Online Estimation and Adaptive Temperature Control of Polymerization Reactor

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Abstract: The temperature control of a semi-batch polymerization reactor described by Chylla and Haase, a control engineering benchmark problem is considered. The process is nonlinear and time varying in nature. There is significant change in heat transfer coefficient, during a batch due to changes in the viscosity of the polymer and also from batch to batch due to surface fouling. Also change in ambient temperature during summer and winter makes the temperature control of this process a challenging task. The conventional cascade control provides robust operation, but often lacks in control performance concerning the required strict temperature tolerances. Hence an adaptive control design by employing a self tuning cascade with feed forward control concept is proposed in this paper to provide excellent control. This design calculates a trajectory for the cooling jacket temperature in order to follow a predefined trajectory of the reactor temperature. The reaction heat as well as the heat transfer coefficient required for the proposed controller is estimated online by using Unscented Kalman Filter (UKF). Simulation results under model uncertainties show the effectiveness of the proposed adaptive control concept.

Keywords: On-line estimation, Unscented Kalman filter, Self tuning cascade with feedforward control

1. INTRODUCTION

Polymerization is the process of reacting monomer molecules together in chemical reactions to form three dimensional networks of polymer chains. The widely used reactors in chemical industry for the production of fine pigments, chemicals, polymers and pharmaceuticals are batch and semi batch reactors. Often the reactions show exothermic behaviour and tight specifications have to be met. Therefore an exact temperature control is required. In many cases conventional linear control algorithms are reported. Industrial Polymerization reactors are usually controlled by a cascade structure consisting of a master controller for the reactor temperature and a slave controller for cooling circuit. The cascade controller gives a robust operation but fails to meet the strict temperature tolerances (Chylla.R.W. and Randall Haase.D,1993). Hence there is a need to employ advanced control techniques which satisfy the control requirements.

Therefore various control concepts have been used in the literature to deal with the benchmark problem. A model predictive controller is used in (Helbig O.Abel, M'hamdi.A and Marquardt.W, 1996) combined with an extended Kalman filter for the estimation of the reaction heat and heat transfer coefficient. A non linear adaptive controller is designed in (Tracy Clarke-Pringle and John F. MacGregor, 1997), to adjust the cooling jacket temperature, which serves as the set point for an underlying PI controller of the cooling jacket. A

further approach (Knut Graichen, Veit Hegenmeyer and Michael zeit, 1996) illustrates the potential of feed forward control by extending the conventional cascade control concept in the frame work of two degree of freedom control concept. The self tuning control concept presented in this contribution solves the problem for polymer B by calculating a trajectory for the cooling jacket temperature in order to follow a predefined trajectory of the reactor temperature. The reaction heat as well as the heat transfer coefficient in the energy balance is estimated online by using Unscented Kalman Filter (UKF). Similar control technique for polymerA of the Chylla Haase polymerization process was implemented (Vasanthi.D, Pranavamoorthy.B and Pappa.N, 2012).

The paper is organized as follows: section 2 describes the Chylla Hasse control problem and the reactor model, in section 3 Self tuning cascade control scheme used for temperature control is discussed and finally section 4 gives the simulation studies for the first batch of summer season.

2. CHYLLA-HAASE BENCHMARK REACTOR

2.1 Polymerization Process

The polymer is produced based on the typical recipe. Generally the process can be divided into heating period, feed period and hold period. The industrial polymerization process described by Chylla and Haase consists of a stirred tank reactor with a cooling jacket and a coolant recirculation, is presented in Fig.1. The reactor temperature is controlled by manipulating the temperature of the coolant which is recirculated through the cooling jacket of the reactor. The slave controller can act in two modes: in cooling mode, cold water is inserted into the recirculation loop, whereas in heating mode, steam is injected into the recirculating water stream.



