Dynamic Simulation for Risk Analysis: Application to an Exothermic Reaction

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Abstract
Currently, there is a strong demand for quantitative process risk analysis. There is a challenge in describing the process dynamic behaviour in case of failures. We suggest a methodology that combines dynamic simulation (Aspen Plus Dynamics tool), risk analysis (HAZOP review) and risk matrices. The hazardous scenarios leading to major accidents are identified, some of them are simulated which allows the determination of consequences and quantification of severity. Moreover, the knowledge of the process dynamic behaviour and the evolution of the operating parameters during a degraded mode permits adequate safety barriers recommendation. In this paper, the aim is to apply this methodology to a case study concerning an exothermic reaction in a semi-batch reactor. The chosen reaction is the oxidation reaction of sodium thiosulphate by hydrogen peroxide. Advantages and limitations of the proposed approach are revealed and discussed.

Keywords: Process safety, Dynamic simulation, Risk assessment, HAZOP method, Runaway scenario.

1. Introduction

The risk assessment is a major requirement in the industrial context. Risk identification is essential for ensuring safe design and operation of a process. In chemical industry, chemical reactors involving an exothermic reaction are potentially the most hazardous unit operations (Markos et al., 2005). One major concern is the potential for thermal runaway which can have severe consequences (Stoessel, 2008; Zhang et al., 2014). This scenario has several possible triggers such as cooling loss or wrong reactant concentration (Ni et al., 2016).

In fact, several techniques are available to analyse hazardous scenarios (Marhavilas et al., 2011). Among them, the HAZard and OPerability study (HAZOP) is a well-known technique largely applied (Fuentes-Bargues et al., 2016; Galante et al., 2014; IEC, 2016; ISO 31010, 2010; Kletz, 1999; Saada et al., 2015). Initially, HAZOP was a qualitative method. Since its inception in the 1960’s, it has been increasingly used and has evolved to a semi-quantitative method (Trujillo et al., 2015), because risk quantification is decisive for appropriate decision-making. The determination of the effects of failure scenarios is a real challenge (Baybutt, 2015a).

Consequently, there is a real interest in knowing the system behaviour during malfunctions for safety analyses. For this purpose, dynamic simulation is an efficient tool to predict the evolution of variables in chemical processes during deviations from normal
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