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Development of a Software Tool for Hazard Identification Based on Process Simulation

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Computer-aided process engineering provides industrially widely applied software solutions that can be successfully exploited for safety analysis. In this work, simulation-based hazard identification tool with demonstrative applications is proposed. HAZOP study was selected as the base methodology and commercial simulator Aspen HYSYS was employed as the simulation environment. Two case studies, ammonia synthesis plant and propylene glycol production, differing in employed unit operations were selected to determine robustness and reliability of the proposed tool. Hazards and operability problems were identified utilizing advanced mathematical algorithms such as parametric sensitivity analysis coupled with runaway effect detection and steady state multiplicity identification. Reactive systems of both case studies are well known for their nonlinear behavior and the presence of steady state multiplicity. This phenomenon was successfully simulated using Aspen HYSYS built-in solver.

1. Introduction

During the last decade, industry has undergone a considerable change. The requirement of higher yields caused by economic pressure led to the modification of manufacturing processes towards extreme operating conditions. Therefore, robust process safety becomes even more important step in process design and optimisation. Hazard and operability (HAZOP) study is a highly efficient process hazard identification technique frequently used in chemical industry (Dunjó et al., 2010). The goal of HAZOP study is to investigate the causes, propagation and consequences of process deviations created by combining guide words with process parameters. The standard HAZOP study report contains all possible deviations, their causes and consequences, present system barriers to prevent hazards and operability problems and recommendations for process safety improvement (Kletz, 2001).

The lack of time and sufficient experiences of human expert teams are often the main problem in a HAZOP execution. The most frequently proposed solution of this problem is the introduction of computer-aided tools. There are two possible approaches: knowledge-based and model-based. Typical knowledge-based software tools, i.e. tools using a huge knowledge base containing information about past accidents including the failure mode, causes and consequences of process deviations, are HAZOPExpert (Vaidhyanathan et al., 1996) and TOPHAZOP (Khan and Abbasi, 1997). However, the knowledge-based approach has one significant disadvantage: the identification of all possible hazardous events relies only on large databases of experience which can lead to overlooking hazards in novel industrial technologies that are usually lacking vast experience with nonstandard operating regimes. This demand for more robust tools is one of the reasons, why the model-based approach has gained more attention in academic and industrial sphere in recent years (Pasman et al., 2018).

The model-based HAZOP study is based on the implementation of a mathematical model of a chemical process. Employed mathematical models strongly vary in their depth and detail. One of the possible approaches represents simplified mathematical model where mass, energy and information flows are interconnected in form of logical interactions, i.e. functional model (Rossing et al., 2010). This approach is more suitable for an early process design phase when quantitative models are not yet available and if complex potentially hazardous behaviour is expected, use of rigorous mathematical models based on conservation

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equations and equation of state is recommended (Wu et al., 2015). Advantages of the rigorous mathematical modelling use in hazard identification were demonstrated e.g. by Molnár et al. (2003) and Labovský et al. (2007). These works analysed chemical processes employing own mathematical models specifically developed for the unit operation under review. Such mathematical models are not generally applicable to other case studies. One of the possible solutions is the use of commercial process simulators which enable simulation of a chemical plant by adding and removing available predefined mathematical models of unit operations widely used in industrial practice (heat exchangers, distillation columns, reactors, etc.). A variety of commercial process simulators has been used in hazard identification, e.g. Aspen Plus (Jeerawongsuntorn et al., 2011), K-Spice (Enemark-Rasmussen et al., 2012), Aspen HYSYS (Janošovský et al., 2016) and Aspen Dynamics (Berdouzi et al., 2017).

The aim of this work is to propose the application of a model-based HAZOP study tool in identification of process hazards caused by perturbation in process parameters. The proposed tool implements Aspen HYSYS as the simulation environment to analyze process parameter deviations and their consequences. Firstly, description of software methodology is presented. In the second part, two case studies are introduced, ammonia synthesis plant and propylene glycol production, to demonstrate the applicability of the proposed software tool in hazard identification of complex chemical processes and to highlight advantages of the use of rigorous mathematical models in computer-aided approach to safety analysis.

