NONLINEAR CONTROL OF CONTINUOUS POLYMER REACTORS VIA PASSIVATION

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Abstract: A nonlinear passive control to stabilize continuous free-radical solution polymer reactors is presented, with temperature, level and flow measurements. First, the state-feedback problem is addressed with a constructive control framework via passivation by backstepping, yielding the solvability conditions and the attainable closed-loop behavior, or the recovery target for the output-feedback (OF) design. The resulting OF control consists of volume and cascade temperature controllers, a ratio-type monomer controller, and an inventory-type MW controller. The temperature and monomer control components do not need polymerization kinetics and heat transfer models. The MW controller component only requires initiation and transfer rate constants. The proposed control technique has a systematic construction and a simple tuning scheme, and is tested with an industrial size reactor via simulations.

Keywords: Polymerization reactor control, nonlinear geometric control, chemical process control, feedback control, material balance control, continuous process control.

1. INTRODUCTION

Motivated by the need of designing processes with better compromises between safety, productivity, and quality, and by the development of nonlinear control methods, in the last two decades the polymerization reactor problem has been the subject of extensive theoretical, simulation and experimental studies. The related state of the art can be seen elsewhere (Congalidis and Richards, 1998), and here it suffices to mention that: (i) only parts of the overall multi-input multi-output (MIMO) control problem have been addressed, (ii) a diversity of control techniques have been employed, including linear PI decoupling (Padilla and Alvarez, 1997) and model predictive (MPC) (Maner and Doyle, 1997) as well as nonlinear geometric (Daoutidis et al., 1990; Soroush and Kravaris, 1993; Alvarez et al., 1994; Alvarez, 1996; Gauthier and Kupka, 2001), MPC (Mutha et al., 1997), and calorimetric (Alvarez et al., 2004) control techniques, and (iii) the nonlinear controllers have been implemented with open-loop (Soroush and Kravaris, 1993), extended Kalman filter (EKF) (Mutha et al, 1997), and Luenberguer (Alvarez, 1996; Gauthier and Kupka, 2001) nonlinear observers. Eventhough valuable insight has been gained in the understanding of the complex polymer reactor control problem, the resulting nonlinear controllers are strongly interactive and model dependent, and these features signify complexity and reliability drawbacks for their applicability. In particular, the temperature and MW feedback regulation schemes with heat exchange, monomer feed, and initiator (and/or chain transfer agent) dosage rates as control inputs have been underlain by non-passive controllers with second-order relative degrees (RD), and this is an obstacle for control robustness (Sepulchre et al., 1997).

These observations rise the issue that constitutes the motivation of the present work: the design of a passive controller to regulate a (possibly open-loop unstable) polymerization reactor, on the basis of level, temperature and flow measurements in conjunction with mass and energy balances, in the understanding that controller must perform the stabilization task without needing the (typically

uncertain) polymerization kinetics and heat transfer models.

In this work the problem is addressed via passivation. First, the state-feedback (SF) problem is studied, identifying the solvability conditions with physical meaning, and establishing that the problem is not solvable with static feedback, but with a non-passive dynamic controller with RD equal to two. To remove this high RD obstacle for robustness, a backstepping approach (Sepulchre et al., 1997; Alvarez et al., 2004) is employed to passivate the SF controller and design its observer-based counterpart. The result is an OF scheme made by the combination of: volume and cascade temperature controllers, a ratio-type monomer dosage controller, and an inventory-type MW controller. The component that ensures the stability of the reactor, does not need polymerization kinetics and heat exchange models, and the component that regulates the MW only needs initiation and transfer rate constants. The proposed approach is tested with an industrial size reactor through numerical simulations.

