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

Reaction optimisation in safe conditions using the normalised thermal potential

Y. Dupasquier[a], C. Guinand[b], B. Roduit[b], M. Dabros[c], O. Vorlet[c]

yan.dupasquier@master.hes-so.ch

Introduction

In fed-batch operation, the control of accumulation is a key step to reach safe operating conditions [1].

Once the system (reactor and reaction dynamics) is characterised, how can we find the best operating conditions in order to remain inherently safe?

Guinand et al. introduced a new parameter, the normalised thermal potential θ_{Gu} [2]. Through it, the thermal safety of an operation can be assessed at any given time of the process. When applied to fed-batch operations, this dimensionless parameter enables to control the feed rate during the feeding stage, as well as the temperature setpoint along the post-feeding stage, maintaining productivity and safety at any time as shown in the following application, involving the simulation of the heat released by a chemical reaction in a real system.

The normalised thermal potential θ_{Gu}

The normalised thermal potential is a dimensionless parameter helping to ensure thermally safe operating conditions, as well as optimising the productivity (Fig.1) [2].
The temperature reached in case of cooling failure T_{cf} at time t is evaluated as follows:

$$T_{cf}(t, t_{pred}) = T_r(t) + \Delta T_{ad}(t, t_{pred})$$

where ΔT_{ad} is the adiabatic temperature rise for a considered time range t_{pred} which typically amounts to 8 or 24 h.

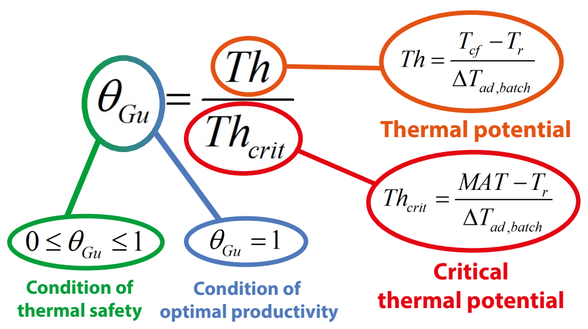

Figure 1: The normalised thermal potential, where MAT is the maximum allowed process temperature, $\Delta T_{ad,batch}$ is the adiabatic temperature rise of a batch reactor in case of cooling failure and T_r is the temperature of the reaction mixture.

The following points are necessary for the implementation of θ_{Gu}:

- The kinetic and thermodynamic parameters,
- The temperature of the reaction mixture $T_r(t)$,
- Determination of T_{cf} at $t+t_{pred}$,
- Control of both feed and $T_r(t)$.

Method

Using AKTS-Thermokinetics software, the total amount of heat released by hypothetical chemical reactions (Figs. 3, 4) can be imitated by a Joule heating element in any type of reactor. As an example, a 1L reactor is used, containing an initial mass of 750 g of water where 250 g are fed. The concentrations and temperature reached in case of cooling failure are computed continuously from the reactor temperature T_r and the reaction kinetic model (Figs. 2, 3).
The feed is controlled via an on/off command in order to maintain θ_{Gu} at a value of 1.
The temperature setpoint is controlled using the following equation:

$$T_{r,set} = MAT - \frac{T_{cf} - T_r}{\theta_{Gu,set}}$$

where $\theta_{Gu,set}$ is a setpoint value of the normalised thermal potential maintained during the post-feeding stage. In the framework of this study, the values of θ_{Gu} and MAT are set at 1 and 60 °C, respectively.

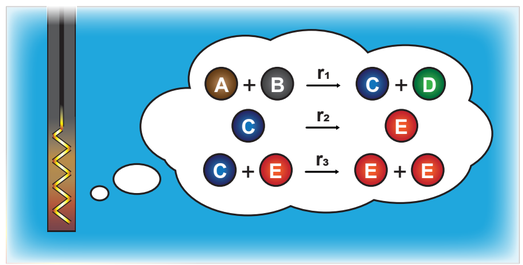

Figure 3: Scheme of the reaction system simulated by the heater.

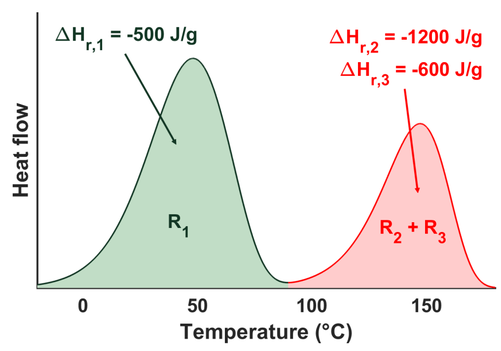

Figure 4: Simulated DSC signals obtained for equal initial masses of A and B at a heating rate of 3.3 K/min.