2. Software methodology

The presented software tool consists of two independent modules. The first one, Process simulation module, provides data transfer between the presented tool and the simulation engine (Aspen HYSYS). In this module, the connection of our tool with the simulation engine is established and process parameter deviations from design intent are created and sent to the selected simulation engine for their steady state simulation. In contrast to conventional HAZOP study, simulation-based approach requires not only presence of the deviation, but also definition of its size. Currently, quantitative guide words NONE, MORE, LESS and REVERSE are implemented for the deviation creation. Qualitative HAZOP deviations are implemented partially by applying guide words MORE and LESS to the process parameters representing composition of material streams, e.g. mole and mass fractions. After the successful simulation of individual deviations, their consequences, i.e. simulated steady states, are stored for further analysis of their severity. For data storage, SQLite database engine is used. The second module, Simulation data analysis module, serves for the consequences investigation. Two different hazard identification approaches are applied. The first one is based on predefined advanced numerical methods that are fully automated. Methods such as runaway conditions identification, parametric sensitivity analysis, steady state multiplicity investigation, etc., are applied to simulation data to identify hazardous events and operability problems. These methods are discussed in more detail in our previous works (Danko et al., 2018; Janošovský et al., 2017). The second one requires user intervention and enables the customization of hazard identification procedure by defining the process- or equipment-specific threshold values that can be either determined by technical specifications or by operating staff experiences. Results of the hazard identification can be accessed through several visualization techniques and they are cleanly summarized in a simplified HAZOP report. Both modules and the data transfer logic of the whole software tool are more comprehensively explained in our recent paper (Janošovský et al., 2018). The presented software methodology is schematically depicted in Figure 1.

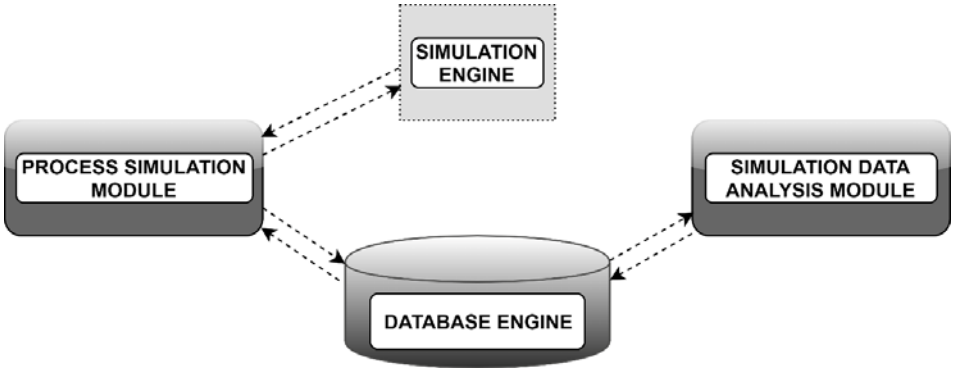

Figure 1: Simplified scheme of the presented software tool

3. Case studies

3.1 Case study 1 – Ammonia synthesis plant

As a first case study, ammonia synthesis plant is presented. The model of the plant consisted of syngas production from natural gas by steam reforming, syngas purification to produce hydrogen and ammonia synthesis loop that was represented by an adiabatic fixed-bed reactor composed of three beds in series with fresh feed quenching between each bed to adjust the optimum temperature profile in the reactor. The ammonia separation unit was also a part of the model. The analyzed plant flowsheet in Aspen HYSYS simulation environment is shown in Figure 2. Details of ammonia synthesis loop configuration were taken from the real industrial accident reviewed by Morud and Skogestad (1998) and appropriately implemented into Aspen HYSYS (Janošovský et al., 2015). Operating parameters of other segments of the presented plant model were firstly introduced in detail in our recent paper (Janošovský et al., 2018).

