operation are initially simulated in order to ascertain that the process operates under a steady-state condition. Then, the steam temperature is reduced in the reboiler of C-1 from 212 °C to 192 °C and 19 additional hours are simulated for the analysis of the deviation propagation.

4.1 Propagation effects in the column C-2

Figure 3 shows the overpressures and vent flowrates that are established at the top of the column C-2 due to the loss of heating efficiency in the upstream column. The permanent reduction of the steam temperature leads to a continuous opening in all the relief device configurations. In spite of the similar tendencies observed in all the simulation scenarios, a difference is evidenced in the dynamic responses since the overpressure induced by the deviation propagation is greater when PSV-2 has a linear opening. Figure 3a also indicates that the overpressure levels can be lower if a configuration based on quick-opening valves is used at the top of the column.

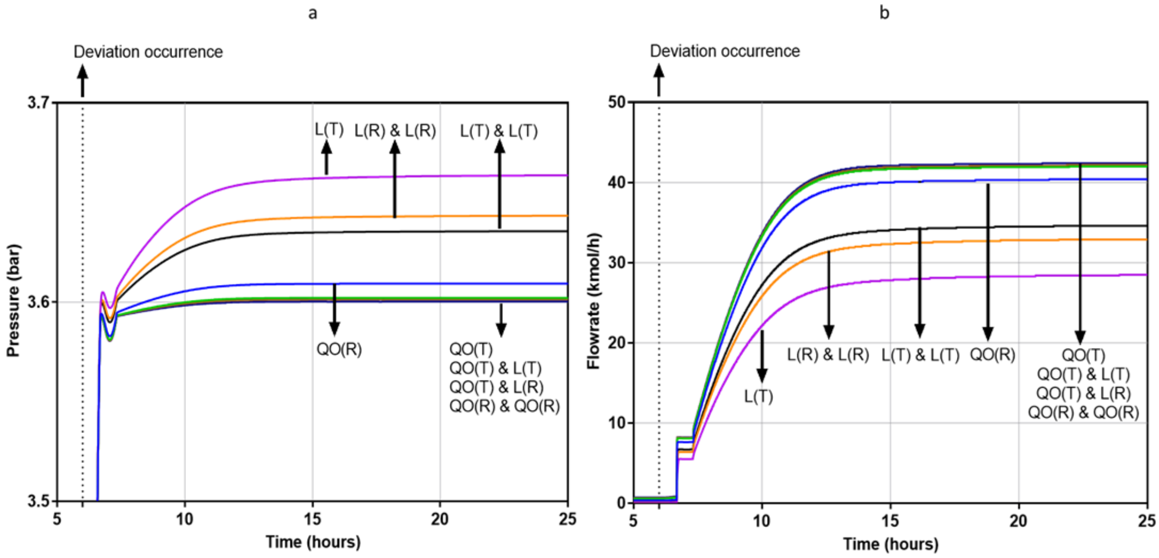

Figure 3: Pressure and vent flowrate at the top of the column C-2 after the loss of heating efficiency in the column C-1 (nominal pressure: 3 bar – PSV set pressure: 3.6 bar)

Moreover, the responses observed with the linear valve configurations are also determined by the total vent area. Hence, the excessive pressurization can be reduced with the installation of an additional safety valve as well. This result can be evidenced in Figure 3b and Table 2 by comparing the vent flowrate of the original safety valve (L(T)) with that observed with two linear process safety valves (L(R) & L(R) and L(T) & L(T)). The simulation results show that the introduction of additional safety valves can also be considered as an appropriate measure for the column operation. On the contrary, with the quick-opening configurations, the vent area does not have a significant effect on the flowrate value. Hence, the vent flowrate through these safety valves is not significantly affected by the addition of complementary safety valves or an increase of the nozzle dimensions.

