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Automated Model-based HAZOP Study in Process Hazard Analysis

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In the age of chemical processes operated at extreme pressures and temperatures it is necessary to perform a detailed process safety analysis. Hazard and operability study (HAZOP) is one of the most used and highly efficient techniques for the identification of potential hazards and operability problems. Model-based HAZOP study is based on the implementation of a detailed mathematical model of chemical productions. Possibilities and limitations of model-based HAZOP study using Aspen HYSYS are discussed in this work. Results of numerical simulations are collected and directly transformed into standard HAZOP tables. Advantages and disadvantages of the presented software tool are shown in the process hazard analysis of a chemical production with strong nonlinear behavior, an ammonia synthesis reactor system.

1. Introduction

Chemical industry together with other industrial sectors is subject to modernisation and automation. These considerable changes push the chemical processes towards extreme operating conditions (pressure, temperature, etc.). Therefore, conventional hazard analysis methods may not be sufficient anymore. There are several process safety analysis techniques such as checklist (CL), what-if (WI) analysis, failure modes and effects analysis (FMEA), fault tree analysis (FTA), and hazard and operability (HAZOP) study. HAZOP study is currently recognised as one of the most used and frequently modified process safety analysis methods (e.g. determination of the required safety instrument level (Dowell, 1998), blended hazard identification (BLHAZID) methodology (Seligmann et al., 2012), HAZOP analysis based on structural model (Boonthum et al., 2014), innovative LOPA-based methodology with integration of a HAZOP study (Argenti et al., 2015), etc.). HAZOP study is a highly sophisticated technique of hazard identification based on monitoring process parameter deviations. The process parameter deviation is created by combination of the guide word (more, less, etc.) and process parameter (temperature, pressure, flow, etc.). The principal task of HAZOP analysis is to investigate the causes, propagation and consequences of process variable deviations. The standard output of "hazoping" is a list of all possible deviations, their causes and consequences, installed levels of protection and recommendations for process safety improvement. (Kletz, 1997) The main disadvantages of conventional process safety analysis methods including HAZOP are their time consuming character, cost requirements and the demand for experienced and skilled human expert team including safety engineers and process engineers for successful execution of process hazard analysis.

Development of computer technology has created new possibilities to eliminate or reduce the disadvantages of conventional process hazard analysis techniques. As indicated by the literature review presented by Dunjó et al. (2010), approximately 40 % of HAZOP-related research is focused on HAZOP automation. It is impossible to completely eliminate the presence of a human expert team in the HAZOP execution process, but there are several attempts to create a robust support tool that is able to automate some of the procedures necessary to perform a HAZOP study. There are two basic approaches in HAZOP automation: knowledge-based and model-based. Knowledge-based approach, dominant in the 20th century, uses large knowledge databases containing information about the failure mode, causes and consequences of various process units and/or pieces of equipment. Typical knowledge-based expert systems are e.g. HAZOPExpert, a HAZOP automation tool developed by Venkatasubramanian and Vaidhyanathan (1994), projects of OptHAZOP, TOPHAZOP and EXPERTOP (Khan and Abbasi, 2000), integration of knowledge-based and mathematical

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programming approaches for process safety verification by Srinivasan et al. (1997) or Automatic Hazard Analyzer (AHA) - an expert system based on multi-model approach presented by Kang et al. (1999).

The model-based approach has gained more attention and importance in the 21st century. This approach is based on the implementation of a detailed mathematical model of chemical productions. The main benefit of using the model-based hazard analysis tool is the possibility of complex overview of the analysed process limited only by the reliability of the mathematical model. Mathematical modeling allows the user to consider not only the presence of the deviation, but also its value and duration. Several benefits of model-based HAZOP automation are demonstrated by combining the HAZOP technique with dynamic simulations employing MATLAB in the work of Eizenberg et al. (2006) and in the article about the integration of human-machine interface with automated HAZOP analysis using Aspen Plus® version 2006.5 proposed by Jeerawongsuntorn et al. (2011). Principal issues of safety analysis utilizing mathematical modeling have been discussed by Molnár et al. (2005) and several attempts of combining a HAZOP study with mathematical models of process equipment based on this article were made. Articles about mathematical model of chemical reactors as a useful complement in the HAZOP study (Švandová et al., 2005) have been published. The use of a mathematical model of a chemical reactor in safety analysis using the HAZOP methodology is also presented in the work of Labovský et al. (2007a). The research of this team was later focused on HAZOP studies of real chemical plants with nonlinear behavior, e.g. a MTBE plant (Labovský et al., 2007b). The possibilities of model-based hazard identification in chemical reactors were summarised and discussed by Labovská et al. (2014). Reliability of model-based HAZOP is strongly dependent on the selection of an appropriate mathematical model and its parameters describing the physicochemical behavior of individual components and their mixtures. These issues were investigated by Laššák et al. (2010).

