The study of reaction kinetics using Design of Experiments and numerical simulation

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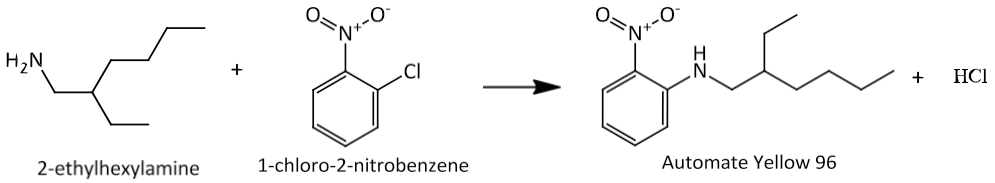
Understanding and controlling the chemical reactions is one of the most important and challenging aspects of chemical process development and risk assessment. From this perspective, it is necessary to acquire sufficient understanding of the reaction kinetics and process behavior both under normal and failure conditions [1].

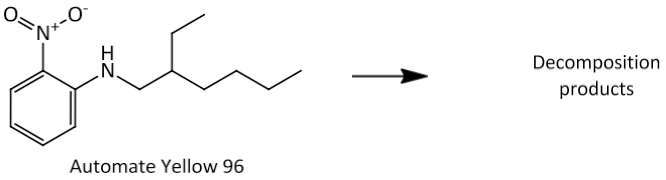
In order to achieve this goal efficiently, the dynamics of the system can be studied using numerical simulations where parameters are estimated from a series of representative measurements. Such models are based on ordinary differential equations describing the reaction system (reaction kinetic model) and the process behavior (process model) [2]. However, even with this method, the calculation time can be very long due to the potentially complex models, involving a large number of parameters and requiring a large amount of measurements to ensure adequate reliability and precision. Therefore, a new approach to solve these problems needs to be investigated.

The proposed approach can be summarized in two points: the first step one is to plan the required measurements in a systematic way to optimally cover the experimental space with a minimum of experiments [3, 4]. The second step involves developing a numerical algorithm capable of extracting the kinetic parameters from the acquired measurements [5].

The proposed method was studied on the reaction system (Synthesis reaction



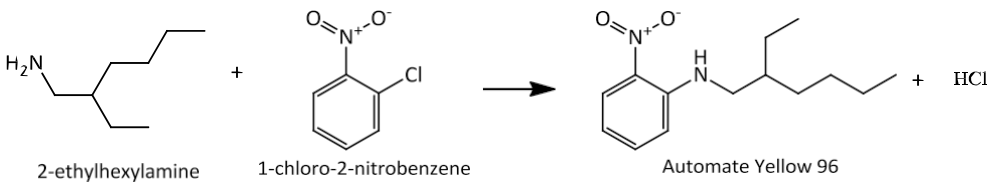
(1) Decomposition reaction



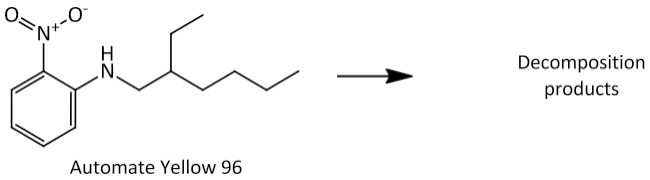
Scheme 1 - The Morton case reactions (synthesis and decomposition)

) involved in the Morton accident in New Jersey (1998). The reaction system is composed of a synthesis reaction (1) followed by an autocatalytic decomposition of the product (2), the latter being the root-cause of the incident.

(2) Synthesis reaction



(3) Decomposition reaction



Scheme 1 - The Morton case reactions (synthesis and decomposition)

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