JOINT PROCESS AND CONTROL DESIGNS OF A SEMIBATCH EMULSION POLYMERIZATION REACTOR

Fernando Zaldo[1,3], Mauricio Hernández[1,2], and Jesús Álvarez[2]

[1] Centro de Investigación en Polímeros (CIP)
Marcos Achar Lobatón # 2, 55855 Tepexpan Edo. de México, MÉXICO
[2] Universidad Autónoma Metropolitana-Iztapalapa
Depto. de Ingeniería de Procesos e Hidráulica
Apdo. 55534, 09340 México D.F, MÉXICO
[3] Universidad Nacional Autónoma de México
Depto. de Ingeniería Química, Facultad de Química
04510 México D.F., MÉXICO

Abstract: The problem of jointly designing the equipment, the operation policy, and the calorimetric controller of a semibatch emulsion polymerization reactor is addressed within a nonlinear constructive control framework. A backstepping approach yields a passive cascade control structure, identifying the attainable closed-loop behavior, and the construction of a calorimetric controller. The designs of the equipment and of the operation are obtained from a recursive dynamic inversion in the light of safety, productivity, and quality considerations. The calorimetric controller tracks a prescribed temperature-free monomer profile by manipulating the heat exchange and monomer addition rates. The polymerization of vinyl acetate in an industrial size reactor is considered as application example with numerical simulations. *Copyright© 2003 IFAC.*

Keywords: Calorimetric estimator, on-line control, polymerization reactors, non-linear observer, batch process control, process design, process and control design.

1. INTRODUCTION

The industrial design of a semibatch emulsion polymerization reactor amounts to finding a suitable compromise between safety, productivity, and quality attributes in the light of investment-operation costs (Álvarez et al., 1995; Zaldo and Álvarez, 1998). The interplay between the process and control designs is handled with some dosage of experience in conjunction with industrial process, control, laboratory-to-plant testing and scaling tools. Thus, the development of systematic process-control designs should lead to more effective semibatch emulsion operations.

In the last two decades, the calorimetric control problem has been extensively studied mostly in laboratory scale reactors, with EKF (MacGregor, 1985), and Luenberguer (Schuler and Schmidt, 1992; McKenna et al., 2000; and references there in) calorimetric estimators and several (adaptive inferential, model-based predictive, geometric) nonlinear control techniques (Othman et al., 2000; Mutha et al., 1997; Sáenz de Buruaga et al., 1997; and references there in). The temperature is controlled with a standard or commercial controller, the heat generation rate is controlled by manipulating the monomer feedrate, and recently, an override supervisory controller has been incorporated to stop the monomer addition when its concentration surpasses a certain bound (Sáenz de Buruaga et al., 1997). For industrial applicability, these calorimetric controllers have several drawbacks: (i) an *a priori* (Sáenz de Buruaga et al., 1997) or occasionally calibrated (McKenna et al., 2000) heat transfer-solid content correlation is required, (ii) an override controller to resolve the conflicting tasks of the heat generation and free monomer control objectives is questionable because it requires on-line free monomer measurements, and implies a saturated (i.e., discontinuous) controller that could upset the semibatch operation. With emphasis on the equipment and operation policy design aspects, Álvarez et al. (1995) and Zaldo and Álvarez (1998) addressed the joint process-control design problem via dynamic inversion, identifying the tracking of temperature and free monomer concentration as the main task of the control scheme. The control scheme consisted of a cascade temperature controller with a preprogrammed monomer addition. However, the connection between the process and control designs was not formally discussed.

In this work, a constructive nonlinear control approach (Kristic et al., 1995) is employed to connect the process and calorimetric designs of semibatch emulsion polymer reactors. A backstepping scheme (Álvarez-Ramírez et al., 2002) yields a passive dynamic inverse, identifying the attainable closed-loop behavior with any nonlinear SF (state-feedback) controller, and yielding the construction of the calorimetric observer-based controller without needing a heat transfer-solid content correlation (Zaldo et al., 2002). The nominal operation is obtained with a tractable recursive dynamic inversion in the light of safety, productivity, and quality considerations. As the first step of an experimental study underway, in this work the polymerization of vinyl acetate in an industrial size reactor (Álvarez et al., 1995) is considered as an application example with numerical simulations.

