Comparison of Two Different Strategies to Control Particle Size Distribution in Batch Emulsion Polymerization Using PID Controller

Parul Arora*, Alok Gupta[1]

Chemical Engineering Department, Malaviya National Institute of Technology,

Jaipur (Rajasthan), India

parul.arora07@gmail.com

Abstract : *This paper describes the PID control of a batch polymerization reactor concluding after comparison of two different mode of control. The main objective of any control system is to attain target value within minimum time. To achieve this goal we compared split range control with controller using heat load as manipulative variable. Both provide good control but after study of performance index we found PID controller with heat load as manipulative variable performs better than split range controller.*

Keywords: Control Particle size distribution, PID, Split range, Heat load.

Introduction : Emulsion polymerization can be described mathematically by accounting particle number, particle volume, number of radicals and chain length. Smith and Ewart were the first who gave the population balance equation to describe the complete particle balance in the system Katz and his co-workers were the first who solve the population balance equation. These population balance equations are used to predict the vigorous behaviour of the particle size distribution.

The control objective in a batch reactor is to reach specific target product quality with the help of different parameters as manipulative variable. In this paper we compare two algorithms having different strategy. Control of a batch process is very complicated as compared with continuos process, being highly non-linear in nature and absence of equilibrium condition.

A far-reaching model was given by the authors (Coena and Gilberta 1998) for the particle size distribution (PSD), particle number, particle size and amount of secondary nucleation in emulsion polymerization. In this model the initiator decomposes in the water phase, forming radicals which then react with monomer to form oligomeric radicals in the water phase. These oligomeric radicals can propagate in the water phase; terminate with another radical of degree of polymerization. Size dependence of various parameters was considered by the authors such as the rate coefficients above and the concentration of monomer in particles. They found particle number as functions of variations in concentration of surfactant and initiator, that model reproduce experiments adequately. Effect of monomer feed rat (Zeaiter, Romagnoli et al. 2002),initiator (Chern, Lin et al. 1998) and temperature (Meadows, Crowley et al. 2003) on particle size distribution have been studied experimentally(Abedini and Mohammad Shahrokhi 2010).

Mathematical model : Evolution of particle size distribution is mathematically explained by population balance equations. The model used is Zero- One model as taken from literature. The particle size population is divided into a population containing one and zero radical. This population balance equation can be solved by using orthogonal collocation method. These equations given below are derived from general population balance equation.

$$\frac{\partial \eta_0(r)}{\partial t} = \rho(r)[n_1^p(r) + n_1^m(r) - n_0(r)] + k_0(r) - n_1^m(r)$$

$$\frac{\partial n_1^p(r)}{\partial t} = \rho_{ini}(r) - n_0(r) - \rho(r) - n_1^p(r) - k_{tr}[M]_0 n_1^p(r) + \sum_{j=z}^{jcri} k_{em,i}[micelles][p_i^z]\delta(r - r_{nuc})$$

Quasi –steady state assumption is applied and we get

$$n_1^m = \frac{k_{e,t}(r)[E] n_0(r) + k_{tr}[M]_p n_1^p}{\rho_r + k_{p,e}[M]_p + k_0(r)}$$

From equation 1, 2 and 3 we get total particle size population balance as give below in equation 4

$$n(r) = n_0(r) + n_1^m + n_1^p$$

Min and ray were the first to model the entire PSD, they characterized the particles by their population density, function F(x,t) was the measure of the concentration of particles having n growing radicals, where x is the measure of particle size like mass, volume, time and radius(Min and Ray 1974).