Fig. 1. Schematic diagram of the Polymerization Reactor

The recipe for the polymer B comprises of the following steps:

- 1. Place initial charge of solids and water into the reactor at ambient temperature
- 2. Raise temperature of the initial charge to the reaction temperature set point
- 3. After 1800 s feed pure monomer into the reactor at 6.048×10^{-3} Kg/s for 3600 s
- 4. After the feed addition period is complete, hold at reaction temperature for 1800 s
- 5. Feed pure monomer into the reactor at 6.048 x 10⁻³ Kg/s for 2400 s
- 6. After the second feed addition period is complete, hold at reaction temperature for 2700 s

Thereby, the monomer feed starts and ends abruptly at specified time points. The polymer is produced in five subsequent batches, and is removed between the batches. However, the reactor is only cleaned after the fifth batch. The control tasks are complicated by several features of the polymerization process:

- Changing ambient temperatures in winter and summer
- The heat transfer coefficient decreases significantly during a batch due to an increasing batch viscosity, and from batch to batch due to surface fouling
- The reaction kinetics is nonlinear
- Impurity of the monomer
- Semi batch operation
- Production of multiple products
- Variation of delay times θ_1 and θ_2

2.2 Polymerization Reactor Model

A dynamic model of the polymerization reactor has been derived by Chylla and Haase based on simplified kinetic relations. The corrected model given by (Knut Graichen, Veit Hegenmeyer and Michael zeit, 1996) is used for simulation. The temperature dynamics are captured by considering energy balances for the reactor and the cooling jacket. The reactor model comprises the material balances (1) and (2) for the monomer mass $m_M(t)$ and the polymer mass $m_P(t)$, the energy balance (3) with the reactor temperature T(t), as well as the energy balances (4) and (5) of the cooling jacket and the recirculation loop with the outlet and inlet temperatures of the coolant C. Further variables and the parameters of the reactor model are listed in Table I.

$$\frac{dm_{M}}{dt} = m_{M}^{in}(t) + \frac{Q_{rea}}{\Delta H}$$
(1)

$$\frac{dm_p}{dt} = -\frac{Q_{rea}}{\Delta H}$$
(2)

$$\frac{dT}{dt} = \frac{1}{\sum_{i} m_{i} C_{p,i}} [m_{M}^{in}(t) C_{p,M} (T_{amb} - T) - UA(T - T_{j}) - (UA)_{loss} (T - T_{amb}) + Q_{rea}] (i = M, P, W)$$

$$\frac{dT_{j}^{out}}{dt} = \frac{1}{m_{c}C_{p,c}} [m_{c} C_{p,c}(T_{j}^{in}(t-\theta_{1})-T_{j}^{out}) + UA(T-T_{j})]$$
(4)

$$\frac{dT_{j}^{in}}{dt} = \frac{dT_{j}^{out}(t-\theta_{2})}{dt} + \frac{T_{j}^{out}(t-\theta_{2}) - T_{j}^{in}}{\tau_{p}} + \frac{K_{p}(c)}{\tau_{p}}$$
(5)

The available measurements of the process are the temperatures of the reactor and cooling circuitry. The heating/cooling function $K_p(c)$ is influenced by an equalpercentage valve with valve position c(t) and the following split-range valve characteristic as shown in equation (6)

$$K_{p}(c) = \begin{cases} 0.8 \times 30^{-c/50} \left(T_{inlet} - T_{j}^{in}(t) \right), & c < 50\%, \\ 0, & c = 50\%, \\ 0.15 \times 30^{-c/(50-2)} \left(T_{stream} - T_{j}^{in}(t) \right), & c > 50\% \end{cases}$$
(6)

For c < 50%, ice water with inlet temperature T_{inlet} is inserted in the cooling jacket, whereas a valve position c > 50% leads to a heating of the coolant by injecting steam with temperature T_{steam} into the recirculating water stream.

Table III summarizes the empirical relations for R_p , A, and U. A detailed description of these relations is given in (Knut Graichen, Veit Hegenmeyer and Michael zeit, 1996). The parameter values of the model and the polymer B are listed in Table II and Table IV.