Table 2: Maximum vent flowrate through PSV-2 after the temperature deviation at the reboiler of C-1

Simulation scenario	Reference	Maximum vent flowrate through PSV-2 (kmol/h)	Vent flowrate variation with regard to the L(T) configuration (%)
1	L(T)	28.5	--
2	QO(R)	40.4	+42
3	QO(T)	42.0	+47
4	L(R) & L(R)	33.0	+16
5	L(T) & L(T)	34.7	+22
6	QO(R) & QO(R)	42.4	+49
7	QO(T) & L(R)	42.1	+48
8	QO(T) & L(T)	42.2	+48

Finally, the simulations results indicate that vent flowrates can be increased by replacing the linear valve with a quick-opening one and increasing the vent area. Hence, the replacement of the L(T) valve with a QO(R) & QO(R) configuration is recommended. This option provides a better pressure relief capacity thanks to a greater vent flowrate (+49 %).

4.2 Propagation effects in the column C-3

The vent flowrate generated by the complete opening of PSV-2 is insufficient to release the light hydrocarbons. Hence, the deviation propagates to the column C-3. Figure 4 shows that different overpressure levels are also reached in this column since its operating pressure is lower than that of C-2. Unlike the second column, C-3 only evidences temporary effects during the deviation propagation due to the action of the control loops and the vent flow through PSV-2.

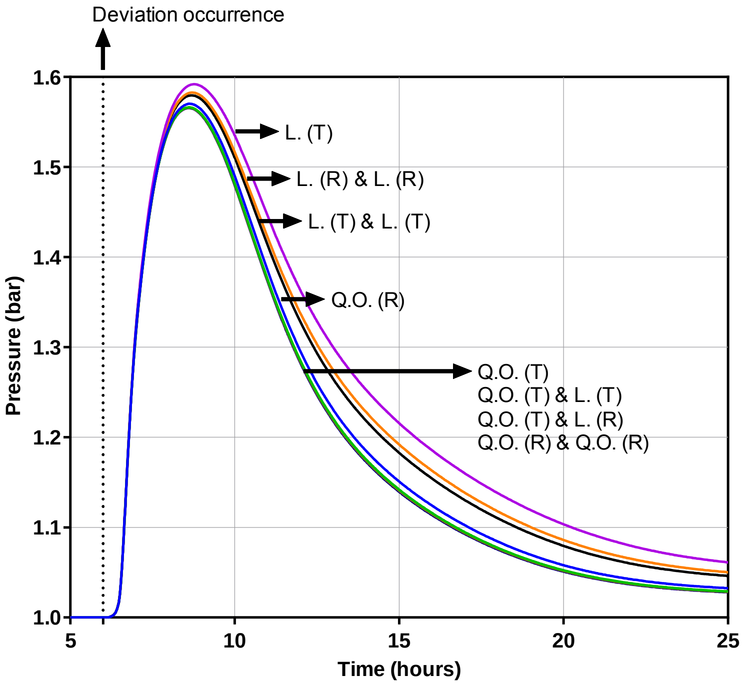

Figure 4: Pressure at the top of the column C-3 after the loss of heating efficiency in the column C-1 (nominal pressure: 1 bar – PSV set pressure: 2 bar)

Moreover, Figure 4 indicates that the abnormal column pressurization is not high enough to open PSV-3. Nevertheless, the pressure profiles show a tendency that agrees with the behaviour observed in Figure 3a. In fact, the maximum overpressure is reached by the L(T) configuration whereas the minimum one is obtained with the installation of quick-opening process safety valves. In addition, the use of linear safety valves in C-2 requires longer periods for the pressure reduction in C-3. For instance, the QO configurations stabilize at 1.05 bar approximately 14 hours after the deviation occurrence whereas L configurations require 5 additional hours to reach this condition. These results allow establishing how the various relief device configurations can generate different propagation effects in downstream equipment. For this reason, vent sizing calculations must not only consider an isolated equipment but also consider the influence of deviations occurred in other process units.

