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Key Performance Indicators for Chemical Plants

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Abstract: Knowing the adiabatic temperature rise can improve safety in chemical processes in case of cooling failure. This study shows firstly how the temperature rise can be calculated online according to a mass and energy balance and secondly that the required accuracy of the desired values can only be attained by having additional temperature sensors.

Keywords: Accumulated energy · Adiabatic temperature rise · Online energy and mass balance · Semi-batch procedure · Thermal process safety

Introduction

Chemical plants are often controlled by process control systems which register a lot of information and values. However, only a part of this data is needed directly for process control. From the already available data, the key performance indicators are calculated automatically on the basis of process models, without making additional work for the operator.[1] The concept of the key performance indicators was first used in the project 'Lean Maintenance' carried out with industrial partners and the Confederation's innovation promotion agency (CTI). In this CTI-project[2] the slow fouling of the wall of a chemical reactor used for vitamin A production was predicted by calculation from the heat transfer coefficient. The latter was automatically calculated by means of a process model from an energy balance for a reflux period at the end of each batch process. Based on the predicted time-dependent value of the heat transfer coefficient, it was possible to optimise the timing of plant cleaning, thus improving plant availability.

Improvement of Process Safety for Exothermal Reactions

The aim of this project is the improvement of process safety for exothermal reactions.

If the cooling system of the reactor breaks down during exothermic reactions, a runaway of the chemical reaction is likely.[3] Depending on the chemical substance, this temperature rise can initiate thermal decomposition and lead to an explosion of the reactor. The potential of chemical reactions is characterized by the adiabatic temperature rise ΔT_{ad} (complete conversion under adiabatic conditions).

To avoid a runaway, chemical processes are performed according to the semi-batch procedure, which means that for a bimolecular reaction only one reactant A and solvent are fed into the reactor while the second reactant B is added slowly. In the case of cooling failure, the addition of reactant B is stopped automatically by the control system. Thus only those reactants already added can react completely and the heat production and the temperature rise are limited.

The semi-batch procedure is satisfactory for fast reactions. Slower reactions can be accelerated by increasing the process temperature, provided the selectivity of the reaction remains acceptable. In the case of a really slow reaction, however, there might be a lot of non-reacted, accumulated reactant B depending on the ratio of the feed rate to the reaction rate. If the cooling system or the stirrer breaks down, these accumulated reactants react completely and can, in the case of exothermal reaction, lead to a dangerous temperature rise (= $\Delta T_{ad,acc}$).

Limiting the Accumulation of Reactants and the Temperature Rise

There are three ways of limiting the accumulation of the reactants and therefore of keeping the temperature rise at an acceptable value:
1) reducing the feed rate (the process takes longer);
2) diluting with solvent (reduces the production amount);
3) setting the feed rate according to the possible adiabatic temperature rise $\Delta T_{ad,acc}$ and the accumulation of the reactants, respectively.

Calculation of the Accumulated Energy and the Resulting Adiabatic Temperature Rise

For the best option 3, the current possible adiabatic temperature rise $\Delta T_{ad,acc}$ must be known. This can be calculated once the accumulation of the reactants has been determined from the energy and mass balance:

$$\Delta T_{ad,acc} = \frac{m_{acc}\,(-\Delta H_r)}{m_{tot}\,\bar{c}_p} \qquad (1)$$

$$m_{tot} = m_{start} + \int \dot{m}_{dos}\,dt \qquad (2)$$

$$m_{acc} = \int \dot{m}_{dos}\,dt - m_r \qquad (3)$$

$$m_r = \frac{Q_r}{(-\Delta H_r)} \qquad (4)$$

$$Q_r = \int q_r\,dt \qquad (5)$$

$\dot{m}_{dos}$ mass feed rate of B; m_{acc} mass B accumulated; m_r reacted mass B; m_{start} mass at beginning; m_{tot} total reaction mass; ΔH_r reaction enthalpy; Q_r energy produced by reaction; q_r heat release rate due to reaction.

