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Model-Based Linear Control of Polymerization Reactors

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Abstract

This work addresses the design and performance evaluation of a control system for a class of continuous stirred tank reactors to produce homopolymers via free radicals. The control system claims to be of practical implementation in the sense that: (i) it manages both measurement types existing in this class of processes: continuous-instantaneous, and discrete-delayed with a periodic sampling-time; and (ii) its designing exploits the linear systems theory on the basis of the reactor model. The behavior of the control system, achieving stabilization of an open-loop unstable steady state, in spite of disturbances and parametric model errors, is discussed and illustrated via simulation highlighting the effect of the sampling time.

Keywords: linear control, discrete-delayed measurements, polymerization reactor

Introduction

The polymerization reactors, because of their industrial importance and highly nonlinear nature, have represented excellent study cases to evaluate and develop different control techniques [1]. In fact, as it can be observed in the open literature, considering the challenge that the nonlinear feature places in front, the studies follow nonlinear advanced approaches; most of them are based on the process model. However, nowadays the industrial polymerization reactors are typically operated through linear controllers that automatically maintain nominal levels of temperature and volume, and supervisory schemes that control the production rate and product quality; and, it can be said that these reactors still are not being fit with advanced control schemes. It can be argued that the nonlinear nature of most of advanced control systems makes them seem complex and of expensive implementation; besides, polymerization reactors are also monitored by discrete-delayed measurements, and the advanced control systems are designed in a framework of continuous measurements, except when model predictive control technique or Kalman filters are applied.

The above mentioned has motivated a research line of automatic control systems of polymerization reactors that: (i) are based on deterministic models, (ii) manage both continuous-instantaneous and discrete-delayed measurements, and (ii) are of technically feasible and non-expensive implementation. Methodologically speaking, a linear approach must firstly be followed, but this kind of study is missing in the open literature; and even though controlling temperature and volume does not represent a challenge for linear controllers, automatically controlling production rate and product quality does.

Then, in this work, on the basis of linear control elements, and regarding the discrete-delayed nature of the measurement related to the production rate, a control system was designed for the class of free-radicals homopolymerization continuous stirred tank reactors. Next, the performance was evaluated emphasizing the effect of the sampling-time.

The Polymerization Reactor and its Control Problem

In this work, the class of continuous stirred tank reactors, where a free radical homopolymerization takes place, was considered. This class of processes encloses most of the phenomenological characteristics of any polymerization reactor. Their dynamics, with respect to the production rate and safety aspects, are described by a set of four highly nonlinear equations [2]:

$$\dot{I} = -r_I(I,T) + \varepsilon \cdot r_P(I,M,T) \cdot I + (W_I/V) - (q_e/V) \cdot I := f_I(\cdot), \quad t_{i+1} = t_i + \delta_t \tag{1a}$$

$$\dot{M} = (1-\varepsilon M) \cdot r_P(I,M,T) \cdot M + (q_e/V)(M_e - M) := f_M(\cdot), \quad y_M(t_i) = M(t_{i-1}) \tag{1b}$$

$$\dot{T} = (-\Delta H_P) r_P(I,M,T) - U \cdot (T - T_J) + (q_e/V)(T_e - T) := f_T(\cdot), \quad y_T(t) = T(t) \tag{1c}$$

$$\dot{V} = -\varepsilon \cdot r_P(I,M,T) \cdot V + q_e - q_s := f_V(\cdot), \quad y_V(t) = V(t) \tag{1d}$$

These equations result from material and energy balances, and polymerization arguments, and point up the reactor state is given by the initiator (I) and monomer (M) concentrations, and by the temperature (T) and volume (V) of the reactor content; and the inputs are the initiator (W_I) and monomer (q_e) feed rates, the jacket temperature (T_J), and the output flow rate (q_s). Considering a practical case, the reactor is monitored via monomer (y_M), temperature (y_T) and volume (y_V) measurements. It must be noticed y_M, at the sampling time instant t_i, takes the value of M at t_{i-1}, and δ_t is the periodic sampling time ($t_i = t_{i-1} + \delta_t$); say, y_M is a discrete-delayed measurement resulting from a sampling-analysis activity along the reactor operation. The functionalities r_I and r_P represent the consumption rate of I and the polymerization rate, respectively; ε is the volume contraction factor, and U represents the heat transfer capabilty of the jacket. Then, the objective is controlling the reactor in a certain (possibly open-loop unstable) nominal state ($\overline{I}, \overline{M}, \overline{T}, \overline{V}$) by the manipulation of q_e, T_J, and q_s, on the basis of the continuous measurements of T and V ($y_T(t)$, $y_V(t)$), and the discrete-delayed measurement of M ($y_M(t_i)$).

