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# Optimal nonlinear control of an industrial emulsion polymerization reactor

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## ABSTRACT

In this paper, the modelling, dynamic optimization and nonlinear control of an industrial emulsion polymerization reactor producing poly-vinyl acetate (PVAc) are proposed. The reaction is modeled as a two-phase system composed of an aqueous phase and a particle phase according to the model described in our previous work (Gil et al., 2014). The case study corresponds to an industrial reactor operated at a chemical company in Bogotá (Colombia). An industrial scale reactor (11 m<sup>3</sup> of capacity) is simulated. Three different dynamic optimization problems are solved from the more simplistic (only one control variable: reactor temperature) to the more complex (three control variables: reactor temperature, initiator flow rate and monomer flow rate) in order to minimize the reaction time. The results show that it is possible to minimize the reaction time while some polymer desired qualities (conversion, molecular weight and solids content) satisfy defined constraints. The optimal temperature profile and optimal feed policies of the monomer and initiator, obtained in a dynamic optimization step, are used as optimal set points for reactor control. A nonlinear geometric controller based on input/output linearization is implemented for temperature control.

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## 1. Introduction

The purpose of dynamic optimization studies is to determine a set of variables of a dynamic system, such as flow rates, temperatures, pressures, heat duties, etc., that optimize a given cost function or criterion (costs, productivity, time, energy, selectivity) subject to specific constraints (dynamic model, operating conditions, safety and environmental restrictions). Some of the common problems of chemical engineering addressed by means of dynamic simulation and optimization include startup, upset, shutdown and transient analysis, safety studies, control and scheduling of batch and semi-batch processes, and the validation of control schemes (Biegler, 2007; Cervantes and Biegler, 2008). In all cases, it is important to possess a dynamic model sufficiently representative of the real process by means of mass and energy balances, and algebraic equations for physical and thermodynamic relations, but with a moderate complexity in order to get a

mathematical and numerical solution without difficulty (Corriou, 2004, 2012).

Some of the most important objectives in resins and polymer production plants are related to the improvement of safety, quality and productivity, minimum operating costs and respect of environmental constraints (Gentric et al., 1999). These make the optimization and control of polymerization reactors of great interest. In most cases, an optimization problem for a polymerization system requires the definition of an objective function and constraints which are defined by the reaction time and/or polymer molecular characteristics, together with operating conditions. In terms of polymerization reactors, the main contributions concern homogeneous reactions and some multiphase considerations trying to minimize the batch period, improve quality control and minimize the molecular weight distribution. In these cases, nonlinear models are essential to accurately describe the dynamics of the process. The solution of this kind of optimal control

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### Nomenclature

$C_{pj}$	specific heat of component $j$ [ $\text{J K}^{-1} \text{kg}^{-1}$ ]
$I$	moles of initiator in the reactor [mol]
$k_{fm}$	rate constant for chain transfer to monomer [ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$ ]
$k_{fp}$	rate constant for chain transfer to polymer [ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$ ]
$k_t$	termination rate constant [ $\text{m}^3 \text{mol}^{-1} \text{s}^{-1}$ ]
$k_I$	overall initiation rate constant [ $\text{s}^{-1}$ ]
$M_M$	moles of monomer in the reactor [mol]
$\bar{M}_n$	number average molecular weight [ $\text{g mol}^{-1}$ ]
$\bar{M}_w$	weight average molecular weight [ $\text{g mol}^{-1}$ ]
$M_t$	total moles of monomer fed to the reactor [mol]
$MW_M$	monomer molecular weight [ $\text{kg mol}^{-1}$ ]
$m_w$	mass of water in the reactor jacket [kg]
$\bar{n}$	average number of radicals per particle [-]
$q_I$	flow rate of initiator fed to the reactor [mol/s]
$q_M$	flow rate of monomer fed to the reactor [mol/s]
$\mathcal{R}_{pol}$	overall reaction rate [mol/s]
$T$	reactor temperature [K]
$T_j$	jacket temperature [K]
$U$	overall heat transfer coefficient [ $\text{W m}^{-2} \text{K}^{-1}$ ]
$V_{pol}$	total volume of polymer generated in the reaction [ $\text{m}^3$ ]
$V_w$	total volume of aqueous phase [ $\text{m}^3$ ]
$\alpha$	probability of propagation [-]
$\Delta H_r$	heat of reaction [ $\text{J kg}^{-1}$ ]
$\lambda_0$	total concentration of zeroth moment for growing chains [-]
$\mu_0$	concentration of zeroth moment for dead chains [-]
$\mu_1$	concentration of first moment for dead chains [-]
$\mu_2$	concentration of second moment for dead chains [-]
$\phi_S$	solids content [-]
$\rho_{pol}$	polymer density [ $\text{kg m}^{-3}$ ]

problems can be obtained by means of various optimization methods such as variational calculus, Hamilton-Jacobi equations, Pontryagin's maximum principle for continuous time systems and Bellman dynamic programming for discrete time systems, among others (Corriu, 2004, 2012; Kameswaran and Biegler, 2006; Biegler, 2007).

