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The role of a commercial process simulator in computer aided HAZOP approach

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ABSTRACT

Process safety is one of the key pillars of sustainable industrial development. In combination with the increasing use of computer aided process engineering, the demand for an appropriate model-based safety analysis tool capable to identify all hazardous situations leading to a major accident has increased. Commercial process simulators are equipped with extensive property databases and they employ high accuracy mathematical models providing the capability to simulate real behavior of a process operated within the area of the mathematical model validity. The main focus of this work is to improve standard hazard identification methods by the combination of hazard and operability (HAZOP) study and process simulation in commercial process simulator Aspen HYSYS. Software tool consisting of modules for computer simulation and complex analysis of simulation data will be proposed. The developed tool was applied to modern chemical productions exhibiting strong nonlinear behavior, where proper prediction of consequences can be very difficult. In the first case study, hazard identification in continuous glycerol nitration employing user-dependent analysis is presented. Mathematical methods of simulation data analysis independent of the user is demonstrated in the second case study of ammonia synthesis. Possibilities and limitations of the proposed tool are revealed and discussed in this work.

1. Introduction

Several serious industrial accidents (e.g. Flixborough, Seveso, Bhopal and Tianjin disasters) in the past have underlined the importance of loss prevention approach in chemical industry. Dynamic development of industry has not only resulted in more efficient and profitable chemical productions, but also in the increase of plants complexity as well as the variety of chemicals and processes used in the plant. In addition, the majority of modern processes exhibit strong nonlinear behavior. Therefore, the task of identifying potential sources of hazards has become more complex (De Rademaeker et al., 2014). In combination with the ever growing use of computer aided process engineering, the demand for an appropriately detailed safety analysis tool capable to identify all hazardous situations leading to a major accident has increased. The safety point of view should be implemented not only in the design stage of any chemical plant, but also during the entire plant life cycle. Identification of all possible fault propagation paths is thus, for example, the key feature of proper design of control systems (Leveson and Stephanopoulos, 2014; Parmar and Lees, 1987; Seider et al., 2014).

Actual trend in computer aided loss prevention is to improve standard hazard identification methods by employing mathematical modeling and process simulation in commercially available simulators. Commercial process simulators are equipped with extensive property databases and utilize high accuracy mathematical models thus providing the capability to simulate real behavior of a process operated within the area of the mathematical model validity. Model-based hazard identification also benefits from the fact that mathematical modeling of the analyzed process is usually employed as a part of process design and optimization activities, e.g. optimization of biorefinery downstream processes employing SimSci PRO/II (Corbetta et al., 2016), design of hydrocarbons separation unit using Aspen Plus (de Riva et al., 2016) and Aspen HYSYS supported design of syngas production proposed by Sunny et al. (2016). If the use of process simulators is well implemented in the company policy, successful adoption of safety extensions for these simulators is more likely.

Model-based approach was applied not only in hazard identification, but also in reliability engineering (Favarò and Saleh, 2016) and quantitative risk assessment (Labovský and Jelemenský, 2011; Qi et al., 2014). While mathematical modeling in these areas is accepted by

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Nomenclature

a	Reaction order of glycerol
A	Pre-exponential factor
b	Reaction order of nitric acid
c	Molar concentration, $l\,mol^{-1}$
E_a	Activation energy, $J\,mol^{-1}$
p	Partial pressure, bar
r	Reaction rate
R	Universal gas constant, $J\,K^{-1}\,mol^{-1}$
Greek symbols	
β	Enhancement factor
ρ_c	Catalyst bulk density, $kg\,m^{-3}$

the safety engineering community, model-based hazard identification is still subject of discussion because of model validity and its input parameters uncertainty (Labovská et al., 2014; Švandová et al., 2009). Published model-based tools vary in the complexity of mathematical models and simulation data evaluation methods. The complexity of mathematical models depends on whether they were constructed specifically for the analyzed system or the developed tool employed a group of mathematical models, e.g. a commercial process simulator. Although the computing time increases with the increase of model complexity, several efforts were made towards shortening the time required for the solution of large nonlinear systems, e.g. utilization of parallel computing (Danko et al., 2015; Labovský et al., 2015). The simulation data can be evaluated manually, automatically or by a combination of both ways. The majority of published works benefited from the robustness and complexity of the hazard and operability (HAZOP) study that belongs to the most used process hazard analysis procedures worldwide and is recognized as an effective and accurate hazard identification method in chemical industry (Dunjó et al., 2010; Kletz, 2001).

