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Computer Aided HAZOP Study Implementation Bottlenecks in Chemical Industry

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Implementation of computer aided approach into hazard and operability (HAZOP) study is one of the most researched topics in the field of hazard identification improvement. However, acceptance of an automated HAZOP tool in the industrial practice is limited. This contribution provides retrospective analysis of application issues connected with the use of process simulations in computer aided HAZOP studies. As case studies, mathematical models utilising different sets of unit operations, e.g. plug flow reactor, continuous stirred-tank reactor, phase separator, heat exchanger etc. were analysed. Two different simulation platforms, commercial process simulator Aspen HYSYS and our own mathematical models in MATLAB, were employed. Relevant concerns regarding the use of process simulations in the HAZOP study such as model reliability and its parameter uncertainties effect on the HAZOP study output and interpretation variability of quantitative HAZOP deviations for process simulations are discussed. It is demonstrated that the application of process simulation is a feasible way to perform precise safety analyses of processes widely used in chemical industry. However, proper attention has to be paid to the construction and use of mathematical models in order to develop a suitable software solution.

1. Introduction

Constant growth of chemical industry has led to the increase of manufacturing processes complexity in order to achieve higher production efficiency at lower costs. Therefore, appropriate process safety analysis has become one of the most challenging tasks in sustainable plant design and operation (Tugnoli et al., 2012). With the development of computer aided process engineering and process systems engineering tools, the demand for computer aided hazard identification has also increased. Implementation of suitable software solutions improving conventional process hazard analyses is also a part of the Industry 4.0 initiative (Kagermann et al., 2013).Several hazard identification techniques are well established in industrial companies' policies such as What-If analysis, Checklist, Failure modes and analysis (FMEA) and Hazard and operability (HAZOP) study (Mannan, 2012). However, the HAZOP study is clearly identified as the most used and highly efficient technique for the identification of potential hazards and operability problems in modern chemical plants (Dunjó et al., 2010). In addition, systematic approach and robustness of the HAZOP study qualify it for implementation into software solution (Taylor, 2017). In the past, several proposals of sophisticated software tools for computer aided hazard identification were published such as combination of HAZOP study principles with dynamic simulations in MATLAB for educational purposes (Eizenberg et al., 2006), dynamic simulations in Aspen Dynamics used to improve risk analysis of oxidation processes (Berdouzi et al., 2017), implementation of Aspen HYSYS simulation into hazard identification of an ammonia synthesis reactor system (Janošovský et al., 2016), integration of Aspen Plus simulation into safety instrumented system evaluation (Jeerawongsuntorn et al., 2011) etc. As it was shown in these works, utilisation of proper mathematical models represents a feasible way of performing precise hazard identification in modern complex nonlinear processes used in chemical industry.In this paper, critical review of results provided by a smart software solution utilising HAZOP principles and mathematical modelling of common chemical processes is introduced. The examined software was tested in combination with the simulation platforms represented by predefined mathematical models in Aspen HYSYS, a commercial process simulator widely used in chemical industry, particularly in oil and gas industry, and our own mathematical models developed in the environment of

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MATLAB. The HAZOP methodology was used for the generation of simulation inputs (HAZOP deviations). Consequent multilevel simulation data analysis determined the severity of simulated process states corresponding to HAZOP deviations, i.e. HAZOP consequences. The goal of this study is to identify the main obstacles in the implementation of computer aided HAZOP study based on process simulations in chemical industry. To illustrate the issues associated with its use, mathematical models of alkylpyridine N-oxidation and ammonia synthesis plant were selected as case studies. It will be demonstrated how interpretation variability of quantitative HAZOP deviations, and model reliability and its parameter uncertainties can alter hazard identification results.

2. Case studies

Case study A is a novel approach to alkypyridine N-oxidation in a continuous stirred-tank reactor (CSTR) system. The process of N-oxidation was conducted in liquid phase and in the presence of phosphotungstic acid as the catalyst and aqueous hydrogen peroxide solution as the oxidising agent. Two reactions were considered in this particular case study: N-oxidation of 3-methylpyridine to 3-methylpyridine-N-oxide and decomposition of hydrogen peroxide to water and gaseous oxygen. The process had to be conducted in a small temperature range of 110 – 125 °C under elevated pressure to suppress evaporation and hydrogen peroxide decomposition. Significant influence of the uncertainty of the N-oxidation reaction enthalpy value on the position of safe operating points is discussed. An illustrative process flowsheet is depicted in Figure 1. Feed 1 represents 3-methylpyridine and Feed 2 represents water solution of hydrogen peroxide. Mathematical model of the process constructed in MATLAB environment and its parameters have been described in detail by Danko et al. (2018).

