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Nonlinear Observer for Copolymerization Processes

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Abstract

The difficulties encountered in chemical engineering arise from the lack of reliable and robust sensors. Several works deal with the design of software sensors in order to estimate the unavailable/non-measured variables. However the theoretical convergence of these state estimators is not often proven. This paper concerns nonlinear state estimation in a semi-batch polymerization reactor where free radical solution copolymerization of methyl methacrylate (MMA) and vinyl acetate (VAc) takes place. We propose two estimation methods whose convergence is theoretically shown and which allow the estimation of the live polymer concentration. The first method consists of combining a Kalman like observer with an optimization algorithm, and the second one is based on dynamic programming. The convergence of these observers is shown by numerical simulations.

Keywords : Moving Horizon Estimation, Polymerization Process, Kalman-Like observer, Optimization

1. Introduction

Polymerization reactors are a class of processes in which many essential process variables related to product quality cannot be measured at high sampling rates and with significant time delays. The lack of reliability-available, frequent on-

line measurements, from which polymer properties can be inferred, has motivated a considerable research effort in the following research directions : (a) the development of new on-line sensors [1]; (b) the development of qualitative and quantitative relations between readily-available on-line measurements and polymer properties [2]; (c) the development of state estimators/observers that are capable of estimating unmeasurable polymer properties [3]. In most of these studies, extended Kalman filters (EKFs) have been used for state estimation.

In summary, the available nonlinear observer design methods are still inadequate, either because they are applicable to a very restricted class of non linear systems or the global asymptotic stability of their error dynamics cannot be proven. The main objective of this paper is to propose two state estimation strategies based on an optimization algorithm and whose convergence is proven theoretically. The first method consists of a coupling between a Kalman like observer and an optimization algorithm. The second method is a moving horizon estimation approach. These methods involve a formulation of state estimation as a minimization problem. The performance of these two methodologies proposed is illustrated taking as case study a semi-batch copolymerization reactor, where the live polymer concentration and the number of moles of monomers (two different monomers) are estimated using continuous measurements of monomer conversion.

2. Nonlinear model of copolymerization reactor

Polymerization reactors are highly nonlinear processes. In these reactors, many of the essential process variables related to the polymer product quality cannot be measured readily on-line.

In this paper, we consider a semi-continuous reactor where free radical copolymerization takes place. The feed to the reactor consists of two monomers. The reactor model is based on a kinetic mechanism [4] that describes the reactions involved in propagation. This stage involves growth of the polymer chain by the addition of monomer molecules to active chains. We assume that the live polymer (active chains) concentration [$M^{\bullet}$] is constant.

The model assumes perfect mixing and long chains. A material balance for each species present in the reactor can be written to represent its evolution during the reaction. The dynamic behavior of the number of moles of monomer (N_1) and number of moles of monomer (N_2) are described by the following equations:

$$\dot{N}_1 = F_1 - (k_{p11}\varphi_1 + k_{p21}\varphi_2)[M^{\bullet}]N_1 \qquad (1)$$

$$\dot{N}_2 = F_2 - (k_{p12}\varphi_1 + k_{p22}\varphi_2)[M^\bullet]N_2 \tag{2}$$

where φ_1 and φ_2 are the mole fractions of radicals terminating by a radical of monomers 1 and 2 respectively :

$$\varphi_1 = \frac{k_{p21}N_1}{k_{p21}N_1 + k_{p12}N_2} \text{ and } \varphi_2 = 1 - \varphi_1 \tag{3}$$

We suppose that the monomer conversion is measured either by calorimetry or by near infrared spectroscopy. Based on the monomer overall conversion and using the total number of moles of monomer introduced into the reactor the total mass can be calculated. The overall conversion X_m is defined by :

$$X_m = \frac{\sum_i M_{wi}N_i^{tot} - \sum_i M_{wi}N_i}{\sum_i M_{wi}N_i^{tot}} \tag{4}$$

The residual mass of monomer is therefore,

$$y = (1 - X_m)\sum_i M_{wi}N_i^{tot} = M_{w1}N_1 + M_{w2}N_2 \tag{5}$$

3. Estimation strategies

In practice, the feedback control strategy require the knowledge of the state of the system. Because the on-line measurement of the concentration of radicals $[M^\bullet]$ is not possible, we have chose to estimate it together with N_1 (the number of moles of monomer 1) and N_2 (the number of moles of monomer 2) using two different observers.

3.1. Estimation based on a Kalman-Like observer

The first strategy consists of a coupling between a Kalman like observer and an optimization algorithm. Our main result consists to immerse the initial model into a higher dimensional one for which an estimator can be designed. The estimation of the original state can be achieved using an optimization technique.

Consider the following nonlinear system :

$$\begin{aligned} \dot{\zeta} &= f(\zeta) + g(\zeta, u) \\ y &= h(\zeta) \end{aligned} \tag{6}$$

where $\zeta(t) = [N_1; N_2]$ is the state of the system (6) to be estimated using the output measurements $y(t) = h(\zeta) = M_{w1}\varsigma_1 + M_{w2}\varsigma_2$ and the inputs $u(t) = [F_1; F_2]$.

Assuming that there exists a one to one map $\begin{matrix}\phi : \Re^n \to \Re^N \\ \varsigma \to z = \phi(\varsigma)\end{matrix}$, (N≥n) which transforms system (6) into the system :

$$\begin{cases} \dot{z} = A(u)z + B(u) + \varepsilon(t) \\ \qquad Y = Cz \end{cases} \tag{7}$$

where A(u) is a n×n matrix, which depends continuously on u and C is a p×N constant matrix. ε(t) may depend on z(t) and u(t), but assumed to be bounded. The fact that ϕ is one to one means that for every trajectory of (6); there exists a unique trajectory z(t) of (7), s.t. z(t)= ϕ(ζ(t)).

