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MW CONTROL OF CONTINUOUS POLYMER REACTORS

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Abstract: In this work, the problem of controlling (possibly open-loop unstable) continuous free-radical solution polymer reactors with continuous measurements of temperature, level and flows, and discrete-delayed measurements of molecular weight (MW) is addressed. The point of departure is a previous control scheme with linear-decentralized PI volume and temperature components, and a material balance conversion component. Here, the problem of designing and incorporating a MW component driven by discrete-delayed MW measurements is considered within a constructive framework. The result is a four-input four-output control scheme that: (i) has linear decentralized PI-type components with reduced model dependency, and (ii) recovers the behavior of a controller driven by continuous measurements. The proposed approach is tested with a representative example through simulations.

Keywords: Polymerization reactor control, decentralized control, discrete measurements, discrete estimator, chemical process control.

1. INTRODUCTION

A wide class of materials is produced in continuous free-radical polymer reactors, which are highly nonlinear dynamical systems with complex behavior: strong and asymmetric input-output coupling, multiplicity of steady-states, and parametric sensitivity (Hamer *et al*. 1981). Industrially, these reactors are controlled with volume and temperature PI loops, and the conversion and molecular weight (MW) are regulated by adjusting the monomer and initiator (and/or transfer agent) dosages via supervisory control schemes. The production rate, stability, safety and quality indicators are met by controlling the temperature, volume, conversion, and MW. In particular, the control of MW is important to met product quality specifications.

The MW control problem has been the subject of theoretical, simulation and experimental studies over the past decades. The state-of-the-art can be seen elsewhere (Richards and Congalidis, 2006), and here it suffices to mention that several control approaches have been employed, including linear PI controllers (Ellis *et al*., 1994) as well as nonlinear geometric (Adebekun and Schork, 1989; Niemiec *et al*., 2002), model predictive (MPC) (Mutha *et al*., 1997), and calorimetric (Alvarez *et al*., 2004) control techniques, including open-loop (Adebekun and Schork, 1989), extended Kalman filter (EKF) (Ellis *et al*., 1994; Mutha *et al*., 1997), and Luenberger (L) (Tatiraju *et al*., 1999) nonlinear observers. Most of the MW control and/or estimation schemes have been driven by size exclusion chromatography (SEC) (Ellis *et al*., 1994) and gel permeation chromatography (GPC) (Niemiec *et al*., 2002) measurements, which typically involve low sampling rates and long delays. This feature and the detailed-model dependency of the control schemes affect the functioning, and imply complexity, reliability, and cost drawbacks for industrial applicability.

Recently, based on inversion and feedforward (FF) - feedback (FB) control ideas, González and Alvarez (2005) presented a PI-inventory controller that combines industrial-like linear and decentralized PI volume and temperature components, with material balance (MB) monomer and MW controllers. This scheme is driven by continuous-instantaneous measurements of volume, temperature and flows, addresses the complete MIMO control problem (volume, temperature, conversion and MW), and regulates the MW with an offset that depends on the accuracy of the initiator decomposition-chain transfer model, and with a speed that is about twice faster than the one of the open-loop response. The same tasks and results were obtained by a robust control scheme (Alvarez and González, 2006) drawn from the application of constructive control ideas (Sepulchre *et al.*, 1997).

In this work, the problem of controlling (possibly open-loop unstable) continuous free-radical solution polymer reactors with continuous measurements of temperature, level and flows, and discrete-delayed (DD) MW measurements is addressed within a constructive control framework. In particular, we are interested in: (i) designing a MW control component with linearity, decentralization and reduced model dependency features, (ii) the coordination of this component with previously designed volume, temperature and monomer components (González and Alvarez, 2005; Alvarez and González, 2006), and (iii) the capability of handling low sampling rates and long delays, typically encountered in an industrial setting. The proposed approach is illustrated and tested with a representative example through simulations.