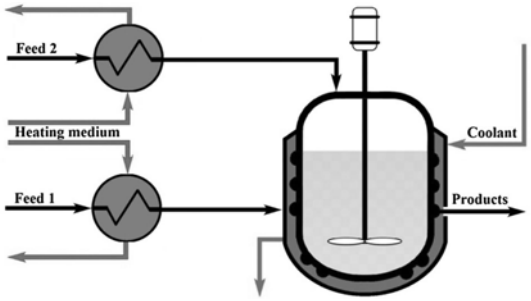

Figure 1: Illustrative process flowsheet as presented by Danko et al. (2018)

Case study B considers an ammonia synthesis process in an adiabatic fixed-bed reactor. Mathematical model constructed in the Aspen HYSYS environment has been thoroughly discussed by Janošovský et al. (2016). The mathematical model included a fixed-bed reactor with three beds, a feed preheater and a refrigeration unit with a vapour–liquid flash separator. The fixed-bed reactor system consisted of three segments – beds in series with feed quenching between each bed to adjust the optimal temperature profile in the reactor system. The feed preheater was modelled as a heat exchanger, where feed is preheated by the outlet product stream from the fixed-bed reactor. The outlet product stream leaving the feed preheater was additionally cooled to the desired temperature in the refrigeration system. In the flash separator, the outlet stream from the refrigeration system was separated to liquid ammonia and gaseous purge. This reactor system corresponds to an industrial ammonia synthesis reactor, where multiple steady states and temperature oscillations were observed in past (Janošovský et al., 2015; Morud and Skogestad, 1998). The process flowsheet in Aspen HYSYS is depicted in Figure 2.

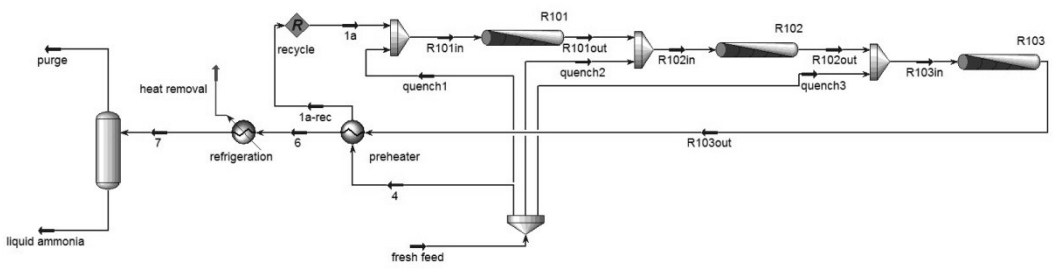

Figure 2: Process flowsheet in Aspen HYSYS as presented by Janošovský et al. (2017)

3. Results and discussion

Computer aided HAZOP study based on process simulations was carried out for the proposed case studies (Danko et al., 2018; Janošovský et al., 2017). In this section, results of the conducted HAZOP study are retrospectively investigated and critically analysed. Two issues associated with the selected case studies are thoroughly discussed:

- HAZOP deviation interpretation variability,
- model reliability.

3.1 HAZOP deviation interpretation variability

In a conventional HAZOP study, logical combination of guide words (more, less, etc.) and process parameters (temperature, pressure, etc.) is used to create HAZOP deviations, e.g. combination of “more” and “temperature” generates “higher temperature”. However, for the implementation of mathematical modelling into a HAZOP study, such information is not sufficient. How much higher temperature is “higher temperature”? How long does the deviation last? Such questions have to be answered to perform computer aided HAZOP study based on process simulations. In the safety analysis of case study B presented by Janošovský et al. (2017), multiple steady states phenomenon leading to potentially dangerous temperature oscillations was revealed. However, depending on HAZOP deviation interpretation, hazardous behavior of the reactive system could be possibly overlooked.In Figure 3, the effect of temperature deviation in material stream “fresh feed” on the ammonia synthesis reactor outlet for case study B is depicted for the temperature range from 210 °C to 400 °C. An increase in the “fresh feed” temperature led to a slight continuous increase of temperature in the synthesis reactor. A decrease of the “fresh feed” temperature led to continuous, but steeper temperature decrease in the synthesis reactor. Additional analysis of material streams composition had, in fact, shown a small increase in the ammonia production. However, such steep temperature decrease indicated the proximity of switching between two solution branches associated with parameter oscillations which are characteristic for systems exhibiting steady state multiplicity. In fact, decrease of “fresh feed” temperature below 210 °C led to a rapid reactor temperature drop (Figure 4). Consequent analysis of reactor outlet stream composition confirmed the termination of the ammonia synthesis reaction. In addition, when the “fresh feed” temperature was corrected, a different solution branch was observed. Such simulated behavior demonstrated the presence of steady state multiplicity in the modelled ammonia synthesis plant. Although the HAZOP study is considered to be a qualitative safety analysis method, with the introduction of computer simulations, also quantitative aspect has been incorporated. Same conventional HAZOP deviations “higher temperature” led to different qualitative consequences – first one (Figure 3) led to a harmless slight change in reactor temperature and the second one (Figure 4) led to a rapid temperature drop potentially associated with hazardous events and operability problems.Results of the HAZOP study without software assistance thus strongly depend on the operational experience of process engineers and operators. The analysis of “fresh feed” temperature deviation in an insufficiently small range could lead to neglecting potentially disastrous events. With the aid of software tools based on process simulations, quantitative aspect of the HAZOP deviations can be considered and such neglect can be avoided.

