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Mass & energy balances coupling in chemical reactors for a better understanding of thermal safety

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ABSTRACT

Process safety is an important topic in the curriculum vitae of a chemical engineer. It can be a difficult course for the students and professors, because it is a frontier course between chemical engineering and safety. How to introduce this course? We think that this course should be introduced during the chemical reaction engineering, and more particularly during the mass and energy balances lectures. Thus, the students can more easily understand the concept of isoperibolic mode, secondary reactions, heat-flow rate due to chemical reactions, Semenov curves, etc. In this manuscript, we propose a pedagogical method to introduce this concept by using numerical simulation. In the first section, the roots of energy balance for the different reactors is derived. In the second section, mass and energy balances coupling is derived for the different chemical reactors. In the third section, the different thermal modes, i.e., isothermal, isoperibolic and adiabatic are described. Then, a tutorial by using a batch reactor with several exothermic reactions is treated and corrected. At this moment of the course, the instructor can introduce the last section about safety criteria by using the zero-order approximation. The rigorous mass and energy balances coupling should be introduced to the students before the current approximation made by the safety community, i.e., zero order, in process safety.

1. Introduction

The introduction of safety and risk assessment during a chemical engineering curriculum is recommended by different associations (Favre et al., 2008; Shallcross, 2013; Perrin and Laurent, 2008; Dee et al., 2015; Spicer et al., 2013). Process safety for chemical engineers can be a difficult course for the students and for the professors, because it includes several concepts from thermodynamics, reaction kinetics, chemical reaction engineering, process design, accident scenario development and even sociology.

A chemical engineer should appreciate the risk of thermal runaway which can cause a pressure elevation and an explosion of the vessel. The evolution of heat-flow rate due to chemical reactions should be known, thus kinetics and thermodynamics of the chemical system should be determined. When the behavior of the heat-flow rate due to chemical reactions is known, the chemical engineers could design a system to remove the excess of heat to diminish the risk of thermal runaway. For that reason, different Chemical Reaction Engineering (CRE) books have integrated one chapter on process safety or on thermal stability of reactor (Coker, 2001; Fogler,

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2016; Rawlings and Ekerdt, 2013; Villermaux, 1999). We should also mention the book of Francis Stoessel on thermal process safety assessment (Stoessel, 2008). By segregating this lecture of thermal safety from CRE, students could use some formulae to calculate safety criteria based on zero-order reaction.

We are also convinced that this course can be introduced as a chapter in chemical reaction engineering (CRE) courses. More particularly, during the lectures on mass and energy balances. During our lectures of CRE and reactor stability at Åbo Akademi University or at INSA Rouen, we have noticed that we should spend more time to illustrate properly the strong coupling of mass and energy balances. Thus, students learn how to determine the different heat-flow rates in a chemical reactor which illustrates the dynamic of the system. The thermal safety criteria are often introduced with a static approach: by assuming full accumulation, adiabatic conditions, single reaction and zero-order reaction. The main drawback with that approach is those students do not study properly the determination of heat-flow rate under different thermal modes in presence of multiple reactions. This static approach, based on the worst case scenario, could lead to some confusion for the future chemical engineers. The different concepts of time to maximum rate under adiabatic conditions TMR_{ad}, or adiabatic temperature rise ΔT_{ad} during process safety lectures can be abstract to understand and handle (Stoessel, 2008). Based on our experience, we have developed a pedagogical strategy including numerical simulation to ease the understanding of such concept during a CRE course for undergraduate and master students (Antunes et al., 2011; Lindfors, 1971; Taipa et al., 2015). The use of simulation is an efficient pedagogical tool to understand the dynamic of a chemical reaction system (Coker, 2001; Finlayson, 2006; Fogler, 2016; Law, 2013; Rawlings and Ekerdt, 2013; Salmi et al., 2010). However, the instructors should spend time to explain correctly the program to the students. Furthermore, due to the introduction of simplification, the results of the simulation should be viewed with caution, essentially during the stage of design (Levenspiel, 1999).