The Control System

The control system for the polymerization reactor is depicted in Figure 1; it can be observed that the defined control structure is the following: M is controlled through q_e, which is driven by an estimate of M (M^E); T is controlled through T_J, driven by y_T; and V is controlled through q_s, driven by y_V. Then, the essential control elements are a controller, and an estimator; regarding to the discrete-delayed characteristic of y_M, the estimator is added in order to provide $M^E(t_i)$ each sampling time instant (t_i).

The Controllers

The linear controllers for monomer, temperature and volume are:

$$q_e(\tau) = \overline{q}_e + k_P^{MC} \cdot (M^E(t_i) - \overline{M}) + k_I^{MC} \cdot \sum_{i=0}^{n} (M^E(t_i) - \overline{M}) \cdot \delta_t, \quad \tau \in [t_i, t_{i+1}] \tag{2a}$$

$$u(t) = \overline{u} + k_P^X \cdot (y_X(t) - \overline{X}) + k_I^X \cdot \int_0^t (y_X(s) - \overline{X}) \cdot ds \tag{2b}$$

where $u = T_J$, q_s, and $X = T$, V, respectively; the '¯' symbol refers to a nominal value of the variable. The controllers have proportional and integral (sumatorial for the monomer controller) actions, where $k_P^{MC}, k_P^X, k_I^{MC}, k_I^X$ are the tuning gains. It is noticed that q_e becomes a stepwise function that depends on the sequenece of the monomer estimate values $\{M^E(t_0), M^E(t_1), M^E(t_2), \ldots\}$.

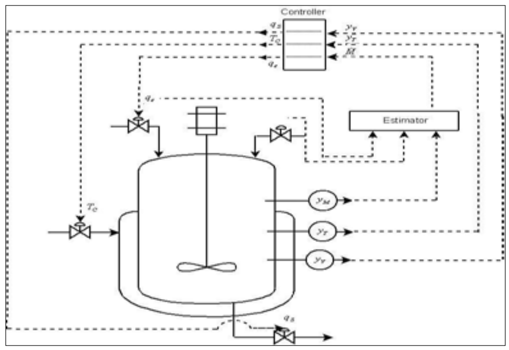

Figure 1. Control System of the Polymerization Reactor

The Estimator

The estimator construction followed the straightforward application of the procedure given in [3] on the basis of the linearized version, at the nominal contidition, of the *I* and *M* dynamics of the reactor model (Eq. 1a, b),

$$\dot{\tilde I} = a_{II}\tilde I + a_{IM}\tilde M + a_{IT}\tilde y_T + a_{IV}\tilde y_V + a_{Iq_e}\tilde q_e + a_{IW_I}\tilde W_I, \quad a_{mn} = (\partial f_m / \partial n)\big|_{\bar x, \bar u} \tag{3a}$$

$$\dot{\tilde M} = a_{MI}\tilde I + a_{MM}\tilde M + a_{MT}\tilde y_T + a_{MV}\tilde y_V + a_{Mq_e}\tilde q_e, \quad \tilde y_M(t_i) = \tilde M(t_{i-1}) \tag{3b}$$

where the '~' symbol indicates a deviation variable between the actual and nominal values (i.e. $\tilde M = M - \overline{M}$). *T* and *V* dynamics are not considered since y_T and y_V equal *T* and *V*, respectively, and only *I* and *M* are necessary to estimate, in a reduced order estimation scheme [4]. The possibilty of the estimator construction is provided by the stable feature of the sole *I*-dynamics (Eq. 3a), and by the trivial observability property of the coefficients pair (a_{MM}, 1). The estimator takes the following form:

$$\tilde I^E(t_{i+1}) = \Theta_I(\tilde I^E(t_i), \tilde M^E(t_i), \tilde y_T(t), \tilde y_V(t), \tilde W_I(t), \tilde q_e(t)) \tag{4a}$$

$$\tilde M^E(t_{i+1}) = \Theta_M(\tilde I^E(t_i), \tilde M^E(t_i), \tilde y_T(t), \tilde y_V(t), \tilde q_e(t)) + k_P^{ME} e_M(t_i) + k_I^{ME} i_M(t_i), \tag{4b}$$

$$i_M(t_{i+1}) = i_M(t_i) + k_I^{ME} e_M(t_i), \quad e_M(t_i) = \tilde y_M(t_i) - \tilde M^E(t_i) \tag{4c}$$

where Θ_I and Θ_M are the transition maps of the linear differential equations (3a, b). Besides the proportional action, the estimator has a sumatorial one accounted by the variable i_M. k_P^{ME} and k_I^{ME} are the estimator tuning gains.

