

Optimization of PID Controller Parameters in the Case of Batch Styrene Suspension Polymerization

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The highly exothermic polymerization reaction needs an efficient cooling system in order to avoid thermal runaways. The thermal agent flowrate or inlet temperature may represent the manipulated variable (MV) that the controller should adjust according to a set of laws to achieve a suitable goal. The laws the controller observes determine the class it belongs to: proportional (P), integral (I), derivative (D) or a combination of them. Due to its versatility and better performances, the PID controller was our choice. Its parameters can be set either by applying a set of rules, like Ziegler-Nichols' or Cohen-Coon's, or by searching for the optimal values fulfilling a performance criterion concerning the polymerization process, the optimization algorithm being suitably selected. One possible choice as performance criterion could be the distance between the actual reactor operating temperature and a set point. An interesting case study for applying this solution strategy is the batch reactor for the polymerization of styrene in suspension due to the two-step heat transfer: a) directly, from the monomer-polymer drops of given distribution to the continuous phase and b) indirectly, from the latter to the thermal agent, through the reactor wall. This way, the monomer/polymer drop temperature (which is function of drop's size as well and determines the polymer characteristics) can be influenced by the way the system responds to the adjustments made by the controller. The drop-water interface acts like a heat sink, but the average temperature of the drop is maintained at a higher level as compared to water by the ongoing polymerization reaction. The larger the drops, the higher the temperature differences between them and the continuous medium, with implications, as is to be shown by this contribution, on the optimized PID controller parameters.

1. Introduction

The thermal control of polymerization processes has received much attention in literature, both for product quality and for process safety reasons. Since the polymerizing systems, with very few exceptions, are capable of releasing large amounts of heat, a way to control them had to be found, which should be both reliable and simple in design. The PID controller meets these requirements due to its three components, proportional, differential and integral; the former two are responsible for the cancellation of the present and future fluctuations of the process variable from its set-point while the latter accounts for the system's past. Control structures such as fuzzy-hybrid PID (Ni et al., 1997) and predictive control (Ye et al., 2012) were reported to perform well, and, moreover, the generalized Takagi-Sugeno fuzzy controller (Solgi et al., 2006) and the PD type fuzzy controller (Abonyi et al., 1997) were successfully applied in batch polymerization processes. In spite of these more advanced and efficient control techniques, the ideal PID controller preserves the advantage of straightforward design, while still yielding satisfactory results (Seki et al., 2001), being advocated in more recent studies (Vahidi et al., 2008) as well. Its parameters can be adjusted according to a series of methods (Skogestad, 2003), but optimization, although highly time-consuming, allows for more precise tuning.

In their turn, the parameters of the controller depend on the process particularities, such as the thermal effect and the operating conditions; for instance, the same combination of values for the three factors will yield a different temperature profile for a bulk process as compared to the suspension polymerization of

the same monomer. Similarly, a suspension with large drops is expected to require different values for the PID controller's parameters than a suspension that is initially formed of small drops.

Such size differences from one polymerizing system to another may originate from the use of different stirrers, from variable stirring rate caused by malfunctioning or from wrong initiator dosage. However, the existing literature does not provide enough information on the extent to which the differences in drop size affect the results yielded by the PID controller. The objective of this paper therefore consists in showing that the optimum values for the parameters of the PID controller depend on the drop size. It is within the scope of this contribution to compare the P, I and D gains obtained for suspensions containing differently-sized polymerizing drops. For this purpose, optimization runs using genetic algorithms have been conducted for the cases of uniform large- and small-drops suspension polymerization.

