Annals of DAAAM for 2010 & Proceedings of the 21st International DAAAM Symposium, Volume 21, No. 1, ISSN 1726-9679
ISBN 978-3-901509-73-5, Editor B. Katalinic, Published by DAAAM International, Vienna, Austria, EU, 2010
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DAAAM Symposium

STUDY OF A SEMI-BATCH TO BATCH PROCESS CONVERSION

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Abstract: *In this paper two types of reactors, batch and semi-batch reactor, are analysed. They are compared from the point view of their control by simulation means mainly. For the study the same real process is used – chromium sludge recycling technology. This process is strongly exothermic, so the temperature control is necessary. At first, semi-batch processing, secondly the batch processing is studied. This study can be useful for efficiency of these processes comparison (like time demands, cost savings) and for processes optimization.*
Key words: *semi-batch, batch, process, modelling, simulation*

1. INTRODUCTION

Batch reactors provide flexible means of producing high value-added products in specialty chemical, biotechnical, and pharmaceutical industries.

In the past, authors have controlled a chemical reactor by feeding one of the reaction components, so the reactor was treated as a semibatch reactor (Macků, 2005). As can be seen from literature, same papers deal with batch reactors using for control heating medium in the reactor jacket as a manipulating value. For example Cho Wonhui et al. (Cho et al., 2008) improved robustness of dual-mode controller with an iterative learning technique. Full heating is applied first to raise quickly the reactor temperature and then full cooling is followed to reduce the rate of temperature increment and for reactor temperature to approach the set point smoothly. Also Graichen at al. (Graichen et al., 2006) or Škrjanc (Skrnajc, 2007) control the reactor temperature by manipulating the setpoint of the cooling jacket temperature.

The same idea as was meant above we applied to the reactor for chromium sludge processing. We have converted the semibatch process to batch process, using for the reactor control not any longer the reaction component feeding, but we put there the whole batch (or part of batch) and tried to control the reactor using heating medium in the reactor jacket as a manipulating value. We were observing the total processing time and other important values.

2. BATCH AND SEMIBATCH REACTOR MODEL

The chromium sludge is processed in a chemical reactor by an exothermic chemical reaction with chrome sulphate acid (Kolomazník, 1996). During this reaction a considerable quantity of heat is developing so that control of the reaction is necessary. In order to investigate main properties of the real process, a mathematical model of the chemical reactor was derived based on Fig.1 (Macků, 2005).

2.1 Mathematical model

Under usual simplifications, based on the mass and heat balance, the following 4 nonlinear ordinary differential equations can be derived (Macků, 2005):

$$\dot{m}_{FK} = \frac{d}{dt} m(t)$$
$$\dot{m}_{FK} = k\, m(t)\, a_{FK}(t) + \frac{d}{dt}[m(t)\; a_{FK}(t)]$$
$$\dot{m}_{FK} c_{FK} T_{FK} + \Delta H_r k\, m(t)\, a_{FK}(t) =$$
$$= K\, S[T(t) - T_V(t)] + \frac{d}{dt}[m(t)\, c_r\, T(t)]$$
$$\dot{m}_V c_V T_{VP} + K\, S[T(t) - T_V(t)] =$$
$$= \dot{m}_V c_V T_V(t) + m_{VR} c_V \frac{d}{dt} T_V(t) \qquad (1)$$

The first equation expresses the total mass balance of the chemical solution in the reactor. The symbol $\dot{m}_{FK}$ [kg.s^{-1}] expresses the mass flow of the entering chromium sludge and $m'(t)$ [kg.s^{-1}] describes the accumulation of the in-reactor content.

The second equation represents the chromium sludge mass balance. The input is $\dot{m}_{FK}$ [kg.s^{-1}] again, the accumulation is given by the last term $[m(t)\; a_{FK}(t)]'$ [kg.s^{-1}], where $a_{FK}(t)$ [-] the mass concentration of the chromium sludge in the reactor denotes and $m(t)$ [kg] describes weight of the reaction components in the system. The expression $k\, m(t)\, a_{FK}(t)$ [kg.s^{-1}] defines the chromium sludge extinction by the chemical reaction. Here k [s^{-1}] is the reaction rate constant expressed by the Arrhenius equation (2) where A [s^{-1}], E [J.mol^{-1}] and R [J.mol^{-1}.K^{-1}] are pre-exponential factor, activation energy and gas constant.

$$k = A e^{-\frac{E}{RT(t)}} \qquad (2)$$

The third equation describes the enthalpy balance. The input heat entering the reactor in the form of the chromium sludge is expressed by the term $\dot{m}_{FK} c_{FK} T_{FK}$, the heat arising from the chemical reaction is given by the expression $\Delta H_r k\, m(t)\, a_{FK}(t)$ and the heat transmission through the reactor wall is expressed by the formula $K\, S[T(t) - T_V(t)]$. The individual symbols used above mean: c_{FK} [J.kg^{-1}.K^{-1}] – chromium sludge specific heat capacity, c_R [J.kg^{-1}.K^{-1}] – specific heat capacity of the reactor content, T_{FK} [K] – chromium sludge temperature, ΔH_r [J.kg^{-1}] – reaction heat, K [J.m^{-2}. K^{-1}.s^{-1}] – conduction coefficient, S [m2] – heat transfer surface, $T(t)$ [K] - temperature of reaction components in the reactor, $T_V(t)$ [K] – temperature of a coolant in the reactor double wall.