2. CONTROL PROBLEM

Consider a CSTR where an exothermic free-radical solution homopolymer reaction takes place. Monomer, solvent and initiator are fed to the tank, and heat exchange is enabled by a cooling jacket. Due to the gel effect (Chiu *et al*, 1983), the reactor can present steady-state multiplicity (Hamer *et al.*, 1981). From standard free-radical polymerization kinetics (Hamer *et al.*, 1981), and viscous heat exchange considerations (Alvarez *et al.*, 1996), the reactor dynamics are given by the following mass and energy balances:

$$\dot{T} = \{\Delta_h r - U(T - T_j) + (\rho_m q_m c_m + \rho_s q_s c_s)(T_e - T)\}/C := f_T, \qquad y_T(t) = T \qquad (1a)$$

$$\dot{T}_j = \{U(T - T_j) + \rho_j q_j c_j (T_{je} - T_j)\}/C_J := f_j, \qquad y_j(t) = T_j \qquad (1b)$$

$$\dot{V} = q_m + q_s - (\varepsilon_m/\rho_m)\, r - q := f_V, \quad y_V(t) = V \qquad (1c)$$

$$\dot{m} = - r + \rho_m q_m - (m/V)\, q := f_m \qquad (1d)$$

$$\dot{\iota} = (- r\,\iota + r_0)/p := f_\iota, \qquad y_\iota(t_k) = \iota(t_{k-1}) \qquad (1e)$$

$$\dot{I} = - r_i + w_i - (I/V)\, q := f_i \qquad (1f)$$

$$\dot{s} = \rho_s q_s - (s/V)\, q := f_s \qquad (1g)$$

$$\dot{Q} = - (r/p)\{[2 - (r_0/r)/\iota]Q - [2(r/r_0) + W_m]\iota\} := f_Q \qquad (1h)$$

$$u = (q_j, q, q_m, w_i)', \qquad z = (z_T, z_V, z_m, z_\iota)'$$

$$r = f_r(T, V, m, I, s) \qquad (2a)$$

$$U = f_U(T, T_j, V, m, s), \qquad \rho = f_\rho(V, m, s) \qquad (2b)$$

$$C = f_C(V, m, s), \qquad p = V\rho - m - s \qquad (2c)$$

$$r_i = E(T)\, I := f_{r_i}(T, I), \qquad r_0 = f_0(T, V, m, I, s) \qquad (2d)$$

The *states* (x) are: the reactor (T) and jacket (T_j) temperatures, the volume (V), the free (i.e., unreacted) monomer (m), solvent (s) and initiator (I) masses, as well as the (number-average) MW inverse ($\iota = M_n^{-1}$) and its polydispersity (Q). The *measured exogenous inputs* (d) are: the reactor (T_e) and jacket (T_{je}) feed temperatures, and the solvent (q_s) volumetric flowrate. The *regulated outputs* (z) are: the temperature (T), the volume (V), the monomer content (m), and the MW inverse (ι). The *continuous-instantaneous measured outputs* (y_c) are: the temperature (y_T), the volume (y_V), and the jacket temperature (y_j). The *DD measured output* (y_d) is the MW inverse (y_ι). The *control inputs* (u) are: the coolant (q_j), exit (q) and monomer (q_m) volumetric flowrates, and the initiator mass feedrate (w_i). Δ_h is the heat of polymerization per unit monomer mass, W_m is the monomer molecular weight, ε_m is the monomer contraction factor, ρ_m (or c_m), ρ_s (or c_s) and ρ_j (or c_j) are the monomer, solvent and coolant fluid densities (or specific heat capacities), C and C_J are the reacting mixture and cooling system heat capacities, p is the polymer mass; U, ρ, r, r_i and r_0 are the heat transfer coefficient, the reacting mixture density and the rates of polymerization, initiator decomposition, and change of the zeroth moment (Hamer *et al.*, 1981), and E is the initiation rate constant.

Having as point of departure our previous studies on the reactor without MW measurements (González and Alvarez, 2005; Alvarez and González, 2006), our problem consists in: (i) designing the measurement-driven (MD) MW component with linearity, decentralization and reduced-model dependency features, (ii) the coordination of the MW component with the previously developed volume, temperature and conversion components, (iii) the capability of handling of low sampling rates and long delays, and (iv) drawing easy-to-apply tuning guidelines that include the sampling period-time delay.

3. MW CONTROL WITH CONTINUOUS MEASUREMENT

In this section, the MW control problem with continuous MW measurements is addressed. The objectives are: (i) the setting of a point of departure for the case with DD measurements, and (ii) the determination of the behavior recovery target for the DD-measurements control design.