4.3 Propagation effects in the packed bed reactor

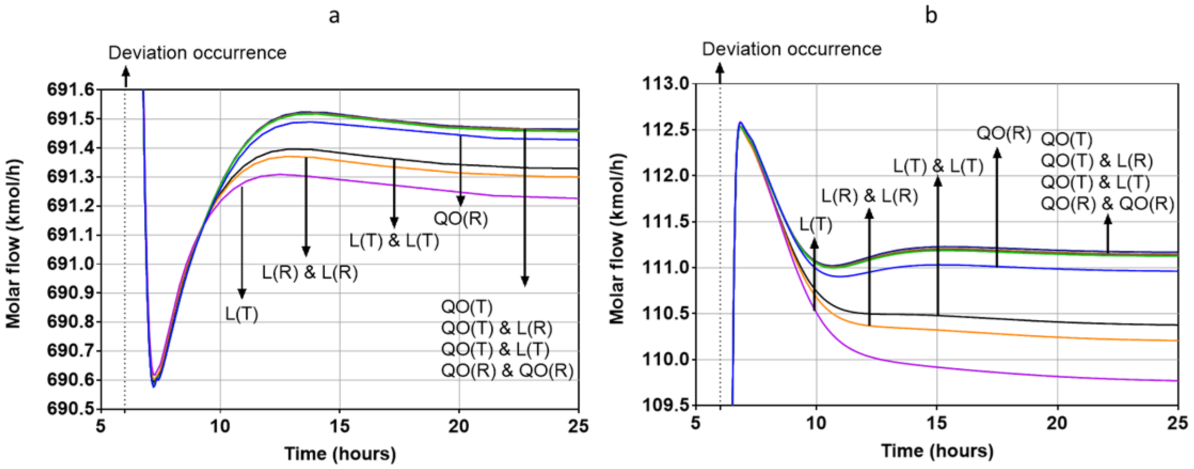

Figure 5: Variation in the reagent flowrates in the reactor feed
a. Benzene (nominal flowrate: 700 kmol.hr^{-1}); b. Propene (nominal flowrate: 100 kmol.hr^{-1})

The propagation effects can also be observed in the equipment upstream C-2. Figure 5 shows the variations of the reagent flowrates in the reactor feed. The action of the flow control loop after the deviation occurrence induces an increase of the propene flowrate and a decrease of the benzene flowrate. In consequence, the selectivity to cumene of the reaction process is affected negatively since the benzene/propene molar ratio reduces from its nominal value (7:1) (Murillo et al., 2018). Figure 5 indicates that the amplitude of this effect is also associated with the relief capacity of PSV-2. Indeed, the permanent variations of the recycle stream cannot be completely mitigated by the flow control of the makeup streams. This aspect constitutes the variation of the flowrates and compositions through all the chemical process and defines different operating conditions in all the process equipment. This fact confirms not only the importance of an appropriate specification of the relief devices but also the necessity of complementary safety barriers. At this moment, a safety instrumented system can be considered to place the plant in a safe condition if the process deviation leads to a hazardous event.

5. Conclusions

This study shows how the technical specifications of the process safety valves determine the propagation effects of a process deviation. In this case, the loss of heating efficiency in a distillation column (C-1) generates different overpressures in downstream columns (C-2 and C-3). The major effects are observed in the column C-2 since it is directly fed with the bottoms stream of the column C-1. The safety valve that is installed at the top of C-2 (PSV-2) opens to generate a vent release due to an excessive accumulation of light hydrocarbons. In the same manner, the performance of upstream equipment is also affected due to flowrate and composition variations of the reactor feed stream that are generated by the recycle of the distillate of C-2.

Moreover, the simulation results show that the amplitudes of the propagation effects are directly associated with the relief capacity of PSV-2. This variable is defined by the technical specifications of the safety valve. On the one hand, linear PSV configurations evidence a greater relief capacity when the vent area is increased. This can be achieved by increasing the nozzle diameter or including additional relief devices. On the other hand, quick-opening PSV configurations have the greatest relief capacities but do not evidence any improvement of their performance when the vent area is increased. For this case study, the major relief capacity was obtained with two quick-opening valves whose size reference is R (QO(R) & QO(R)).

Finally, this influence of the PSV specifications on deviation propagations shows that dynamic simulations can be considered as a decision-making tool for PSV specifications. This aspect must be considered since the overpressure in an equipment can be determined by the dynamic response of surrounding units or even the global process.

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