2. REACTOR CONTROL PROBLEM

Consider the class of continuous stirred-tank reactors 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; Padilla and Alvarez, 1997). From standard free-radical polymerization kinetics (Hamer et al., 1981), and viscous heat exchange considerations (Alvarez et al., 1994; Padilla and Alvarez, 1997), the following energy and material balances describe the reactor dynamics:

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

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

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

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

$$\dot{\pi} = (r - \pi r_0)\pi/(V\rho - m - s) := f_\pi \qquad z_\pi = \pi \quad (1e)$$

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

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

$$\dot{\mu}_2 = r_2 - (\mu_2/V) q := f_{\mu 2} \quad (1h)$$

$$u_j = q_j, \; u_V = q, \; u_m = q_m, \; u_i = w_i$$

where:

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

$$U = f_U(T, T_j, V, m, s), \qquad H = U(T - T_j) \quad (2b)$$

$$C = f_C(V, m, s), \qquad \rho = f_\rho(V, m, s) \quad (2c)$$

$$r_i = f_{ri}(T, I), \quad (r_0, r_2)' = (f_0, f_2)'(T, V, m, I, s) \quad (2d, e)$$

$$\varpi_s = (V\rho - m - s)/V\rho \quad (3a)$$

$$c = (V\rho - m - s)/(V\rho - s) \quad (3b)$$

$$\theta = W_m \mu_2/[(V\rho - m - s)\pi] \quad (3c)$$

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) molecular weight (π) and second moment (μ_2) of the MW distribution. 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 (number-average) molecular weight (π). The *measured outputs* (y) are: the temperature (y_T), the volume (y_V), and the jacket temperature (y_j). The *control inputs* (u) are: the coolant volumetric flowrate (q_j) through the jacket circuit, the exit flowrate (q), the monomer flowrate (q_m) and the initiator mass feedrate (w_i). From a practical viewpoint, one is interested in looking and (indirectly) controlling the conversion (c), the solid fraction (ϖ_s), and the MW polydispersity (θ).

Δ 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; U, ρ, r, r_i, r_0, and r_2 are the heat transfer coefficient, the reacting mixture density and the rates of polymerization, initiator decomposition, and change of the zeroth and second moments (Hamer et al., 1981). The moment rates r_0 and r_2 can be expressed in terms of initiation and monomer and solvent transfer rates (Flory, 1953).

In vector notation, the reactor model (1) is given by:

$$\dot{x} = f(x, d, u), \qquad y = C_y x, \qquad z = C_z x \quad (4)$$

where:

$$x = (T, T_j, V, m, \pi, I, s, \mu_2)'$$
$$f = (f_T, f_j, f_V, f_m, f_\pi, f_i, f_s, f_2)'$$
$$d = (T_e, T_{je}, q_s)', \; y = (y_T, y_j, y_V)'$$
$$u = (q_j, q, q_m, w_i)', \; z = (z_T, z_V, z_m, z_\pi)' \quad (5)$$

Our problem consists in designing a robust controller that, driven by the measurements (y and d), regulates the reactor operation about a (possibly open-loop unstable) nominal steady state $\bar{x}$. For applicability purposes, the control design should minimize the dependency on the kinetics and heat transfer model functions (2), especially for the components which perform the stabilizing task.

3. NONLINEAR STATE-FEEDBACK CONTROL

In this section the nonlinear SF control problem is addressed under the assumption that the states and exact reactor model are known and available for control. The purpose is two-fold: to identify the solvability conditions and the attainable closed-loop behavior, or equivalently, the recovery target of the proposed OF controller.

3.1 Passivation

Following the approach employed in previous polymer reactors control studies (Daoutidis et al., 1990; Soroush and Kravaris, 1993; Alvarez et al., 1994; Alvarez, 1996; Gauthier and Kupka, 2001; Alvarez et al., 2004), the direct application of the standard geometric control method (Isidori, 1995) leads to the conclusion that the control problem is solvable with RD equal to two and dynamic extension for the monomer feed (q_m) and exit (q) flow controls:

$$(\kappa_T, \kappa_V, \kappa_m, \kappa_\pi) = (2, 2, 2, 2)$$
$$\dot{x} = f(x_a, d, \upsilon),\ \dot{q} = u_q,\ \dot{q}_m = u_{qm} \qquad (6)$$
$$x_a = (x', q, q_m)',\ u = (q_j, w_i, u_q, u_{qm})'$$

