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Model-based hazard identification in multiphase chemical reactors

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ABSTRACT

Chemical productions operated in extreme conditions (high pressure, high temperature) require a detailed analysis of all potentially dangerous situations that can lead to a major industrial accident and thus cause a loss of life and property. Many accidents in the near or distant history underline the need of a detailed safety analysis in process industries, not only in the phase of plant design but also during the operation of the plant. It would be shown that simulation of a chemical unit using an appropriate mathematical model and the nonlinear analysis theory can be a suitable tool for safety analysis. This approach is based on mathematical modeling of a process unit where both the steady-state analysis, including the analysis of the steady states multiplicity and stability, and the dynamic simulation are used. Principal objective of this paper is to summarize problems regarding the model-based hazard identification in processes. A case study, focused on phenomena of multiple steady states in ammonia synthesis reactor will be presented. The influence of the model complexity and model parameters uncertainly on the quality of safety analysis would be underline.

1. Introduction

Chemical units include a wide range of hazards arising from the process itself, properties of the chemicals and their handling, such as fire, explosion and exposure to toxic substances. Statistics show that modern chemical industry is one of the safest industries in the world (Kletz, 2001); however, there still is real potential of major industrial accidents with catastrophic impact. This fact suggests that the role and responsibility of chemical engineers are mainly in providing reliable operation, optimization of material and energy consumption in the production and to minimize losses due to accidents.

Chemical productions operated in extreme conditions (high pressure, high temperature) require a detailed analysis of all potentially dangerous situations that can lead to a major industrial accident and thus cause a loss of life and property. Many accidents in the near or distant history underline the need for a detailed safety analysis in process industries, not only during plant design but also in the operation phase of the plant (AICHE, 1992; Mannan & Lees, 2005). It is also very important to note that safety analysis is often subject of official approval of constructions by the national government authorities.

Most of the major process units were developed based on the scale up of smaller (laboratory or pilot) units operated with minimal attention to safety. The design of a real industrial unit is always a compromise between technological, economic and safety requirements. To find a compromise between the number of installed safety elements and the planned investment costs is particularly problematic.

Currently, there are two basic approaches that can be applied to safety analysis and hazard identification in process industries. The first group of hazard identification method is based on theoretical approaches considering expert examination of the technological process in order to identify potential sources of hazard (HAZOP, What-if FMEA, FMECA, FTA, HRA and their modifications, or combination) (Crawley & Tyler, 2003). The strength of the standard methods is in considering also trivial errors that could trigger undesired events. Furthermore, many efforts have been recently made to improve the effectiveness of HAZOP, exploiting, for instance, the strength of plant digital representation and the utilization of the knowledge-based approach.

The established methods are mostly carried out manually and thus still involve many disadvantages which can be summarized in several points:

- these methods are time consuming and expensive;
- there is a possibility of overlooking a potentially dangerous situation and its consequences especially when a particular situation (deviation) has never occurred before;

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- requirements on the cooperation of engineers who have experience with the particular type of the process.

The introduced limitations of "standard" hazard identification methods can be eliminated (at least partially) by the second approach based on mathematical modeling and simulation of chemical processes and technologies used to identify known but mainly unknown hazards which have never occurred in practice (Labovský, Švandová, Markoš, & Jelemenský, 2007a, 2007b; Molnár, Krajčiová, Markoš, & Jelemenský, 2004; Molnár, Markoš, & Jelemenský, 2005; Švandová, Markoš, & Jelemenský, 2006). This second approach is a progressive and economically advantageous hazard evaluation method transferring real chemical processes to virtual reality to identify and then simulate the development of a possible accident from its beginning to the final state in the process of risk assessment. Principal advantage of this approach is based on deep knowledge of the physical and chemical phenomena, and the behavior of the processes of chemical technology and equipment, which allows predicting the system's behavior in situations that are exceptional and unlikely to occur (Seveso, Bhopal), thereby avoiding dangerous situations, or developing effective measures (means) to minimize the impact on humans, environment and property. Mathematical modeling is used as a tool for the description of the processes and equipments behavior under designed conditions and the simulation of system behavior (processes and equipments) on the change of the system parameters due to a failure. The effect of parameter changes depends on the parameter deviations from the designed values and on the duration of the deviations. Deviations from the expected values of the parameters lead to two types of response: a reversible change (returning the system to its original state after returning to the original parameter value), and irreversible changes (system settles in another steady state after the restoration of parameter values).