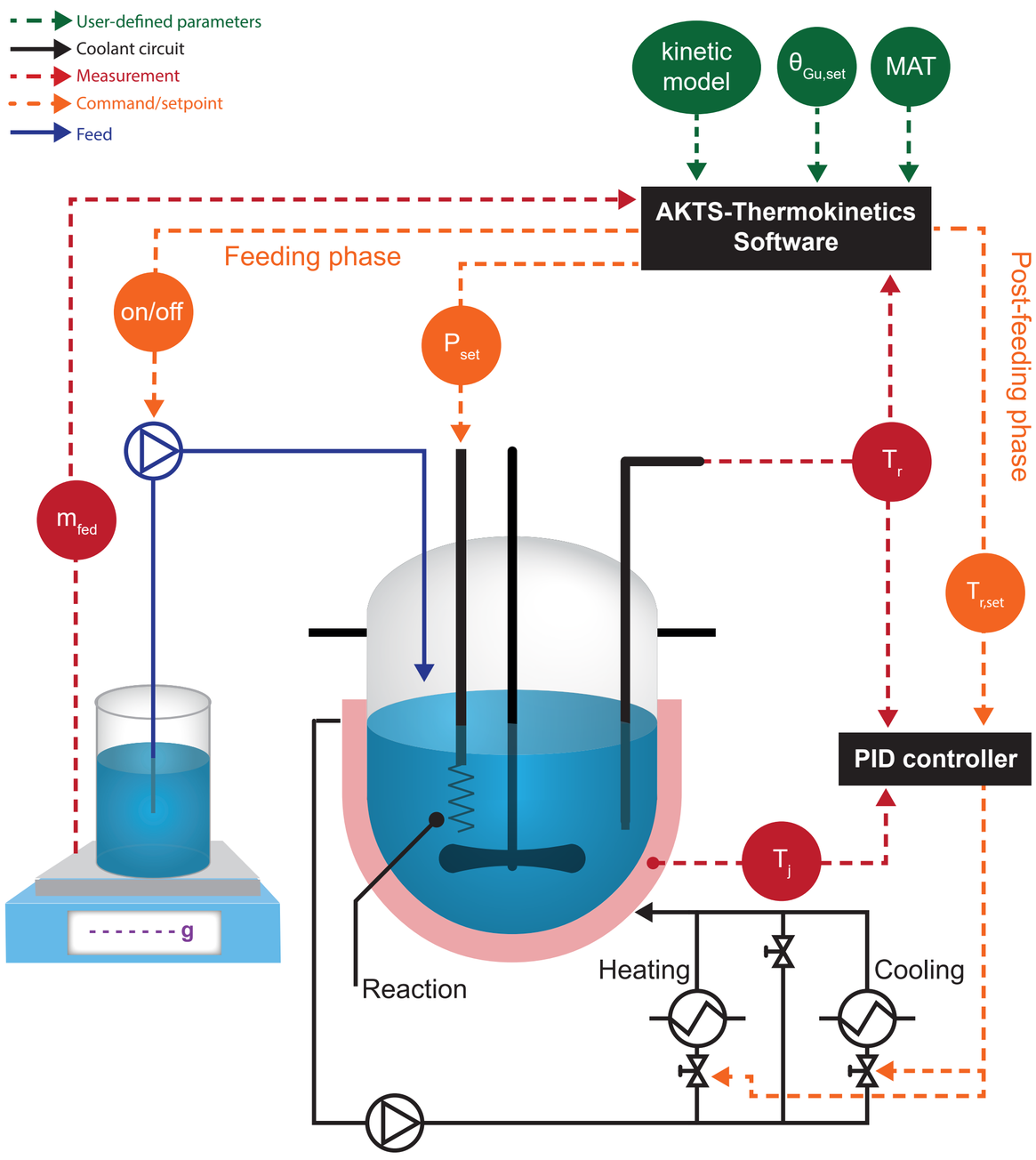

Figure 2: Scheme of the experimental setup and representation of the interactions. $\theta_{Gu,set}$ is a setpoint of the desired value of normalised thermal potential and MAT is the maximum allowed temperature. The commands (orange) at different phases of the process are computed by the AKTS-Thermokinetics software as a function of user-defined parameters (green) and reaction data (red) in order to maintain a desired value of normalised thermal potential θ_{Gu}.