The goal of the presented paper is to propose the fundamentals of combining model-based HAZOP analysis with the simulation environment optimised for process safety engineering including the use of Aspen HYSYS v8.4 process modelling. Aspen HYSYS provides one of the most extensive property databases and the possibility of data transfer between external software and internal simulation environment. It will be shown, that presented software tool facilitates and accelerates the execution of a process safety analysis. After the process deviation effect is simulated, the simulation data are collected and processed applying the principles of the HAZOP methodology. It will be demonstrated that the presented automated model-based HAZOP tool is able to handle and examine processes operated in parametrically sensitive region that can lead to process hazards and operating problems such as the ammonia synthesis reactor incident in 1989 (Morud and Skogestad, 1998).

2. Software methodology

The proposed software tool consists of two separate parts with shared classes and databases (Figure 1). The first part is used for the actual simulation of the analysed system. In this software module, the connection of our tool with the Aspen HYSYS simulation environment is established and when the simulation case is open and active, individual streams and operation units are checked for the possibility of performing a HAZOP study. After this primary control, the user can select the desired material streams and create process variable deviations. When the final list of process variable deviations is created, the simulation section is initiated. The list is transferred to the internal database where deviations are stored.

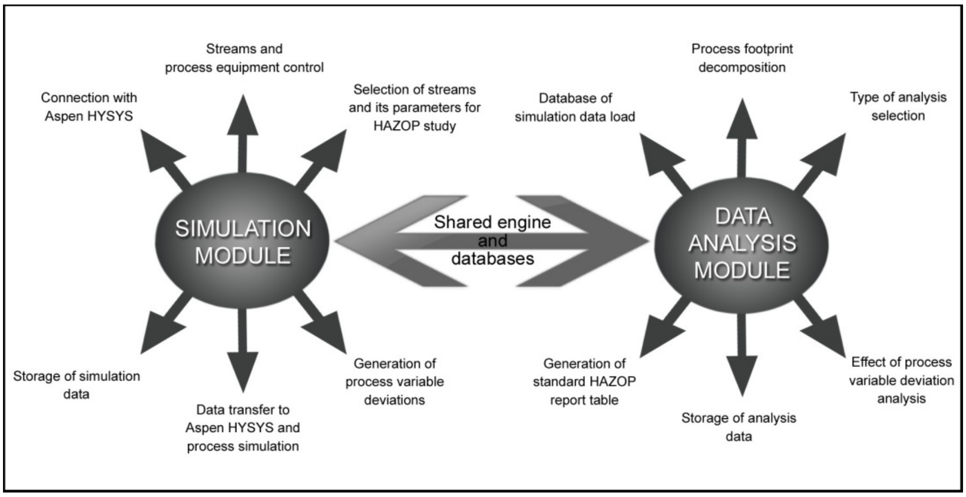

Figure 1: Schematic description of the presented automated model-based HAZOP analysis tool

After this procedure, the user is allowed to start the simulation. The information containing the stream identification number, its parameter and deviation value is sent from the analysis tool to the internal environment of Aspen HYSYS v8.4, where the process simulation is done. After each simulation of variable deviation, the footprint of the current process state is created. This footprint contains values of important process variables such as temperature, pressure, flow, composition etc. of each stream and the live reference to the HYSYS environment. When all selected process variable deviations are investigated, the investigation part of the presented HAZOP analysis tool is finished.
The second part of our analysis tool is designed for the simulation data analysis. The depth of the analysis is optional and depends on the user's choice. In this part, the shared internal database belonging to the analysed system is loaded. Process footprints for each simulated deviation are decomposed and user is able to investigate the system response to the deviated parameter. Examination questions can be formulated as: Is the reaction terminated? Is the runaway effect possible? Which stream is the most parametrically sensitive? Is there a possibility of unexpected vapor fraction occurrence in the process? After the analysis, a HAZOP-like report is generated.
The possibilities and limitations of both modules of our analysis tool are demonstrated on one example. The demonstrational example is a case study of a complex ammonia synthesis reactor system focused on the ammonia synthesis nonlinearity and providing insight into the robustness and advantages of our automated model-based HAZOP analysis tool.