2. Model equations

Batch suspension polymerization of styrene was taken as a case study. The reaction was considered to develop in a cylindrical reactor, equipped with a mechanical stirrer, and cooled by water flowing through the jacket. The flowrate of the latter is manipulated by the PID controller as a response to the thermal effect of the polymerization. The assumptions used in model development are summarized as follows (Paláu et al., 2012):

- a. Initiation takes place by peroxide initiator decomposition and, above 90 °C, by self-initiation of the monomer, with third-order kinetics with respect to the latter. The overall initiation rate is computed as the sum of the two individual initiation rates.
- b. The termination reaction only takes place by recombination.
- c. The chain transfer reaction only takes place with the monomer molecules.
- d. Active centres obey the quasi-steady-state assumption.
- e. All the reactions take place in the suspended drops.
- f. Drops are isotropic.
- g. Diffusion is the only mass transport mechanism acting along the drop radius.
- h. Suspended drops of monomer/polymer solution and polymer particles are of spherical shape.
- i. The distribution of the suspended drops is uniform.
- j. The geometry of the reactor is cylindrical, that of the jacket is annular.
- k. The physical properties of the suspension change with conversion and drops/particles composition and distribution.
- l. The reaction volume varies with the polymer-monomer fraction.

2.1 Conservation equations

Assumptions e. - i. above are of particular importance, since they underline the monomer drops as distinct entities subjected to changing composition. They therefore represent a set of independent micro-reactors where polymerization occurs simultaneously, generating important amounts of heat. A detailed description of the material and thermal balances within the drops, as well as on the kinetic model, is to be found in (Paláu et al., 2012).

The aqueous phase in which the drops are suspended plays an active role in heat removal: once the heat is received from the drops, it is transferred to the thermal agent that flows through the jacket. The mathematical model is given by Eq. (1), where Q_{id} represents the rate of heat transfer from drops through their interface, while Q_{ta} stands for the rate of heat transfer to the thermal agent; T , m , and C_p represent the temperature (T), mass (kg), and heat capacity (J/kg/K), respectively, while the subscript w designates the water in the reactor, seen as a heat carrier.

$$\frac{dT_w}{dt} = \frac{Q_{id} - Q_{ta}}{m_w C_{p_w}} \quad (1)$$

$$Q_{id} = 4 \pi R_{drop}^2 N_{drop} k_T (T_{ds} - T_w) \quad (2)$$

$$Q_{ta} = K \pi d_r \left(h_r + \frac{d_r}{4} \right) (T_w - T_{aa}) = D_{ma} \frac{C_{p_w}(T_w) + C_{p_w}(T_{ai})}{2} (T_w - T_{ai}) \quad (3)$$

The two heat transfer rates are defined by Eqs. (2) and (3). The drops are able to transfer heat at a rate proportional to their interface, while the jacket can remove as much heat as allowed by its contact surface

with the suspension. N_{drop} is the number of drops in the suspension, T_{ds} is the temperature at the surface of the drop, d_r and h_r are the diameter and the height of the reactor, respectively, D_{ma} , T_{aa} , and T_{ai} represents the flowrate, the average and inlet temperature of the thermal agent, respectively.

2.2 Tuning of the controller's parameters

Figure 1 shows the variations in the thermal agent flowrate corresponding to the cases of a small and of a large drop suspension, respectively. The small-drop system is characterized by a higher interfacial area, thus the continuous phase is capable to quickly remove the heat of polymerization. The temperature of the aqueous medium increases, forcing the PID controller to act accordingly; consequently the flowrate of the thermal agent (MV) is raised. The heat being removed, the temperature of the continuous phase (the process variable, PV) is brought near the set-point value (SP), and so the MV starts decreasing. This in turn allows for heat to accumulate and for the PV to increase again. The MV is consequently augmented and the system is thus forced to develop a pseudo-cyclic behaviour; this is an indicator of an over-responsive controller with a too high derivative gain.