2. PROCESS-CONTROL DESIGN PROBLEM

In a semibatch emulsion homopolymer reactor, monomer is converted into polymer via a strongly exothermic reaction (Dubé et al., 1997). First, water, surfactant, and initiator are loaded into the reactor. Then, monomer and heat are added to start the reaction, and after some period of time (in which the reaction sites have been formed), heat generated by the polymerization is removed in order to have an adequate reactor temperature control. Once the entire monomer load has been added, the temperature is increased to exhaust the monomer down to a small prespecified value. The monomer addition and heat exchange rates must be coordinated so that the batch is finished as soon as possible with adequate safety margin and product variability. The process is described by the following nonlinear equations over the finite-time interval $0 \le t \le t_f$:

$$\dot{T}_j = C_j^{-1}[U(T-T_j) - U_J(T_j-T_s) + Q_J], \qquad T_j(0)= T_{jo} \tag{1a}$$

$$\dot{T} = C^{-1}[\Delta R + wc_m(T_e-T) - U(T-T_j)], \qquad T(0)= T_o \tag{1b}$$

$$\dot{M} = w, \qquad M(0) = W + M_s := M_o \tag{1c}$$

$$\dot{P} = R, \qquad P(0) = P_o \tag{1d}$$

$$\dot{I} = - R_I, \qquad I(0) = I_o \tag{1e}$$

$$\dot{N} = R_N, \qquad N(0) = 0 \tag{1f}$$

$$y_T = T, \qquad y_j = T_j, \qquad y_m = m \tag{1g}$$

$$m = 1 - (M_o + P)/M := \alpha(P, M) \tag{1h}$$

The *states* of the reactor are: the emulsion (T) and jacket (T_j) temperatures, the emulsion (M) and polymer (P) masses, the water-soluble initiator concentration (I), and the number (N) of latex particles per unit volume of water phase. The initial condition M_o is made by the masses of loaded water (W) and surfactant (M_s). The *measured exogenous inputs* are: the monomer feed (T_e), the cold water feed (T_{je}), and the surroundings (T_s) temperatures. The *tracked outputs* for the nominal operation design are the emulsion temperature (T), and the mass fraction (m) of free (i.e., unreacted) monomer. The *measured outputs* for on-line control are: the emulsion (T) and jacket fluid temperatures (T_j). The *manipulated inputs* are the monomer (mass) feedrate w, and the heat rate Q_J exchanged through the jacket. The input Q_J is realized via a heating-cooling system with a recirculation loop that admits either the cold water flow supplied by a chiller (using ammonia as a coolant media) w_j or the heat rate $w_s\lambda_s$ (w_s and λ_s are the steam flow and its latent heat of vaporization):

$$Q_J = \theta(w_J,T, T_j, T_{je}), \qquad w_J = (w_j, w_s)' \tag{1i}$$

$$\theta(w_J,T, T_j, T_{je}) = \begin{cases} w_s\lambda_s & \text{if } T<T_j \\ 0 & \text{if } T = T_j \\ w_j[c_j(T_{je} - T_j)] & \text{if } T > T_j \end{cases}$$

$$w_j, w_s \ge 0, \quad w_j = 0 \text{ if } T \le T_j, \; w_s = 0 \text{ if } T \ge T_j$$

Thus, the manipulation of the scalar input Q_J is equivalent to the coordinated manipulation of the vector w_J, and the inverse map υ of θ is given by:

$$w_J = \upsilon(Q_J,T_j,T_{je})$$

$$w_J = \begin{cases} (0, Q_J/\lambda_S)' & \text{if } Q_J > 0 \\ (0, 0)' & \text{if } Q_J = 0 \\ [Q_J(c_j(T_{je} - T_j))^{-1}, 0]' & \text{if } Q_J < 0 \end{cases} \tag{2}$$