We apply a like Kalman-like observer on the state affine system (7) :

$$\begin{cases} \dot{\hat{z}} = A(u)\hat{z} + B(u) - S^{-1}C^T(C\hat{z} - y) \\ \dot{S} = -\theta S - A(u)^T S - SA(u) + C^T RC \end{cases} \tag{8}$$

where S(0) is a N×N symmetric positive definite matrix and R is a p×p constant matrix.

In order to determine the estimated value of the state x, we use a quadratic problem formulation which minimizes the 2-norm of the difference between the state of observer ($\hat{z}$) and the functions Z which depend on the estimated state $\hat{x}$. The current formulation solves the problem :

$$J = \min_{\hat{x}} \left\| m(\hat{z}(t) - z(\hat{x}(t))) \right\|^2 \tag{9}$$

where t is the current time and m is a scaling vector for weighting or normalizing the error.

3.2. Estimation based on a moving horizon observer

For the second strategy, we reformulate the estimation in term of optimization. It is a question of determining the states of the system which minimize a nonlinear criterion on a moving horizon. This strategy is thus based on a moving horizon estimation (MHE).

The first step is the discretization of the model (Euler's method). The second step concerns the optimization algorithm. The method produces an estimate of the state of the nonlinear system at time t by minimizing a cost function over the preceding interval (horizon) [t-T,T]; as t advances so does the horizon. The cost function employed is a measure of the distance between the output of the system and the output of the estimator over some time interval preceding the time instant in which the state estimate is required. The current formulation solves the problem :

$$\operatorname{argmin}\theta \sum_{l=k-N}^{k}(\hat{y}_l - y_l)_2 \tag{10}$$

with N the length of the moving horizon, y_l is the process measurement vector and $\hat{y}_l$ is the vector of process model estimates.

The computation algorithm is given below :
[1.] Initialization of the state x
[2.] Computation loop
For t=0 to Tmax
If k≤ N

$$\hat{x}_k = x_k$$

If k > N, θ> 0

$$\hat{x}_{k-N} = \operatorname{argmin}\theta \sum_{l=k-N}^{k}(y_l - y_l)_2$$

[3.]We initialize the optimization with the preceding states $\hat{x}_{k-N}$.

3.3. Results & discussions

The estimation strategies developed above were tested by simulation during the methyl methacrylate (MMA) and vinyl acetate (VA) copolymerization. The reaction was assumed to take place under isothermal conditions at 333K. The kinetics of this system are given in [6].

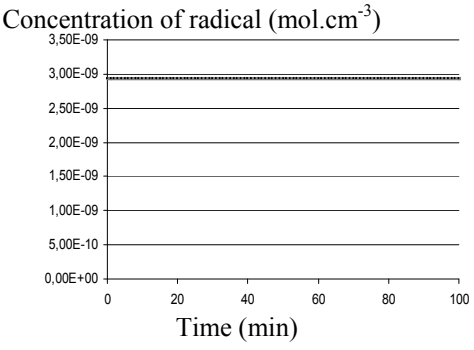

Figure 1 : Estimation by MHE of radical concentration (mol.cm^{-3})

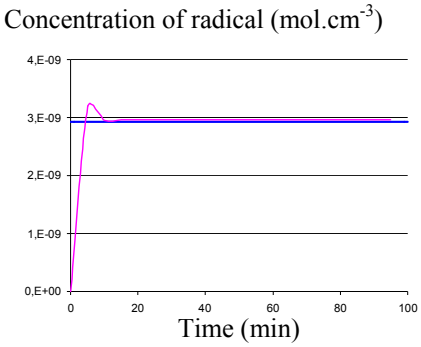

Figure 2 : Estimation based on Kalman like observer of radical concentration (mol.cm^{-3})

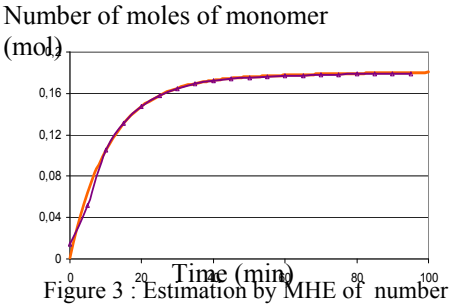

Figure 3 : Estimation by MHE of number of moles N1 and N2 (mol)

Simulations results are reported in Fig. 1 to Fig. 3 that shows the estimated values compared to the real values. The optimization works good. And a rapid convergence to the real values could be detected.

4. Conclusions

In this paper, we develop two estimation strategies whose convergence are theoretically proven. These strategies perform very well. The difficulty of the first method concerns the choice of the scaling vector. The second method is more delicate because of the cascade of two optimization algorithms.

Nomenclature

F_i : Feed flow of monomer i ($mol.s^{-1}$)
k_{pij} : Propagation rate of a radical with the ultimate unit of type i with monomer j ($cm^3.mol^{-1}.s^{-1}$)
N_i : Number of mole of monomer i (i=1,2) (mol)
$[M^{\bullet}]$: Concentration of radicals (living polymer chain) ($mol.cm^{-3}$)
V : Volume of the reacting mixture (cm^3)
N_i^{Tot} : Total number of moles of monomer i introduced to the reactor (mol)

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