This model is zero-one model referring instantaneous bimolecular radical termination followed by some assumptions-

1. All reactions are irreversible.

2. The reactions are independent of chain length.

3. The quasi-steady state assumption is stated for free radical chain.

4. There is no chain transfer.

The energy balance for the reactor and the jacket used in split range is tabulated in table no-1 and for heat load in table no 2

Design of controller

The polymerization kinetic model explained above was simulated in matlab. The PID controller was first used in 1939 and is the most widely used controller in the market till today. PID controller is a feedback controller as shown in figure 1 below, using a block diagram representation. As shown in the figure, the process is the objective to be controlled. The purpose of the control is to make the process variable y follow the set-point r. To achieve the purpose, the manipulative variable u is changed by the controller.

$$G_c = K_p \left(1 + \frac{1}{sTi} + T_d s \right)$$

$$= K_p + \frac{K_i}{s} + K_d s$$

First controller strategy used is split range and second is heat load. Split range is a controller configuration where a single PID controller outputs to two control valve. In our case PID output signal controls the hot-water and cold water steam as per required. As shown in fig.2 below how the hot water and cold water streams changes with output signal. The range of signal is constrained between 0-1.Flow rates are used as manipulative variable and reactor temperature is used as control variable.

In second strategy heat load is used as manipulative variable, which may vary from 40-140 W in our case optimum value is 90W. Heat load value is highly correlated with flow rate of stream. The generated results were first compared with experimental data and then further proceeds towards comparison of strategy.

Before implementing the controller tunning parameters should be optimised first to achieve the good performance of the controller. The parameters were optimized and used given in table no-3

Result and Discussion

Particle size distribution of the emulsion polymer or product is convincingly influence polymer's rheological, chemical, physical, mechanical, film forming properties.

Batch reactor was used for production of PMMA.A measured amount of MMA, emulsifier and water was charged to the reactor. The reactor was bubbled with nitrogen gas to purge oxygen from the reactor. The reactor was brought to the initial temperature and then required amount of initiator was supplemented to the reactor. Comparison of experimental value of reactor temperature with simulation without controller and with controller was studied and the result found was shown below. PID controller is successfully operated; performance of controller was studied with different parameters. After this we compared two methods which will be explained later.

The temperature profile in batch polymerization reactor follows:-
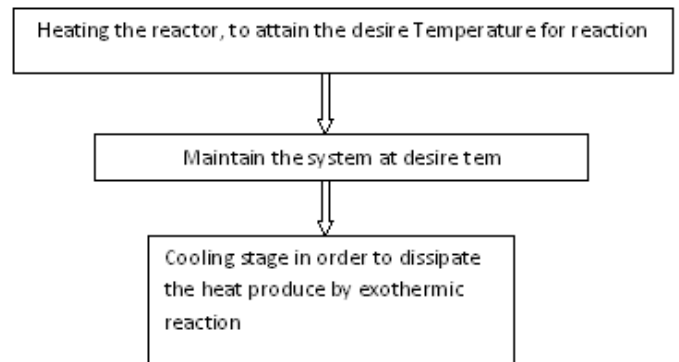
In our study first strategy uses split range controller as explained above and second one uses heat load as a manipulative variable. Both two are capable to maintain the desire reactor temperature with load changes and suddenly set point changes. Performance index is calculated for the system, results are discussed in table no 4 and 5.The comparison of result of both controller is given in fig.3

Green line is showing the heat load method and blue shows split range. As clearly shown in fig 4 split range controller requires minimum time to settle down at set-point i.e 343K and heat load takes ample of time (4000 sec) but there is small oscillations in split range controller. Split range controller uses both hot water stream and cold water stream as its manipulative variable (fig 5) and is capable to maintain set-point better than heat load. The performance index for both the controller were studied and discussed in table 4.As the data of Performance index provide evidence that split range perform better than the heat load fig 5 shows the flow rates of hot water and cold water stream in split range controller. The value of Absolute error for split range is 3.833×10^6 which is enormously lesser than heat load method having value 1.4137×10^7.Both the controllers behave well at load change and suddenly set-point change in system. Performance index were compared in table 5.A contradictory results were found. Performance index shows heat load as manipulative variable is capable to handle load change and set-point change better than split range, which means heat load as manipulative variable is much better strategy to be used since physically or practically there may be load at any time to the controller. A better controller is who handle the load change and set-point change efficiently along with set-point. Figure 6 and 7 shows set-point change in both the controllers. In split range after set point change there are some oscillations before settling down on change but in heat load set point change is very smooth.