3.1 Nonlinear FF-FB control

Let us re-write MW inverse (ι)-initiator (I) subsystem (1e-f) with the following modification: the initiator mass state (I) is replaced by the state ν that represents the rate of change of the MW inverse, this is,

$$\nu := \dot{\iota} = f_\iota(V, T, m, \iota, I, s) \qquad (3)$$

This coordinate change can be performed because f_ι is I-monotonic ($\partial_I f_\iota > 0$) (Alvarez and González, 2006), and physically speaking, the last inequality is fulfilled because the free-radical population increases with the initiator content (Flory, 1953), which causes that the MW decreases. Thus, the MW inverse (ι)-initiator (I) subsystem (1e-f) can be expressed into the phase canonical form (4) associated with a standard Hamiltonian mechanical formulation (Slotine and Li, 1991; Sepulchre *et al*., 1997)

$$\dot{\iota} = \nu, \qquad y(t) = \iota \tag{4a}$$

$$\begin{aligned}\dot{\nu} = &- \kappa_v(T, V, m, I, s, q)\, \nu \\ &- \kappa_\iota(T, T_j, V, m, I, s, q_s, T_e, q, q_m, w_i)\, \iota \\ &+ \alpha_\iota(T, V, m, s)\, w_i \\ &+ \theta_\iota(T, T_j, V, m, I, s, q_s, T_e, q, q_m, w_i)\end{aligned} \tag{4b}$$

$$\kappa_v = \lambda_r + \lambda_i > 0, \quad \lambda_r = r/p, \quad \lambda_i = E + \theta, \quad \theta = q/V$$

$$\kappa_\iota = \lambda_r\lambda_i > 0, \qquad \alpha_\iota = c_d\, E/p$$

$$\theta_\iota = c_d\, (\dot{E}/p)I + (\iota_t - \iota)\dot{\lambda}_r + \dot{\iota}_t\lambda_r + \lambda_r\lambda_i\iota_t$$

and ι_t (or c_d) is a chain transfer function (or initiation constant) (Alvarez and González, 2006). Introduce the Lyapunov function (5a) and enforce the negative dissipation rate (5b)

$$V_{SF} = (\kappa_\iota\tilde{\iota}^2 + \nu^2)/2 > 0, \qquad \tilde{\iota} = \iota - \bar{\iota} \tag{5a}$$

$$\dot{V}_{SF} = - (\kappa_v + k_v)\nu^2 < 0, \qquad k_v > 0 \tag{5b}$$

to obtain the *nonlinear FF-FB passive controller*

$$w_i = (1/\alpha_\iota)(\kappa_\iota\bar{\iota} - \theta_\iota - k_v\nu) \tag{6}$$

Observe that the implementation of this controller needs the detailed reactor model.

3.2 Linear output-feedback passive control

As a step to reduce the model dependency, let us re-write the MW control model (4) as follows

$$\dot{\iota} = \nu, \qquad y(t) = \iota \tag{7a}$$

$$\dot{\nu} = - c_v\, \nu - c_\iota\, \iota + a_\iota\, w_i + b_\iota \tag{7b}$$

$$b_\iota = \beta_\iota(T, T_j, V, m, \iota, \nu, I, s, q_s, T_e, q, q_m, w_i) \tag{7c}$$

$$c_v = \bar{r}/\bar{p} + \bar{E} + \bar{\theta} = 2\, \bar{\theta} + \bar{E}$$

$$c_\iota = (\bar{r}/\bar{p})(\bar{E} + \bar{\theta}) = (\bar{\theta})(\bar{E} + \bar{\theta}), \qquad a_\iota = c_d\, \bar{E}/\bar{p}$$

$$\beta_\iota = - (\kappa_v - c_v)\, \nu - (\kappa_\iota - c_\iota)\, \iota + (\alpha_\iota - a_\iota)\, w_i + \theta_\iota$$

where $(\bar{\cdot})$ denotes the steady-state approximation of $(\cdot)$, and b_ι is regarded as a nonlinear disturbance load generated by the nonlinear map β_ι. Equation (7a-b) [or (7c)] is a linear decentralized dynamic (or nonlinear interactive and static) component, and (7) is an (exact) representation of the MW model (4). Accordingly, the SF control (6) is written as follows

$$w_i = (1/a_\iota)(c_\iota\bar{\iota} - b_\iota - k_v\nu), \qquad b_\iota = \beta_\iota(x, d, u) \tag{8}$$

and the substitution of this controller in the MW dynamics yields the *closed-loop dynamics under SF control*:

$$\ddot{\tilde{\iota}} + (c_v + k_v)\, \dot{\tilde{\iota}} + c_\iota\tilde{\iota} = 0, \tag{9}$$

