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Use of LOPA Concept to Support Automated Simulation-Based HAZOP Study

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This paper discusses the relation between hazard and operability study – HAZOP, mathematical modeling of processes and process control presented as the first layer of protection within general Layer of protection analysis (LOPA). In this work, these aspects are integrated in a new concept of hazard identification and operability study of the investigated process and both, steady state and dynamic, analyses are integrated in the methodology. The concept is able to identify hazardous regimes caused by parameter disturbances itself and also those when inappropriate control loop actions act synergic with already present disturbances. Thus, validation of the applied process control is provided. The concept is applied for the CSTR chemical process of catalyzed propylene glycol production under Proportional-Integral-Derivative (PID) actions. Under the investigated conditions, the process is characterized by the presence of strong nonlinearity and multiple steady state phenomena, which unpredictably affect the process control actions. Some hazardous events and operability issues were identified by the presented methodology and corrective actions were proposed.

1. Introduction

Hazard and operability (HAZOP) study is one of the best and highly disciplined techniques for identification of hazards and operability problems in chemical plants. Unfortunately, even such widely used systematic method has drawbacks and is often also time-consuming and labor-intensive, thus a computer-support tool to guide the study is needed. The latest overview of recent developments including support by CAPE (computer aided process engineering) methods and combination of HAZOP with other PHA has been provided by Pasman and Rogers, (2016). However, only a minority of such extended HAZOP studies are case studies based on mathematical modeling supported by dynamic simulations and other risk assessment techniques (Antonello et al., 2016). Regarding simulation part of published automated safety analyses, the use of commercial process simulators appears as an effective option. However, especially those discussing possible dangerous situations resulting from the existence of multiple steady states of the investigated chemical system (Li and Huang (2011) and Janošovský et al., 2016) refer about strong limitations for the simulation of processes operated near or within these nonlinear behavior regimes. To be rigorous, control and regulation systems need to be also integrated to the simulation environment. Basic process control is the first of various protection layers used to lower the frequency of undesired consequences (AICHE 2001). Here, LOPA provides a consistent basis for judging whether there are sufficient IPLs (Independent Protection Layers) to control the risk of an accident for a given scenario. Problem is that feed forward and feedback control as well as other safety loops unpredictably affect the propagation of disturbances mainly within the nonlinear behavior regimes of the process. Testing only processes with implemented process control in a commercial simulator by HAZOP deviations and their consecutive evaluation can bring situations where it is not possible to identify the root cause of a dangerous consequence. In other words, in these situations it is difficult to distinguish consequences caused by parameter disturbance itself from those caused by inadequate process control loop intervention. Thus, it is very important to test both layers: process itself and basic process control individually - layer by layer. Subsequent classification of root causes reveals parameter disturbances for which the investigated protection layer failed.

2. Methodology

The proposed hazard identification methodology combines two unique approaches of standard safety analysis study. Upper part of scheme in Figure 1 represents a typical onion diagram of LOPA with its IPLs. Second down-part shows simulation-based approach for automated HAZOP in many research studies of the last years, completed with simulation and hazard identification techniques proposed in this work. Strategy of the hazard identification methodology in this work is based on the integration of these two aspects by systematical testing of the process and first IPL in LOPA (control system) by HAZOP deviations, individually. These numerical deviations define parameter disturbances propagating through the investigated system during simulation testing. Testing of relevant IPLs is performed individually - layer by layer. First, generated deviations are simulated and applied just to the production process itself, providing reliable prediction of parameter disturbance effect on the process. Then, the same deviations simulation is applied to the process "covered" by a basic process control system while recording the control loop intervention. Testing of the first IPLs in this methodology can bring valuable information about the process operability safety and so support higher IPLs in the LOPA diagram e.g. Alarms and operator's actions.