We study the load change in second method it requires 402 seconds to overcome with load change in system shown in fig 8 below.
It is explained above that the controller using heat duty is performs better than the other controller. The optimization of the controller for better performance is shown in fig 9 and 10 .

It is found while using split range controller, there is critical zone when switching from heating to cooling. To avoid both heating cooling together is required, there is also a small dead zone where both heating and cooling is absent. Switching between both the modes of control may cause oscillations and difficulties. Comparison of density function of two controllers along with experimental result is shown in fig 11.

Conclusion

The batch polymerization reactor used for PMMA production has been successfully operated under the control of PID. Controller performance was studied under different optimal conditions. Based on results it is concluded that PID performs very well at tracking the optimal temperature trajectory. In this article two control strategies were compared and found spit range controller is better in settling down towards set-point (343k) but better disturbance rejection was found in second strategy where heat load is used as manipulative variable. In split range controller, switching between heating and cooling mode creates difficulties and oscillations.

References

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" Chem Eng Sci. 57: 2955-2969.

Tables

Process energy equation	$\rho V C_P \dfrac{dT}{dt} = \Delta H R_P - h_i A_i \left(T - T_M \right)$
Energy equation for metal wall	$\rho_M C_{PM} V_M \dfrac{dT_M}{dt} = h_i A_i \left(T - T_M \right) - h_{os} A_o T_M - T_J$
Energy equation for hot water	$V_J \dfrac{dU_J \rho_J}{dt} = F_S \rho_S H_S - h_o A_o \left(T_J - T_M \right) - W_C h_C$
Energy equation for cold water	$C_J \rho_J V_J \dfrac{dT_J}{dt} = F_W C_J \rho_J \left(T_{J0} - T_J \right) - h_o A_o \left(T_M - T_J \right)$
Energy equation for jacket	$\dfrac{dT_J}{dt} = \dfrac{F_{hot} T_{hot} + F_{cold} T_{cold}}{V_J} - \dfrac{\left(F_{hot} + F_{cold} \right) T_J}{V_J} + \dfrac{UA_J (T_R - T_J)}{V_J \rho_J C_J}$

Table 1: Energy balance for split range controller.

| Equation for Reactor	$Q + (-\Delta H) R_m$ $V - UA(T-T_J)/VC_p \rho - (T/V dV/dt)$
Jacket dynamics	$M_c C_{pc}(T_{ji} - T_{jo}) + UA(T-T_j)/V_c \rho_c C_{pc}$

Table 2: Energy balance for controller having heat load as manipulative variable.

Parameter	Split range	Heat load
Kc	5.29	10
TauI	0.31	0.01

Table 3: Control parameters.

Performance Criteria	Split Range controller	Controller using Heat duty
ITAE	3.8333e+006	1.4137e+007
IAE	3.1993e+002	1.6120e+004
ISE	4.2969e+004	1.8296e+005
ITSE	5.1468e+007	7.4853e+007

Table 4: Performance at set-point (343 K) using two different control strategy.
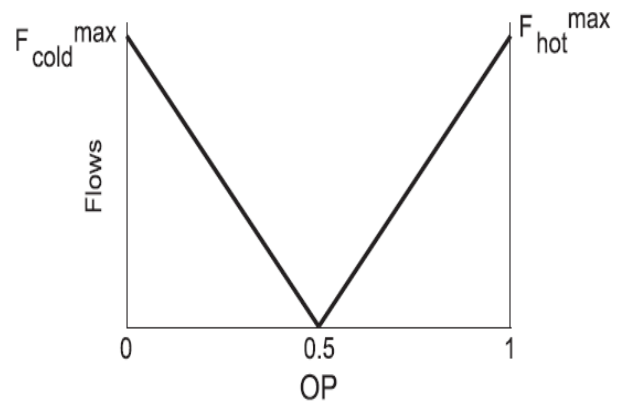
Controller	Split Range controller				Controller using Heat duty			
Parameter	ITAE	IAE	ISE	ITSE	ITAE	IAE	ISE	ITSE
Positive Load Change	2.2805 e+008	1.906 e+003	3.5205 e+005	4.2102 e+007	1.0387 e+008			
Negative Load change	2.7642 e+008	2.311 e+003	4.2346 e+005	5.0635 e+007	1.0403 e+008			
Positive set-point change	4.8527 e+010	3.643 e+005	5.0364 e+006	6.6920 e+010	3.7422 e+010			
Negative set-point change	1.5279 e+010	3.152 e+005	2.09 e+006	2.1469 e+010	3.7422 e+010			