Due to the instantaneous observability property of system (7), the pair (ν, b_ι) can be reconstructed by means of a linear reduced-order observer (10a-b) (Stefani *et al*., 2001). The combination of this observer (10a-b) with the passive controller (8) yields the *linear output-feedback (OF) passive MW controller*:

$$\begin{aligned}\dot{\chi}_v = &- (c_v + \omega_1)\chi_v + \chi_b + [\omega_2 - \omega_1(c_v + \omega_1) - c_\iota]\, y_\iota \\ &+ a_\iota w_i, \qquad \hat{\nu} = \chi_v + \omega_1\, y_\iota\end{aligned} \tag{10a}$$

$$\dot{\chi}_b = - \omega_2\chi_v - \omega_1\omega_2 y_\iota, \qquad \hat{b}_\iota = \chi_b + \omega_2\, y_\iota \tag{10b}$$

$$w_i = (1/a_\iota)(c_\iota\bar{\iota} - \hat{b}_\iota - k_v\hat{\nu}) \tag{10c}$$

This linear MD dynamic controller recovers, with fast estimator convergence rate, the behavior of its exact model-based nonlinear passive counterpart (6), and constitutes the recovery target for its DD counterpart.

4. MW CONTROL WITH DISCRETE-DELAYED MEASUREMENT

In this section, a linear-decentralized output-feedback MW controller is constructed on the basis of DD MW measurements and a suitable discrete model, with reduced model-dependency.

4.1 Discrete MW model

Sometimes nonlinear chemical process and polymer reactor estimation and control problems are addressed on the basis of Euler-type discretization (Tatiraju *et al*., 1999; Niemiec *et al*., 2002). By doing so, the implementation is simplified at the cost of limiting the estimation and/or control capability to handle DD MW measurements. Given the linear form of our MW continuous model (7), the model prediction, or equivalently, the capability to handle measurement delay can be enhanced by performing an analytical integration of the model (7) with the enforcement of the step control specification $u(t) = u_k\ \forall\ t \in [t_k, t_{k+1}]$. The result is the following MW discrete model:

$$\iota_{k+1} = \gamma_{11}\, \iota_k + \gamma_{12}\, \nu_k + \beta_1(u_k + b_k), \quad u_k = a_\iota w_i(t_k) \tag{11a}$$

$$\nu_{k+1} = \gamma_{21}\, \iota_k + \gamma_{22}\, \nu_k + \beta_2(u_k + b_k) \tag{11b}$$

$$\gamma_{11} = [1 + (\bar{\theta}/\bar{E})(1-e^{-\Delta\bar{E}})]e^{-\Delta\bar{\theta}}, \quad \gamma_{12} = [(1-e^{-\Delta\bar{E}})e^{-\Delta\bar{\theta}}]/\bar{E}$$

$$\gamma_{21} = - \bar{\theta}[1+(\bar{\theta}/\bar{E})](1-e^{-\Delta\bar{E}})e^{-\Delta\bar{\theta}}$$

$$\gamma_{22} = [e^{-\Delta\, \bar{E}} + (\bar{\theta}/\bar{E})(1 - e^{-\Delta\, \bar{E}})]\, e^{-\Delta\, \bar{\theta}}$$

$$\beta_1 = - [1 - e^{-(\bar{\theta} + \bar{E})\Delta}]/[\bar{E}(\bar{\theta} + \bar{E})] + (1 - e^{-\Delta\bar{\theta}})/(\bar{\theta}\, \bar{E})$$

$$\beta_2 = [(1 - e^{-\Delta\bar{E}})\, e^{-\Delta\bar{\theta}}]/\bar{E}, \qquad \Delta = t_{k+1} - t_k$$

where Δ is the *sampling period-delay*, and the term b_k is reconstructible from the DD MW measurements. In input-output form, the discrete model (11) is expressed as:

$$\iota_{k+2} - \tau\iota_{k+1} + \delta\iota_k = \beta_1(u_{k+1}+b_{k+1}) + \beta_p(u_k+b_k) \quad (12)$$
$$\tau = \gamma_{11} + \gamma_{22},\quad \delta = \gamma_{11}\gamma_{22} - \gamma_{12}\gamma_{21},\quad \beta_p = \gamma_{12}\beta_2 - \gamma_{22}\beta_1$$

