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Observer-based nonlinear control law for a continuous stirred tank reactor with recycle ☆

M.P. Di Ciccio [a,*], M. Bottini [b], P. Pepe [a], P.U. Foscolo [b]

[a] Department of Electrical and Information Engineering, University of L'Aquila, 67040, Poggio di Roio, L'Aquila, Italy

[b] Department of Chemical Engineering, University of L'Aquila, 67040, Poggio di Roio, L'Aquila, Italy

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ABSTRACT

This paper proposes new results concerning the problem of the control of a continuous stirred tank reactor with recycle. The novelty of the proposed results consists of a new nonlinear observer-based controller which is found by means of recent results of differential geometry for time-delay nonlinear systems, without using linear approximations of the model. Local convergence of the system state to the arbitrarily chosen operating point is theoretically proved. The significance of the proposed control law is shown by many simulations, which show high performances with any initial conditions, even at the start-up, and with critical cases of mismatched parameter values.

1. Introduction

The control of the operation of chemical reactors has attracted the attention of researchers for a long time. The underlying motivation relies on the fact that industrial chemical reactors are frequently operated at unstable operating conditions, which often corresponds to optimal process performance (Adebekun, 1996; Aguilar et al., 2001; Alvarez-Ramirez and Morales, 2000; Jana, 2007; Assala et al., 1997; Chang and Chen, 2004; Chen and Peng, 2006; Daaou et al., 2008; Fissore, 2008; Gibon-Fargeot et al., 2000; Hashiimoto et al., 2000; Iyer and Farell, 1994; Kosanovich et al., 1995; Kravaris et al., 1994; Pierri et al., 2006; Prakash and Senthil, 2008; Senthil et al., 2006; Soroush, 1997; Wright and Kravaris, 2006). Polymerization processes (Assala et al., 1997) and bio-reactors fermentors (Soroush, 1997) are important examples of large-scale chemical reactors operated at unstable conditions. In addition there exist many process control strategies, in which the information about the internal state of the process is necessary to calculate the control input. Consequently, the presence of unknown state variables becomes a difficulty which can be overcome with the inclusion of an appropriate state estimator (Aguilar et al., 2001; Chang and Chen, 2004; Daaou et al., 2008; Fissore, 2008; Adebekun, 1996; Salehi and Shahrokhi, 2008; Iyer and Farell, 1994; Jana, 2007; Kosanovich et al., 1995; Kravaris et al., 1994; Biagiola and Figueroa, 2004; Hashiimoto et al., 2000).

The above papers do not consider the problem of state estimation in the presence of the time-delays in the state variables. Other papers propose methodologies borrowed by time-delay systems nonlinear control theory (Wu, 1999; Pepe, 2009; Cao and Frank, 2000), but it is assumed that all the state variables are available for measure, thus a nonlinear observer for state variables estimation is not employed. In the paper Antoniades and Christofides (1999), an observer-based nonlinear control law for chemical reactors with recycle time-delay is presented. The observer gain is computed by means of the linearized model. A model with only two state variables (reagent concentration and reactor temperature) is used, and the dynamics of jacket refrigerant temperature is not taken into account. Also, the manipulated input is the inlet reagent concentration in the fresh feed, which can arise some further complications in the accuracy of the practical implementation of the control law.

In this paper we deal with the controller design, by means of partial state measurements, for a continuous stirred tank reactor, where an irreversible, exothermic, liquid-phase reaction $A \rightarrow B$ evolves. In order to reduce reaction waste, a separation volume is added to the reaction volume, and the exit flow is partially recycled to the feeding stream. Such recycle is responsible of a

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* Corresponding author. Tel.: +39 0862 434422; fax: +39 0862 434403.
E-mail addresses: diciccio@ing.univaq.it (M.P. Di Ciccio), massimo.bottini@gmail.com (M. Bottini), pepe@ing.univaq.it (P. Pepe), foscolo@ing.univaq.it (P.U. Foscolo).

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non-negligible time-delay due to the fluid transport. The model of the plant is given by three nonlinear delay differential equations (the dynamics of the jacket temperature is considered too). The control input consists of the cooling water flow-rate. The controlled output is the reactor temperature. The measured output consists of the reactor and jacket temperatures. Here we do not use the measurement of the reactor concentration, which is expensive to obtain by techniques, for instance, of gas-chromatography. The reactor concentration is estimated by means of a nonlinear observer for time-delay systems (Germani et al., 2001; Germani and Pepe, 2005). The state feedback control law is obtained by means of the method of the exact input–output linearization, with delay cancellation, of nonlinear time-delay systems (Germani et al., 2000, 2003). If the states were available, the state feedback control law yields the convergence of the state variables to the operating point. In the spirit of the separation principle, the controller is here implemented by using the state estimations provided by the observer instead of the unavoidable full state measurements. First-order approximated linearization methods are not used here. The control law is actuated by means of a pneumatic valve which regulates the cooling water flow-rate. This actuation process is easier to implement than the ones based on the use of the inlet reactor concentration or of the jacket temperature as manipulated inputs. It is proved theoretically that the observer-based control law yields the asymptotic stability of the chosen operating point. Many performed computer simulations show the high performance of the proposed observer-based controller. Saturation effects have been taken into account in simulations. The convergence of the state variables to the arbitrarily chosen operating point is always obtained with the many considered system initial conditions (even start-up initial conditions) and initial estimation error, and with different values of the recirculation coefficient. As well, the convergence of the estimated state variables to the true state variables is always obtained in such simulations. If parameters mismatch occurs, all the many performed simulations show that a steady-state value is still obtained, with a steady-state error (with respect to the chosen operating point). The steady-state error for the reactor temperature is always tolerable, in the performed simulations. No instability occurs for the considered significant mismatch (see the simulations section).