Energy Balance for the Calculation of the Actual Heat Release Rate q_r

The heat release rate due to the reaction q_r is calculated from the individual energy flows by means of an energy balance (details see below). Similarly, the individual energies and the total energy produced by reaction Q_r can be calculated by integration of the individual energy flows. In contrast to the usual procedure in reaction calorimetry,[4] the energy losses cannot be compensated by calibration heating but must be calculated individually. The mathematical formulas for the calculation of the individual energy flows and for the accumulation of energy from the electronic sensors are not given in detail.

Input = Output + Accumulation + Loss

Input: q_r heat release rate due to reaction; q_{dos} energy flow by mass feed of B; q_{stir} energy flow due to stirrer.

Output: q_{hm} energy flow through the heating/cooling jacket; q_{wt} energy flow by condenser; q_{kond} energy flow by distillate taken off.

Energy accumulation in: q_{rm} reaction mass; q_{re} reactor jacket, cover and frame; q_e reactor inserts; q_K column and packing (four sectors), condenser, piping; $q_{hm,M}$ heating/cooling media.

Energy losses through convection and radiation: $q_{ab\ re}$ reactor jacket, cover and frame, partly non-isolated; $q_{ab\ K}$ column und packing (four sectors, condenser), partly non-isolated; $q_{ab\ L}$ tubing/piping and fittings, partly non-isolated; $q_{ab\ wt}$ condenser non-isolated.

Pilot Plant and Control System

The R 340 pilot plant consists of a 400-litre steel enamel reactor with an impeller stirrer, DN 150 packing rectification column, condenser with inert cooling media, several tanks and dosing systems (Fig. 1).

For this project, several temperature sensors, a mass flow meter for the heating/cooling device and a rotary flow meter for the condenser cooling media were installed additionally.

As process control system the Freelance from ABB was used. The implementation of the process models and the calculation of the heat released and the $\Delta T_{ad,acc}$ from the values of the electronic sensors were carried out with the Labview-System.[5–7] Additionally, several temperature-dependent values for the heating/cooling media and the condenser cooling media were required. The values indicated were registered in a selectable time cycle and the power and energy of each term subsequently calculated online. The automatic setting of the feed rate of the second reactant B according to the possible adiabatic temperature rise $\Delta T_{ad,acc}$ has not yet been realised.

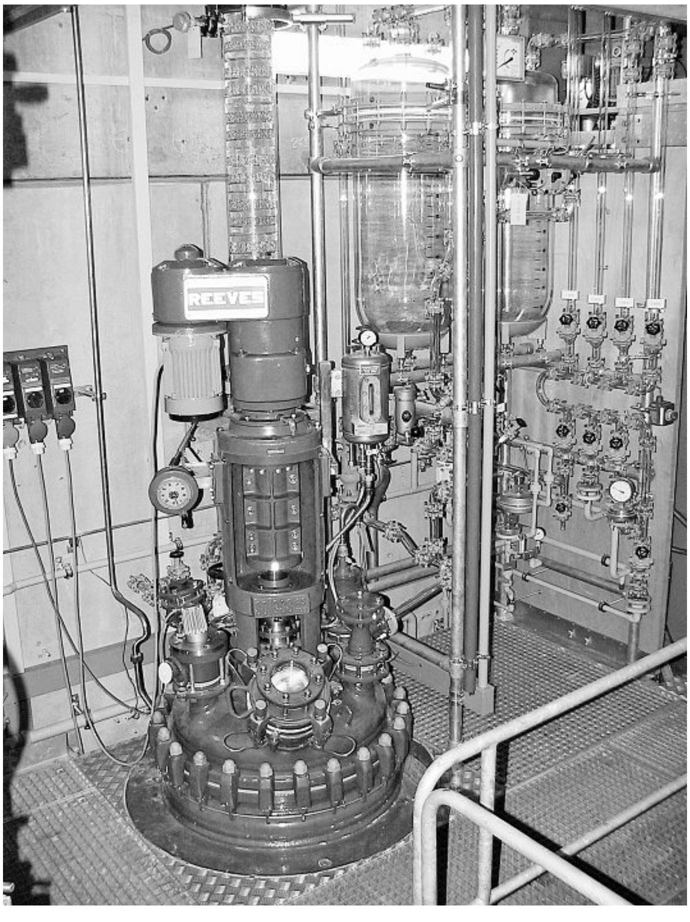

Fig. 1. Pilot plant device R 340 with 400 l steel enamel reactor

Experimental Work and Results

To use the adiabatic temperature rise $\Delta T_{ad,acc}$ – calculated online – for the control of the feed system, an adequate degree of accuracy is required. Estimations show that the energy produced by the reaction Q_r must be measured with a maximum deviation of 1600 kJ, since $\Delta T_{ad,acc}$ should have an accuracy of ±1 K (= ±1% from ΔT_{ad} = 100 K).