R, R_I, and R_N are respectively the polymerization, initiator decomposition, and latex particle generation rates, and U is the heat transfer coefficient between the emulsion and the jacket fluid, according to the nonlinear equations (Dubé et al., 1997):

$$R = f_R(T, P, M, I, N), \qquad R_N = f_N(T, P, M, I, N) \tag{3a}$$

$$R_I = f_I(T, I), \qquad U = f_U(T, T_j, P, M) \tag{3b}$$

U_J is the heat transfer coefficient associated to the heat lost to the surroundings. Δ is the heat of polymerization per unit monomer mass. C is the emulsion heat capacity, and C_j is the one of the jacket system made by the reactor (R), jacket (J) and insulator (I) walls as well as by the jacket fluid (F):

$$C = (M - P - M_o)c_m + Pc_p + Wc_w := f_C(P, M)$$

$$C_j = C_R + C_F + C_J + C_I$$

$$C_S = M_S c_S, \qquad S = R, F, J, I$$

where M_S is the mass of component S, and c_S is its specific heat capacity. c_m, c_p, c_w, c_j are respectively the specific heat capacities of the monomer, polymer, water, and jacket fluid. The rate (Q) of heat generation by chemical reaction, and the monomer conversion (χ) are given by (M_L is the monomer mass fed over the semibatch period):

$$Q = \Delta R, \qquad \chi = P/M_L, \qquad M_L = \int_0^{t_f} w(\tau)d\tau$$

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

$$\dot{x} = f(x, d, u, p), \qquad 0 \le t \le t_f, \qquad x(0) = x_o \qquad (4a)$$
$$\psi = g(x), \qquad y = h(x) \qquad (4b)$$

with state (x), exogenous input (d), control input (u), measured output (y), tracked output (ψ), model function (f), model parameters (p), kinetics-heat transfer model function F(x), and data D

$$x = (T, T_j, P, M, I, N)', \qquad d = (T_e, T_{je}, T_s)'$$
$$u = (w, w_j)', \qquad \psi = (y_m, y_T)', \qquad y = (y_T, y_j)'$$
$$f = (f_T, f_j, f_P, f_M, f_I, f_N)'$$
$$F(x) = (f_R, f_I, f_N, f_U)'(x), \quad D = [x_o, d(t), u(t), p] \qquad (5)$$

For a given D, the model has a unique (possibly open-loop unstable) solution motion x(t), with unique output trajectories $\psi(t)$ and y(t):

$$x(t) = \tau[x_o, d(\cdot), u(\cdot), p], \qquad 0 \le t \le t_f \qquad (6a)$$
$$\psi(t) = g[x(t)], \qquad y(t) = h[x(t)] \qquad (6b)$$

The *operation-control problem* consists in designing: (i) the *nominal operation* O (i.e., the equipment and the operation policy)

$$O = [\bar{x}(t), \bar{d}(t), \bar{u}(t), \bar{\psi}(t), \bar{y}(t), p], \quad 0 \le t \le t_f \qquad (7)$$

so that the closed-loop process takes place as fast as possible with an adequate compromise between safety, operability, and quality measures, and (ii) the dynamic *calorimetric controller*

$$\dot{x}_c = f_c[x_c, d(t), y(t), \bar{\psi}(t), p_c], \quad u(t) = h_c(x_c, p_c) \qquad (8)$$
$$p_c = (c_m, c_p, c_w, C_j, \Delta, W, M_s, U_J)'$$

so that the closed-loop reactor robustly tracks the nominal motion $\bar{x}(t)$ of O, with adjustable linear temperature error dynamics, and bounded free monomer error. The construction of the calorimetric controller must be based on the calorimetric parameters (p_c), and not on the uncertain kinetics-heat transfer model function F(x) (Eq. 5).

3. NOMINAL OPERATION DESIGN

In this section is recalled the dynamic inversion-based nominal equipment-process design presented in Álvarez et al. (1995) and Zaldo and Álvarez (1998), with two additional considerations to connect the process and calorimetric control designs: the jacket dynamics are included, and the resulting reactor dynamics are inverted with a backstepping passivation scheme (Kristic et al.,1995).

The dynamic inversion problem consists in determining the unique control trajectory u(t) associated to a given input-output realization [d(t), y(t)] over [0, t_f]. Take the time derivative of the output map $\psi = g(x)$ (Eq. 6b), substitute $\dot{x}$ by f (Eq. 4a), and obtain the algebraic equation pair

$$\dot{y}_m = [-R + (1 - y_m)w]/M \qquad (9a)$$
$$\dot{y}_T = C^{-1}[\Delta R + c_m (T_e - y_T)w - U(y_T - T_j)] \qquad (9b)$$