provided that the zero-dynamics (presented in the next subsection) are stable, and that the RD conditions are met:

$$f_U > (T_j - T)\partial_{T_j} f_U \qquad (7a)$$
$$V f_\rho > m + s, \qquad \partial_I f_r > \pi\, \partial_I f_0 \qquad (7b, c)$$

meaning that the construction of the related SF controller requires partial derivatives of the (typically uncertain) model functions (f_r, f_U, f_0). To remove this obstacle for robustness, let us apply the passivation scheme via backstepping employed in the constructive control design (Sepulchre et al., 1997) according to the physically-drawn rationale:

(i) As it is done in the industrial design of cascade temperature controllers for jacketed reactors (Alvarez-Ramírez et al., 2002; Alvarez et al., 2004), regard the measured (y_j) jacket temperature state (T_j) as a virtual control ($T_j = T_j^*$) to decompose the second-order RD coolant flow(q_j)-to-temperature(z_T) path into the series interconnection of two first-order RD paths: the coolant flow(q_j)-to-jacket temperature(T_j) path, and the jacket temperature(T_j)-to-reactor temperature(z_T) path.

(ii) In a similar manner, regard the initiator state (I) as a virtual control ($I = I^*$) to decompose the second-order RD initiator feedrate(w_i)-to-MW(z_π) path into the series interconnection of two first-order RD paths: the initiator feedrate(w_i)-to-initiator(I) path, and the initiator(I)-to-MW(z_π) path.

3.2 Passive controller and zero-dynamics

Recall (1a) [or (1e)], regard its state T_j (or I) as a primary or virtual control T_j^* (or I^*), enforce the primary closed-loop LNPA (linear, noninteractive, pole assignable) regulation dynamics for the temperature, volume, free-monomer and MW

$$\dot{T} = -k_T(T - \bar{z}_T), \qquad \dot{V} = -k_V(V - \bar{z}_V)$$
$$\dot{m} = -k_m(m - \bar{z}_m), , \qquad \dot{\pi} = -k_\pi(\pi - \bar{z}_\pi)$$

and solve the equation set (1a, c, d, e) for (T_j^*, q, q_m, I^*) to obtain the *primary SF controller*:

$$T_j^* = T - [f_C(x)k_T(T - \bar{z}_T) + \Delta f_r(x) + (\rho_m q_m c_m + \rho_s q_s c_s)(T_e - T)]/f_U(x) := \gamma_j^*(x, d) \qquad (8a)$$
$$q = [-k_m(m - \bar{z}_m) + \rho_m k_V(V - \bar{z}_V) + (1 - \varepsilon_m) f_r(x) + \rho_m q_s]/(\rho_m - m/V) := \gamma_V(x, d) \qquad (8b)$$
$$q_m = [-k_m(m - \bar{z}_m) + f_r(x) + (m/V)q]/\rho_m := \gamma_m(x, d) \qquad (8c)$$
$$I^* = f_\pi^{-1}[T, V, m, \pi, s, -k_\pi(\pi - \bar{z}_\pi)] := \gamma_i^*(x) \qquad (8d)$$

where T_j^* (or I^*) is the jacket temperature (or initiator) time-varying setpoint, and its time derivative is given by

$$\dot{T}_j^* = (\partial_x \gamma_j^*) f + (\partial_d \gamma_j^*) \dot{d}, \qquad \dot{I}^* = (\partial_x \gamma_i^*) f \qquad (9a,b)$$

Enforce the secondary closed-loop LNPA tracking dynamics for the jacket temperature and initiator mass

$$\dot{T}_j = \dot{T}_j^* - k_j(T_j - T_j^*), \qquad \dot{I} = \dot{I}^* - k_i(I - I^*)$$

and solve the equation set (1b, f) for (q_j, w_i) to obtain the *secondary SF controller*:

$$q_j = \{C_J[\dot{T}_j^* - k_j(T_j - T_j^*)] - f_U(x)(T - T_j)\} / [\rho_j c_j (T_{je} - T_j)] \qquad (10a)$$
$$w_i = \dot{I}^* - k_i(I - I^*) + f_{ri}(T, I) + (I/V)\, q \qquad (10b)$$