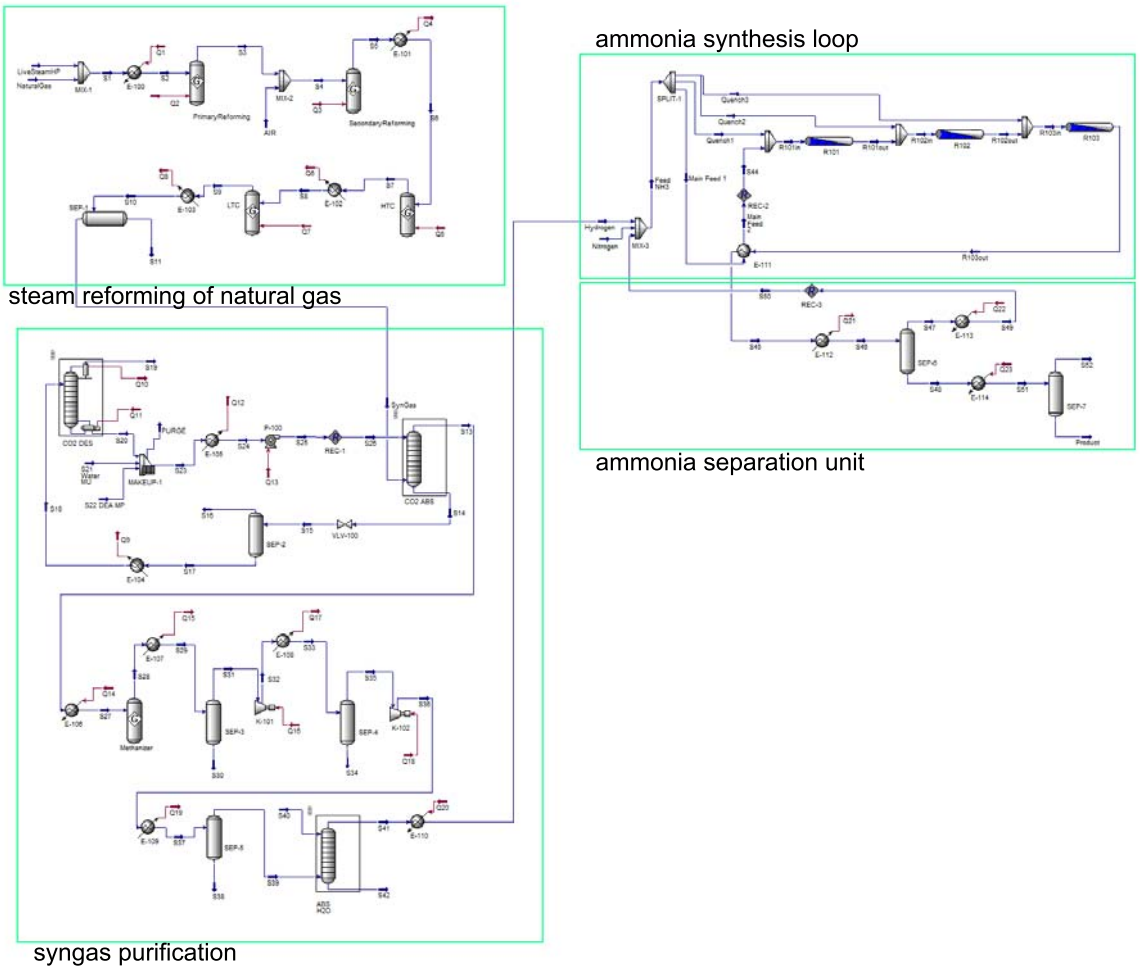

Figure 2: Ammonia synthesis plant flowsheet in Aspen HYSYS simulation environment

3.2 Case study 2 – Propylene glycol production

As a second case study, simplified model of propylene glycol production in continuous stirred tank reactor (CSTR) is presented. The model of CSTR was adapted from the prearranged Aspen HYSYS simulation template and additionally verified by data from scientific literature (Molnár et al., 2003, 2004). The reaction of propylene glycol production can be written as Eq(1). The reaction kinetics follows standard Arrhenius equation with the first order with respect to propylene oxide and water and reaction kinetics parameters were not altered from the Aspen HYSYS template. The process flowsheet is depicted in Figure 3. Vapor output stream as the second output stream from CSTR “reactor” was only required to authorize the simulation of CSTR in Aspen HYSYS. Its mole flow was zero in the design intent. Key operating parameters are summarized in Table 1. To increase the bubble point of the reaction mixture, process is carried out under elevated pressure

and methanol is added into the reactor. The reaction conversion achieved in this reactor configuration was 94.2 %. As a cooling medium, water with temperature of 10 °C and mass flow of $37.2x10^3$ kg/h was used. Total heat flow from reactor (the size of energy stream "Coolant") was $3.6x10^6$ kJ/h. Cooling was simulated via combination of "Reactor" and heat exchanger "E-100" connected by heat flow "Coolant". This configuration did not take heat transfer into account.