Table 5: Performance of controllers for set-point change and load change.

Figures

Fig 1: PID control Logic

Fig 2: Split range temperature control (manipulative variables Vs control signal).

Fig 3: Comparison of Reactor Temperature.

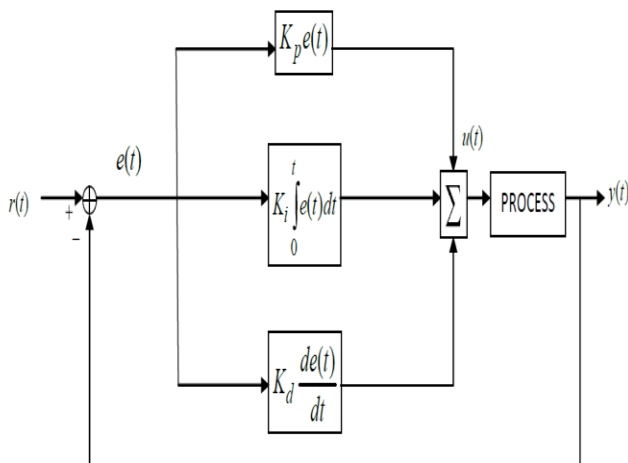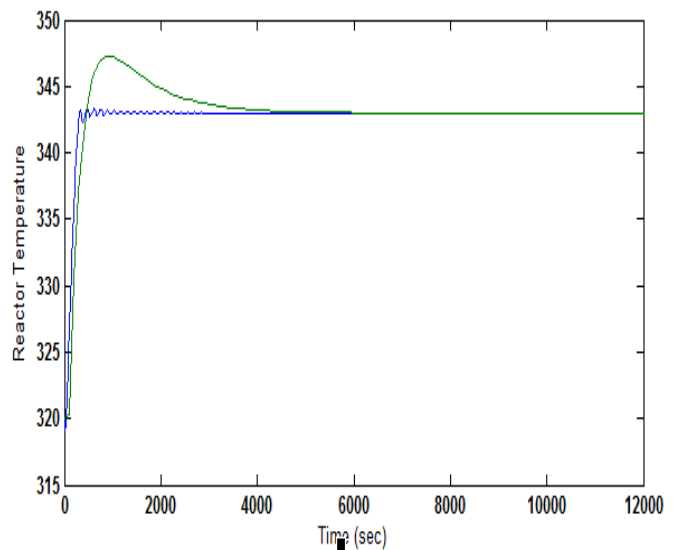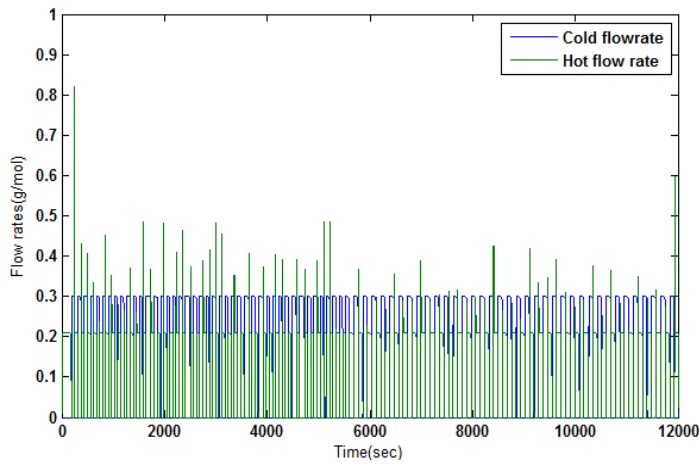Fig 4: Control Variable (split range- blue, Heat load- Green).