The application of the preceding *cascade SF controller* (8, 10) to the reactor (1) with the restriction $z = \bar{z}$, yields the reactor *zero-dynamics*:

$$\dot{x}_{II} = f_{II}(x_{II}, d), \qquad x_{II}(0) = x_{IIo} \qquad (11)$$
$$x_{II} = (s, \mu_2)'$$
$$f_{II}(x_{II}, d) = (f_s, f_{\mu 2})'(\bar{T}, \bar{V}, \bar{m}, I^*, s, \mu_2, q_s\, q)$$
$$I^* = \gamma_i^*(\bar{T}, \bar{V}, \bar{m}, \bar{\pi}, s),\ q = \gamma_V(\bar{T}, \bar{V}, \bar{m}, I^*, s)$$

3.3 Solvability assessment

According to the preceding developments the non-passive dynamic (discussed in subsection 3.1) and the passive static reactor SF control problems are

solvable due to the fulfillment of the following conditions:

i) The reactor has RD = 2 because there is heat exchange via the diathermal wall (7a), there is converted monomer (7b), and the MW balance (1e) is met with a unique initiator content I (7c), or equivalently, there is a one-to-one correspondence between the live polymer chain and the initiator concentrations (Flory, 1953).
ii) The reactor is a minimum phase process, or equivalently, its zero-dynamics (11) has a unique steady-state $\bar{x}_{II}$ which is asymptotically stable. This condition is met because fixing the reactor temperature, volume and monomer content at their nominal values implies that the instability by gel effect (Alvarez et al., 1994) is precluded.

As expected (Sepulchre et al., 1997), the backstepping treatment introduces intermediate virtual controls and differentiators (9), whose analytic representation requires the partial derivatives of the kinetics (f_r, f_0) and heat exchange (f_U) nonlinear functions. The partial derivatives grouped into the differentiators mean a simplification in the cascade control scheme. As we shall see in the next section, the estimation of the time derivatives (9) via linear filters will considerable simplify and robustify the controller design by avoiding the need of the partial derivative computation.

4. OUTPUT-FEEDBACK CONTROL

From the application (Alvarez et al., 2004) of the PI geometric estimator technique (López and Alvarez, 2004), the heat generation (Q) and the heat exchange (H) rates (2a, b) can be estimated from the reactor and jacket temperatures measurements (y_T, y_j) in conjunction with the energy balances (1a, b). This signifies that in the reactor model (1), the kinetics [$r = f_r$ in (2a)] and heat transfer rate [$U(T - T_j)$ in (2b)] model equations can be replaced by the augmented dynamical states Q and H,

$$\dot{Q} \approx 0, \quad \dot{H} \approx 0 \tag{12}$$

implying that a passive (in the paths Q-y_T and H-y_j) state observer can be designed and coordinated with the passive controller (8, 10).

4.1 Measurement-driven cascade controller.

The combination of the state estimator (13a) with the controller (8, 10) expressed (13b, c) in terms of the estimator states, yields the *OF controller* in Internal Model Control (IMC) form:

Estimator (13a)

$$\dot{\hat{T}} = [\hat{Q} - \hat{H} + (\rho_m q_m c_m + \rho_s q_s c_s)(T_e - \hat{T})]/f_C(\hat{V}, \hat{m}, \hat{s}) + 2\zeta\omega(y_T - \hat{T})$$

$$\dot{\hat{T}}_j = \{\hat{H} + \rho_j q_j c_j(T_{je} - \hat{T}_j)\}/C_J + 2\zeta\omega(y_j - \hat{T}_j)$$

$$\dot{\hat{Q}} = \omega^2[C_J(y_j - \hat{T}_j) + f_C(\hat{V}, \hat{m}, \hat{s})(y_T - \hat{T})]$$

