Reaction kinetic and safety investigation of the Morton case based on calorimetric methods

Haute école d'ingénierie et d'architecture Fribourg
Hochschule für Technik und Architektur Freiburg

June 2015

CHEMISTRY

Introduction

In 1998, within the firm Morton international, the synthesis of dye AY96 produced an explosion due to a runaway reaction and caused extensive damage. Indeed, the product of decomposition was an autocatalytic reaction.

The aim of this project was to determine the kinetic model of this reaction using calorimetric methods (DSC,C80) and AKTS software. In addition, a study on the safety of this process was performed.

Method

The kinetic model of the reaction was investigated using the method of Reaction Kinetic Investigation (RKI) and the AKTS software.

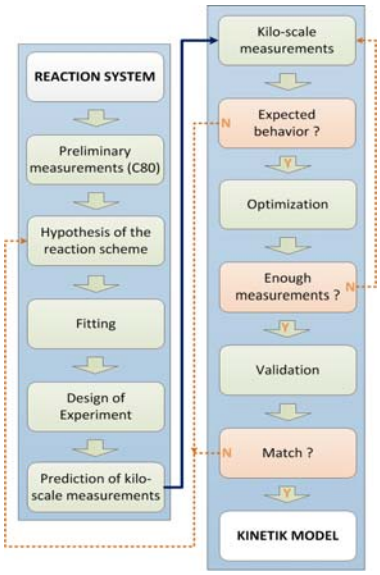

Figure 1 : *RKI method*

Conclusion

- The kinetic model of the synthesis of the AY96 has been determined.
- The model was validated using the calorimetric experiments and simulations.
- The reaction is qualified as criticality class 5.
- Adapting the reaction in continuous mode would be a good alternative.

Reaction

The synthesis of the AY96 is highly exothermic and the decomposition is autocatalytic.

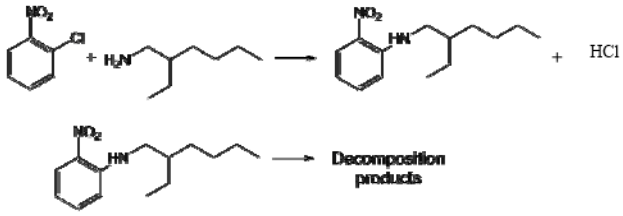

Figure 2 : Synthesis reaction of AY96 and its decomposition

Model of the reaction scheme

$$A + B \longrightarrow C + D$$

$$C \longrightarrow E$$

$$C + E \longrightarrow 2E$$

The kinetic model is described using Arrhenius and power rate laws :

$$k_j = A \cdot \exp\left(-\frac{E_{a,j}}{RT_r}\right) \qquad r_j = k_j \cdot \prod_{i=1}^{I} C_i^{mi}$$

Results

As the simulations fit well with the experimental measurements, the model can be considered as valid.

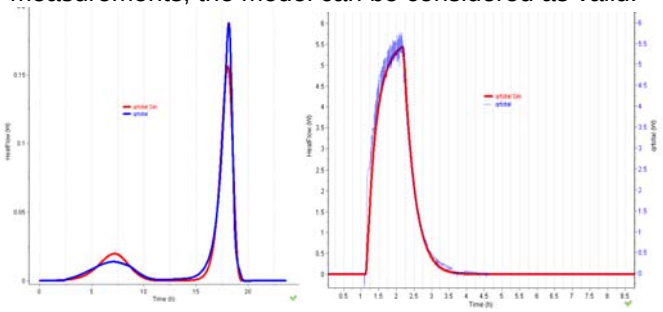

Figure 3: *comparison of the DSC (0.2 K / min ; left) and RC1 (right) measurements with their respective simulation.*

Using the kinetic model of the reaction, the Stoessel diagram can be drawed :

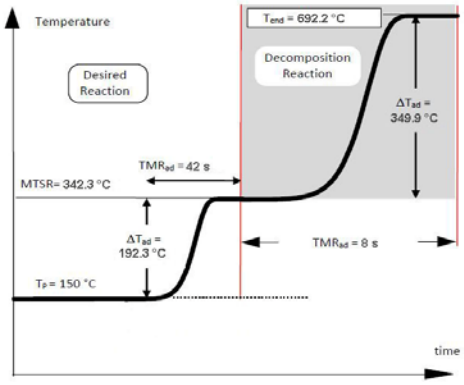

Figure 4 : Stoessel diagram for the Morton case

Students:
Mohammed Biya &
Sylvie Mathieu

Professor:
Dr. Christophe Alleman

Project proposed by:
Charles Guinand