3. Application to a case study - ammonia synthesis unit

Ammonia synthesis unit is well known for its nonlinear character documented e.g. by Morud and Skogestad (1998). The mathematical model of an ammonia production plant consists of fixed-bed reactor divided into three separate beds, a feed preheater and a refrigeration system with a vapor-liquid separator (Figure 2). The feed stream is transferred to the splitter where the feed is divided into four outlet streams. One outlet stream is led to the feed preheater as the cool medium and three other outlet streams are parts of fresh feed quenching between each bed to achieve the optimal temperature profile. As the hot medium in the feed preheater, the product stream leaving the reactor system is used. The cooled product stream is led into the refrigeration unit with a phase separator, where the products are separated into two phases, gaseous purge and liquid ammonia. Relevant parameters of the selected material streams and their design values are presented in Table 1.

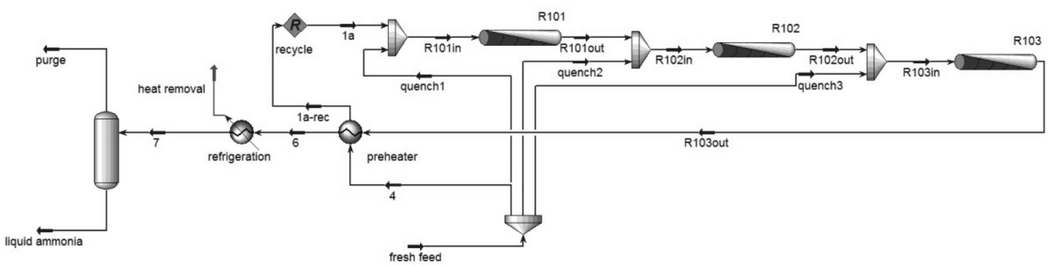

Figure 2: Ammonia synthesis unit in Aspen HYSYS v8.4 simulation environment

Table 1: Design parameters of the ammonia synthesis unit

Stream name	fresh feed	4	quench 1	quench 2	1a	R101out	R102out	R103out	6	liquid ammonia
Temperature [°C]	250	250	250	250	424	520	530	525	436	8
Pressure [MPa]	20	20	20	20	20	20	20	20	20	20
Mass flow [10^3 kg/h]	252	127	58	35	127	185	220	252	252	50
Mole fraction										
Nitrogen	0.239	0.239	0.239	0.239	0.239	0.215	0.210	0.209	0.209	0.003
Hydrogen	0.719	0.719	0.719	0.719	0.719	0.645	0.630	0.625	0.625	0.015
Ammonia	0.042	0.042	0.042	0.042	0.042	0.140	0.160	0.166	0.166	0.982

The conventional process hazard analysis of this chemical plant can be carried out using a standard HAZOP study. The human expert team should hold meetings where the possibilities and consequences of every potential process variable deviation have to be considered. This part of "hazoping" is the most time consuming part. Some of the team members can adapt incorrect conclusions and overlook potentially hazardous consequences resulting from the lack of experience. Also some consequences can be overlooked completely because of insufficient knowledge of the examined process (like the Seveso disaster) or too complicated failure propagation. With the use of our analysis tool, these inconveniences are significantly reduced. Our model-based HAZOP tool directly helps the human expert team with answering the majority of the important questions. After selecting the target streams, their parameters and the deviation range, the deviation list is generated and the process simulation takes place. Then, simulation data are evaluated with the assistance of the human expert team. For this case study, the effect of temperature, pressure and composition of each material stream was investigated. Because of the huge amount of the simulation data, the stream “fresh feed” and its parameter temperature were selected for the demonstration in the next section.