The last equation describes coolant heat balance. The input heat is given by $\dot{m}_V c_V T_{VP}$, the heat entering the coolant by the reactor wall is expressed by $K\,S\,[T(t) - T_V(t)]$, the heat going out with the coolant is described as $\dot{m}_V c_V T_V(t)$ and the heat accumulated in the double wall describes the last term $m_{VR} c_V\, T_V'(t)$. The symbols mean: $\dot{m}_V$ [kg.s^{-1}] – coolant mass flow, c_v [J.kg^{-1}.K^{-1}] – coolant specific heat capacity, T_{vp} [K] – input coolant temperature, m_{vr} [kg] – coolant mass weight in the reactor double wall.

3. CONTROL THEORY POINT OF VIEW

From the systems theory point of view the reactor has four for semibatch reactor (or three if we exclude $\dot{m}_{FK}$ for batch reactor) input signals $\dot{m}_{FK}$, $\dot{m}_V(t)$, $T_{FK}(t)$ and $T_{vp}(t)$, four state variables $m(t)$, $a_{FK}(t)$, $T(t)$, $T_V(t)$ and one output signal to be controlled given by the temperature inside the reactor $T(t)$. Hence, it can be generally seen as a Multi Input – Multi Output (MIMO) system of 4th order. In addition it possesses strongly nonlinear behaviour. Practically, the only manipulated variables are input flow rates of the chromium sludge $\dot{m}_{FK}(t)$ and of the coolant $\dot{m}_V(t)$, or $\dot{m}_V(t)$ and $T_{vp}(t)$ for batch reactor eventualy. Therefore, input temperatures of the filter cake $T_{FK}(t)$ and of the coolant $T_{vp}(t)$ can be alternatively seen as disturbances, or set as a constant.

4. SIMULATION RESULTS

4.1 Semibatch reactor

The results of semibatch reactor control using PID control were following: the upper-most in-reactor temperature *T* reached 370.22 K, the maximum chromium sludge concentration *a* was 0.0439 and the total batch time made 25491 seconds. The maximum and minimum actuating variable values were 1.546 kg.s^{-1} or 0 kg.s^{-1} respectively. The steady state actuating variable value made 0.032 kg.s^{-1} approximately. The PID control diagram is displayed in figure 2.

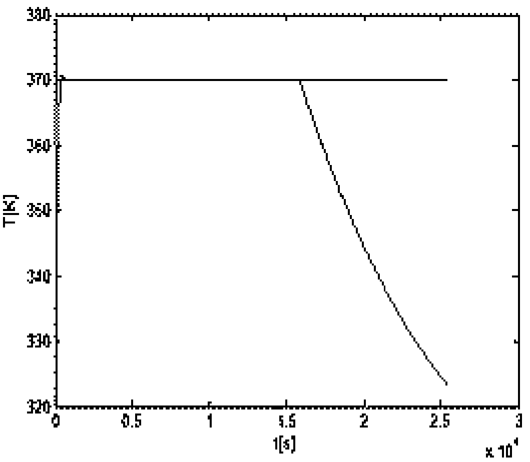

Fig. 2. The in-reactor temperature – semibatch reactor

4.2 Batch reactor

The results of batch reactor control can be seen further: the upper-most in-reactor temperature *T* reached 372.00 K, the maximum chromium sludge concentration *a* was 0.2233 and the total batch time was less than 16000 seconds. The in-reactor temperature development is displayed in figure 3.

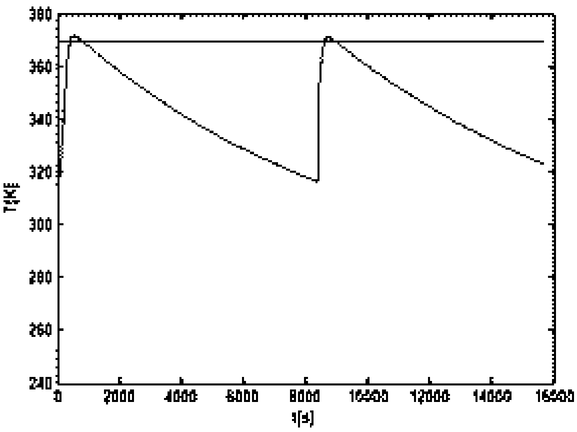

Fig. 3. The in-reactor temperature – batch reactor

4.3 Discussion

As can be seen from simulations, the total process time was reduced on a half using batch process (the batch process was divided to two sequent batches) compared to semibatch process. But, the in-reactor temperature spread was unsatisfactory and also the initial conditions of variables were inconvenient.

5. CONCLUSION

The above mentioned simulations were just first attempt for the semibatch to batch process conversion. There are still a lot of unsolved possibilities how to improve this process. In the future work, some other approaches will be applied to the batch process to find out other possible ways to eliminate these disadvantages.

6. ACKNOWLEDGEMENTS

This work has been supported by the Ministry of Education, Youth and Sports of the Czech Republic under grant MSM 7088352102 and by the Tomas Bata University under grant IGA/40/FAI/10/D. These supports are gratefully acknowledged.

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