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An optimal control-based safety system for cost efficient risk management of chemical processes

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ABSTRACT

The design of conventional safety systems is based on failure likelihood and accident severity, which is normally obtained empirically, leaving the system vulnerable to process nonlinearities. To ensure process safety, control actions are conservative and small deviations from setpoints may lead to shutdown, generating economic losses. In this work, periodic simulations of system behavior against failures is proposed in order to determine the potential risk to which the system is subjected. Depending on this potential, preventive actions can be taken in order to guarantee the system safety and integrity and avoid potential shutdown. These actions are calculated to provoke least possible disturbance in order to reduce impact on product quality, while keeping the process operating. The goal is to increase annual operating time of the plant without compromising safety and product quality. Results show that the proposal is feasible to real time applications and unnecessary shutdowns can be avoided.

1. Introduction

Although the chemical industry has operated on a large scale for decades, only in the last two decades the subject of safety has gained the attention it deserves. Several accidents have marked the history of the chemical industry, such as Chernobyl, Bhopal, Seveso and Sandoz. Important lessons have been learned from these tragedies. Among them, the deep knowledge of the chemical process can be emphasized. During development of a new process, even after the tests on a pilot scale, the scale-up to industrial scale can bring serious changes in the dynamic behavior of the system. Besides these changes, the control structure can modify the stability of the system at various operating points. In this case, the use of mathematical models is essential for reliable dynamic analysis. Moreover, with the rapid advancement of computing in recent years, the use of rigorous phenomenological models becomes increasingly feasible (Manenti, 2011). Their penetration in the industrial environment, however, is still limited. The situation is similar in security systems. Despite the obvious gains that non-linear mathematical models can bring regarding the reliability of the analysis, their use still faces difficulties in implementation and hesitancy for industrial sites to replace traditional linear models. In the area of process safety, the scenario is even worse because, traditionally, the analyses are based on process empirical knowledge. Often qualitative models are used for that purpose, which are still quite lagged in respect to alternative proposals found in the scientific literature, which has suggested the use of more accurate models and techniques (Venkatasubramanian and Rengaswamy, 2003).

In addition to the difficulties faced during the design of safety systems, new obstacles arise during industrial operation. Detecting the origin of unwanted events can constitute a complex task, but once found, can be decisive in determining the actions of the security system (Venkatasubramanian and Rengaswamy, 2003). Another important issue is that operators, whose subjectivity considerably reduces the reliability of the security system, take many decisions involving hazardous situations. All of that makes the design and operation of these systems very conservative, with tight and narrow tolerances for deviations from the setpoints and often using the emergency shutdown as a way to ensure safety (Luyben, 2012). These actions, however, lead to considerable loss of production and, consequently, financial losses, since the plant can idle for days before it is ready for the new startup.

1.1. The safety problem

Security is an issue of paramount importance, especially in the chemical industry, where tons of hazardous substances are processed daily. To ensure a safe process, reduce environmental impacts and avoid major changes later, the security must be taken

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Nomenclature

C_p	reaction mixture heat capacity [J mol^{-1} K^{-1}]
E_a	activation energy [J/mol]
F	flow [mol h^{-1}]
H	safety system prediction horizon
H_{rec}	reconciliation horizon
k	equivalent kinetic constant [mol h^{-1}]
k_0	Arrhenius pre-exponential factor [m^3 mol^{-1} h^{-1}]
M	NMPC control horizon
M	amount of substance [mol]
P	NMPC prediction horizon
P	safety system convergence horizon
$\mathbf{Q}$	controlled variables tracking error weighting matrix
R	universal gas constant [J mol^{-1} K^{-1}]
$\mathbf{R}$	control actions weighting matrix
r	chemical reaction rate [mol h^{-1}]
$\mathbf{S}$	manipulated variables tracking error weighting matrix
T	temperature [K]
t	time [h]
UA	overall heat transfer coefficient [J h^{-1} K^{-1}]
$\mathbf{u}$	manipulated variables vector
V	volume [m^3]
$\mathbf{X}$	safe state weighting matrix
x	molar fraction
$\mathbf{x}$	model state variables vector
x	safety system predicted state
$\mathbf{y}$	model output variables vector
y	measured variables vector

Greek symbols

ΔH_r	reaction heat [J/mol]
κ	equivalent heat transfer coefficient [h^{-1}]
$\boldsymbol{\theta}$	dynamic model parameters vector
ω	process failure

Subscripts and superscripts

Cat	catalyst
in	input
j	jacket
Mon	monomer
max	maximum
Pol	polymer
Sol	solvent
t	total

into account from the process design to the daily operating practices (Howell, 2010; Woodcock and Au, 2013).