4. Results and discussion

4.1 Effect of feed temperature on simulated ammonia synthesis unit

Temperature in the fixed-bed reactor affects the overall conversion of reactants and the total production of ammonia respectively. The reaction in every bed of the reactor was carried out at a constant pressure of 20 MPa. The feed temperature deviation list was generated using the classic HAZOP approach of combining guide words "more" and "less" with the parameter "temperature" resulting in classic HAZOP deviations "higher feed temperature than design value" and "lower feed temperature than design value". The developed model-based HAZOP analysis tool required to consider the value of the parameter deviation D_P defined in Eq(1), where P_O is the original non-deviated value of the parameter P and P_N is the new value of parameter P after the deviation is applied to the process.

$$D_P = \frac{P_N - P_O}{P_O} \times 100 \qquad (1)$$

The range of feed temperature deviation D_T was from + 30 % to - 30 % in this case study, which means that the feed temperature varied from 175 °C to 325 °C. Figure 3a shows the effect of the feed temperature on the “R103out” (see Figure 2) temperature, the absolute response. Figure 3b presents the effect of the feed temperature deviation on the “R103out” temperature deviation, the relative response. In Figure 3c, the effect of the feed temperature on the rate of “R103out” temperature change defined as the change of the “R103out” temperature divided by the corresponding change of the feed temperature is depicted.

As shown in Figure 3, an increase of the feed temperature causes gradual increase of the reactor outlet temperature. Since the exothermic reaction is enhanced at lower temperatures, when the temperature in the reactor system was decreased, the overall ammonia production increased. However, a step change (a decrease of ca. 60 %) of the operating temperature of “R103out” in the region of the feed temperature deviation of around 18 % was observed. This step decrease of the reactor outlet temperature indicates the system switch to a steady state with lower reaction rates. The shift between different steady states led to the termination of the reaction and a new reactor start-up was required. The phenomnenon of multiple steady states in the ammonia synthesis similar to that one described by Morud and Skogestad (1998) was observed.

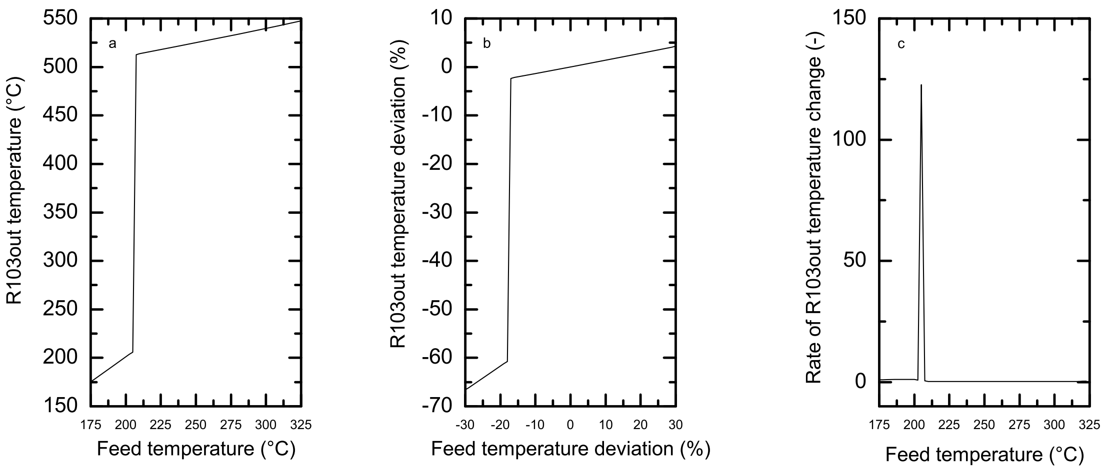

Figure 3: Effect of feed temperature deviation on the temperature of stream “R103out” (a –absolute response, b –relative response, c –rate of “R103out” temperature change, see Figure 2)

Similar behavior was exhibited by the operating temperatures of the reactor beds outlet and inlet streams and the feed preheater outlet and inlet streams. For the analysis of the overall process response, the effect of the feed temperature deviation on the temperatures of material streams in the process is depicted in Figure 4. The color intensity is dependent on the parameter deviation value according to the color scale in the right section of Figure 4. The temperature change of streams "quench1", "quench2", "quench3" and "4" directly mirrored the feed temperature deviation, because these streams are outlet streams from a splitter where the only input stream is the fresh feed. Temperature of streams "7", "purge" and "liquid ammonia" is not affected, because the heat removal in the refrigeration unit is set to the output temperature of 8 °C.