In the case of emulsion polymerization, several studies deal with dynamic optimization. For example, Jang and Yang (1989) report the dynamic minimization of the final time of a batch emulsion polymerization of vinyl acetate using initiator flow rate as control variable, and the maximum allowable reaction rate together with the total amount of initiator as constraints. Gentric et al. (1999) calculate the optimal temperature profile that minimizes the batch time of a copolymerization reactor of styrene and  $\alpha$ -methylstyrene using orthogonal collocation coupled with a sequential quadratic programming method. As constraints, they used the final conversion and the final number average molecular weight. Sayer et al. (2001) and Vicente et al. (2002) calculated the optimal monomer and chain-transfer agent feed profiles for the semi-batch methylmethacrylate (MMA)/*n*-butylacrylate (*n*-BA) emulsion copolymerization, using iterative dynamic programming with an objective function that included a term for the copolymer composition and also a term for the molecular weight distribution, in a way close to multiobjective optimization. Araújo and Giudici (2003) used variable time intervals with an iterative dynamic programming procedure to minimize the reaction time while composition and molecular weight are controlled at specific

values. Paulen et al. (2010) worked on the dynamic optimization of the emulsion copolymerization of styrene and  $\alpha$ -methylstyrene applying control vector parameterization (CVP) method in order to minimize the total reaction time. Recently, batch and semibatch operation of copolymerization of styrene and MMA (Ibrahim et al., 2011) were studied in order to maximize the monomer conversion in one case and the average molecular weight in a second case by means of CVP techniques solved by successive quadratic programming. Multiobjective optimization refers to simultaneous optimization of more than one objective function, which is typical in most real-life optimization problems encountered in industry (Benyahia et al., 2011). Multiobjective dynamic optimization has been also studied for a semibatch styrene polymerization process in order to establish optimal operating temperature and feeding policies, which maximize monomer conversion and minimize the residual initiator in the final product (Silva et al., 2004).

In the present work, the dynamic optimization of the industrial emulsion polymerization of vinyl acetate is performed with respect to three different optimization scenarios, 1: with temperature, 2: with temperature and initiator flow rate, 3: with temperature, initiator flow rate and monomer flow rate as control variables respectively. In the three cases, the objective is to minimize the reaction time by varying separately or simultaneously the reactor temperature, initiator flow rate and monomer flow rate. After optimization, some open loop optimal results obtained are used for comparison with closed loop simulations. The nonlinear geometric controller coupled with state estimation is used for tracking the optimal reaction temperature profile found by dynamic optimization. The results show the potential of dynamic optimization in finding optimal feed policies and operating temperature to improve the productivity. Also, it is demonstrated that the optimal temperature trajectory is well followed by means of a nonlinear controller.

## 2. Dynamic optimization of vinyl acetate emulsion polymerization

### 2.1. Experimental validation of the model

The dynamic state space model of the process has been described in a previous work (Gil et al., 2014). Nine states are used [ $I$ ,  $M_t$ ,  $M_M$ ,  $V_{pol}$ ,  $\mu_0$ ,  $\mu_1$ ,  $\mu_2$ ,  $T$ ,  $T_j$ ] standing respectively for the initiator concentration  $I$ , total added monomer  $M_t$ , remaining monomer  $M_M$ , total volume of polymer  $V_{pol}$ , three first moments of polymerization  $\mu_i$ , reactor temperature  $T$  and jacket temperature  $T_j$ . The first seven equations correspond to the reaction kinetics and the two following equations to the energy balances for the reactor and jacket. Algebraic equations for the polymerization reaction rate  $\mathcal{R}_{pol}$ , average number of radicals per particle  $\bar{n}$ , and monomer phase distribution, are not included here because are completely described in our previous study (Gil et al., 2014)

Kinetic model:

$$\frac{dI}{dt} = q_I - k_I I \quad (1)$$

$$\frac{dM_t}{dt} = q_M \quad (2)$$

$$\frac{dM_M}{dt} = q_M - \mathcal{R}_{pol} \quad (3)$$

$$\frac{dV_{pol}^p}{dt} = \mathcal{R}_{pol} \frac{MW_M}{\rho_{pol}} \quad (4)$$

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