In order to heat-up the reactor to the specified set point T^{set} before the monomer feed $m_M(t)$ starts, a trajectory is planned for the desired reactor temperature $T^*(t)$ by the polynomial set-up as given by equation (7)

$$T^{*}(t) = \begin{cases} T_{amb} + (T^{set} - T_{amb}) \sum_{i=3}^{5} a_{i} \left(\frac{t}{t^{heat}}\right)^{i}, & \text{if } t \le t^{heat} \\ T^{set}, & \text{if } t > t^{heat} \end{cases}$$
(7)

With $a_3 = 10, a_4 = -15$, $a_5 = 6$. In this first interval $t \le t^{heat}$, the reactor is heated up to the set point T^{set} . For $t > t^{heat}$, the temperature $T^{*}(t)$ is kept constant at T^{set} . In the

following, the heat-up time is set to $t^{heat}=30$ min corresponding to the time instant when the monomer feed $m_M^{in}(t)$ starts.

3. PROPOSED SELF TUNING CASCADE WITH FEED FORWARD CONTROLLER DESIGN

A very tight temperature control is necessary in order to produce polymer of a desired quality. The controller should be able to maintain the reactor temperature T within an interval of ± 0.6 K around the desired set point under all operation conditions and disturbances. Commonly used for chemical reactors is a PI cascade control structure, which provides a robust operation but often lacks in control performance. The cascade control structure is shown in Fig.3. The master controller regulates the reactor temperature T by manipulating the set point T_j^{set} of the mean cooling jacket temperature T_j . The slave controller adjusts the valve position c in order to control the mean jacket temperature T_j^{set} by the



Fig. 2. Block diagram of Convention Cascade control scheme

In order to get accurate response, it is desirable to calculate the self tuning parameters online. However, this requires the estimation of the time-dependent quantities reaction heat, Q_{rea} and heat transfer coefficient, U during the successive batches. Fig.3. shows the block diagram of the considered adaptive control scheme with an unscented Kalman filter (UKF) which uses the available temperature measurements to estimate the

reaction heat Q_{rea} and the heat transfer coefficient U (Eric A. Wan and Rudolph Vander Merwe, 2000).



Fig.3. Block diagram of proposed self tuning Cascade with Feed Forward control scheme

The uncertainties of the system are modelled as the system noise in the state error covariance matrix and the uncertainties in the measurement are modelled as the measurement noise in the measurement error covariance matrix. The information on the monomer additions are accounted in the first principle model used inside the estimator. The estimated output not only estimates the Q_{rea} and U which cannot be measured online, but also gives a filtered output of the various parameters required for taking

the control action. The parameter adjustment mechanism receives these estimates and calculates a desired trajectory for the cooling jacket temperature which makes the controller adaptive. The respective set point for slave controller is adjusted by master controller in case of conventional cascade control whereas the respective set point is generated by parameter adjustment mechanism in case of this proposed self tuning control scheme. The proposed scheme acts as self tuned primary controller along with feed forward control action.

$$T_{j}^{*} = T^{*} + \frac{1}{\hat{U}.A} \begin{bmatrix} \sum_{i} m_{i}^{*} C_{p,i} \dot{T}^{*} - \dot{m}_{M}^{jn}(t) C_{p,M}(T_{anb} - T^{*}) \\ -\hat{Q}_{rea} + (UA)_{loss}(T^{*} - T_{anb}) \end{bmatrix}$$
(8)

Thus T_j^* is found with the help of equation (8) and this T_j^* is compared with the present jacket temperature, T_j and control action is taken by manipulating the control valve which in turn maintains the reactor temperature at its set point and the error is kept within the tolerance limit.

4. SIMULTION RESULTS AND DISCUSSIONS

The process is simulated with the conventional PI cascade control structure as well as the self tuning control structure and the performance of both the control schemes are compared. Fig.4. (a) – (c) shows the simulation results for the process with conventional cascade control for batch 1 and 5 for summer season.