Tuning
The tuning scheme was constructed through the following procedure:
(i) for the continuous controllers (Eq. 2b), the coefficients of the corresponding second-order closed-loop linearized dynamics of T and V, in a decoupled structure, were matched with the ones of the characteristic polynomial of the stable linear dynamics of reference $\ddot{x} + 2\xi\omega\dot{x} + \omega^2 x = 0$; where (ξ.- damping factors, and ω.- characteristic frequencies
(ii) for the discrete M-controller (Eq. 2a) and M-estimator (Eq. 4), first a characteristic polynomial of reference was constructed on the basis of the eigenvalues (γ) that result from mapping the eigenvalues (λ) of the above continuos reference dynamics into the unit circle: $\gamma = \exp(\lambda\ \delta_t)$; next, the coefficients of the characteristic polynomials of the corresponding second-order closed-loop discrete linear dynamics of M, and convergence error dynamics of the M-estimator, were matched with the reference characteristic polynomial.
In this way, the gains are given in terms of the well-known parameters (ξ.- damping factor, ω.- characteristic frequency) of a stable dynamics:

$$k_P^X = -(1/a_{Xu})(a_{XX} + 2\xi_X\omega_X), \quad k_I^X = -({\omega_X}^2/a_{Xu}), \quad a_{Xu} = (\partial f_X/\partial u)\big|_{\bar{x},\bar{u}} \tag{6a}$$

$$k_P^{M,Z} = (c_1(\delta_t, \xi_M^Z, \omega_M^Z) + p_1(\delta_t) + 1)/p_2^Z(\delta_t), \qquad X = T,\ V \quad u = q_e,\ T_J \tag{6b}$$

$$k_I^{M,Z} = (c_1(\delta_t, \xi_M^Z, \omega_M^Z) + c_2(\delta_t, \xi_M^Z, \omega_M^Z) + 1)/(\delta_t \cdot p_2^Z(\delta_t)), \quad Z = C,\ E \tag{6c}$$

$$p_1(\delta_t) = \exp(a_{MM} \cdot \delta_t), \quad p_2^C(\delta_t) = a_{Mq_e}(1 - p_1(\delta_t))/a_{MM}, \quad p_2^E = 1$$

$$c_1(\delta_t, \xi, \omega) = -2\exp(\delta_t \xi\omega)\cos(\delta_t\sqrt{1-\xi^2}\,\omega), \quad \text{if} \quad \xi \le 1;$$

$$c_1(\delta_t, \xi, \omega) = -(\exp(2\delta_t\sqrt{\xi^2 - 1}) + 1)\exp(-\delta_t(\xi + \sqrt{\xi^2 - 1})\omega), \quad \text{if } \xi > 1,$$

$$c_2(\delta_t, \xi, \omega) = \exp(-2\delta_t\xi\omega).$$

Consequently, the controllers and the estimator are tuned in a framework of convergence rate manipulation by firstly setting the sampling time; next, choosing damping factors, and varying desired settling times with the characteristic frequencies.

Control System Performance

The test of the control system was based on the study case of Alvalrez [2]. The nominal operation conditions associated to an open-loop unstable steady state were considered, $(\bar{I}, \bar{M}, \bar{T}, \bar{V}, \bar{q}_e, \bar{T}_c, \bar{q}_s, \bar{W}_I, \bar{T}_e)$ = (0.001831 gmol/L, 0.5809, 349.58 K, 40 L/min, 315 K, 34.94 L/min, 0.08 gmol/min, 300 K); with these conditions, the polymerization is carried out at high solid fraction with gel effect, making the control system test extreme. In order to emulate the operational problems that appear in an industrial framework (i.e. change in the heat transfer capability of the reactor due to jacket fouling, and changes in the kinetics efficiency due to different raw material providers), parameter errors were introduced to the reactor model. Besides, disturbances on W_I (+10% of the nominal value) and T_e (+2% of the nominal value) were introduced.
In Figure 2 the performance of the control system is shown for two sampling time situations: (i) δ_t = 5 min, with the tuning parameters (ξ_M^C, ξ_T, ξ_V, ξ_M^E) = (2, 0.7071,

0.7071, 2), and (ω_M^C, ω_T, ω_V, ω_M^E) = (0.04, 0.15, 0.4, 0.4); and (ii) δ_t = 15 min, with the tuning parameters (ξ_M^C, ξ_T, ξ_V, ξ_M^E) = (2, 0.7071, 0.7071, 2), and (ω_M^C, ω_T, ω_V, ω_M^E) = (0.004, 0.15, 0.4, 0.04). It can be observed that the performance of the control system with a δ_t = 5 min is adequate and fast, and the required effort on the control inputs is smooth. In the case of δ_t = 15 min, the nominal state is still maintained; however, it takes a longer settling time and requiere more control effort (even the temperature and volume controllers) than in the case of frequent monomer mesurement.
In fact, it must be said that for a δ_t greater than 17 min, the control system does not achieve stabilization; but, in the ideal case of non parametric errors, the control system does with a δ_t up to 25 min.