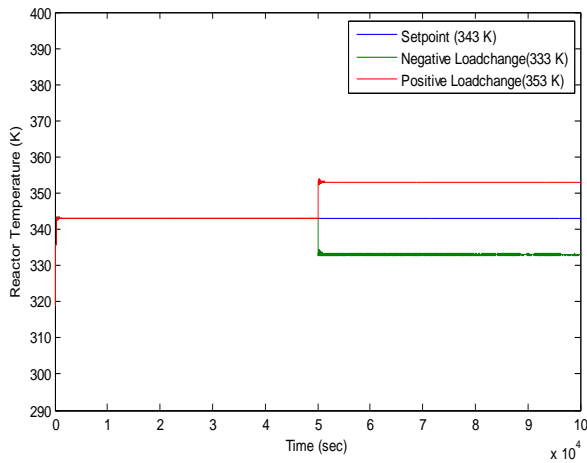Fig 5: Manipulative variable of split range controller.

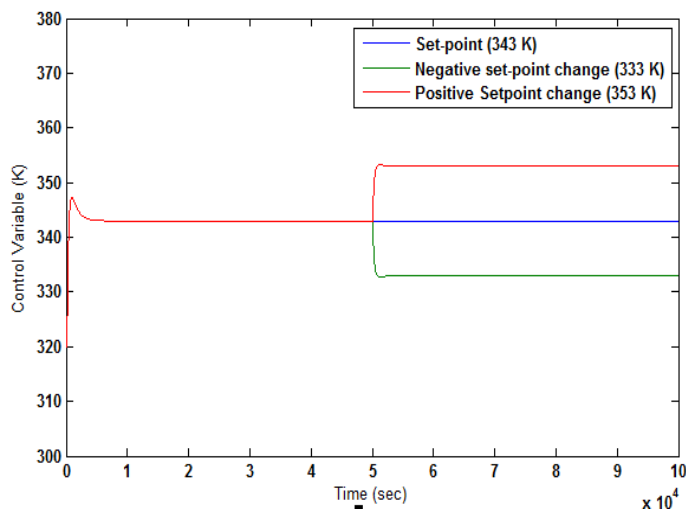Fig 6: Set point change in split range controller.

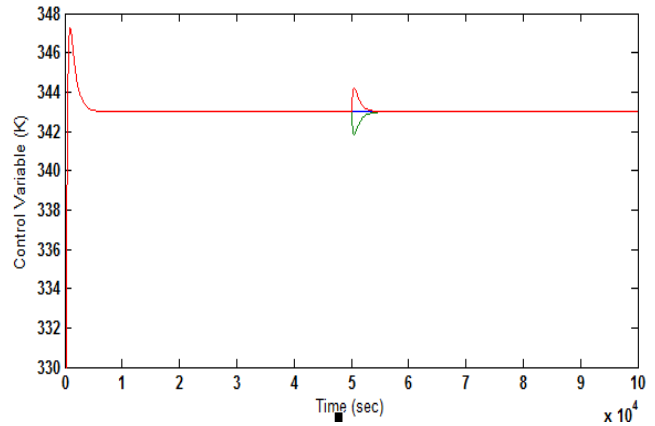Fig 7: Set point change in Second controller.
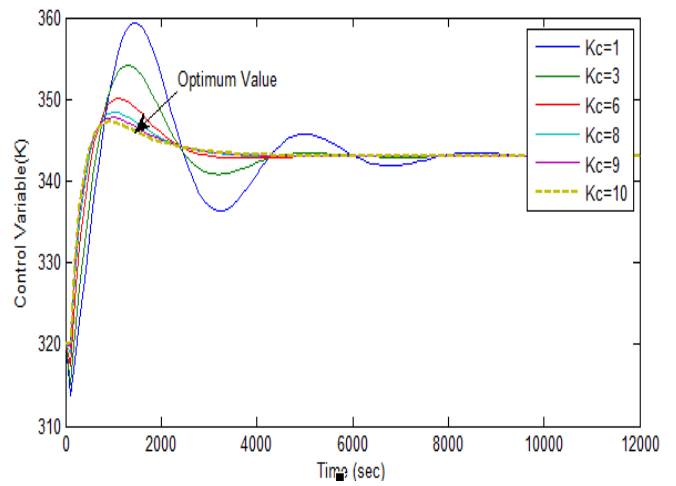

