An early warning criterion for semibatch reactors.

Francesco Maestri[1]*, Renato Rota[1], Sabrina Copelli[2]

1 Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria chimica "G. Natta"
piazza L. da Vinci 32, 20133 Milano, Italy; 2 Università degli Studi dell'Insubria, Dipartimento di Scienza e Alta Tecnologia
via G.B. Vico 46, 21100 Varese, Italy

**Corresponding author: francesco.maestri@polimi.it*

Highlights

- Potential runaway fine chemical reactions are performed in semibatch reactors (SBRs).
- The safe SBR operating regime must be determined with the minimum experimental effort.
- A criterion is implemented for the kinetic-free monitoring of the SBR.
- The criterion allows for an early warning prevention of unsafe scenarios.

1. Introduction

The safe operation of chemical reactors in which potential runaway reactions are performed is of crucial importance to avoid accidents resulting in plant damages and losses of human lives. If the rate of heat generation by the exothermic chemical reaction exceeds the rate of heat removal by the cooling system, the temperature of the reacting mass will begin to rise with a self-accelerating behavior: as a consequence very fast and exothermic decomposition reactions could be triggered, generating dangerous reactor overpressures. Early warning systems are useful to promptly detect such hazardous scenarios and to allow plant operators to adopt the necessary actions to keep the process safe [1], [2].
In this work the industrial implementation of the general energy criterion developed by Maestri and Rota [3] is discussed, with the aim of early detecting during the SBR normal operation reactivity losses and resulting accumulation phenomena at the origin of severe runaway phenomena.

2. Methods

The criterion is based on the following easy to measure Key Process Indicators (KPIs):

$$\Psi = \frac{(m\hat{C}_P)_{dos}(T-T_{dos})+(m\hat{C}_P)_{cool}(T_{cool,OUT}-T_{cool,IN})}{(-\Delta\hat{H}_r)m_{dos}\omega_A/\nu_A}\times 100$$

$$X = \frac{(m\hat{C}_P)_0(T-T_0)+(m\hat{C}_P)_{fed}(T-T_{dos})+\int_0^t(m\hat{C}_P\Delta T)_{cool}dt}{(-\Delta\hat{H}_r)m_{fed}\omega_A/\nu_A}\times 100$$

$$MTSR_{ad} = T + (1 - 9X/100)\Delta T_{ad}$$

Ψ measures the degree of approach of the SBR regime to pseudo steady state conditions with respect to both the coreactant accumulation and the reaction temperature, X is a direct measure of the conversion degree of the dosed coreactant and $MTSR_{ad}$ accounts for the residual energy release potential of the system due to the conversion of the coreactant still to be dosed as well as of its accumulated amount.
The use of the energy criterion does not require a kinetic characterization of the system, but is based on information available from simple laboratory scale measurements. Moreover, the involved KPIs can be easily measured during the reactor operation, through the elaboration of fully available process variables.

3. Results and discussion

When the SBR is safely operated, the conversion rate is fully determined by the coreactant supply rate and the reaction heat is removed from the system at a much lower time scale than that at which it is evolved. Under such conditions Ψ and X quickly approach values close to 100, which are then kept for most of the dosing period.

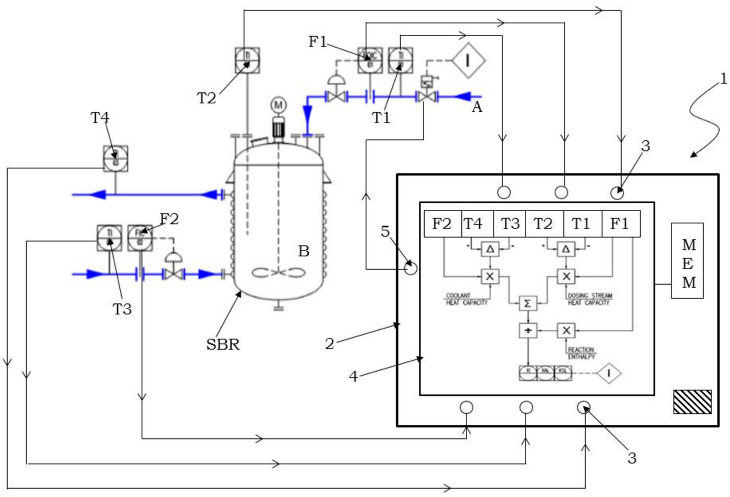

Figure 1. SBR monitoring system through the energy criterion.

The present work describes the system interconnected with the SBR for implementing the previous criterion (schematically shown in Figure 1) as well as its operation logic.

System 1 consists of a housing 2 enclosing the components for performing the signal elaboration and parameters calculation. Moreover, it comprises a unit MEM storing the target operating conditions of the SBR in terms of coreactant accumulation and reaction temperature behaviors.

The process variables, such as the temperature T1 of the feed stream, the temperature T2 of the reaction mass, the inlet and outlet temperatures of the coolant, T3 and T4, the feed stream flowrate F1, as well as the coolant flowrate F2, are measured in time through sensors and their values are transmitted to system 1. The system is then equipped with device 3 for receiving the measured process variables, to be then processed through e.g. digital and/or analog inputs.

In particular, system 1 consists of a processing unit 4 for calculating the Ψ and X parameters and of a device 5 able to generate a trigger signal (for example a TTL signal) to interrupt the feed of the coreactant A in case of displacement of the SBR operation from the target operating conditions stored in the unit MEM.

If at a given time a Ψ number lower than its threshold limit (e.g. 80) is detected, a reaction inhibition or a heat transfer efficiency decay could have occurred. If at such a time the maximum attainable temperature $MTSR_{ad}$ is higher than a maximum allowable limit, MAT, the feed is immediately interrupted. Otherwise a final check on the X value is performed, which again triggers the feed stop only if its value is lower than a threshold limit (e.g. 90), as a consequence of a system reactivity drop that would lead to an undesired coreactant accumulation.

4. Conclusions

The energy criterion allows for early detecting dangerous scenarios on exothermic SBRs due either to reactivity losses or to an early decay of the heat removal efficiency. The monitoring strategy on which the criterion is based can be easily implemented on an existing plant on the basis of the elaboration of fully measurable process variables.

References

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Keywords
Runaway Reactions; Semibatch Reactors; Early Warning; Key Process Indicators.