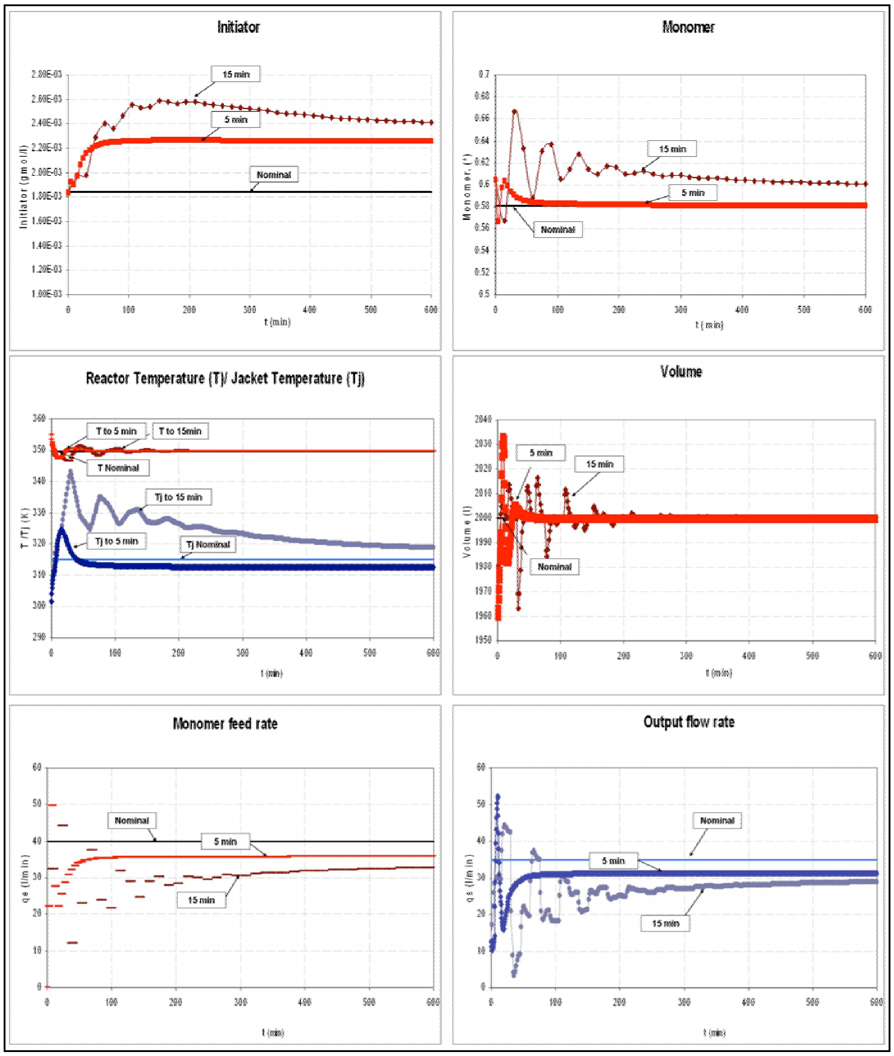

Figure 2. Control System Performance

Although this control system only deals with the variables related to the production rate and safety (*M*, *T*, *V*), it fits to say that the control of the product quality is also achieved, but its convergence rate, and offset, is not handled in a direct form, as the *I*-dynamics (Figure 2). In the light of the attained performance, the approach can be extended to control the product quality; for example, driving the initiator feed rate or a transfer agent with discrete-delayed measurements of the average molecular weight of the polymeric product.

Conclusions

In this work, it was designed a control system for a polymerization reactor whose linear control elements had the capability to adequately ensure its nominal operation, managing continuous-instantaneous and discrete-delayed measurements. The control system includes a systematic model-based tuning scheme that takes in account the sampling time, and whose conventional parameters provide insight into desired convergence rates. This system of linear controllers presents the least implementation cost, and a comparison of its performance with systems of nonlinear controllers would be worthwhile.

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