These equations say that the output ψ has a relative degree pair (1, 2), and that the construction of the inverse requires the nonlinear function F (Eq. 5) and its Jacobian matrix $\partial_x F$. To circumvent this obstacle for the construction of an F-independent controller, let us regard the jacket temperature T_j as the "virtual" control input (instead of Q_J), solve Eq. (9) for (w, T_j), and obtain the *primary (m, T_j)-control*:

$$w = \iota_w(x_I, \psi_m), \qquad T_j = \iota_j(x_I, \psi_m, \psi_T, T_e) \qquad (10a, b)$$

where

$$x_I = (M, I, N)' \ , \quad \psi_m = (y_m, \dot{y}_m)' \ , \quad \psi_T = (y_T, \dot{y}_T)'$$
$$\iota_w(x_I, \psi_m) = (R + M\dot{y}_m)/(1 - y_m),$$
$$\iota_j(x_I, \psi_m, \psi_T, T_e) = y_T + U^{-1}[C\dot{y}_T - \Delta R - wc_m(T_e\text{-}y_T)]$$
$$\pi(y_m, M) = (1 - y_m)M - M_o$$

(R, U) = $(f_R, f_U)(x)$ (Eq. 3) with $T = y_T$, $m = \alpha(P, M)$ (Eq. 1h), and $P = \pi(y_m, M)$.

Recall the jacket heat balance [Eq. (1a)], solve it (Eq. 11c) for Q_J with $\dot{T}_j$ replaced by its estimate $\hat{\upsilon}_j$ drawn from a standard T_j-driven fast second-order filter (Eqs. 11a, b), substitute into Eq. (2), and obtain the *secondary T_j-control*

$$\dot{\hat{T}}_j = \hat{\upsilon}_j + 2\zeta\omega(T_j - \hat{T}_j), \qquad \hat{T}_j(0) = y_{jo} \qquad (11a)$$
$$\dot{\hat{\upsilon}}_j = \omega^2(T_j - \hat{T}_j), \qquad \hat{\upsilon}_j(0) = \hat{\upsilon}_{jo} \qquad (11b)$$
$$Q_J = C_j\hat{\upsilon}_j - U(T - T_j) + U_J(T_j\text{-}T_s) \qquad (11c)$$
$$w_J = \upsilon(Q_J,T_j,T_{je}) := \iota_J(x_I, \psi_m, \psi_T, \hat{\upsilon}_j, d) \qquad (11d)$$

where ω and ζ are the adjustable observer frequency and damping factor. The enforcement of the restriction $g(x) = \bar{\psi}(t)$ on the reactor model followed by the application of the primary (Eq. 10) and secondary (Eq. 11) controllers into the reactor model (Eq. 1) yields the *dynamic inverse*

(Primary inverse)

$$\dot{x}_I = \phi_I(x_I, \psi_m, y_T), \quad x_I(0) = x_{Io} \qquad (12a)$$

$$w = \iota_w(x_I, \psi_m), \quad T_j = \iota_j(x_I, \psi_m, \psi_T, T_e) \qquad (12b)$$

(Secondary inverse)

$$\dot{\hat{T}}_j = \hat{v}_j + 2\zeta\omega(T_j - \hat{T}_j), \quad \hat{T}_j(0) = y_{jo} \qquad (12c)$$

$$\dot{\hat{v}}_j = \omega^2(T_j - \hat{T}_j), \quad \hat{v}_j(0) = \hat{v}_{jo} \qquad (12d)$$

$$w_J = \iota_J(x_I, \psi_m, \psi_T, \hat{v}_j, d) \qquad (12e)$$

where

$\phi_I = (\phi_i, \phi_N, \iota_w), \quad \phi_i(y_T, x_I) = - f_I(y_T, I)$

$\phi_N(y_m, y_T, x_I) = f_N[y_T, M, \pi(y_m, M), I, N]$

By construction (ζ, $\omega > 0$), the secondary inverse dynamics (Eqs. 12c-e) are stable, and therefore the stability property of the cascade dynamic inverse (Eq. 12) is determined by the same property of the (unique) solution motion

$$x_I(t) = \tau_I[x_{Io}, \psi_m(\cdot), \psi_T(\cdot), d(\cdot)] \qquad (13)$$

of the primary inverse dynamics (Eq. 12a). The stability of the nonautonomous motion $x_I(t)$ is not generic in the sense that it holds for one particular data D (Eq. 5) (Álvarez et al., 1995). A formal consideration of the important subject of robust motion stability goes beyond the scope of this work. Here it suffices to mention that the present study is underlain by the definition of motion finite-time exponential (increasing or decreasing) stability employed in Zaldo et al.'s (2002) geometric calorimetric estimation technique. It must be pointed out that the inverse dynamics represents the high-gain limiting behavior attainable with any calorimetric-observer based controller.