To verify the accuracy of the energy balance, the reactor was filled with solvent (160 kg methanol) and heated to reflux. The evaluation of the heat balance (Fig. 2 and 3) results in a total deviation of *ca.* 9000 kJ with a drift of *ca.* 500 kJ/h. The total deviation is the result of an unsatisfactory calculation of the accumulated energy of the heating/cooling media during the extremely unsteady heating and cooling period at the beginning and the end of the experiment respectively. Additional temperature sensors and an improved process model for the heating/cooling jacket are needed. To reduce the drift, additional terms in the process model for energy losses are needed.

Further experiments (the dilution of sulphuric acid and subsequently the neutralisation with aqueous sodium hydroxide) showed results similar to those from the experiment with methanol. The energy produced by the dilution and by the neutralisation reaction

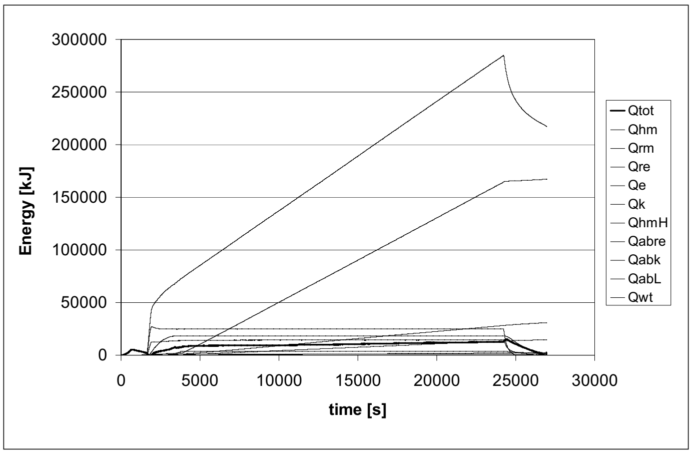

Fig. 2. Time-dependent behaviour of the energies Q_i ($Q_{tot} = Q_r$).

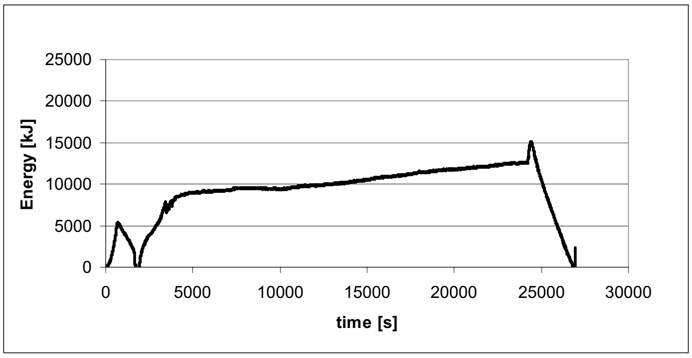

Fig. 3. Time-dependent behaviour of $Q_{tot} = Q_r$ only.

showed reasonably satisfactory values if the total deviation of the energy balance already mentioned was taken into account.

Conclusion

To avoid a runaway of a chemical process, the process is performed as a semi-batch procedure. In the case of cooling failure, the addition of the second reactant is stopped immediately by the control system. Nevertheless, in a slow reaction there might be a sufficient amount of non-reacted, accumulated reactant to lead to a dangerous temperature rise ($\Delta T_{ad,acc}$) with a dangerous decomposition of the reaction mass.

This adiabatic temperature rise can be calculated online once the energy and mass balance has been determined using process models. The addition of the second reactant can take place in such a way that even in the case of cooling failure, the resulting temperature rise is limited to a safe value.

The performed experiments showed that the acceptable accuracy has not yet been attained and that the pilot plant must be equipped with additional temperature sensors and an improved process model for the heating/cooling jacket. To reduce the drift, additional terms in the process model for energy losses are needed.

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