4.2 State-feedback control

Let us introduce the synthetic input μ, with feedforward (μ_k^*) and feedback ($\tilde{\mu}_k$) components:

$$\beta_1(u_{k+1}+b_{k+1})+\beta_p(u_k+b_k) := \mu_k,\quad \mu_k = \mu_k^* + \tilde{\mu}_k \quad (13)$$

Assume that the MW inverse (ι) is at its setpoint value ($\iota_{k+2} = \iota_{k+1} = \iota_k = \bar{\iota}$), and obtain the FF discrete component

$$\mu_k^* = (1 - \tau + \delta)\,\bar{\iota} \quad (14)$$

Enforce the following closed-loop output regulation error difference equation:

$$\tilde{\iota}_{k+2} - (\tau + k_1)\,\tilde{\iota}_{k+1} + (\delta + k_2)\,\tilde{\iota}_k = 0,\quad \tilde{\iota}_k = \iota_k - \bar{\iota} \quad (15)$$

and obtain the discrete FB component ($\tilde{\mu}_k$)

$$\tilde{\mu}_k = k_1\,\tilde{\iota}_{k+1} - k_2\,\tilde{\iota}_k \quad (16)$$

$$k_1(\Delta, \omega_c, \zeta_c) = -\tau + [\lambda_1(\Delta, \omega_c, \zeta_c) + \lambda_2(\Delta, \omega_c, \zeta_c)]$$
$$k_2(\Delta, \omega_c, \zeta_c) = -\delta + [\lambda_1(\Delta, \omega_c, \zeta_c)\,\lambda_2(\Delta, \omega_c, \zeta_c)]$$
$$\lambda_n(\Delta, \omega_c, \zeta_c) = \exp\{-\Delta\omega_c\,[\zeta_c \pm (\zeta_c^2 - 1)^{1/2}]\},\ n = 1, 2$$

ω_c (or ζ_c) is the control characteristic frequency (or damping factor) associated to the mappings of the control design poles from the continuous representation in the LHS of the complex plane to the unit circle (Hernández and Alvarez, 2003). The combination of (13), (14) and (16) yields the *discrete MW SF controller*

$$w_i(t_k) = -(\beta_p/\beta_1)w_i(t_{k-1}) - [b_k + (\beta_p/\beta_1)b_{k-1}]/a_\iota$$
$$+ [(1-\tau+\delta)/\beta_1]\bar{\iota}/a_\iota + [k_1(\iota_k-\bar{\iota}) - k_2(\iota_{k-1}-\bar{\iota})]/(a_\iota\beta_1) \quad (17)$$

In eq. (17): (i) the first term is an integral-like action due to discretization, (ii) the first three terms represent feedforward action, on the basis of present and past load estimates, and (iii) the last term is a feedback correction driven by present (ι_k) and past (ι_{k-1}) values of the MW inverse.

4.3 Output-feedback control

The implementation of the discrete controller (17) needs present and past estimates of the MW inverse. For the continuous measurements case, the state estimation can be adequately performed with a reduced order observer (10a-b), but this is not convenient for the discrete-measurements case. A reduced-order discrete observer yields present estimates (ι_k) from an open-loop (i. e., without correction) difference equation (Ogata, 1994), but this estimate can degrade the controller performance. Thus, the application of the full-order discrete observer technique yields the state observer (18a-c), and its combination with the discrete controller (17) yields the *discrete MW OF controller*:

$$\hat{\iota}_k = \gamma_{11}\hat{\iota}_{k-1} + \gamma_{12}\hat{v}_{k-1} + \beta_1(u_{k-1}+\hat{b}_{k-1}) + k_1^o(\Delta,\omega_o,\zeta_o)(y_k - \hat{\iota}_{k-1})$$
$$\hat{v}_k = \gamma_{21}\hat{\iota}_{k-1} + \gamma_{22}\hat{v}_{k-1} + \beta_2(u_{k-1}+\hat{b}_{k-1}) + k_2^o(\Delta,\omega_o,\zeta_o)(y_k - \hat{\iota}_{k-1})$$
$$\hat{b}_k = \hat{b}_{k-1} + k_3^o(\Delta,\omega_o,\zeta_o)(y_k - \hat{\iota}_k),\quad u_k = a_\iota w_i(t_k) \quad \text{(18a-c)}$$
$$w_i(t_k) = -(\beta_p/\beta_1)w_i(t_{k-1}) - [\hat{b}_k + (\beta_p/\beta_1)\hat{b}_{k-1}]/a_\iota$$
$$+ [(1 - \tau + \delta)/\beta_1]\bar{\iota}/a_\iota$$
$$+ [k_1(\hat{\iota}_k - \bar{\iota}) - k_2(\hat{\iota}_{k-1} - \bar{\iota})]/(a_\iota\,\beta_1) \quad \text{(18d)}$$