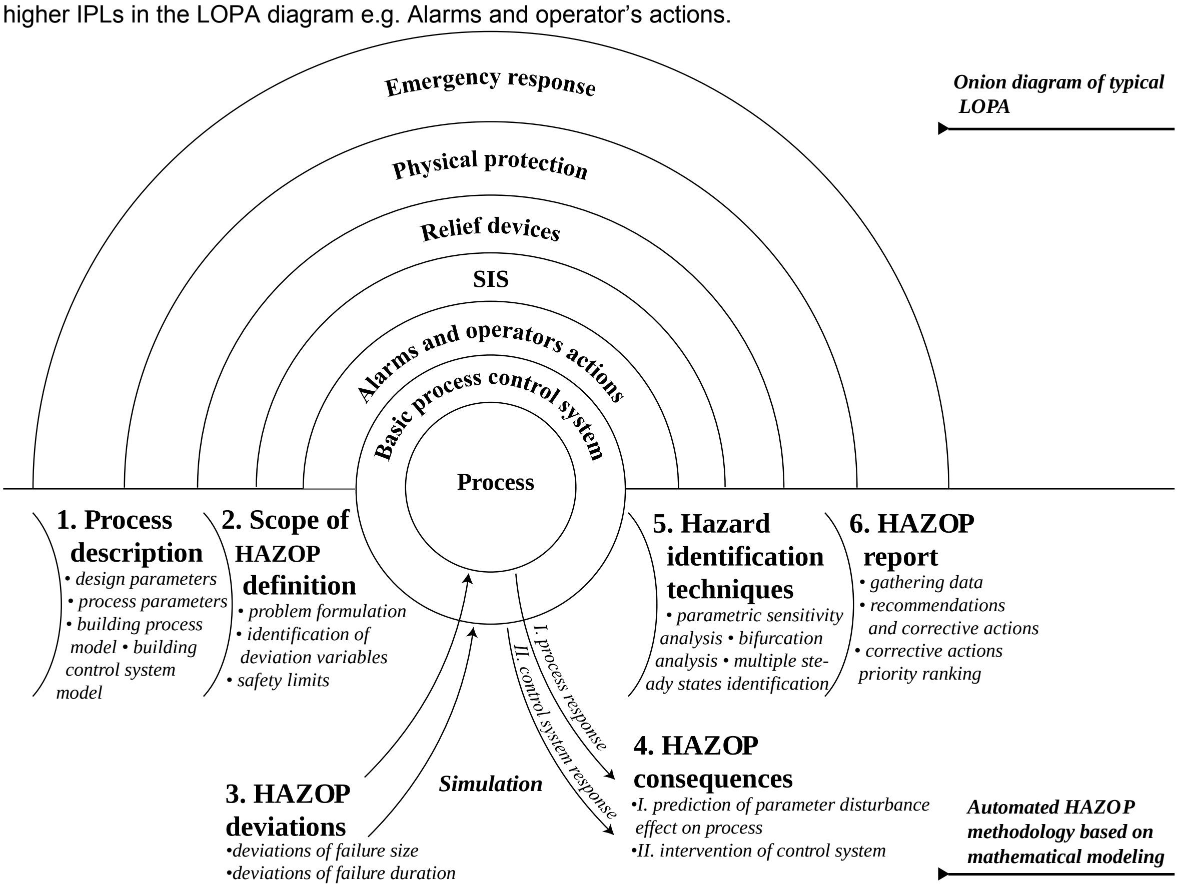

Figure 1. Proposed methodology diagram.

2.1 Process and control system description

Mathematical model of the process investigated in this work consists of standard material balances of compounds, enthalpy balances of the reactor and the cooling medium for CSTR. Mathematical model of steady-state simulation is represented by a standard system of nonlinear algebraic equations:

$$F(X, X^f, \alpha) = 0 \tag{1}$$

where X^f represents the vector of inlet conditions as concentrations of components and inlet temperatures of the reactor and cooling medium, X represents the vector of reactor outlet conditions in the same manner and α the vector of investigated operating parameters. Dynamic simulation of the effect of process parameter fluctuations on the reactor behaviour can be modelled using a system of ordinary differential equations:

$$\frac{dX}{dt} = G(X, X^f, \alpha) \tag{2}$$

with the initial conditions in Eq.3, where t is the time and X^0 the vector of initial conditions.

$$t = 0 : X = X^0 \tag{3}$$

To model actions of the control system layer, Eq. 4 as a classic interpretation of PI control actions, with controller gain k_c and integral time constant τ_I, was used. Controller functions minimizing any unexpected disturbances that may upset the process by introducing appropriate changes in the system manipulated inputs MI from its default value, MI0 and measuring output variable that has to be controlled, and compare it to a desired value T_{SP} (set point). The difference between measured output and T_{SP} is the error signal, i.e (Eq. 5).