$$\dot{\hat{H}} = \omega^2 C_J(y_j - \hat{T}_j)$$

$$\dot{\hat{V}} = q_m + q_s - (\varepsilon_m/\rho_m)\,\hat{Q}/\Delta - q + \omega(y_V - \hat{V})$$

$$\dot{\hat{m}} = -\,\hat{Q}/\Delta + \rho_m q_m - (\hat{m}/\hat{V})\,q$$

$$\dot{\hat{\pi}} = [\hat{Q}/\Delta - \hat{\pi}\, f_0(\hat{T}, \hat{V}, \hat{m}, \hat{I}, \hat{s})]\hat{\pi}/(\hat{V}\, f_\rho(\hat{V}, \hat{m}, \hat{s}) - \hat{m} - \hat{s})$$

$$\dot{\hat{I}} = -\,f_{ri}(\hat{T}, \hat{I}) + w_i - (\hat{I}/\hat{V})\,q, \qquad \dot{\hat{s}} = \rho_s q_s - (\hat{s}/\hat{V})\,q$$

$$\dot{\hat{T}}_j^* = \hat{v}_j^* + 2\zeta\omega(T_j^* - \hat{T}_j^*), \qquad \dot{\hat{v}}_j^* = \omega^2(T_j^* - \hat{T}_j^*)$$

$$\dot{\hat{I}}^* = \hat{v}_i^* + 2\zeta\omega(I^* - \hat{I}^*), \qquad \dot{\hat{v}}_i^* = \omega^2(I^* - \hat{I}^*)$$

Primary controller (13b)

$$T_j^* = \hat{T} - (H^*/\hat{H})(\hat{T} - \hat{T}_j)$$

$$H^* = \hat{Q} + (\rho_m q_m c_m + \rho_s q_s c_s)(T_e - \hat{T}) + f_C(\hat{V}, \hat{m}, \hat{s})\, k_T(\hat{T} - \bar{z}_T)$$

$$q = [-\,k_m(\hat{m} - \bar{z}_m) + \rho_m k_V(\hat{V} - \bar{z}_V) + (1 - \varepsilon_m)\,\hat{Q}/\Delta + \rho_m q_s]/(\rho_m - \hat{m}/\hat{V})$$

$$q_m = [-\,k_m(\hat{m} - \bar{z}_m) + \hat{Q}/\Delta + (\hat{m}/\hat{V})\,q]/\rho_m$$

$$I^* = f_\pi^{-1}[\hat{T}, \hat{Q}, \hat{V}, \hat{m}, \hat{\pi}, \hat{s}, -\,k_\pi(\hat{\pi} - \bar{z}_\pi)]$$

Secondary controller (13c)

$$q_j = \{C_J[\hat{v}_j^* - k_j(\hat{T}_j - \hat{T}_j^*)] - \hat{H}\}/[\rho_j c_j(T_{je} - \hat{T}_j)]$$

$$w_i = \hat{v}_i^* - k_i(\hat{I} - \hat{I}^*) + f_{ri}(\hat{T}, \hat{I}) + (\hat{I}/\hat{V})\,q$$

This controller consists of components that resemble control and feedforward schemes employed in industrial practice (Shinskey, 1988; Alvarez et al., 2004): (i) volume and cascade temperature controllers that manipulate the exit flow q and the coolant flow q_j, (ii) a ratio-type free monomer controller that sets q_m proportionally to the heat generation rate $\hat{Q}$, and (iii) an inventory-type MW controller that sets w_i proportionally to the estimated MW and material balances.