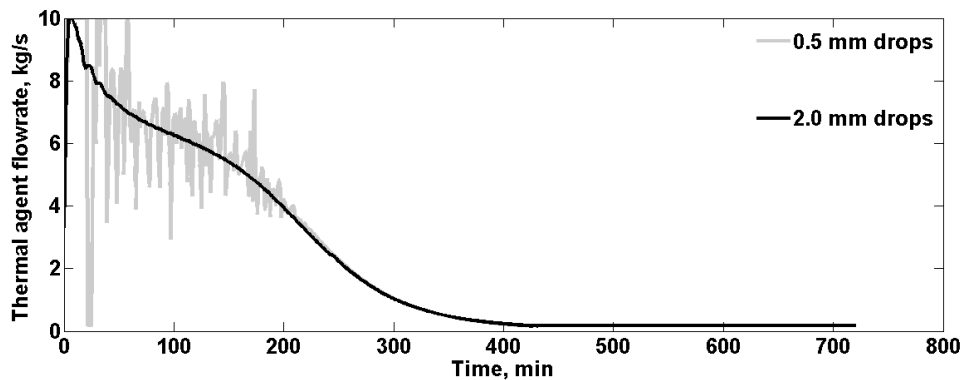


Figure 1: MV profiles for small- and large-drop polymerizing systems, respectively, under the influence of the same values in the PID controller parameters, prior to optimization

However, for the same values of the PID controller's parameters, the large-drop system shows a different behaviour; given the lower drop-water interfacial area, the drops release the heat of reaction at a constant slower pace to the continuous phase, thus it accumulates more in the organic phase; this type of system is thus characterized by a higher thermal inertia and the MV is not subject to sudden variations as in the previous case. The PID controller is, in turn, capable of finding a much smoother profile for the thermal agent flowrate.

These dissimilar performances of the two systems lead to the need for differentiated adjustment of the parameters of the PID controller. The objective of the latter's use consists in diminishing the difference ε between the PV and the SP. For this purpose, the MV is adjusted with the value obtained from Eq. (4), where T_{ref} denotes the set-point. The algorithm that the PID controller obeys is schematically shown in

Figure 2. The flowrate of the thermal agent also has to observe a series of restrictions and the system is therefore forced to operate in a range of MV. The upper boundary is given by the power of the pumps and by the maximum flowrate allowed through the jacket, while the lower limit is necessary due to safety considerations.

$$CO = K_r (T_w - T_{ref}) + \frac{\int_0^t (T_w - T_{ref}) dt}{\tau_i} + \tau_d \frac{dT_w}{dt} \quad (4)$$

The parameters K_r , τ_i , and τ_d of the controller were adjusted by optimization using the genetic algorithms ("ga") built-in function of the R2012b version of Matlab®. Because of its evolutionary nature, this method does not guarantee finding the global optimum; on the other hand, it can skip local traps and is suitable for large search domains, given its ability to consider mutation as a population-changing random operator. The routine was used with the default parameters, except for the number of generations and the population size. Simulations were conducted with 5 generations with populations of 25 individuals (sets of

parameters). The objective function $FOB = \frac{\sqrt{\|\varepsilon\|}}{N}$ was defined in connexion to the distance ε between the values of the suspension temperature and its set-point $\varepsilon = T_w - T_{ref}$, computed for each integration step; here, N represents the length of ε .

The SP value was defined as the initial reaction temperature. The instantaneous position of the PV relative to the SP leads to the identification of two successive time intervals for the process. During the first of these, the high monomer concentration contributes to the enhanced rate of propagation, and ultimately to large amounts of heat being generated into the polymerizing system; the PV is in this situation above SP and the PID controller is forced to increase the MV up to its superior limit (see Figure 1). As the monomer is slowly depleted, the overall thermal effect starts decreasing, and the flowrate of the thermal agent is gradually diminished to its minimum value (see Figure 1) – this is the interval of interest in which the temperature should stay as close as possible to SP. After that moment, the PV still continues to decrease below the SP, since the generated heat becomes too low to balance the transferred heat, even for the lowest MV value – from this point on, the PID controller becomes useless.

Since the error yielded during the first time-interval is less prominent than that in the second time-interval, when temperature drop is around 10-15 K, the optimization algorithm tends to focus on adjusting the three parameters with respect to the latter case. This, however, presents no runaway risks, and should not contribute to FOB. Therefore, when the rate of monomer consumption drops under a sufficiently low value giving only residual generated heat (this defines the end of the first time-interval, which is not the same for two different sets of PID parameters), the computation of the FOB ceases.