Fig 8: Load change in second controller.

Fig 9: Optimization of controller gain in second controller.
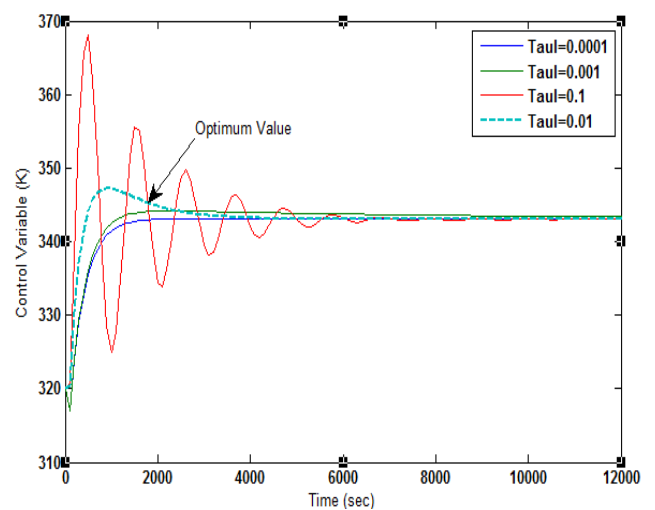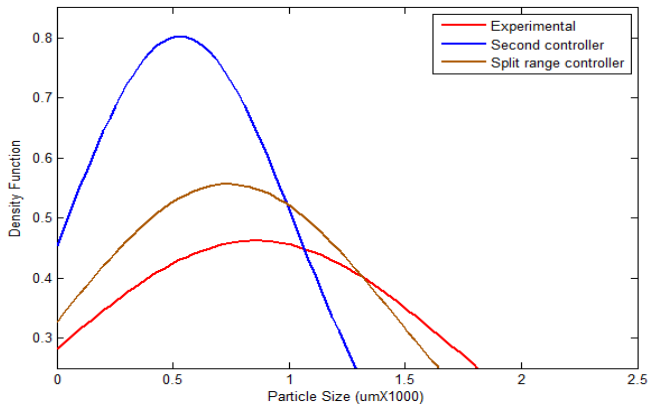

Fig 10: Optimization of TauI in second controller.

Fig 11: Comparison of density function.

Nomenclature

1. η1p= Polymer radicals which would not diffuse out from the particles due to large size.

2. η1m= Population containing one radical.

3. ρ (r)= Overall radical entry rate.

4. n0(r) = Population containing zero radical.

5. δ(r- r nuc) = Nucleation of particle.

6. [Micelle] = (1 x10 -4 ln (exp (1x 104([S]w-[Scmc]))+1.0)/ nag

7. ρ ini= Entry rate of initiator derived polymer radicals only

8. k0= Radical exit rate.

9. ktr= Termination rate

10. ke,m = 4 π rmicelle NA Dw/i1/2

11. NA= 6.0221x 10 23

12. Q= Heat duty

13. Uj = internal energy of hot water in jacket

14. Hs =enthalpy of incoming hot water

15. hc = enthalpy of liquid cooled

16. M = molecular weight of hot water

17. U = overall heat transfer coefficient

18. A_H = heat transfer area

19. Tj=temperature of cooling water in jacket,

20. ρj =density of water

21. Cj =heat capacity of water

22. Tj0 =inlet cooling water temperature

23. Fhot = are the flow rate of the hot

24. Fcold =cold streams fed to the circulating water