OPTIMAL TEMPERATURE CONTROL OF PARTIALLY SIMULATED BATCH REACTOR

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Abstract

A prototype of an industrial batch unit was constructed in our laboratory on the Department of Process Engineering, University of Pannonia, that consists of three main parts, a heatable/coolable autoclave, a monofluid thermoblock containing three different levels of temperature, a condensator for the reactor vapour product, feeding and collector tanks. An electric heater with variable power was attached to the autoclave, which enables extending the physical system with simulated exothermic chemical reactions without using any real chemical compounds [1]. In this paper a control solution with three hierarchy levels is presented, which leads the reactor on an optimal temperature setpoint that provides the exothermic chemical equilibrium reaction to reach the maximum conversion at the least possible time, and reaching the economically optimal reactor operation. On each levels of control, model based control algorithms were implemented.

Key words

model based control, batch reactor, thermometer calibration, reaction heat simulation

1 The Pilot Plant

The P&I diagram of the batch unit can be seen on Fig. 1. The monofluid is circulated in the circulation loop of the reactor's jacket with a pump. The fluid with the appropriate temperature level enters the jacket's loop depending on the state of the six ball valves, the inlet flow rate can be adjusted with the control valve on the outlet. The monofluid thermoblock allows three different temperature levels, the hottest can be controlled with an electric heater, the middle with a tap water cooled heat exchanger, the coolest with a refrigerator. [5], [6], [7]

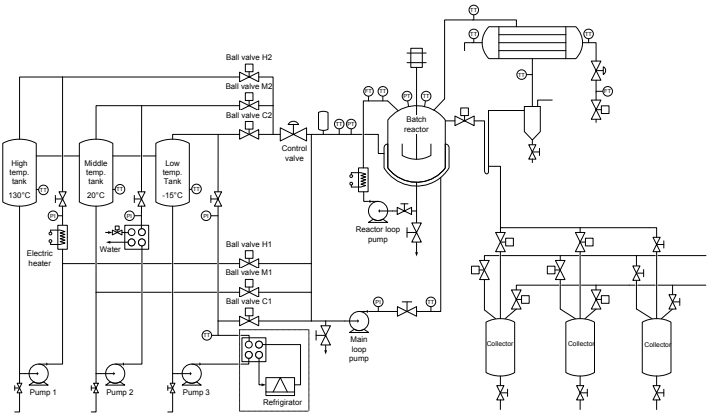

Fig. 1 The P&ID of the pilot plant

In batch systems quick transitions occur in certain periods, where the dynamic behaviour of measuring instruments can be dominant. Therefore the special dynamic calibration of the thermometers in the system had to be done (the performance of the model based controllers can be highly improved with the dynamic calibration of measuring instruments [2]). Fig. 2 shows the characteristics of the electric heater for the reaction heat intake. The heat flow is calculated via the energy balance equation of the heater using the outlet temperature and the reactor's temperature as inlet temperature, and the flow rate measured with a Flexim flow meter. The previously calibrated thermometers measure the temperature with different time constants at different points of the system. Varying the value of the manipulated variable of the heater in the range of [0, 100%] the characteristic is not strictly monotone, that is difficult to explain with first principle knowledge. The faster thermometer's signal filtered with a proper first order filter and with a temperature dependent steady-state difference (bias) between the two thermometers results a linear, pole starting characteristic with an end point equal to the maximum power of the heat exchanger. Hence the reaction heat flow calculated with the simulator can be promoted in to the reaction mixture using a feed forward controller.

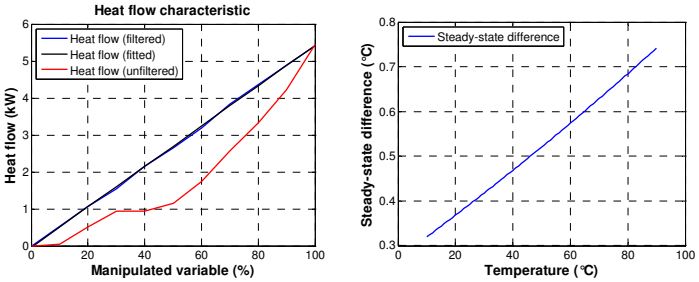

Fig. 2: The characteristics of the electric heater and the temperature dependent steady-state difference (bias) between the thermometers

2 The Control Concept

A model-based control structure with 3 levels was designed for the system.