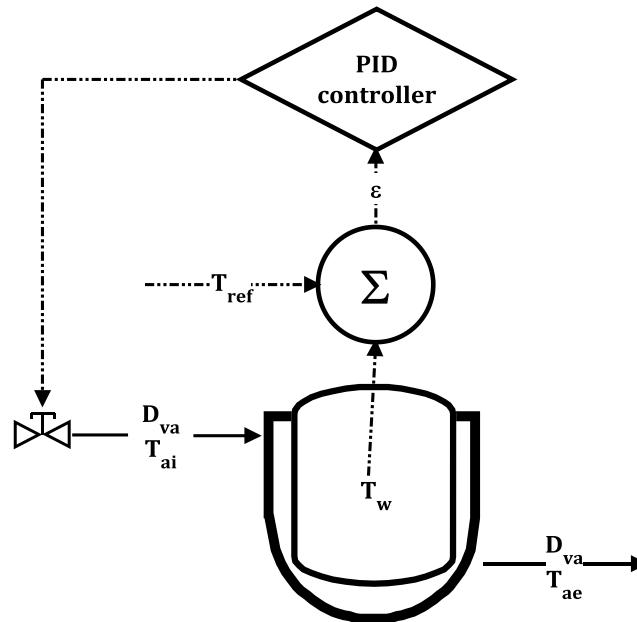


Figure 2: Schematic representation of PID controller's functioning

3. Results and discussions

The starting values of K_r , τ_i , and τ_d gains set to 5, 2, and 2.5, after some preliminary runs. The values of these parameters obtained after optimization considering the two drop sizes are listed in Table 1. The dissimilarities between the two optimized sets of PID parameters are the consequence of different values in the heat transfer surface between the two phases in the reactor. The value of the proportional term K_r reflects the current deviation of the PV from the SP; the integral gain τ_i , on the other hand, is a response to the ε evolution in time, while τ_d , or the derivative parameter, is an indicator of how steep the slope of the PV is.

The large-drop case, characterized by high thermal inertia, is shown to require a lower proportional gain, i.e. a slower response; the integral term is decreased with respect to the starting value, meaning that the past evolution of the system is not as significant as was assumed initially; the value of τ_d is close to the

starting point of the simulation, and the slight need for its adjustment is underlined by the smoothness of the initial MV profile shown in Figure 1.

The small-drop polymerizing system, on the other hand, since it shows sudden PV variations, requires a fast response from the controller, and therefore a larger K_r . The derivative gain is decreased, for reducing the rate of MV variations, while the integral parameter is close to its initial guess.

This shows that, unlike the large drops, the small ones do not present thermal inertia due to their extended heat transfer area; they consequently require larger proportional and integral gains, and a lower value for the τ_d . The obtained value for the objective function, lower for the small drops than for the large ones, shows that the thermal inertia of these latter draws the PV from the reference point, notwithstanding the smooth profile of the MV.

Table 1: Final parameters of the PID controller

Drop size, mm	Proportional gain, K_r , kg/(s K)	Integral gain, τ_i , s ² K/kg	Derivative gain, τ_d , kg/K	Final value of the objective function
2	4.95	1.88	2.48	$5.9 \cdot 10^{-3}$
0.5	5.05	1.98	2.37	$1.5 \cdot 10^{-3}$