$$MI(t) = MI_0 + k_c e(t) + \frac{k_c}{\tau_I}\int_0^t e(t)\, dt \tag{4}$$

$$\mathrm{e(t) = T(t) - T_{SP}} \tag{5}$$

2.2 HAZOP deviations simulating and hazard identification techniques

Multiplicity of steady states is expressed as the number of different sets of state variables for a fixed set of conditions or parameters. This nonlinearity may lead to serious incidents as small disturbances can drive the system away from a stable steady state to an unstable steady state. The aim of a future complex hazard identification tool is sequential testing of all deviations generated in the range of input parameter uncertainty. In regard to the focus and scope of this work, to identify and present weaknesses in the designed process and control system, four limit deviations in the PO feed flow rate (-17%, +30%, +66%, +120%) representing process conditions under which system stability changes were chosen and are further discussed. In terms of hazard identification, also evaluation of the number of dynamic simulations has to be done using the techniques mentioned in Fig. 1. Their combination with the continuation analysis has been successfully applied in previous papers (Danko et al. 2017). To make the hazard identification methodology as rigorous as possible, other issues like human factor related causes, lack of process knowledge or missing data, repeated deviations and scenarios and simultaneous multiple deviations have to be solved and implemented. As promising solutions for the study of situations when two or more process variables change at the same time, Monte Carlo methods together with the sensitivity analysis are applied. Further issues represent limitations in the currently proposed methodology. Their solving and implementation will be also challenge for future work.

3. Case study

The presented safety analysis methodology is demonstrated on a case study of propylene oxide (PO) hydrolysis to mono-propylene glycol (PG) carried out in a continuous stirred tank reactor (CSTR), where PO reacts with water to form PG in one exothermic reaction (Fig. 2). Kinetic parameters of the reaction were taken from Fogler (1999). Complete reaction data are listed in Table 1.

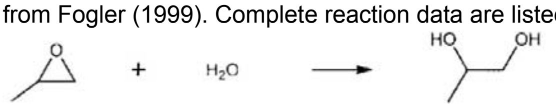

Figure 2. Reaction scheme of the mono-propylene glycol production process.

Table 1: Kinetic parameters for the Arrhenius equation

Variable	Units	Value
Pre-exponential factor	$m^3\ mol^{-1}\ s^{-1}$	96,000
Activation energy	$J\ mol^{-1}$	75,362
Heat of reaction	$J\ mol^{-1}$	-91,360

According Fig. 3, PO and water were fed into the reactor as two separate streams. Inflow temperature of both streams was 26°C. The reaction was carried out in a reactor with the volume of 2 m^3 and at the pressure of 2 MPa. At standard operating conditions, the molar flow rate of PO was 10 mol/s and that of water was 6 mol/s. The reactor was cooled with a jacket; the cooling medium, water, was fed into the jacket at the temperature of 15°C with the flow rate of 150 mol/s. Heat transfer capacity of the cooling system with the value of 7 kW/K was considered. Under these conditions, the reactor was operated at stable steady state at the temperature of 86°C and a 92 % water conversion, which is in agreement with data in Švandová et al. (2005).

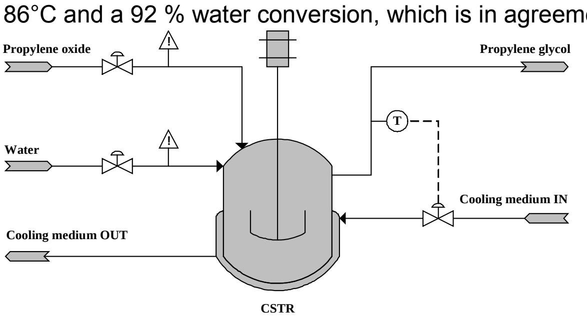

Figure 3. Simple schematic flow diagram of the investigated process.

The main aim of the investigated process is to produce PG with water conversion of above 90%. As conditions in the feed can vary due to different actual production requirements and unexpected failures, the output parameters, can fluctuate and so result in dangerous situations. Considering safe operation, temperature in the reactor should not exceed 97 °C, the point of safety temperature level. At this temperature, evaporation of a large amount of the reaction mixture occurs. Crossing this level is unacceptable. To prevent such situations, the basic control loop mechanism is introduced in the process. If the error signal is not equal to zero, a controller makes appropriate changes in one of the system manipulated inputs, MI (e.g., cooling medium flow rate, m_c) to force the output variable, T, to return to its set point, T_{sp} set to 86°C.