Model dependency. Since: (i) the function pair (f_r, f_U) was replaced by the estimate ($\hat{Q}$, $\hat{H}$), and (ii) the pair ($\dot{T}_j^*$, $\dot{I}^*$) (whose analytic computation require the partial derivatives of f_r, f_U and f_0) was replaced by the estimate ($\hat{v}_j^*$, $\hat{v}_i^*$) drawn from a standard (T_j^*, I^*)-driven linear filter, the modeling requirements of the OF controller (13) are considerably smaller than the ones of the observer-based nonlinear controllers employed in previous polymer reactor studies (Soroush and Kravaris, 1993; Alvarez, 1996; Gauthier and Kupka, 2001). Here, (i) the stabilizing component that regulates the temperature, volume and free monomer by manipulating (q_j, q, q_m) only requires mass-heat capacity and thermodynamic

parameters (2c), and (ii) the component that regulates the MW by manipulating w_i, requires initiation and transfer constants (2d, e). In general, the mass-heat capacity and thermodynamic parameters are less uncertain than the ones of the kinetic rates, meaning that the critical stabilization task for safety and operability purposes should be rather robust, and that the regulation of the MW for product quality purposes should not affect the stabilization function.

Convergence and tuning: The formal consideration of the closed-loop stability issue goes beyond the scope of the present work, and here it suffices to mention that the application of the existing tools for the stability assessment of nonlinear controllers with high-gain observers (Alvarez, 1996) and of nonlinear high-gain calorimetric observers (Alvarez et al., 2004) leads to the following results: The observer gain (ω) should not be set faster than the dominant frequency (ω_J) of the jacket dynamics, the secondary (k_j) and primary (k_V, k_T) control gains, as well as the initiator gain k_i, should set sufficiently separated and slower than the one (ω) of the observer, and the ratio control gains (k_m, k_π) should set equal to the inverse of the residence time (τ_R) (i.e., smaller than k_j):

$$k_T, k_i < k_V, k_j < \omega \le \omega_J = (\bar{U} + \rho_j \bar{q}_j c_j)/C_J$$
$$k_m, k_\pi \approx 1/\tau_R$$

This tuning should yield a closed-loop stable reactor with non-wasteful control inputs, and with the following features: (i) The measured volume and temperature are regulated asymptotically with almost linear error dynamics and convergence rate fixed by the designer, and (ii) the unmeasured monomer and MW are regulated asymptotically with convergence rate fixed by the reactor residence time.

5. APPLICATION EXAMPLE

To subject the controller to a severe test, let us consider an extreme case of an industrial situation: the operation of a reactor at high-solid fraction with the potentially destabilizing gel-effect at play, about a nominal steady-state which is open-loop unstable. The monomer is methyl methacrylate, with ethyl acetate (solvent) and AIBN (initiator). The residence time is τ_R = 220 minutes and nominal volume $\bar{z}_V \approx$ 2000 L. The functionalities and parameter values were taken and/or adapted from Alvarez et al. (1994), and the nominal inputs were adapted from a previous solution copolymer reactor study (López and Alvarez, 2004). The reactor has three steady states $\bar{x}_i = [\bar{T}$ (K), $\bar{c}$, $\bar{\varpi}_s$, $\bar{\pi}$ (Kg/Kmol), $\bar{\theta}]$':

$\bar{x}_1$: (373.88, 0.7954, 0.5997, 29395.15, 1.9966)'

$\bar{x}_2$: (351.62, 0.5672, 0.4269, 110384.75, 1.999)'

$\bar{x}_3$: (329.72, 0.1072, 0.08066, 399149.03, 1.9997)'

The first ($\bar{x}_1$) and third ($\bar{x}_3$) steady states correspond to ignition and extinction stable operations, and the second steady-state, which is unstable, was chosen as the nominal operating point of the control scheme. Following the tuning guidelines discussed in section 4, the observer and control gains were set as follows:

$\zeta = 0.71$, $\omega = \omega_J = (1/5)$ min^{-1}, $k_j = k_V = \omega/8$
$k_T = 2/\tau_R$, $k_i = 4/(3\tau_R)$, $k_m = k_\pi = 1/\tau_R$

The observer damping factor (ζ) was set with an ITAE or Butterworth criterion (López and Alvarez, 2004). In Fig. 1, three closed-loop responses are shown with (i) the cascade SF control (8, 10) with full-model dependency, (ii) the OF control (13) with reduced modeling requirements, and (iii) the OF control with typical parameter errors: -14% error in the frequency factors of the monomer and solvent chain-transfer to propagation rates quotients (Flory, 1953), and -5 % in the initiator efficiency factor.