Fig. 4. Response of the simulated polymerization reactor for polymer B with conventional cascade controller during summer season

The sampling time for the self tuning control is set to 1s which is the same as the sampling time of the cascade controller. Fig.5 (a) - (h) gives the simulation results for the process with self tuning control for summer season for batch 1. The deviations of the reactor temperature between T and T^* (desired reactor temperature) in the conventional cascade control scheme is due to the time delayed response of the slave controller to the respective set point adjusted by the master controller. The simulations with the cascade controlled reactor together with the self tuning control illustrate that the temperature error can be reduced significantly compared to the conventional cascade control scheme. The temperature error stays within the tolerance interval of ± 0.6 K during the heat up as well as the critical time points when the monomer feed starts and stops. There is also significant improvement in the performance of the control valve.





Fig.5. Response of the simulated polymerization reactor for first batch of polymer B with self tuning controller during summer season

A quantitative analysis is done for both the control schemes by calculating ISE and IAE for batches 1 and 5 respectively for summer season and is shown in the TABLE V. It is observed that both ISE and IAE are much lesser for self tuning control scheme compared to the cascade control structure.

Control Schemes	ISE		IAE	
	I Batch	V Batch	I Batch	V Batch
Cascade Control	505.8241	742.8408	1328.4	1603.2
Self Tuning Control	4.8819	4.3823	126.8213	126.8781

Furthermore a robustness analysis is carried out in order to compare the performance of the self tuning control structure

with respect to the conventional PI cascade control structure. It is assumed that the reactor is operated in the winter season where the low ambient temperature posses high demand in the cascade control during the heat up of the reactor. The UKF provides robust estimates of the reaction heat, heat transfer coefficient and the reactor temperature stays within the specified tolerance interval of ± 0.6 K with self tuning control scheme however with increase in monomer feed by 5% in the model, results in increased error in reactor temperature upto ± 0.9 K. Even with this change in monomer feed stable operation is achieved and it is also observed that this proposed adaptive scheme outperforms the conventional cascade controller.

5. CONCLUSION

Self tuning controller with UKF based estimation concept for the temperature control of Chylla and Haase polymerization process is studied in this paper. The estimates for the heat transfer coefficient U and the reaction heat Q_{rea} are obtained using Unscented Kalman Filter. The simulation results shows that on comparison with the conventional cascaded control the proposed adaptive control concept of self tuning control is superior. The proposed controller is able to maintain the reactor temperature with in the interval of ±0.6K from the desired set point through out the production of polymer for all the batches and for different ambient temperature.

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Appendix A. FIRST APPENDIX

Table I Variables and parameters of the polymerization reactor model

Variable	Variable name	Unit
$m_M(t)$	Monomer feed rate	Kg/s
$Q_{rea} = -\Delta H.R_p$	Reaction heat	kW
R _p	Rate of polymerization	Kg/s
$-\Delta H$	Reaction enthalpy	kJ kg^{-1}
U	Overall heat transfer coefficient	$kWm^{-2}K^{-1}$
Α	Jacket heat transfer area	m^2
$(UA)_{loss}$	Heat loss coefficient	kW/K
$C_{p,M}, C_{p,P}, C_{p,C}$	Specific heat at constant pressure	$kJkg^{-1}K^{-1}$
θ_1, θ_2	Transport delay in jacket and recirculation loop	S
$T_j = (T_j^{in} + T_j^{out})/2$	Average cooling jacket temperature	K
$K_p(c)$	Heating/cooling function	K
$ au_p$	Heating/cooling time constant	S

Table II Data of reactor parameters

Reactor parameters	Unit	Values
R	$kJ kmol^{-1}K^{-1}$	8.314
$(UA)_{loss}$	$k W K^{-1}$	0.00567567
$ au_p$	S	40.2
θ_1	S	22.8
θ_2	S	15.0
i		[0.8,1.2]
1 / h _f	$m^2 K k W^{-1}$	[0.000,0.176,0.352, 0.528,0.704]
T _{amb}	K	280.382(winter), 305.382(summer)
T _{inlet}	K	294.26
T _{steam}	K	449.82