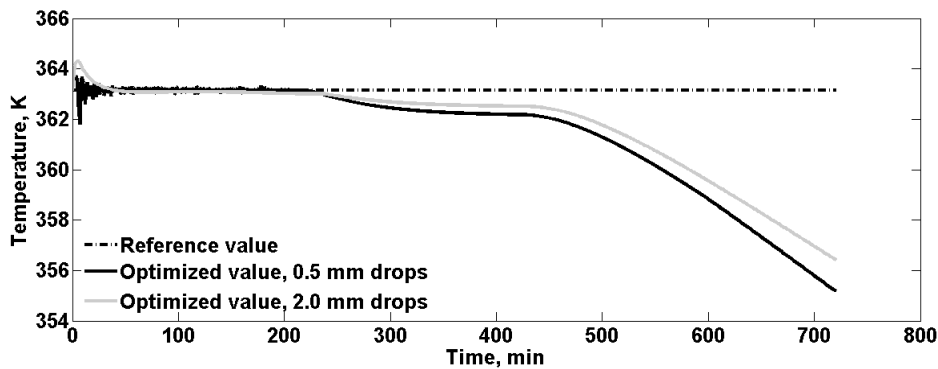


Figure 3: PV profiles under the influence of the optimized values in the PID controller parameters

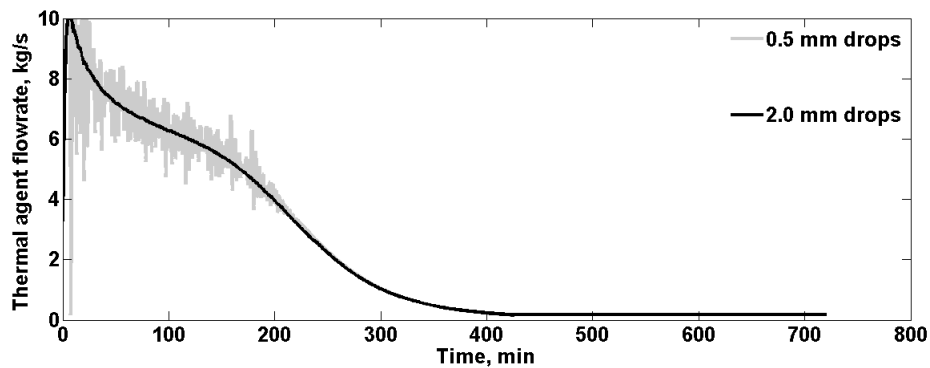


Figure 4: MV profiles under the influence of the optimized values in the PID controller parameters

The PV and MV plots resulted from runs with the optimized PID controller parameters are shown in Figures 3 and 4, respectively. In spite of the lower value of the objective function, it is shown that the parameters of the PID controller lead to an interval in which the MV has bang-bang type behaviour for the small-drop polymerizing system (see the first 200 min, Figure 4). Not only the PV in Figure 3 is subjected to sudden variations, but its departure from set-point is also large. Although no thermal runaway is implied since the most considerable variation is negative, this can have consequences upon the final molecular weight distribution. On the contrary, the large-drop suspension presents one positive deviation; the large value of the objective function is given by the time interval needed for the controller to cancel this larger error, given the higher thermal inertia of this latter system.

4. Conclusions

This work has shown the need for the control system of the suspension polymerization processes to be treated in a specific manner, depending on the size of their dispersed phase. Although the case of a slow-reacting monomer was simulated, the differences between the large-drop system and the small-drop one were shown to be significant in terms of the flowrate variations of the cooling agent. The parameters of the PID controller were therefore tuned separately for each case. A particular methodology was used for this purpose, applied on the optimization procedure of the two cases.

The time profile of the process variable showed larger deviations from the set-point during the monomer depletion interval, which presented no runaway risk. Based on this observation, the objective function was computed using only the data obtained in the first time-interval. Optimization runs were conducted in Matlab®, using the “ga” built-in routine, with 5 generations and population size of 25. The values obtained for the three parameters of the controller reflect the high heat transfer area that characterizes the small-drop system and the high thermal inertia of the suspension containing only large drops. Higher proportional and integral parameters are required for the system to quickly respond to PV variations, while the lower value for the derivative parameter shows the need for a less aggressive controller in the case of small-drop suspension, as compared to those containing large drops. The objective function, on the other hand, reflects the high capacity of the small drops to transfer large amounts of heat; the heat generated inside the large drops is, on the contrary, transferred at a slower rate to the continuous phase acting like a heat carrier.

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