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Early warning detection of runaway initiation using non-linear approaches

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Abstract

We present a method for early detection of runaway initiation in chemical reactors using only temperature measurements and based on the calculation of the divergence of the system. The method is based on state space reconstruction techniques and is illustrated using simulated as well as experimental datasets. The results show that the method is able to distinguish between runaway and non-runaway situations and it does not produce false alarms during controlled heating/cooling experiments.

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1. Introduction

The reliability of a chemical reactor installed in a plant depends on the capability of the control/supervision system to estimate its state and to identify, in time, its operation malfunctions or failure modes. Specifically for chemical reactors carrying out exothermic reactions, the major

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problem is the loss of temperature control. In this situation, when the rate of heat generation by chemical reaction exceeds the rate of heat removal by the cooling system, there is a positive feedback mechanism, since the temperature of the reaction mass will rise, increasing in turn the heat generation rate. In this situation, if no countermeasures are taken, a runaway or thermal excursion may occur.

There are several reasons for which the early detection of dangerous states is important for the correct operation of chemical reactors. Apart from health and environmental considerations, an accident in a chemical reactor is extremely expensive [7]. Furthermore, chemical industries experience a number of near-misses, which could be reduced by the use of an early warning detection system (EWDS). This reduction would also contribute to the reduction of minor and major accidents, since as it has been shown that these values are correlated [12].

Methods for early warning detection can be divided into three main categories depending upon the quantities being used: conventional limit check systems [10,16], temperature derivatives [8], and model-based estimation techniques, i.e. Kalman filtering or equivalent [6,9]. However, despite all the different approaches, the early on-line detection of hazardous states in batch and semibatch processes is still an open problem because of the wide range of processes that are carried out on such equipment; their complexity; strong non-linearities; and time-varying parameters. In this context, the bottlenecks for the development of an effective on-line detection system are the definition of criteria, which distinguish between dangerous and non-dangerous situations; the avoidance of false alarms, since countermeasures may consist on dumping the reactor contents or injecting an inhibitor with the loss of the batch, which means that in practice a trade-off exists between early detection (sensitivity) and number of false alarms (reliability); and the use of few measurements since the number of process carried out batchwise makes it not economically feasible to develop a detailed kinetic model for each process, i.e. the EWDS has to be as independent as possible of the actual process carried out in the plant.

Furthermore, as shown in Fig. 1 the dynamic behaviour of chemical reactors have a high parametric sensitivity [17], i.e. a small change in one of the operating conditions or parameters of

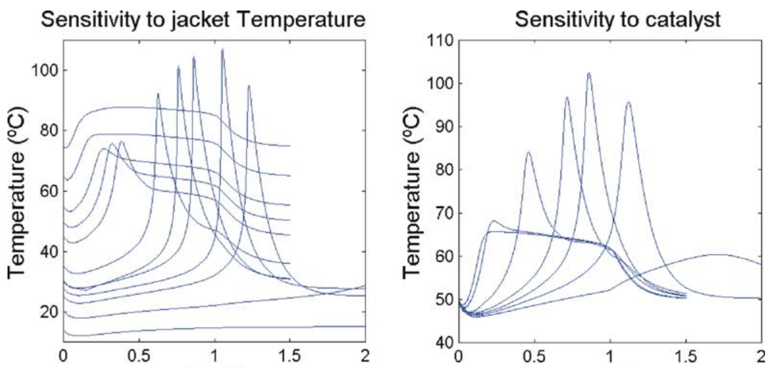

Fig. 1. Reactor temperatures measurements recorded during several semibatch processes using the system 2-butanol–propionic anhydride and sulphuric acid as catalyst in a 2 l bench scale reactor. All the experiments were performed in similar operating conditions but changing in (a) the jacket temperature, from 10 to 80 °C; and in (b) the catalyst concentration, from 0.0 to 2.5 wt.%.