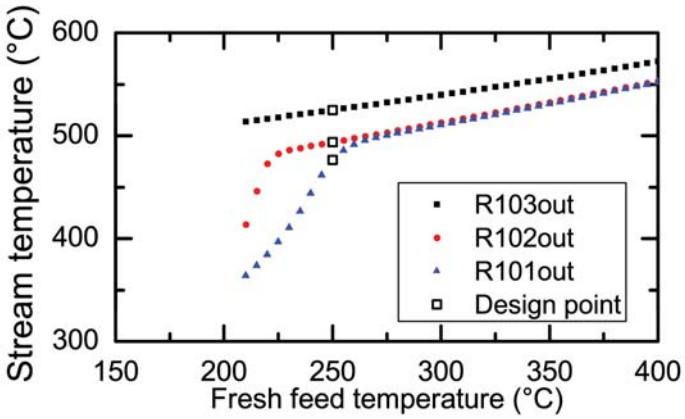

Figure 3: Effect of the deviation “higher fresh feed temperature” and “lower fresh feed temperature” on the temperature of streams “R103out” (black square), “R102out” (red circle) and “R101out” (blue triangle) representing the ammonia synthesis reactor outlet (design point – thick square) in the insufficient value range of HAZOP deviations

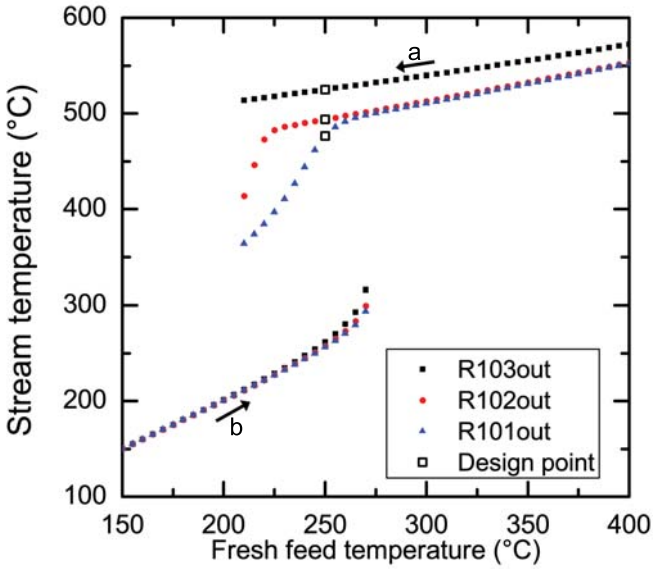

Figure 4: Effect of the deviation "higher fresh feed temperature" and "lower fresh feed temperature" on the temperature of streams "R103out" (black square), "R102out" (red circle) and "R101out" (blue triangle) representing the ammonia synthesis reactor outlet (design point – thick square) with identified higher (a) and lower (b) solution branches (arrows indicate the direction of computer simulation in Aspen HYSYS)

3.2 Model reliability

One of the most discussed issues connected with the implementation of computer aided process engineering and process systems engineering tools into industrial practice is the reliability of the applied mathematical model. Particularly in the chemical engineering practice, there has always been a need to compromise between mathematical model accuracy and complexity as it was colourfully presented by Levenspiel (2002). Selection of mathematical model depth can significantly change the output of computer simulation results and alter the conclusion of the safety and operability analysis (Švandová et al., 2009). Another important problem are the model parameter uncertainties and their impact on the accuracy of simulation results (Laššák et al., 2010). In this contribution, the effect of uncertainty in the value of reaction enthalpy for case study A was analysed. As it was stated, safe temperature range for case study A is from 110 to 125 °C. In Figure 5, temperature in the reactor as a function of the feed temperature (identical temperature was considered for both feeding streams, "Feed 1" and "Feed 2") and the molar ratio of both reactants is shown for two different values of reaction enthalpy.