Exothermic reactions make chemical reactors very dangerous pieces of equipment in the chemical industry. Knowledge of all the chemical reactions involved in the process is critical to the design of a safe reaction system. It is also important to know the kinetics of reactions that can occur in abnormal process conditions such as higher temperatures, the possibility of accumulation of any contaminant present in feed, or the effect caused by contact between the jacket fluid (often water, which is a potentially reactive substance) and the reaction mass.

The runaway is one of the most serious problems in exothermic systems (Gygax, 1988). This phenomenon is characterized by the uncontrolled self-sustained increase of reactor temperature. This quick rise in temperature increases the vapor pressure of the reactants in the reactor and hence increases the pressure inside the vessel. In addition, the temperature rise may trigger secondary reactions, producing more heat and non-condensable gases that also cause increased pressure in the vessel. In this scenario there is a great risk of leakage of flammable gases or even rupture of the reactor walls (Manders et al., 2011).

According to Maschio et al. (1992) the majority of accidents in reaction systems were due to:

- lack of knowledge about the chemistry and thermodynamics of the process;
- inadequate reactor design (heat exchange devices, agitation, scale up);
- inadequate control and safety systems;
- inadequate operating procedures and training of operators.

1.2. Safety systems design

In order to organize the main topics of process safety area, in this paper we propose the division of safety system design in three basic steps: (i) identify the hazards; (ii) determine how often failures occur and the severity of these failures; and (iii) size equipment and define operating and emergency procedures. The first step is generally qualitative. The hazards, their causes and consequences are mapped through hypothetical situations and empirical knowledge of the process. Similarly, the spread of abnormal events can be mapped. However, with increasing complexity of the process, the reliability of this type of analysis is considerably reduced. In these cases, techniques based on mathematical process models are recommended, combining qualitative analysis with quantitative elements (Graf and Schmidt-Traub, 2001). The most used method in this first step is called HAZOP – hazard and operability study – with important results reached by Vaidhyanathan and Venkatasubramanian (1995) and Labovský et al. (2007).

The result of the first stage is a map with all the possible hazards of the process, ranging from minor problems to huge disasters. However, statistically, for each catastrophe, there are thousands of possible small incidents. Thus, these hazards must be weighed according to their frequency, resulting in a matrix similar to Fig. 1. The risk is the product of frequency and severity, resulting in three regions: acceptable risk, moderate risk and unacceptable risk (Baradits, 2010). This matrix is the result of the second stage of the safety system design. The most widely used technique for the determination of events frequency is QRA – quantitative risk

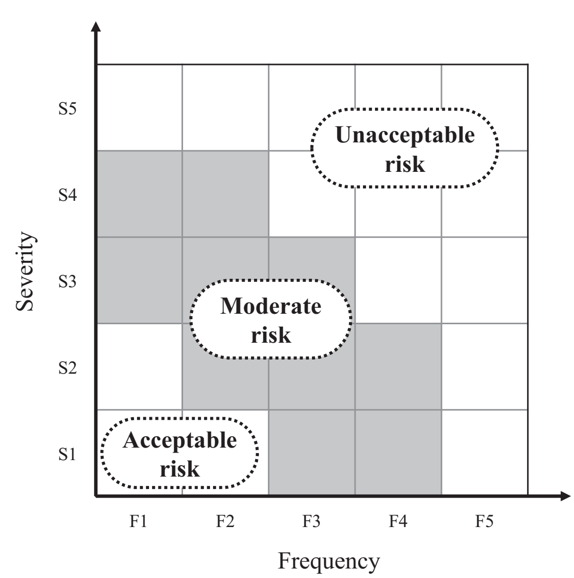

Fig. 1. Risk matrix.

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