The main objective of this manuscript is to propose a dynamic view of safety criteria by using simulation. Fig. 1 illustrates the pedagogical approach. It is not a course on process safety, which should take place after this course. Some articles have modeled some accidents or scenarii, but these case studies are for master or post-graduate students (Eizenberg et al., 2006; Willey et al., 2011; Dixon and Kohlbrand, 2015). We

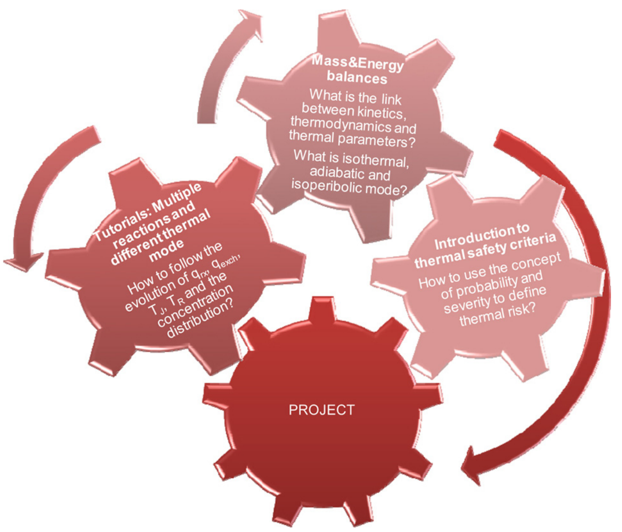

Fig. 1 – Schematic view of the pedagogical approach.

did not simulate the evolution of the pressure in the reactors head space during this course. During the lecture, we mention that pressure increase can be due to the evaporation of the reaction mixture and decomposition reactions producing non-condensable products. We think that this part can be seen during the safety course and particularly during practices. As illustrated by Willey et al. (2011), the example of an industrial accident can be used by using VSP 2 technology.

The course (around 20 h) includes the following main topics:

- Mass and energy balances (3 h)
- Different thermal mode (3 h)
- Tutorials based on numerical simulation (5 h)
- Thermal safety assessment (4 h)
- Project (5 h)

The first 6 h of the course are dedicated to lectures of mass & energy balances in chemical reactors and the different thermal modes. This introduction is fundamental for students, because they can understand why there is a strong mass & energy balances coupling and the importance of the thermal mode. The personal student work is between 3 and 6 h.

The next part of the course (5 h) is dedicated to practice to simulation by using Matlab. The instructors should explain the skeleton of the Matlab code and the exercises. The instructor can individually adapt the proposed exercises to the students. The students must solve out the different exercises by using Matlab (2 or 1 student per computer). This part of the course can be the most demanding for the students and the instructors. It is essential that the students feel familiar with the code to understand the effect of initial reaction and jacket temperature, initial concentrations, thermal parameters and thermal mode on the evolution of heat-flow rate, concentration distribution and temperature with reaction time. The personal student work is important for this part. Depending on student computing capacity, the personal can be estimated to 5–10 h.

The lecture concerning the thermal safety assessment is a lecture, and the personal student work is typically 4 h.

The project should be done by the students. Several configurations have been tested: personal, pair or group project; liberty for the student to choose their partners or the instructor defines a system to make the groups. Based on our experience, the pedagogical results are better when students work by pair and when they choose their partners. The computer room is reserved for the students one time per week. They have 3 weeks to finish that project.

Due to the space limitation of the journal, we have decided to put as supplementary information different elements of the course. For the sake of simplicity, only a batch reactor is described in this manuscript.

2. Remind of mass balance and kinetics in a reactor

Energy balance for chemical reactors is strongly linked to mass balance. Hence, it is important to refresh the fundamentals of mass balances for chemical reactors. Indeed, this course is after the first course of CRE, where the different ideal reactors were described. The instructor should insist on the fact that mass and energy balance are done on a delimited zone (liquid reaction, gas phase). For example, in case of liquid monophase reaction systems, we should pay attention to the fact that the mass balance is derived for the liquid phase. It is quite