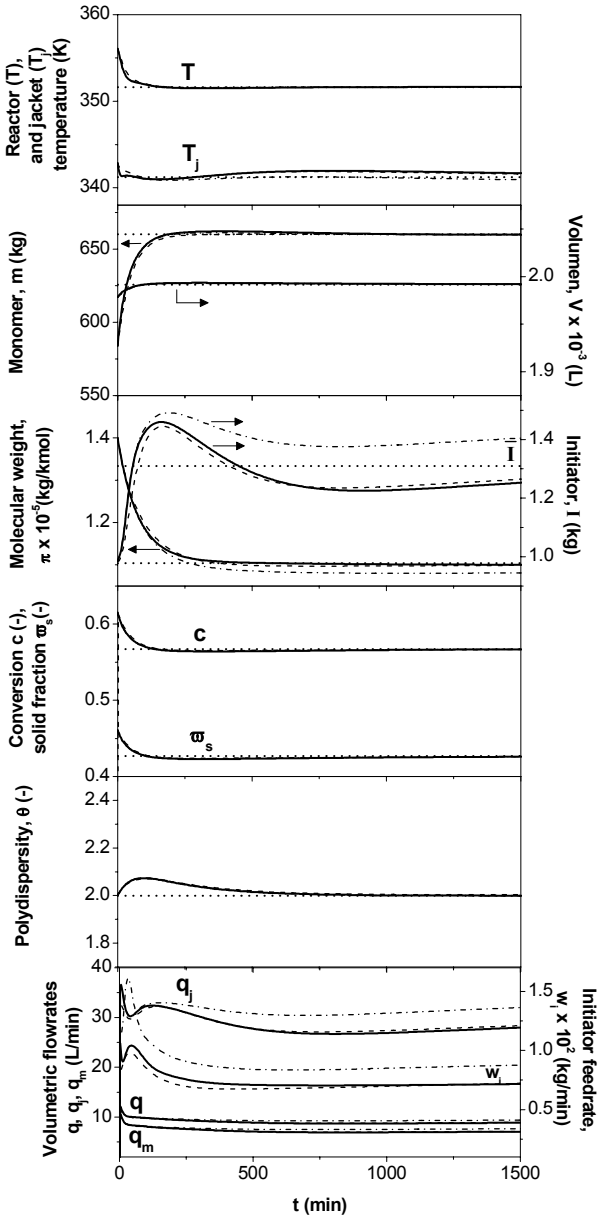

Fig. 1. Reactor behavior with the model-based SF passive control (- - -), OF control (——) and OF control with parameter errors (- · - · -).

Figure 1 shows that: (i) as expected, the OF controller basically recovers the behavior of its exact model-based counterpart, (ii) the volume, temperature and monomer content outputs reach their prescribed set points in about one residence time, in the understanding that the control of these outputs ensures the stability, the production rate level, and to a good extent the product quality, and (iii) the MW reaches its set point in about 2 residence times, (twice faster than the response of a process with the MW in open-loop mode, with a settling time of 4 residence times). As it can be seen from the responses of the OF control with parameter errors, the presence of these errors does not appreciably affect the control behavior, yielding a 3% MW asymptotic offset which is smaller than the measurement device uncertainty. Should this offset be unacceptable larger, the initiator and/or transfer constants should be occasionally recalibrated on the basis of free-monomer, solid fraction and MW measurements which are routinely taken for operation monitoring and product quality assessment purposes. The corresponding control responses are presented in Figure 1, showing that the four manipulated inputs evolve in a smooth and coordinated manner, and reasonably away from saturation phenomena.