4. Results and discussion

4.1 PI parameters design

First task was to find PI parameter values with the best response of the system in the process referred to as controller tuning. Ziegler-Nichols step test method introduced in the MATLAB Simulink toolbox was used as support and the results were verified by the PIDDESIGN tool (Oravec and Bakošová 2012, Bakošová et al. 2011). Final values of PI parameters k_c of 0.2 and integral time constant τ_I of 12.5 were considered.

4.2 Steady state simulations of PO flow fluctuations consequences

In this work, only the PO feed flow was chosen as representative parameter to demonstrate the methodology. To identify possible multiplicity of steady states and their stability, steady states solution diagrams of reactor temperature as a function of the PO feed flow are depicted in Figure 4. First diagram (a) is important for the prediction of parameter influence where the system is under no control loop actions and the cooling medium flow rate is constant. Second diagram provides the whole picture of the influence of cooling medium flow rate dynamic changes as the manipulated variable input in the controller regulating actions. Figure 4 indicates that, for the designed operating feed flow rate of 10 mol/s, only one steady state is possible; however, with uncontrolled fluctuating, other multiple steady states including unstable (bounded by limit points) and oscillating ones (bounded by Hopf bifurcation points) can be achieved.

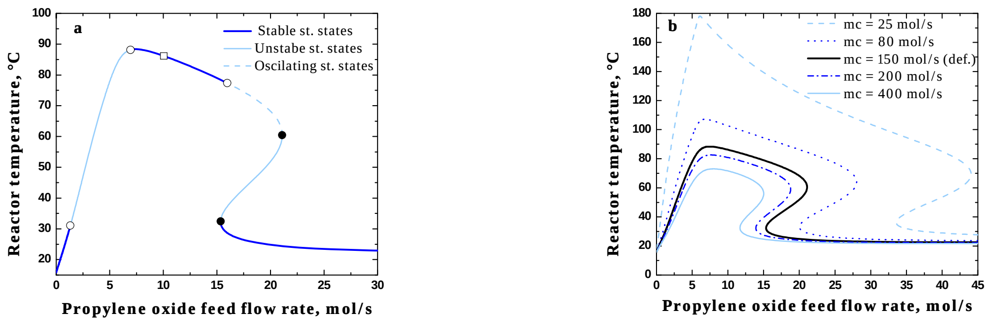

Figure 4. Steady state solutions diagrams: a) at constant value of the cooling medium flow rate of 150 mol/s, solid circle – limit point, empty circle – Hopf bifurcation point, empty square – normal operating point b) at different cooling medium flow as a controller manipulated input variable.

4.3 Dynamic simulations of consequences in a system with no process control

Consequences of PO feed flow fluctuations in a system with no process control were investigated to provide reliable prediction of the parameter disturbance effect on the process. In Figure 5 (first row), different responses of the tested protection layers on parameter disturbance in the process are shown.