Eizenberg et al. (2006) combined a standard HAZOP study and process simulation in MATLAB in order to develop a software tool for better understanding of hazards for the safety education process. Similar approach was adopted in the work of Li et al. (2010). The examined system was a three-phase hydrogenation in an intensified stirred continuous reactor and the simulation results of hazardous cases generated based on the HAZOP principles were presented. HAZOP principles were also applied in the safety assessment based on parametric sensitivity analysis of the key operating parameters in a hydrogen production unit (Ghasemzadeh et al., 2013).

Previously mentioned works focused on safety analysis based on a specific mathematical model of the unit under review. A disadvantage of such an approach is its limited application. If the safety analysis of another unit was required, it was necessary to decompose the current mathematical model and to form and validate a new set of equations describing the behavior of the new unit. Therefore, this approach is not suitable for the development of a universal model-based hazard identification tool. This limitation can be eliminated by involving the use of a commercial process simulation software with predefined and prevalidated sets of unit operations commonly used in industry. In this case, the safety analysis of different units in a plant requires only switching between the generally prepared mathematical models.

A successful combination of the HAZOP study and simulation in Aspen Plus in the case study of biodiesel production was presented by Jeerawongsuntorn et al. (2011). Alternatives including standard and reactive distillation were analyzed for the purpose of the decision-making process improvement and safety instrumented system implementation. The K-Spice software was used for process simulation followed by the HAZOP analysis in the work of Enemark-Rasmussen et al. (2012). Results of the simulated deviations were recorded, evaluated and ranked according to the severity of deviations determined by the sensitivity measure. Tian et al. (2015) introduced the dynamic simulation-based HAZOP (DynSim-HAZOP) methodology employing dynamic simulation in process simulators such as Aspen Dynamics, Aspen Plus and Aspen HYSYS to perform model-based safety analysis of an extractive distillation column and an ammonia synthesis plant. Both Jeerawongsuntorn et al. (2011) and Tian et al. (2015) used monitoring of user defined threshold values (e.g. autoignition temperature or maximum allowed liquid level in the separator) in the simulation data evaluation. Enemark-Rasmussen et al. (2012) partially automated the process of data evaluation by quantifying the deviation effects and their ranking according to the sensitivity measure, i.e. comparing the change of the selected parameter (temperature, pressure ...) to the change of the deviated parameter. The proposed ranking system allowed the elimination of deviations with negligible impact on the process. Systematic approach combining advantages of previously mentioned works applied in process simulation in Aspen HYSYS was proposed by Janošovský et al. (2016a) and it was further analyzed (Janošovský et al., 2016b).

Principal objective of this paper is to summarize issues with the developing computer aided hazard identification tool based on process simulation in the Aspen HYSYS environment. Two case studies focused on modern continuous productions exhibiting strong nonlinear behavior with various levels of complexity are presented. In the first case study, hazards of glycerol nitration in a continuously stirred tank reactor are identified and evaluated. The presence of the multiple steady states phenomenon in an ammonia synthesis reactor with a preheating system and the related numerical complications are discussed in the second case study.

2. Model-based HAZOP tool

Aspen HYSYS v8.4 simulation environment was selected as the commercial simulation tool. Aspen HYSYS is a powerful engineering software tool for steady state and dynamic

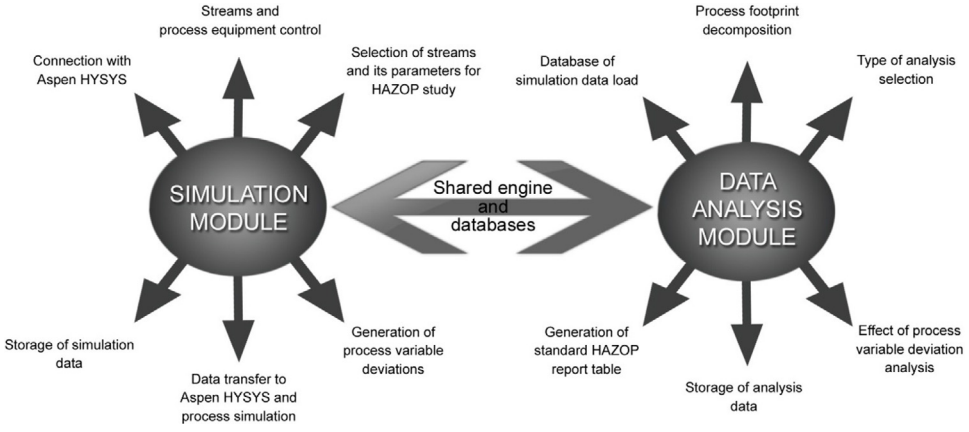

Fig. 1 – Methodology of the proposed software tool.