6. CONCLUSIONS

A constructive approach to the control of continuous solution homopolymerization reactors with flow and temperature measurements has been presented, yielding an output-feedback controller whose behavior recovers the one of an exact model-based state-feedback passive controller. The key robustness oriented passivation step was performed by using some states (jacket temperature and initiator) as virtual (primary) control inputs. The recovery property was accomplished via an inventory-based observer to estimate and compensate the effect of the modeling errors. The proposed controller consists in the combination of elements that resemble well-known industrial controllers: volume and cascade temperature controllers, a ratio-type free monomer controller driven by the heat generation rate, and an inventory-type MW controller driven by the heat generation rate and material balances. The polymerization of MMA in an open-loop unstable industrial size reactor was considered as application example with numerical simulations, yielding a response that recovers the behavior of an exact model-based state-feedback control, and that is robust in the sense that the control performance is not significantly degraded by typical model parameter errors. As a next step towards applicability, studies on the attainment of linearity and decentralization features are underway.

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REFERENCES

Alvarez J. (1996). Output-feedback control of nonlinear Plants. *AIChE J.*, 42(9), 2540.

Alvarez, J., F. Zaldo and G. Oaxaca (2004). *The Integration of Process Design and Control*. Chapter: Towards a joint process and control design framework for batch processes: application to semibatch polymer reactors. Seferlis, P. and M. C. Georgiadis (Eds.), Elsevier, Amsterdam, The Netherlands.

Alvarez, J., R. Suárez and A. Sánchez (1994). Semiglobal nonlinear control based on complete input-output linearization and its application to the start-up of a continuous polymerization reactor. *Chem. Eng. Sci.*, 49(21), 3617.

Alvarez-Ramírez, J. J., J. Alvarez and A. Morales (2002). An adaptive cascade control for a class of chemical reactors. *Int. J. Adapt. Cont. Signal Process*., 16, 681.

Chiu, W. Y., G. M. Carratt and D. S. Soong (1983). A computer model for the gel effect in free-radical polymerization, *Macromolecules*, 16 (3) 348.

Congalidis, J. P. and J. R. Richards (1998). Process control of polymerization reactors: and industrial perspective. *Polym. React. Eng.*, 6(2), 71.

Daoutidis P., M. Soroush and C. Kravaris (1990). Feedforward/feedback control of multivariable nonlinear processes. *AIChE J*., 36(10), 1471.

Flory, P. J. (1953). *Principles of Polymer Chemistry*. Cornell University Press, New York.

Gauthier, J. P. and I. Kupka (2001). *Deterministic observation theory and applications*. Cambridge University Press, UK.

Hamer, J.W., T.A. Akramov and W.H. Ray (1981). The dynamic behavior of continuous polymerization reactors - II. Nonisothermal solution homopolymerization and copolymerization in a CSTR, *Chem. Eng. Sci.*, 36(12), 1897.

Isidori, A. (1995). *Nonlinear Control Systems (3rd ed.)*. McGraw-Hill, Springer-Verlag, New York.

López, T. and J. Alvarez (2004). On the effect of the estimation structure in the functioning of a nonlinear copolymer reactor estimator, *J. Proc. Cont.*, 14, 99.

Maner, B. R. and F. J. Doyle (III) (1997). Polymerization reactor control using autoregressive-plus Volterra-based MPC. *AIChE J.*, 43, 1763.

Mutha, R. K., W. R. Cluett, and A. Penlidis (1997). On-line nonlinear model-based estimation and control of a polymer reactor, *AIChE J.*, 43(11), 3042.

Padilla S. and J. Alvarez (1997). Control of continuous copolymerization reactors. *AIChE J*., 43(2), 448.

Sepulchre, R., M. Jankovic and P. Kokotovic (1997). *Constructive Nonlinear Control*, Springer-Verlag, NY.

Shinskey, F. G. (1988). *Process Control Systems (3rd ed.)*. McGraw-Hill, New York.

Soroush M. and C. Kravaris (1993). Multivariable nonlinear control of a continuous polymerization reactor: an experimental study. *AIChE J*., 39(12), 1920.