1. ***Jacket control level:*** The goal is to compensate the disturbances that affect the temperature of the jacket inlet by utilizing the slave manipulators (jacket mode- 6 ball valves in appropriate state and the appropriate position of the control valve). The temperature of the reactor is considered a measured disturbance. This level works well if the jacket inlet temperature is following the prescribed set point.
2. ***Reactor control level:*** The goal is to compensate any disturbances that affect the reactor temperature by manipulating the slave set point. This level works well if the reactor temperature follows the set point for the reactor temperature.
3. ***Coordinating level:*** On this level the maximal rate of reaction is ensured by calculating the optimal temperature for the reaction, which is the set point of the reactor temperature on the master level.

The schematics of the control concept of the two lower levels can be seen on Fig. 3 [3]. On the grounds of the model we calculate the physical value of the manipulated variable from the set point and the measured disturbances by using constrained inversion technique. During the calculations we also obtain the value of the controlled variable, which will be the reference signal. If the measured value of the controlled variable differs from the reference signal, then model

error is present, and needs to be compensated by a feedback loop. In the IMC structure this means an inversion of the model error.

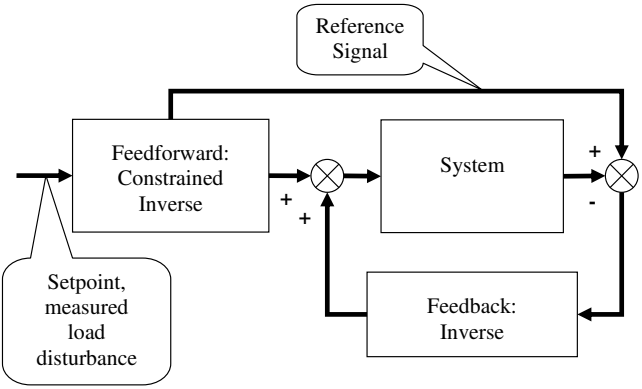

Fig. 3: Control concept at lower levels

On the coordinating level the goal is to determine the value of the optimal temperature for a simple first order equilibrium reaction:

$$A \Leftrightarrow B$$

A is the raw material, B is the product. The reaction takes place in homogenous liquid phase and no catalyst is needed. The equations describing the kinetics of the reaction are:

$$r_1 = k_{01}\exp\left(-\frac{E_{a1}}{RT}\right)c_A \qquad r_2 = k_{02}\exp\left(-\frac{E_{a2}}{RT}\right)c_B$$

Where index 1 marks forward, 2 the backward reaction. k_0 is the preexponential factor of the Arrhenius-equation (1/s), E_a is the activation energy (J/mol), R is the universal gas constant (J/(mol·K)), T is the absolute temperature (K), c_A and c_B are the concentrations of component A and B (mol/m^3).

In a single phase batch reactor the source of change in the concentration of a component is solely the chemical reaction. The time derivatives can be expressed in the following way:

$$\frac{dc_A}{dt} = -r_1 + r_2\,, \qquad \frac{dc_B}{dt} = r_1 - r_2 = -\frac{dc_A}{dt}$$

The initial concentration is $c_{A,0}$ for component A and 0 for component B. The concentration of B can be expressed as:

$$c_B = c_{A0} - c_A$$

Using the above equations an expression for the optimal temperature can be derived. This is the temperature where the change of concentrations is the fastest, thus resulting the highest conversion in a given time.

$$T_{opt} = -\frac{E_{a2} - E_{a1}}{R \cdot \ln\left(\frac{k_{01} c_A E_{a1}}{k_{02}(c_{A0} - c_A) E_{a2}}\right)}$$

The optimal temperature could be calculated from measured concentration data, but in our case no actual reaction is going on. Thus we need to settle for calculating from simulation data. Anyway if the reactor temperature is measured, then reaction speeds can be calculated, from which the actual concentration is also available. Simulation is also needed to calculate the actual rate of heat generated by the reaction:

$$Q_r = V_r \Delta H_r (r_1 - r_2)$$

Where Q_r is the heat generated by the reaction (J/s), V_r is the volume of the liquid inside the tank (m^3), ΔH_r is the absolute value of enthalpy change of reaction (J/mol).

We chose a fictive reaction that takes place between 20 °C and 80 °C with a reasonable speed, and the equilibrium composition depends highly on the final temperature. This way we are able to show that for fast reaction high temperature is needed, but for product-rich final composition low temperature is preferred. The reaction is exothermic. To avoid exceeding the maximal power of the electric heater by the reaction heat $c_{A,0}$ was set low.