On the other hand, the application of mathematical modeling in the identification of hazards is not trivial, which is probably the reason of the absence of a universal and complex system or methodology enabling to perform such an analysis. Many existing applications, as well as the research in this field, can be characterized as a process simulator operated by experts to carry out an extensive series of simulations using the results of the simulations to evaluate the safety of the intended unit (Eizenberg, Shacham, & Brauner, 2006; Labovský, Jelemenský, & Markoš, 2006; Labovský, Laššák, Markoš, & Jelemenský, 2007; Labovský, Švandová, Markoš, & Jelemenský, 2007b; Švandová, Markoš, & Jelemenský, 2006; Švandová, Markoš, et al., 2006; Švandová, Markoš, Jelemenský, & Molnár, 2005), which makes it a very time-consuming task requiring an expert in mathematical modeling, numerical mathematics and safety analysis. It is clear that the identification of hazards by means of mathematical modeling is dependent on the quality of the mathematical model as well as on the quality of the model parameters (Švandová, Labovský, Markoš, & Jelemenský, 2009; Švandová, Markoš, & Jelemenský, 2006; Švandová, Markoš, & Jelemenský, 2008). In addition, the results of safety analysis based on mathematical modeling are very often specific to a particular type of process and therefore it is very difficult (or even impossible) to apply them even for a similar chemical technology. It is also important to point out that mathematical modeling is not an alternative to standard hazard identification methods. The investigated reactor or distillation column must be considered in a very complex plant with interfering problems, e.g. equipment aging, human and organization factors and many other issues, which cannot be included in the mathematical model. Therefore, the process of safety analysis will always require the cooperation of engineers with different expertise even in case a very sophisticated mathematical model is used. Mathematical modeling is valuable for the identification of specific physical hazards and the standard methods are essential for the identification of interfering hazard.

Evaluation of the safety concerns all equipment and technology. In principle, unit operations repeated in multiple technologies can be distinguished and thus considerable information and experience related to such equipments and processes are required. As a rule, the nature of physical processes (e.g. pumping liquids, gas compression, distillation, etc.) is essentially the same and the procedures of safety evaluation are generally established and more or less standard. Another group of processes are associated with chemical transformation specific to the type of reactions taking place under different hydrodynamic and thermodynamic conditions, and which are usually associated with heat and mass transfer, possibly combined with separation processes (e.g. reactive distillation). Chemical reactors in which exothermic reactions take place are probably the key units considering safety. Many accidents in the near history point to the necessity of safety analysis of each chemical reactor, not only after its design but also during its operation, as well as in cases when one of the operating parameters is changed. Based on the statistics presented, the majority of accidents involving chemical interactions occurs in chemical reactors, (Sales, Mushtaq, Christou, & Nomen, 2007); therefore, chemical reactivity is an issue that must be taken into consideration at any stage of the process. To operate a chemical reactor in safe regime it is very important to have qualitative and quantitative knowledge about the limits of the control parameters, at which the reactor operates in a safe regime. Also, it is essential to identify the parameter values potentially leading to a dangerous situation or even to a breakdown of a chemical reactor. When a chemical reactor is operated in the vicinity of multiple steady states, importance of the determination of safe operation increases markedly. However, the information about the presence of multiple steady states is often missing.

Principal objective of the recent work is to summarize problems regarding model-based hazard identification in processes. The existence of the multiple steady states phenomena in an ammonia synthesis reactor is described in the first case study. The influence of the model complexity and model parameters uncertainty on the quality of hazard identification for a reactive distillation column for MTBE production is underlined in the second case study.

2. The first case study – ammonia synthesis reactor and the existence of multiple steady states

One of the most important steps in the process of safety analysis is to qualitatively and quantitatively describe the range between normal operating conditions and conditions at which reactor breakdown can occur. In the process of safety analysis it is very important to identify the boundary between normal operating and potentially hazardous conditions (high temperature, high pressure) which can lead to a breakdown of the reactor. Sometimes, very small disturbances in any process parameter can lead to undesirable hazardous situations. It is therefore very important to know the influence of all process parameters on the reactor behavior. As it was mentioned in (Labovský, Švandová, Markoš, & Jelemenský, 2008; Molnár, Markoš, & Jelemenský, 2005), one of the primary questions concerning safety analysis of chemical units is the knowledge of the existence of multiple steady states. In general, multiple steady states are expressed as the number of different sets of state variables at which the time rate of the change of all state variables is zero for a fixed set of conditions or parameters (Molnár, Markoš, & Jelemenský, 2003). It means that the chemical unit can be operated in different regimes (temperature, conversion, selectivity etc.) under the same input conditions. From the safety analysis point of view, switching from one steady state to another one