propylene oxide + water → propylene glycol (1)

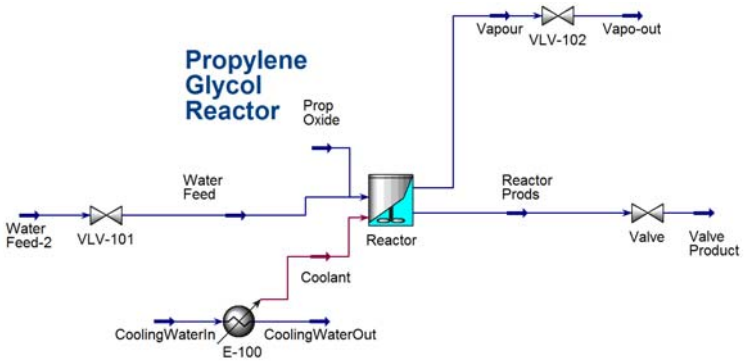

Figure 3: Propylene glycol production flowsheet in Aspen HYSYS simulation environment

Table 1: Operating parameters of propylene glycol production

Stream name	Water Feed	Prop Oxide	Reactor Prods
Temperature [°C]	107.0	23.9	43.5
Pressure [kPa]	130	130	130
Mass flow [kg/h]	4903	1654	6557
Mole flow [10^3 mol/h]	272.2	29.2	275.4
Mole fraction			
Propylene oxide	0.00	0.94	0.01
Water	1.00	0.00	0.89
Methanol	0.00	0.06	0.01
Propylene glycol	0.00	0.00	0.09

4. Hazard identification

Hazard identification of both case studies was carried out by the proposed software tool. Due to the limitations of this paper, only key findings are discussed further. To demonstrate the capabilities of the proposed tool, the figures are taken directly from the software environment.

4.1 Case study 1

Thorough analysis of deviations in every accessible process parameter of case study 1 was performed. Steady state multiplicity was successfully identified for the ammonia synthesis loop for deviations in pressure and temperature of the fresh feed (material stream "Feed NH3" of "ammonia synthesis loop" segment in the scheme depicted in Figure 2) using following simulation approach. Firstly, deviations were sorted by the deviation value in the descending order and simulated sequentially. Secondly, deviations were sorted by the deviation value in the ascending order and simulated sequentially again. This approach enabled mapping of solution branches created by stable steady states in the ammonia synthesis. Figure 4 represents the effect of these deviations on the temperature of material stream "R103out" that was the output stream from the third bed of the adiabatic fixed-bed reactor. Simulated steady states are clearly different based on the order of the deviations (descending – Figure 4a, ascending – Figure 4b). In the descending order, system was shifted in the lower solution branch where ammonia production was practically zero, if the temperature of "Feed NH3" was lower by 25 % and more than the design intent. It was not sufficient to increase the temperature back to its design value to return to the higher solution branch. Therefore, to return to the design intent, new reactor start-up would be required. In addition to the operability problems associated with lower ammonia production, shift from one solution branch to another is associated with parameter oscillations that can be damaging for catalyst as it was observed in the past (Morud and Skogestad, 1998).

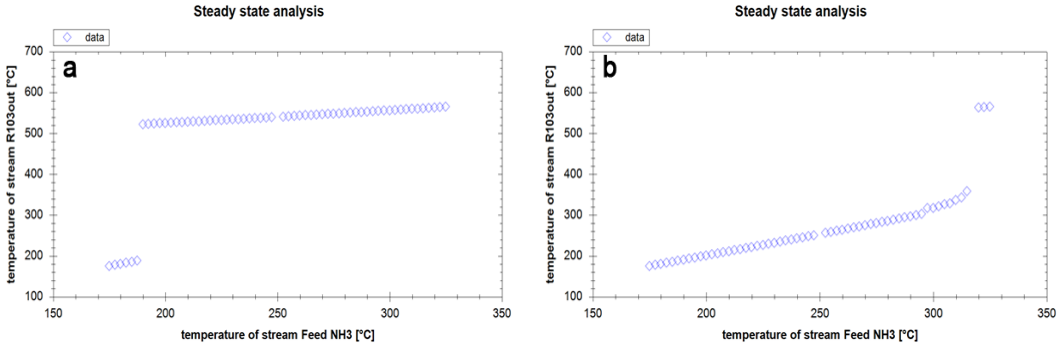

Figure 4: Temperature of material stream R103out for deviation "temperature of material stream Feed NH3 higher and lower than design intent" in the whole simulation range simulated in the descending (a) and ascending (b) order