3 Test of the control solutions

The jacket is more complex in regards of modelling than the reactor, and several unmeasured disturbances are present [4]. The problems of the split-range controller are handled on this stage of control (which temperature level should be active?). The three temperature levels exclude the usage of classical techniques. Fig. 4 shows that the slave level controller works well. If the master level control is attached to the slave-loop, the quality of the control remains excellent (Fig. 5), after changes in the set point, the reactor temperature – with regards to the physical limitations – reaches the new set point fast and without overshoot.

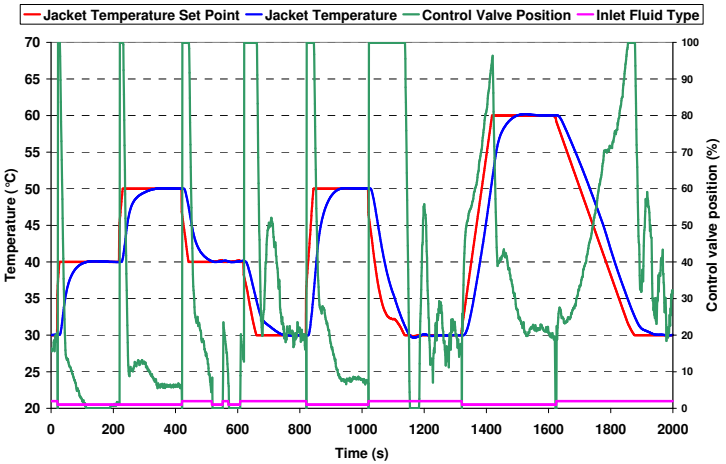

Fig. 4: Jacket temperature control
{Inlet Fluid Type: 1- High temperature fluid (90 °C), 2- Middle temperature fluid (20 °C)}

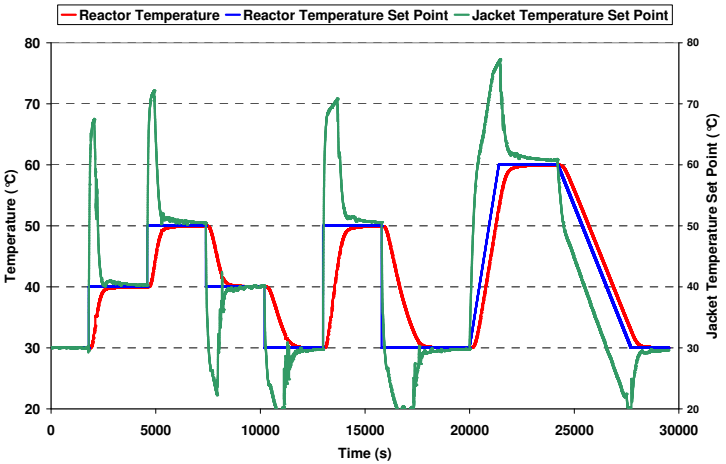

Fig. 5: Reactor temperature control

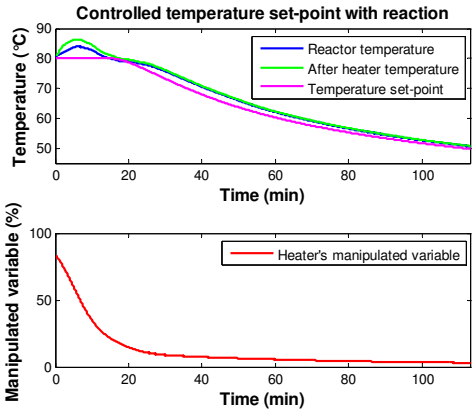

Fig. 6: Temperature control with reaction

4 Conclusion

For operating the partially simulated batch reactor a 3 level hierarchical control structure was applied. The first level (slave) is responsible for controlling the jacket temperature autonomously, choosing the appropriate temperature level and position of the control valve. The key feature of the model-based controller is constrained inversion, which provides a feasible feed forward and a reference signal on the basis of our knowledge of the system. The difference of the actual controlled variable and the reference signal refers to a model error, which can be compensated by feedback. The next level (master) controls the temperature of the reactor, utilizing the above algorithm and manipulating the set point of the previous control level. On the coordinating level a chemical equilibrium reaction is led on the optimal temperature. As the function of the measured reactor temperature and the component mass balance the actual concentrations are calculated, from which the optimal temperature – belonging to the highest rate of reaction – is obtained and used as the master set point. The behaviour of each controller level was tested autonomously and along with the other levels. The structured controller shows excellent control quality, while any changes in the system can be adapted in economically friendly way, and assuring the optimal solution between the physical limitations.

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6 Biography

Miklós Gábor Balaton is a PhD student at University of Pannonia. He has a master degree in chemical engineering. His research area is dynamic simulation is technology operation, and he has experience in UniSim Design and temperature control.

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