where the observer gains (k_1^o, k_2^o, k_3^o) are set according to a root locus-based pole pattern (Hernández and Alvarez, 2003), and ω_o (or ζ_o) is the observer characteristic frequency (or damping factor). The combination of the MW OF controller (18) with the volume, temperature and monomer controllers presented in a previous study (Alvarez and González, 2006) yields the entire OF reactor control scheme:

• *Volume and temperature controllers* (19a)

$$\dot{\chi}_V = -\omega_V\chi_V - \omega_V(\omega_V y_V - q),\qquad \hat{b}_V = \chi_V + \omega_V y_V$$
$$q = \hat{b}_V + k_V(y_V - \bar{V})$$
$$\dot{\chi}_T = -\omega_T\chi_T - \omega_T(\omega_T y_T + a_T y_j),\qquad \hat{b}_T = \chi_T + \omega_T y_T$$
$$T_j^* = -[\hat{b}_T + k_T(y_T - \bar{T})]/a_T$$
$$\dot{\chi}_j = -\omega_j\chi_j - \omega_j(\omega_j y_j + a_j q_j),\qquad \hat{b}_j = \chi_j + \omega_j y_j$$
$$\dot{\chi}_j^* = -\omega_j^*\chi_j^* - \omega_j^*(\omega_j^* T_j^*),\qquad \hat{b}_j^* = \chi_j^* + \omega_j^* T_j^*$$
$$q_j = [\hat{b}_j^* - \hat{b}_j - k_j(y_j - T_j^*)]/a_j$$

• *Monomer controller* (19b)

$$\dot{\hat{m}} = -\hat{r} + \rho_m q_m - (\hat{m}/y_V)\,q,\qquad \dot{\hat{s}} = \rho_s q_s - (\hat{s}/\hat{V})\,q$$
$$\hat{r} = [f_C(y_V,\hat{m},\hat{s})(a_T y_j + \hat{b}_T) + C_J\hat{b}_j]/\Delta$$
$$q_m = [-k_m(\hat{m} - \bar{m}) + \hat{r} + (\hat{m}/y_V)\,q]/\rho_m$$

• *MW controller* (19c)

$$\hat{\iota}_k = \gamma_{11}\hat{\iota}_{k-1} + \gamma_{12}\hat{v}_{k-1} + \beta_1(u_{k-1} + \hat{b}_{k-1}) + k_1^o(y_k - \hat{\iota}_{k-1})$$
$$\hat{v}_k = \gamma_{21}\hat{\iota}_{k-1} + \gamma_{22}\hat{v}_{k-1} + \beta_2(u_{k-1} + \hat{b}_{k-1}) + k_2^o(y_k - \hat{\iota}_{k-1})$$
$$\hat{b}_k = \hat{b}_{k-1} + k_3^o(y_k - \hat{\iota}_k),\qquad u_{k-1} = a_\iota w_i(t_{k-1})$$
$$w_i(t_k) = -(\beta_p/\beta_1)w_i(t_{k-1}) - [\hat{b}_k + (\beta_p/\beta_1)\hat{b}_{k-1}]/a_\iota$$
$$+ [(1-\tau+\delta)/\beta_1]\bar{\iota}/a_\iota + [k_1(\hat{\iota}_k-\bar{\iota}) - k_2(\hat{\iota}_{k-1} - \bar{\iota})]/(a_\iota\,\beta_1)$$

The MW OF controller (19c) amounts to an interlaced estimator-control design, with a second-order SF controller and a third-order discrete observer, and in principle, the analytic solution-based discrete model (11) has better prediction capability than Euler's discretization-based counterparts. Regarded as an individual loop, the preceding MW component, based on a linear input-output model, is considerably simpler than nonlinear sampled-data full-model based estimator-control systems.