4.2 Case study 2

Analogously to the case study 1, thorough analysis of deviations in every accessible process parameter was carried out. Although this reactive system is also well known for the presence of steady state multiplicity (A. Molnár et al., 2003), simulation approach proposed for case study 1 was unable to find position of solution branches formed by stable steady states. In the case study 2, numerical problems and consequent converge issues were encountered. If the region of multiplicity was reached during process simulation, Aspen HYSYS solver was unable to find solution if the reaction was switched on. To ensure convergence, Aspen HYSYS solver switched off the reaction and found solution for the system without reaction. This phenomenon led to unrealistically low temperatures below freezing point of the reactive mixture because of the constant heating flow from reactor caused by cooling system not taking into account principles of heat transfer. It is not the first case reporting convergence issues in Aspen HYSYS for systems exhibiting strong nonlinear behavior (Janošovský et al., 2017). However, hazard identification was still carried out and process hazards were identified for the deviation in cooling water flow. If the heat flow from the reactor was too small, temperature in the reactor crossed the limit value of reaction temperature. The limit value of temperature was set to 97 °C to avoid reaction mixture evaporation. Figure 5 depicts the effect of deviation "mass flow of material stream CoolingWaterIn higher and lower than design intent" on the temperature in the reactor represented by material stream "Reactor Prods".

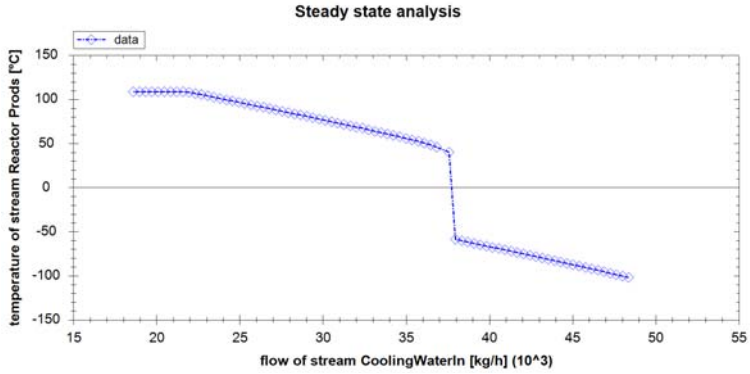

Figure 5: Temperature of material stream Reactor Prods for deviation "mass flow of material stream CoolingWaterIn higher and lower than design intent" in the whole simulation range

Clearly, three regions are visible. The first one is below 0 °C. This region represented aforementioned region with convergence issues where reaction was switched off. Therefore, these steady states were only hypothetical if no reaction was occurring in the reactor. The second region represented operating regime where temperature is below the safety limit of 97 °C. The third region was formed by steady states where temperature is over the safety limit and mixture evaporation was significant. The third region was entered when the mass flow of cooling water was lower by 34 % and more than the design intent.

5. Conclusions

In this work, software tool for computer-aided hazard identification based on process simulation was proposed. Basic description of software methodology and its application to two case studies were presented. It was demonstrated how the safety analysis can benefit from implementation of process simulation into the hazard identification procedure. Process hazards that could be possibly overlooked by conventional methods were simulated utilizing own software tool and Aspen HYSYS as a representative commercial simulator. For the ammonia synthesis case study, steady state multiplicity was exposed and position of solution branches formed by stable steady states were calculated using only built-in Aspen HYSYS solver. In the second case study, propylene glycol production, hazards caused by perturbations in cooling system were identified. In addition, limitations of Aspen HYSYS solving capabilities were also revealed. Convergence issues for systems exhibiting strong nonlinear behavior were encountered. Such numerical problems could hinder the adaptation of computer-aided hazard identification tools based on process simulation into industrial practice. Therefore, future work will be focused on improvement in numerical algorithms and development of simulation environment optimized for the safety analysis purposes.

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