



Framework design for weight-average molecular weight control in semi-batch polymerization



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ABSTRACT

A framework that embraces a state-of-the-art sensor, multi-objective dynamic optimization, nonlinear state estimation and control, is designed and implemented to achieve target weight-average molecular weight trajectories. The Automatic Continuous Online Monitoring of Polymerization reactions (ACOMP) is combined for the first time with a nonlinear state observer for full polymer characterization and signal processing. A hybrid variation of the discrete-time extended Kalman filter (*h*-DEKF) is formulated based on an auto-tuning procedure that uses a stochastic global optimization technique. A number of optimal policies are generated and experimentally tested. Results are provided through investigations into the free-radical aqueous polymerization of acrylamide using potassium persulfate as initiator.

1. Introduction

The competitive landscape of the chemical industry requires practical tools for the Smart Manufacturing of chemicals with desired final properties. Polymers represent a large part of this industry and their synthesis involves complex processes. End manufacturers require raw polymeric materials with uniform characteristics for industrial applications. In the past decades, techniques and strategies for state estimation (Hedengren & Eaton, 2015; Kozub & MacGregor, 1992; Nicholson, López-Negrete, & Biegler, 2014; Romagnoli & Sanchez, 1999; Schuler & Schmidt, 1992; Srinivasan, Kasthurikrishnan, Cooks, Krishnan, & Tsao, 1995; Weiss, Romagnoli, & Islam, 1996) and control (Cho, Chung, & Lee, 2000; Eaton & Rawlings, 1990; Ghadipasha, Romagnoli, Tronci, & Baratti, 2015; Norquay, Palazoglu, & Romagnoli, 1998; Romagnoli & Palazoglu, 2005) have evolved for solving industrial problems in chemical reactors and unit operations. Advanced manufacturing techniques are important as they allow the efficient use of feedstock materials, energy, and labor while also improving safety in a chemical facility. Particularly in the polymer industry the combination of mechanistic model complexity and inadequate real-time characterization techniques present crucial challenges.

A major goal in polymer synthesis is the achievement of a target molecular weight distribution (MWD) as it leads to desired physico-chemical properties. Indeed, MWD is fundamental in the sense that it influences physical, rheological, and thermal characteristics of final

products such as thermal stability, strength, and capability of materials for being processed (Gentekos, Dupuis, & Fors, 2016; Heidemeyer & Pfeiffer, 2002; Isayev, 2011). External disturbances such as temperature, degree of mixing, concentration and purity of reactants affect final MWDs due to the sensitive molecular structure of polymers (McKeen, 2014). The lack of reliable real-time techniques for monitoring MWD, weight average molecular weight (M_w) and number average molecular weight (M_n) makes it difficult to directly control these properties.

A recent state-of-the-art smart sensor for polymerization processes, known as the ACOMP system, provides real-time measurements of different polymer properties and follows the evolution of monomer and polymer concentration along a liquid-phase polymerization (Florenzano, Strelitzki, & Reed, 1998; McAfee et al., 2016; Reed & Alb, 2013). Some examples of the ACOMP applications include the monitoring of polyacrylamide synthesis (Giz, Catalgil-Giz, Alb, Brousseau, & Reed, 2001), prediction of molecular weight in semi-batch free-radical homopolymer reactors (Kreft & Reed, 2009a), and predictive control of average composition and MWDs in semi-batch free-radical copolymerization reactors (Kreft & Reed, 2009b). Although state-of-the-art sensors such as the ACOMP system can overcome many needs, the available measurements are not enough for a complete understanding of the dynamic evolution of the system. Therefore, the implementation of a nonlinear observer is necessary for better comprehension of the evolution of the state variables as well as to improve available measurements.