Process-layer

Process with implemented control-layer

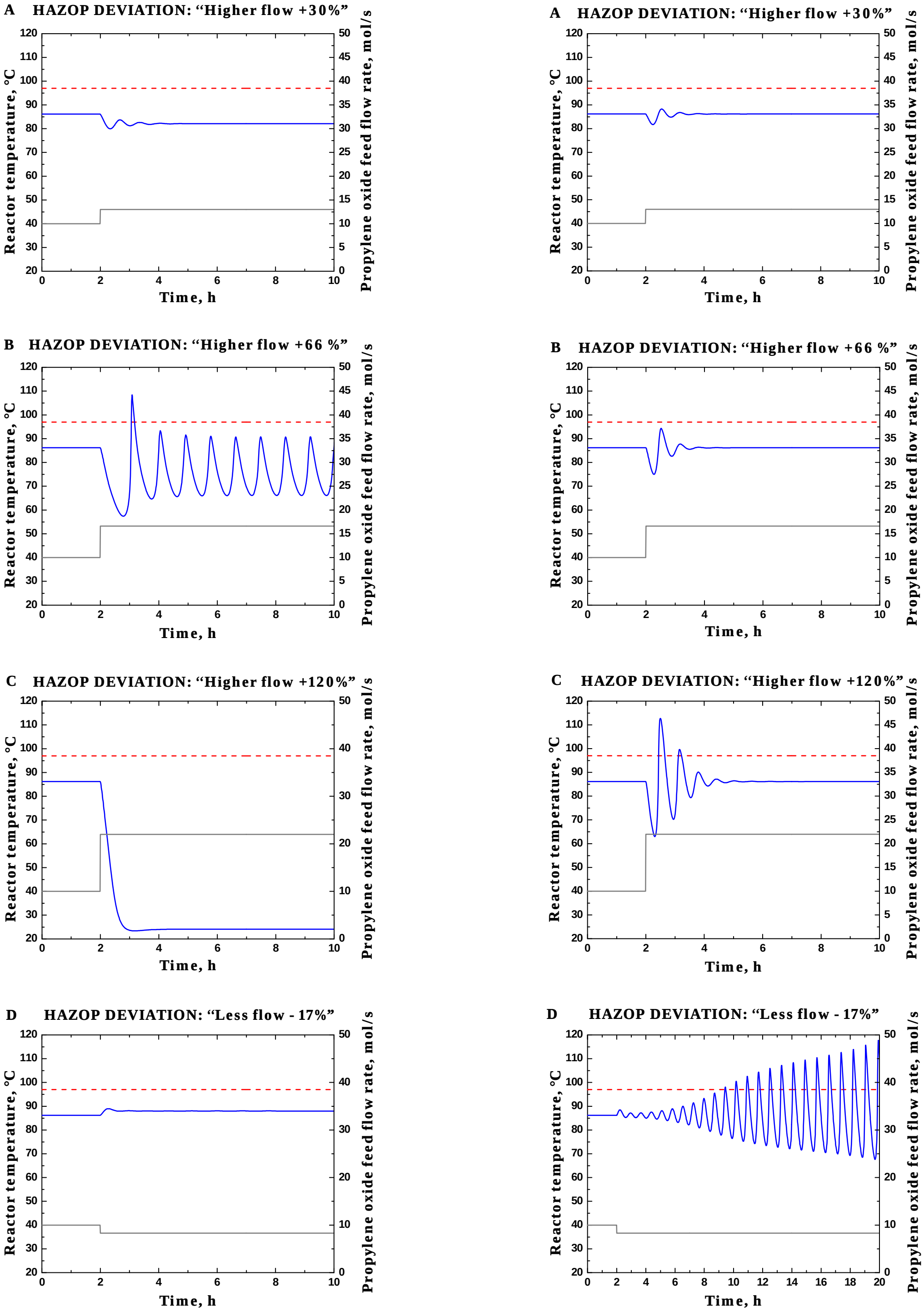

Figure 5.Different responses of tested protection layers on parameter disturbance in the process. Blue line – reactor temperature, gray line – PO feed flow rate (step change), dashed red line – safety temperature level.

4.4 Dynamic simulations of consequences in a system with implemented process control

As shown by the previous analysis of process layer testing, oscillating response and shift to another (lower) steady state were observed in simulation samples B and C, respectively. In the present section, testing of a process with implemented control system-layer, it is important to verify the controller actions especially in these two limit situations. As the controller is set to maintain the reactor temperature at the original steady state value of 86°C, actions are made by changes in the cooling medium temperature. As it can be seen, the control system successfully regulated the first two simulation samples (A and B) to the set point without any expressive overshoots. However, different situation in samples C and D were observed, while the controller acted synergically with the simulated parameter disturbance and worsened the situation. Here, the effect of oscillations initiation by the controller action was proven.

5. HAZOP report and conclusions

A new simulation-based methodology has been developed and used to support and improve the traditional HAZOP study considering also the process control as the first layer of protection. The presented concept is focused on nonlinear systems under basic process control and may potentially lead to the identification of some unexpected hazardous events. Higher PO flow by 120% and Less flow by 17%, are recognised as critical and synergic effect of controller action with a small parameter disturbance and initiation of oscillating behavior were proven. To complete the HAZOP report, recommendations and corrective actions should be suggested. Modifications in the reactor cooling system and using advanced control strategies can bring significant improvement in process safety. The presented concept requires a process model; steady-state analysis used for process stability investigation and dynamic analysis to simulate parameter deviations and process control actions. If such a model is available, the hazard identification concept provides a complementary and valuable input for the HAZOP team and plant operators.

Acknowledgments

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