Given a set of design restrictions D_R and the parameter vector p_e with the equipment design degrees of freedom (this will be illustrated in the section on the application example), the nominal operation O (Eq. 7) is designed as follows: (i) Choose a candidate equipment parameter-output trajectory pair (p_e, $\bar{\psi}$), (ii) Obtain the dynamic inverse $\bar{x}_I(t)$ (Eq. 13), assess its robust stability property, and determine the nominal operation O. If the design restrictions D_R are adequately met, O is accepted as the nominal operation, otherwise, redesign the pair (p_e, $\bar{\psi}$) and go back to step (ii). Typically, with the information, experience, and insight available in an industrial setting, this recursive design takes from three to five iterations (Álvarez et al., 1995), and in principle, can be refined with an optimization scheme.

4. CALORIMETRIC CONTROLLER

Assume that the state x and the model function F (Eq. 5) are available for on-line control, let ω_T (or ω_j) be the primary (or secondary) temperature control gain, enforce the closed-loop output tracking dynamics

$$y_m = \bar{y}_m, \quad \dot{y}_T = \dot{\bar{y}}_T - \omega_T(T-\bar{y}_T), \quad \dot{T}_j = \dot{T}^*_j - \omega_j(T_j-T^*_j)$$

$$T^*_j = T + [C\dot{y}_T - \Delta R - wc_m (T_e - y_T)]/U$$

where T^*_j is the jacket temperature set point. The substitution of these expressions into the primary (Eq. 10) and secondary (Eq. 11) controller of the dynamic inverse (with $T_j = T^*_j$) yields the SF-cascade controller

$$T^*_j = T-\{\Delta f_R(x) + wc_m(T_e-T) - C[\dot{\bar{y}}_T - \omega_T(T-\bar{y}_T)]\}/ f_U(x)$$

$$Q_J = C_j[\dot{T}^*_j - \omega_j(T_j-T^*_j)] - f_U(x)(T-T_j) + U_J(T_j-T_s)$$

$$w = [f_R(x) + M\dot{\bar{y}}_m]/(1-\bar{y}_m), \quad w_J = \upsilon(Q_J, T_j, T_{je}) \qquad (14)$$

The combination of the preceding SF-controller with the calorimetric observer presented in Zaldo et al. (2002) yields the calorimetric controller in IMC form:

Internal model (15a)

$$\dot{\hat{T}}_j = [\hat{H} + \theta(w_J,\hat{T},\hat{T}_j,T_{je}) - U_J(\hat{T}_j-T_s)]/C_j + 2\zeta\omega(y_j-\hat{T}_j), \quad \hat{T}_j(0) = y_{jo}$$

$$\dot{\hat{H}} = \omega^2 C_j(y_j - \hat{T}_j), \quad \hat{H}(0) = \hat{H}_o$$

$$\dot{\hat{T}} = [\hat{Q} + wc_m(\hat{T}-T_e) - \hat{H}]/C + 2\zeta\omega(y_T-\hat{T}), \quad \hat{T}(0) = \hat{T}_o$$

$$\dot{\hat{Q}} = \omega^2[C_j(y_j-\hat{T}_j) + C(y_T-\hat{T})], \quad \hat{Q}(0) = \hat{Q}_o$$

$$\dot{\hat{M}} = w, \quad \dot{\hat{P}} = \hat{Q}/\Delta, \quad \hat{M}(0) = \hat{M}_o, \quad \hat{P}(0) = \hat{P}_o$$

$$\dot{\hat{T}}^*_j = \hat{v}_j + 2\zeta\omega(T^*_j-\hat{T}^*_j), \quad \hat{T}^*_j(0) = \hat{T}^*_{jo}$$

$$\dot{\hat{v}}_j = \omega^2(T^*_j-\hat{T}^*_j), \quad \hat{v}_j(0) = \hat{v}_{jo}$$