Results

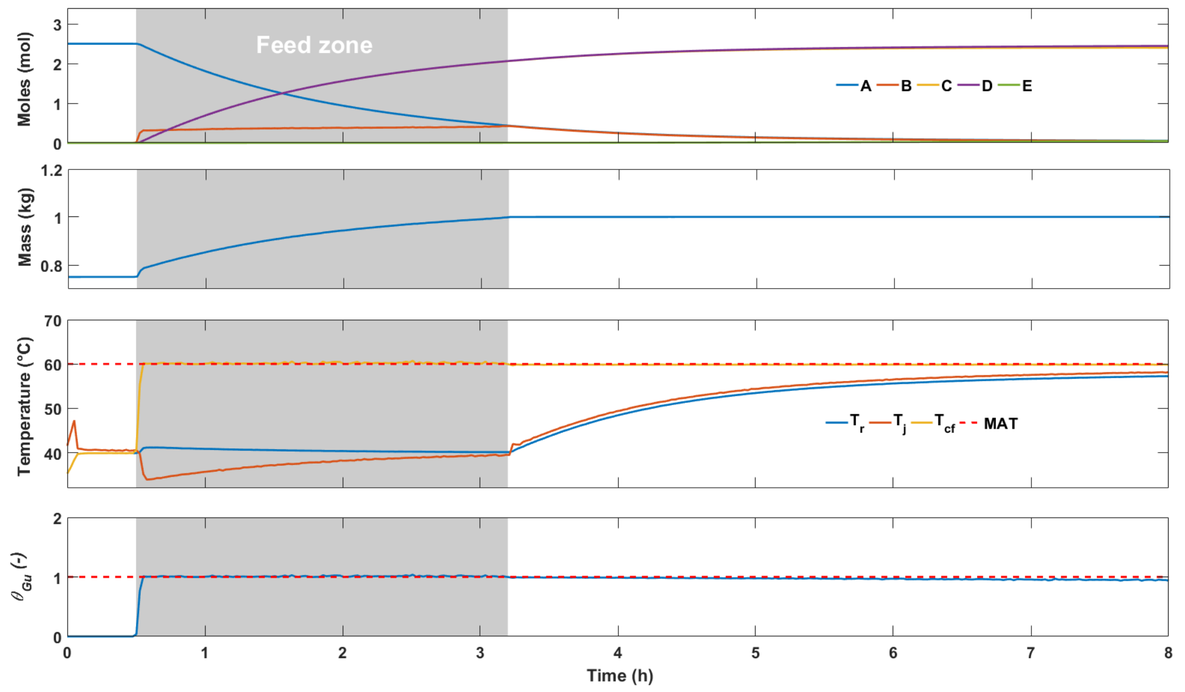

Figure 5: Change of the amount of moles of reactants and products, reaction mass, temperatures (T_r: reaction mixture, T_j: jacket, T_{cf}) and θ_{Gu} as a function of time in a 1 L double jacketed lab reactor. The heat produced by the reaction was estimated for the kinetic scheme presented in Fig. 3 by a Joule heating element.

During the operation, the normalised thermal potential is kept at a value of 1 by adjusting the feed rate (Fig. 5, Feed zone) and then the temperature setpoint $T_{r,set}$ (Fig. 5). To reach 95% of conversion, 8.7 h would be required at a temperature T_r = 40°C, a constant feed rate (250 g in 5 h) and $\theta_{Gu} \le 1$. By setting $\theta_{Gu,set} = 1$, the same conversion could already be reached after ca. 4.8 h (Fig. 5).

Conclusion

Through the heat release of reactions mimicked by the application of a Joule heating element in a 1L reactor, it was shown that the normalised thermal potential enables a real-time design of the feed rate and temperature setpoint profiles. Thus, maximal efficiency is reached, while safe thermal conditions are warranted.
The approach presented in this study can be applied similarly for any type of chemical reactions.

References

[1] Stoessel, F., Thermal safety of chemical processes: risk assessment and process design. 2008, John Wiley & Sons.
[2] Guinand, C., Accumulation in fed-batch reactor with multiple reaction scheme. Thesis. 2017, École Polytechnique Fédérale de Lausanne.

Ackowledgements

Christophe Borgeat - AKTS
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a) Hes·so Haute Ecole Spécialisée de Suisse occidentale
Fachhochschule Westschweiz
University of Applied Sciences and Arts Western Switzerland

b) AKTS Advanced Kinetics and Technology Solution

c) HEIA-FR HTA-FR