4.4 Implementation and tuning

Modeling requirements. The MW controller only needs the approximate constants $\{a_\iota, c_\iota, c_v\}$ (7), or equivalently, the nominal residence time inverse ($\bar{\theta}$) and steady-state approximations of the initiation constant (E) and polymer mass (f_p) functions. The modeling requirements of the volume, temperature and monomer loops (19a-b) are: two steady-state approximated constants (a_T, a_j) for the temperature loop, and calorimetric parameters (densities and heat capacities) for the monomer loop. These modeling requirements are fewer than the ones of previous polymer reactor control studies with MW measurements (Adebekun and Schork, 1989; Ellis *et al*., 1994; Niemiec *et al*., 2002).

Closed-loop dynamics and tuning. The rigorous assessment of the robust closed-loop behavior goes beyond the scope of the present work, and here it suffices to recall previous stability assessments on the same kind of reactor with sampled density measurements (Hernández and Alvarez, 2003) and on the same reactor without MW measurements (González and Alvarez, 2005), to say that, in the present problem, closed-loop stability can be attained by setting the volume, temperature and monomer controllers and then: (i) choosing the observer gain (ω_o) within an interval (ω_o^-, ω_o^+), that depends on the sampling period-delay (Δ), and (ii) setting the control parameter (ω_c) sufficiently smaller than ω_o. The associated tuning guidelines are:

1. Set the MW observer characteristic time ($\tau_o = 1/\omega_o$) three times greater than the MW measurement delay (Δ): $\tau_o = 3\Delta$, and the MW controller characteristic time ($\tau_c = 1/\omega_c$) two times slower than the observer characteristic time: $\tau_c = 2\ \tau_o$.
2. Choose the damping factors greater than one, say (ζ_o, ζ_c) $\in$ (1, 3], to preclude the amplification of the high-frequency unmodeled dynamics (López and Alvarez, 2004).
3. Decrease the observer characteristic time (τ_o) up to its ultimate value τ_o^u, where the response becomes oscillatory, and backoff until a satisfactory response is attained, say at $\tau_o \geq 2\ \tau_o^u$.
4. If necessary, adjust the damping (ζ_o, ζ_c) factors and/or controller characteristic time (τ_c).

In this manner, the MW controller (19c) is set according to prescribed root locus-based pole patterns (inside the unit circle) determined by the damping factors (ζ_o, ζ_c), and the characteristic frequencies (ω_o, ω_c) are the main adjustable parameters.

5. APPLICATION EXAMPLE

To subject the proposed OF controller (19) to a severe test, the operation of a reactor about an open-loop unstable steady-state is considered (via numerical simulations), at high-solid fraction with the potentially destabilizing gel-effect at play. The system is methyl methacrylate (monomer)-ethyl acetate (solvent)-AIBN (initiator). The residence time is $(1/\bar{\theta})$ = 220 minutes with a nominal volume $\bar{V} \approx$ 2000 L. The operating conditions have been given before (González and Alvarez, 2005). The reactor has three steady states $\bar{x}$ = [$\bar{T}$(K), $\bar{m}$(Kg), $\bar{M}_n$ (Kg/Kmol)]':

$\bar{x}_1$:	(373.88, 312.7, 29395.15)'	(Stable)
$\bar{x}_2$:	(351.62, 660.1, 110384.75)'	(Unstable)
$\bar{x}_3$:	(329.72, 1361.1, 399149.03)'	(Stable)

with the unstable steady-state being the setpoint, and the closed-loop reactor-control system was subjected to step changes in the reactor and jacket feed temperatures step changes shown in Figure 1 (at t = 100 min: T_e from 315 to 320 K, and T_{je} from 328 to 330 K). Two sampling periods-delays were tested: (i) Δ = 5 min, to evaluate the recovery target towards the continuous MW measurements case (10), and (ii) Δ = 90 min, in accordance to previous polymer reactor control studies (Niemiec *et al*., 2002) where the long sampling period-delay is about one half of the nominal residence time. Following the tuning guidelines of section 4 and the ones from (Alvarez and González, 2006), the MW control gains were set as follows:

Δ = 5 min,	$\zeta_o = 3$,	$\omega_o = (1/10)\ \text{min}^{-1}$
	$\zeta_c = 1.5$,	$\omega_c = (1/100)\ \text{min}^{-1}$
Δ = 90 min,	$\zeta_o = 1$,	$\omega_o = (1/90)\ \text{min}^{-1}$
	$\zeta_c = 0.71$,	$\omega_c = (1/140)\ \text{min}^{-1}$

In Fig. 1, three closed-loop responses are shown with (i) the OF controller (19a-b) with continuous MW component (10), (ii) the proposed OF controller (19) with DD MW measurements and Δ = 5 min, and (iii) the proposed OF controller (19) with DD MW measurements and Δ = 90 min. As it can be seen in the figure: (i) the behavior of the discrete controller with small sampling period-delay (Δ = 5 min) approaches the behavior of the controller with continuous MW measurements, and (ii) the discrete controller with long sampling period-delay (Δ = 90 min) regulates the MW in about 380 minutes (1.7 residence times). In terms of natural residence time units, the proposed MW controller with Δ = 90 min (about 1 half of the residence time) regulates the MW with similar convergence time than the ones obtained with full-model - based and appropriately tuned control schemes (Niemiec *et al*., 2002). In other words, the proposed MW control scheme can perform the same task with less modeling requirements and more robustness with respect to model uncertainty.

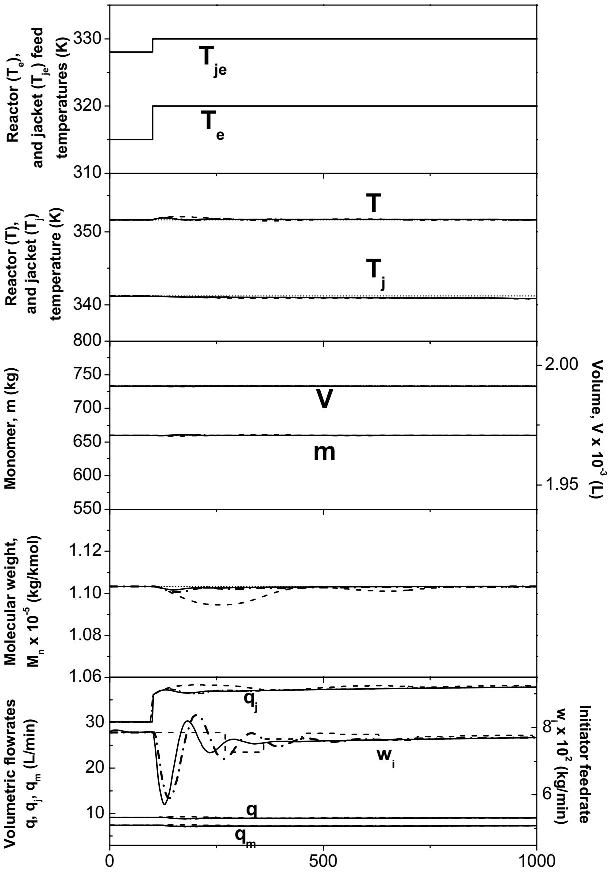

Fig. 1. Reactor behavior with the OF control with continuous MW measurements (—), and DD MW measurements with $\Delta = 5$ min (- · - · -) and $\Delta = 90$ min (- - -), and setpoints (····).

On the other hand, the regulation of the volume, temperature and monomer is not affected by the MW loop, meaning that the control of the last output is performed in a coordinated way with linear decentralized volume, temperature and conversion components. It must be pointed out that controlling these four outputs is an indirect way of attenuating transient polydispersity excursions, with the understanding that its steady-state value is fixed (at 2) and cannot be changed (Flory, 1953).

6. CONCLUSIONS

The control of continuous free-radical solution polymer reactors with continuous measurements of temperature, level and flows, and discrete-delayed measurements of molecular weight (MW) has been addressed within a constructive control framework, with emphasis in the attainment of applicability-oriented features (linearity, decentralization, and reduced-model dependency). The MW component was drawn by combining passivity, discrete model realization, and controllability-detectability considerations. The proposed control technique has a systematic construction and simple tuning guidelines, and its implementation in an open-loop unstable industrial-size case study showed that the proposed controller yields: (i) closed-loop stable dynamics, and (ii) an MW response with convergence time that is similar to the ones obtained earlier with detailed model-based nonlinear controllers.

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