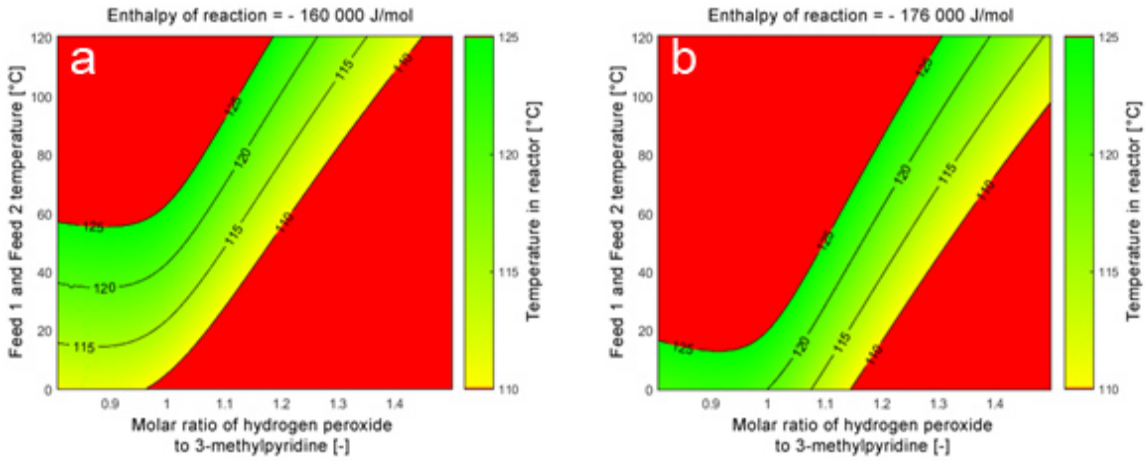

Figure 5: Location of safe operating regimes (green region) as a function of "Feed 1" and "Feed 2" temperature and molar ratio of hydrogen peroxide for the reaction enthalpy value of -160 000 J/mol (a) and -176 000 J/mol (b) (red region represents hazardous operating regimes)

Figure 5a depicts the location of safe operating regimes (shades of green) for the analysed system for the original value of the reaction enthalpy as stated in the work of Danko et al. (2018). However, if the reaction enthalpy was increased by 10 %, the simulated position of safe operating regimes changed dramatically (Figure 5b). Reaction conditions modelled to be safe for one value of the model parameter were completely inappropriate for the model with a small change in the value of this parameter. This phenomenon could lead to false conclusions of the safety analysis. In general, measurement of any variable is always burdened with an error; therefore, uncertainties in model parameters cannot be avoided. In the construction of a mathematical model, this fact must be taken into consideration. To ensure the reliability of the safety analysis utilising process simulations, information on individual model parameter uncertainties should be provided and the appropriate analysis of their impact on the safety analysis results should be performed.

4. Conclusions

In this contribution, computer aided HAZOP study based on process simulations and its application issues in chemical industry were presented. Although the HAZOP study is considered to be a qualitative safety analysis method, with the introduction of computer simulations, quantitative aspect is incorporated which can contribute to significant extension of the HAZOP study scope. Retrospective analysis of two case studies representing frequently used unit operations in chemical industry provided a platform to demonstrate possible bottlenecks of simulation-based hazard identification into industrial practice. Based on the presented results, it is clear that successful implementation of simulation-based HAZOP study is associated with several problems that have to be properly analysed and dealt with.

First problem introduced in this paper was the interpretation variability of HAZOP deviations when mathematical modelling is implemented. In the case study of ammonia synthesis, HAZOP deviation of “lower fresh feed temperature” led to two possible consequences. If the temperature was above 210 °C, slightly lower temperature of the product streams and small increase of ammonia production were simulated. If the temperature was further decreased, practically complete termination of the ammonia production was simulated because of the steady state multiplicity. It was demonstrated how qualitatively the same but quantitatively different HAZOP deviations can cause qualitatively very different HAZOP consequences. The correct method to determine sufficient ranges for every HAZOP deviation must be thus considered in the construction of a suitable software tool for the simulation-based HAZOP study.

Second application issue, reliability of a mathematical model, was studied with the focus on the effect of model parameter uncertainties. Errors in the measurement of model parameter values can lead to critical alterations of the safety analysis results. In the case study of novel process for alkylpyridine N-oxidation, it was shown that the value of reaction enthalpy played a crucial role in proper selection of safe operating points. Increase of its value by only 10 % resulted in significantly different locations of safe operating regimes. An increased attention has to be paid to careful verification of every sensitive model parameter value to avoid misleading conclusions and false safety improvement recommendations.

To summarise the work presented in this contribution, computer aided HAZOP study based on process simulations is a promising concept for the improvement of process hazard identification techniques. As it is evident, human factor cannot be fully excluded from the HAZOP study. The proposed simulation-based approach provides a valuable insight into hazards emerging from process nonlinearity and can significantly reduce the possibility of overlooking hazardous events; however, process simulation results still require appropriate verification and further analysis by experienced process engineers.

Acknowledgments

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