Primary controller (15b)

$$w = (\hat{Q}/\Delta + \hat{M}\dot{\bar{y}}_m)/(1 - \bar{y}_m)$$

$$H^* = \hat{Q} + wc_m(T_e - \hat{T}) - C[\dot{\bar{y}}_T - \omega_T(\hat{T} - \bar{y}_T)]$$

$$T^*_j = \hat{T} - (H^*/\hat{H})(\hat{T} - \hat{T}_j), \quad \text{if } |\hat{H}| \le \varepsilon_H$$

$$\dot{T}^*_j = 0, \quad \text{if } |\hat{H}| > \varepsilon_H$$

Secondary controller (15c)

$$Q_J = C_j[\hat{v}_j - \omega_j(\hat{T}_j - \hat{T}^*_j)] - \hat{H} + U_J(\hat{T}_j - T_s)$$

$$w_J = \upsilon(Q_J, \hat{T}_j, T_{je})$$

where ε_H is a small number specified to circumvent the small-period lack of calorimetric observability and controllability when there is no heat exchange (i.e., $T \approx T_j$). Structurally speaking, this controller is made by the interconnection of two well known industrial controllers: a cascade temperature controller that manipulates the heat exchange rate Q_J for a given monomer feedrate w, and a ratio-type free-monomer controller that sets w proportionally to the heat generation rate $\hat{Q}$. Given that ω_J is the dominant frequency of the jacket dynamics, the study (not presented here due to space limitations) of the closed-loop error dynamics with Zaldo et al.'s (2002) stability approach, choosing the gains $\omega_J = \omega > \omega_j > \omega_T$ with ω_j sufficiently smaller than ω, and ω_T sufficiently smaller than ω_j, yields a closed-loop reactor where: (i) the temperature is tracked asymptotically and the free monomer is tracked with bounded error, and (ii) the nominal motion is tracked with bounded error.

5. APPLICATION EXAMPLE

Consider that a 10,000 liters = V semibatch reactor must process M_L = 4,500 kg of vinyl acetate monomer (supplied at $\bar{T}_e$ = 20ºC) with ammonium persulfate as initiator and sodium lauryl sulfate as a stabilizing agent. The initial values of the reactor, jacket, and surroundings temperatures are: $\bar{T}_o$ = 70°C, $\bar{T}_{jo}$ = 75ºC, and $\bar{T}_s$ = 20ºC. The polymerization temperature is $\bar{T}$ = 80°C while monomer is being fed and is 85ºC in the exhaustion period. The trajectory $\bar{m}(t)$ must be chosen in such a way that a constant amount of unreacted monomer is kept during most of the monomer addition period. The maximum (T_j^+ = 150ºC) and minimum (T_j^- = 5ºC) jacket fluid temperature is fixed by the services considering a safety margin. The reactor operation must finish with a conversion of $\bar{\chi}$ = 0.995. These are the specifications and restrictions referred to as D_R in Section 3. The operation design consists in specifying the heating-cooling system including: the stirrer and emulsion mixing pattern, the volume, the geometry and recirculation of the jacket system, and the jacket fluid-saturated steam heat exchanger. Thus, the adjustable equipment design parameter vector is given by (Álvarez et al., 1995)

$$p_e = (p_h , p_s, w_{rj})' \quad , \qquad p_h= (a_h, b_h, c_h)'$$

where w_{rj} is the recirculation flow, p_h is the vector with three constants set by the choice of stirrer and emulsion mixing pattern, and p_s is the area of the jacket fluid-saturated steam heat exchanger.

The recursive design presented in Section 3 yielded (after three iterations) the nominal operation presented in Figure 1 (dashed lines), with the following observations: (i) the batch productivity is limited by the heat exchange capacity within a standard safety margin, and this in turn is determined by the nominal free monomer concentration output $\bar{y}_m(t)$, (ii) the initial and final free monomer and temperature profiles must be sufficiently smooth (as shown in Figure 1) to preclude control saturation, (iii) a slow semibatch (shown in Álvarez et al., 1995) exhibits an open-loop motion with a large degree of stability and a small product variability, but as the semibatch time is decreased, the degree of open and closed-loop stability decreases, (iv) the semibatch period of t_f = 4 hours shown in Figure 1 represents a suitable compromise between safety, productivity, and product quality, as well as a significant improvement over the reactor before redesign, (v) the initial and monomer depletion periods demand the largest heating duties, whereas the period after the end of the monomer dosage demands the largest cooling duty and represents the most dangerous potential of reactor run away because the cooling effect of the monomer dosage must be abruptly overtaken by the cooling system.