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Notation

A_d	Pre-exponential factor for initiator decomposition, [min ⁻¹]
A_p	Pre-exponential factor for propagation [m ³ mol ⁻¹ min ⁻¹]
A_{td}	Pre-exponential factor for termination by disproportionation [m ³ mol ⁻¹ min ⁻¹]
C_i	Concentration of initiator inside the reactor, [mol m ⁻³]
C_{if}	Concentration of initiator in the initiator flow rate, [mol m ⁻³]
C_m	Concentration of monomer inside the reactor, [mol m ⁻³]
C_{mf}	Concentration of monomer in the monomer flow rate, [mol m ⁻³]
C_s	Concentration of solvent inside the reactor, [mol m ⁻³]
C_{sif}	Concentration of solvent in the initiator flow rate, [mol m ⁻³]
C_{smf}	Concentration of solvent in the monomer flow rate, [mol m ⁻³]
E_d	Activation energy in initiator decomposition, [J mol ⁻¹]
E_p	Activation energy in propagation, [J mol ⁻¹]
E_{td}	Activation energy in termination by disproportionation, [J mol ⁻¹]
e_f	Initiator efficiency, <i>dimensionless</i>
F_i	Flow rate of initiator to the reactor, [m ³ min ⁻¹]
F_m	Flow rate of monomer to the reactor, [m ³ min ⁻¹]
F_{out}	Extraction flow rate out of the reactor for sampling purposes, [m ³ min ⁻¹]
g	Chain length distribution, <i>dimensionless</i>
k_d	Initiator decomposition rate constant, [min ⁻¹]
k_{fm}	Chain transfer to monomer rate constant, [m ³ mol ⁻¹ min ⁻¹]
k_{fs}	Chain transfer to solvent rate constant, [m ³ mol ⁻¹ min ⁻¹]
k_p	Propagation rate constant, [m ³ mol ⁻¹ min ⁻¹]
k_{tc}	Termination by combination rate constant, [m ³ mol ⁻¹ min ⁻¹]
k_{td}	Termination by disproportionation rate constant, [m ³ mol ⁻¹ min ⁻¹]
m	Upper bound for chain length interval, <i>dimensionless</i>
M_n	Number average molecular weight, [kg mol ⁻¹]
M_w	Weight average molecular weight, [kg mol ⁻¹]
n	Lower bound for chain length interval, <i>dimensionless</i>
N_i	Total amount of initiator inside the reactor, [mol]
N_{i0}	Initial amount of initiator inside the reactor, [mol]
N_m	Total amount of monomer inside the reactor, [mol]
N_{m0}	Initial amount of monomer inside the reactor, [mol]
N_{mf}	Total amount of monomer added to the reactor from the flow rates, [mol]
N_s	Total amount of solvent inside the reactor, [mol]
N_{s0}	Initial amount of solvent inside the reactor, [mol]
P_0	Concentration of live polymer in the reactor, [mol m ⁻³]
R_{gas}	Ideal gas constant, [J mol ⁻¹ K ⁻¹]
T	Temperature of the reactor, [K]
t	Time, [min]
V	Volume of the material inside the reactor, [m ³]
w_m	Molecular weight of monomer, [kg mol ⁻¹]
w_i	Molecular weight of initiator, [kg mol ⁻¹]
w_s	Molecular weight of solvent, [kg mol ⁻¹]
X	Monomer conversion, <i>dimensionless</i>

Greek letters

λ_0	Zeroth moment, [mol m ⁻³]
λ_1	First moment, [mol m ⁻³]
λ_2	Second moment, [mol m ⁻³]
α	Probability of propagation, <i>dimensionless</i>
ρ_m	Mass density of monomer, [kg m ⁻³]
ρ_i	Mass density of initiator, [kg m ⁻³]
ρ_s	Mass density of solvent, [kg m ⁻³]

Even though direct measurements from the ACOMP system provide an accurate assessment of the system, the complete state vector can seldom be measured. In addition, mathematical models often become increasingly inaccurate as the reaction proceeds. Thus, a well-adjusted combination of both experimental measurements and mathematical models allows a better understanding of the system dynamics. Developed more than half a century ago, the Kalman filter (KF) (Kalman, 1960; Kalman & Bucy, 1961) provides an elegant basis for incorporating both the available data and a mechanistic model of the process of interest (Qin, 2014). The KF addresses the problem of estimating states of a discrete-time controlled process governed by a linear stochastic difference equation. The assumptions of linearity for both the measurements and the state transitions are crucial for its correctness (Simon, 2006). Nonetheless, state transitions and measurements are rarely linear in practice. For nonlinear systems, the extended Kalman filter (EKF) is one of the most broadly utilized state estimators for the chemical process industry (Hashemi, Kohlmann, & Engell, 2016). A particular configuration of the EKF is the discrete-time extended Kalman filter (DEKF) (Simon, 2006). The method combines the nonlinear model and its linearization to compute the state estimates.

In polymeric systems, many authors have studied a variety of state estimators. Kozub and MacGregor (1992) considered different EKF configurations for semi-batch polymerizations. Ellis, Taylor, and Jensen (1994) implemented a MWD estimator for the methyl-methacrylate using measurements from gel permeation chromatography (GPC) for experimental testing. Tatiraju and Soroush (1997) compared the performance of an EKF with a nonlinear observer for a methyl-methacrylate system in a continuous reactor. Gentric, Pla, and Corriou (1997) and Gentric, Pla, Latifi, and Corriou (1999) proposed an optimal policy formulation integrated with a geometric controller and an EKF for a batch emulsion-polymerization reactor. The trajectories followed by the controller were optimal temperature profiles that lead to desired characteristics of the final polymer. Li, Corripio, Henson, and Kurtz (2004) proposed a framework for online state estimation and parameter estimation. Statistical methods such as the particle filter have achieved a robust performance in nonlinear state estimation (Hashemi et al., 2016). Due to the difficulty of measuring the reactor contents, other authors included the management of delayed and infrequent measurements (Galdeano, Asteasuain, & Sánchez, 2011; Gopalakrishnan, Kaisare, & Narasimhan, 2011). Beyrer, Grote, and Reinig (2008) presented a combined structure for control and state estimation using a sigma-point KF for improving the control action in a Chylla–Haase polymerization reactor. Although results exhibit satisfactory behavior and adequate state estimation capability, some of them are purely simulation results and others lack the advantages provided by the ACOMP system such as directly measuring the control objective.

In this contribution, a framework that combines a state-of-the-art sensor, multi-objective dynamic optimization, nonlinear state estimation and control is proposed for a free-radical polymerization towards full characterization and target polymer production. The ACOMP system is combined for the first time with a nonlinear state observer, taking advantage of its measuring ability in order to obtain better estimates of the underlying model. As a first step, optimal policies are generated by solving a multi-objective dynamic optimization problem targeting polymers with different weight-average molecular weight trajectories

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