A preliminary version of this paper has been presented at the 14th IFAC Conference on Methods and Models in Automation and Robotics, Miedzydroje, Poland, 2009, and is available on IFAC-PapersOnline.

2. The model of the CSTR with recycle time-delay

Here we study a CSTR with jacket cooling in which a first-order irreversible exothermic reaction takes place (Luyben, 2007): $A \rightarrow B$. A separator is considered, which yields a recycle time-delay (see Fig. 1).

If in the reactor out flow an important quantity of not converted reagent is present, the added separator volume reduces the reactant waste and increases the overall conversion of the reaction. The recirculation coefficient, here denoted with Φ, is defined as:

$$\Phi = \frac{\text{Effluent flow-rate}}{\text{Total Reactor flow-rate}}$$

Therefore $\Phi = 1$ means no recycle, $\Phi = 0$ means total recycle. Denoting with F_r the flow-rate of the recirculating stream and with F the total reactor flow rate, it results that

$$\Phi \overset{def}{=} \frac{F - F_r}{F} \Rightarrow F_r = F(1-\Phi)$$

The presence of this recycle loop introduces the associated recycle loop dead time, Δ. In this situation, the inlet stream to the reactor is

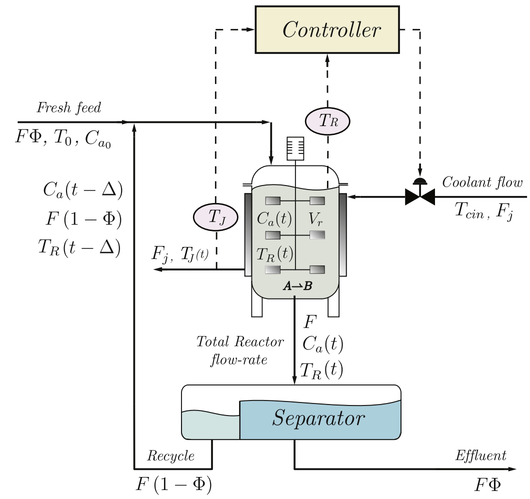

Fig. 1. Schematic CSTR-separator process with recycle.

characterized by fresh feed with pure A, at flow-rate $F\Phi$, concentration C_{a_0}, and temperature T_0 and the recycle stream is characterized by flow-rate $F(1-\Phi)$, concentration $C_a(t-\Delta)$ and temperature $T_R(t-\Delta)$, where C_a and T_R are the reagent concentration and temperature in the reactor, respectively.

The liquids in the reactor and in the jacket are assumed perfectly mixed, that is, with no radial, axial, or angular gradients in properties (temperature, concentrations). This allows to consider reactor and jacket temperatures and reactant concentrations as space invariant variables. If physical properties are assumed constant (densities and heat capacities), the reactor volume is constant and the jacket volume is constant, the mathematical model of the CSTR is given by the following set of nonlinear functional differential equations:

$$\dot{x}_1(t) = \frac{F(\Phi C_{a_0} + (1-\Phi)x_1(t-\Delta) - x_1(t))}{V_r} - x_1(t)k_0 e^{-E/Rx_2(t)}$$

$$\dot{x}_2(t) = \frac{F(\Phi T_0 + (1-\Phi)x_2(t-\Delta) - x_2(t))}{V_r} - \lambda x_1(t)k_0 e^{-E/Rx_2(t)}\rho^{-1}C_p^{-1} - \frac{UA_j(x_2(t)-x_3(t))}{V_r \rho C_p}$$

$$\dot{x}_3(t) = \frac{u(t)(T_{cin} - x_3(t))}{V_j} + \frac{UA_j(x_2(t)-x_3(t))}{V_j \rho_j C_j} \qquad (1)$$

where

$x_1 = C_a$: reactant concentration (kmol/m^3)
$x_2 = T_R$: reactor temperature (K)
$x_3 = T_J$: jacket temperature (K)
$u = F_j$: flow rate of coolant (control input) (m^3/s)
k_0: pre-exponential factor (s^{-1})
E: activation energy (J/kmol)
R: universal gas constant, 8314 J/kmol K
F: flow-rate of feed and product (m^3/s)
T_{cin}: supply temperature of cooling medium (K)
ρ: density of product stream (kg/m^3)
λ: heat of reaction (J/kmol)
C_j: heat capacity of coolant (J/kg K)
C_p: heat capacity of product (J/kg K)
T_0: temperature of feed (K)
V_r: volumetric holdup of liquid in reactor (m^3)
C_{a_0}: concentration of reactant A in feed (kmol/m^3)
U: overall heat transfer coefficient (W/m^2 K)
A_j: jacket heat transfer area (m^2)
ρ_j: density of coolant (kg/m^3)