Following the calorimetric observer tuning guidelines presented in Zaldo et al. (2002), the observer gain parameters were set at ζ = 0.71 and $\omega = \omega_J$ = 40 min^{-1} to have fast heat generation ($\hat{Q}$) and exchange ($\hat{H}$) rate estimates with damped error dynamics and low noise. To ensure the robust functioning of the cascade controller, the gains were chosen to have a typical dynamical separation in industrial processes: the secondary temperature control gain was set ten times slower than the observer dynamics ($\omega_j = \omega/10$), whereas the primary temperature control gain ($\omega_T = \omega_j/10$) was set ten times slower than the secondary. In Figure 1 are shown the closed loop results for the calorimetric (full lines) controller, and the state-feedback (dashed lines) controller (using the uncertain model function F). The robustness of the closed-loop motion was verified numerically, and as it can be seen in the figure, the calorimetric controller (Eq. 15) practically recovers the behavior of the exact SF-controller (Eq. 14).

6. CONCLUSIONS

An industrial application-oriented unified approach to the equipment, operation and calorimetric control designs of semibatch emulsion homopolymerization reactors has been presented. Following the idea of the constructive nonlinear control, the integrated design is based on a structure oriented geometric method, an error propagation stability approach, and the knowledge on the process drawn from industrial experience and polymer reaction engineering modeling and dynamics tools. The nominal equipment-operation design is obtained with a tractable recursive dynamic inversion scheme in the light of process and control design considerations, the controller construction follows from a straightforward step, and its conventional like tuning is simple. The results show that the temperature and free monomer concentration can be reliably tracked with a multivariable calorimetric controller that manipulates the monomer addition and heat exchange rates.

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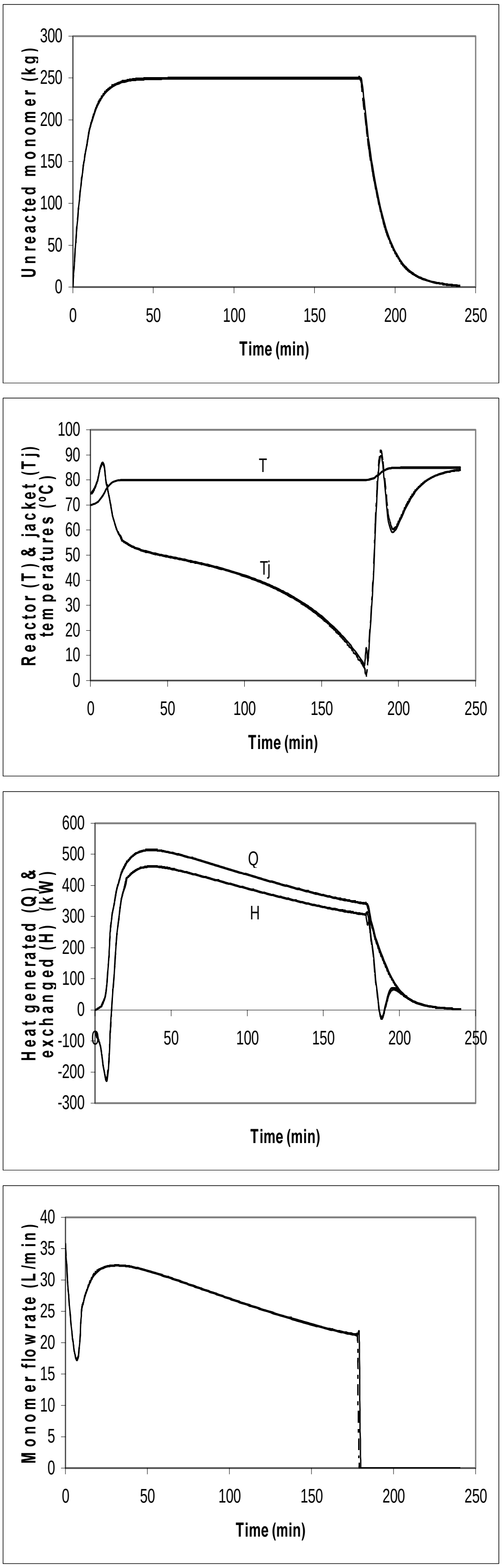

Fig.1. Nominal operation design & closed-loop reactor with SF control (dashed lines), and closed-loop reactor with calorimetric control (full lines).