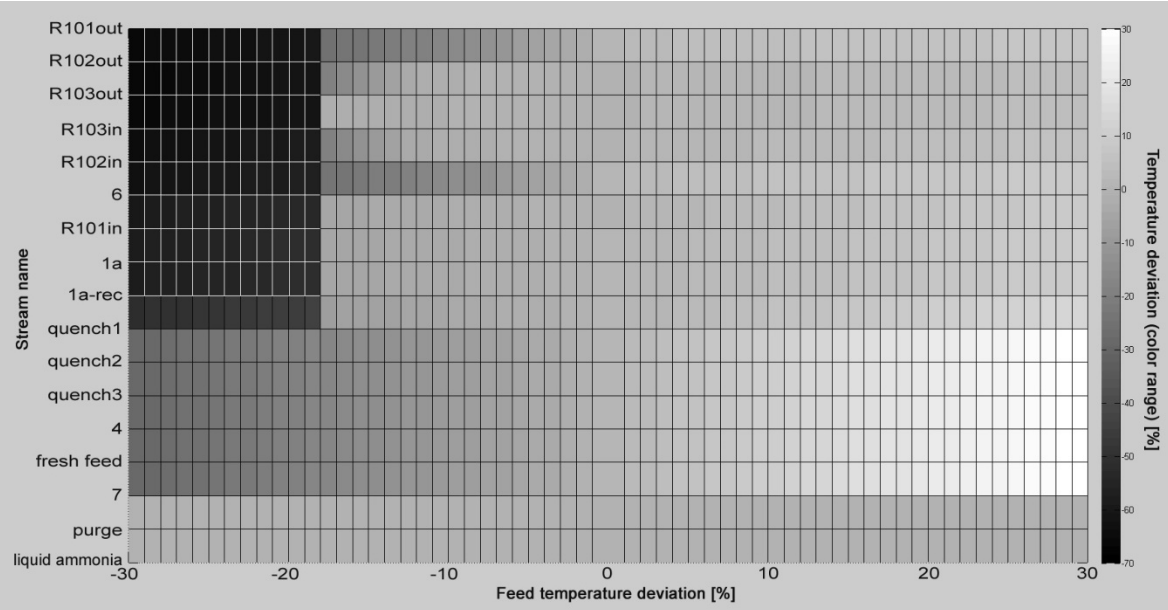

Figure 4: Effect of feed temperature deviation throughout the process

4.2 Model-based process hazard analysis results

Other significant process variable deviations and their detected consequences are summarized in Table 2. As shown, the key consequences of process variable deviations in the process of the presented ammonia synthesis unit are operational problems caused by switching between different steady states. Investigation of the effect of the mole ratio of one component to another one was carried out at a constant mass flow of the analyzed stream.

Table 2: HAZOP report example from model-based process hazard analysis of the ammonia synthesis unit

Deviation from design intent	Deviation value D_P	Detected consequences
"lower feed temperature"	- 18 %	Overall ammonia production decreased by 99,5 %
"lower feed pressure"	- 40 %	Overall ammonia production decreased by 98,2 %
"lower heat removal in refrigeration" ("lower coolant flow")	- 11 %	Yield of ammonia in the phase separator decreased by 45 %
"higher feed mole ratio hydrogen/nitrogen"	+ 54 %	Overall ammonia production decreased by 97,1 %

5. Conclusions

In this work, a software tool combining a chemical unit with model-based HAZOP analysis was presented. The integration of automated model-based HAZOP study can potentially lead to the identification of some unexpected deviations and to the reduction of time required for the process hazard analysis. It can be successfully applied at the beginning stage of the unit design, for the operation of an already existing unit and also for the training of operators. It was demonstrated that the simulation of a chemical unit using an appropriate mathematical model is a suitable tool for safety analysis.

In the presented case study, mathematical modelling of ammonia synthesis in the Aspen HYSYS v8.4 simulation environment was done which allowed identifying parametric zones, where shifting between qualitatively different steady states can be expected. Operational problem of the reaction terminated in a lower steady state was identified. Results of the presented automated model-based HAZOP tool applied to an ammonia synthesis unit were shown to exemplify the application. It is important to note that each uncertainty of a model input parameter can significantly influence the results of a model-based HAZOP study.

Acknowledgments

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