Table III Empirical relations for the Polymerization rate, the jacket heat transfer area and the overall heat transfer coefficient

Variable	Variable	Variable name	Unit
$R_p = ik_{mM}$ with	i	Impurity factor	-
	$k = k_0 \exp\left(\frac{-E}{RT}\right) \cdot \left(k_1 \mu\right)^{k_2}$	First-order kinetic const.	s^{-1}
	$\mu = c_0 \exp(c_1 f) \cdot 10^{c_2(a_0/T - c_3)}$	Batch viscosity	$kgm^{-1}s^{-1}$
	$f = m_P / (m_M + m_P + m_C)$	Auxiliary variable	-
	$k_0, k_1, E, R, a_0, c_0, c_1, c_2, c_3$	Constants	
	R	Natural gas const.	$kJkmol^{-1}K^{-1}$
$A = \left(\frac{m_M}{\rho_M} + \frac{m_P}{\rho_P} + \frac{m_W}{\rho_W}\right) \frac{P}{B_1} + B_2$	ρ_M, ρ_P, ρ_C	Densities	$kg m^{-3}$
	B_1	Reactor bottom area	т
	Р	Jacket perimeter	т
	B_2	Jacket bottom area	
$U = \frac{1}{h^{-1} + h_f^{-1}}$	$h = d_0 \exp(d_1 \mu_{wall})$	Film heat transfer co-efficient	$kWm^{-2}K^{-1}$
	$\mu_{wall} = c_0 \exp(c_1 f) \cdot 10^{c_2(a_0/T_{wall} - c_3)}$	Wall viscosity	$kgm^{-1}s^{-1}$
	$T_{wall} = \left(T + T_j\right) / 2$	Wall temperature	K
	h_f^{-1}	Fouling factor depending on batch no.	$m^2 K / kW$
	d_0, d_1	Constants	

Table IV Data of polymer B

Symbol	Units	Value for polymer
$m_{M,0}$	kg	0.0
$m_{P,0}$	kg	11.227
m_{W}	kg	41.2825
$ ho_{\scriptscriptstyle M}$	kgm ⁻³	900.0
$ ho_{\scriptscriptstyle P}$	kgm ⁻³	1040.0
$ ho_{\scriptscriptstyle W}$	kgm ⁻³	1000.0
$C_{p,M}$	$kJ kg^{-1} K^{-1}$	1.675
$C_{p,P}$	$kJ kg^{-1} K^{-1}$	3.140
$C_{p,W}$	$kJ kg^{-1} K^{-1}$	4.187
MW_{M}	kg kmol ⁻¹	106.0
m _c	kg	42.996
m_c	kg / s	0.9412
$C_{p,C}$	$kJ kg^{-1} K^{-1}$	4.187
k_0	s^{-1}	20

k_1	$m s kg^{-1}$	1000
<i>k</i> ₂		0.4
E	kJ kmol ⁻¹	29,560.89
C ₀	$kg m^{-1}s^{-1}$	3.2×10 ⁻⁵
<i>C</i> ₁		19.1
<i>c</i> ₂		2.3
<i>C</i> ₃		1.563
a_0	K	555.556
$-\Delta H_p$	kJ kmol ⁻¹	-65593.2
d_0	$kW m^{-2} K^{-1}$	0.814
d_1	$m s kg^{-1}$	-5.13
m_{M} in,max m_{M}	kg / s	6.048×10 ⁻³
$\left[t_{M,0}^{in},t_{M,1}^{in}\right]$	min	[30,90]
$\left[t_{M,2}^{in},t_{M,3}^{in}\right]$	min	[120,160]
T^{set}	K	353.160