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Multivariable control of the polymer molecular weight in emulsion polymerization processes

Nida Sheibat-Othman[a,*], Sami Othman[a], Olivier Boyron[b], Mazen Alamir[c]

[a] Université de Lyon, Université Lyon 1, CNRS, CPE Lyon, UMR 5007, Laboratoire d'Automatique et de Génie des Procédés (LAGEP), 43 Bd du 11 Novembre 1918, F-69622 Villeurbanne, France

[b] Université de Lyon, Université Lyon 1, CPE Lyon, CNRS, UMR 5265, Laboratoire de Chimie, Catalyse, Polymères et Procédés (C2P2), LCPP Group, 43 Bd du 11 Novembre 1918, F-69616 Villeurbanne, France

[c] Gipsa-Lab/CNRS, University of Grenoble, Rue de la Houille Blanche, 38400 Saint Martin d'Hères, France

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A multivariable control strategy is developed to control the polymer molecular weight in emulsion polymerization processes while maximizing the reaction rate by manipulating the jacket temperature and the monomer flowrate. In order to take into account the process nonlinearity, input–output linearizing control is considered. A cascade of two nonlinear observers is developed to estimate the heat of the reaction and the number of moles of radicals in the polymer particles. By introducing these estimations and the available measurements into the process model, the polymer molecular weight could be estimated online. The online estimation and control strategy was validated experimentally in seeded emulsion polymerization of styrene for which the model of the molecular weight is well known. It was also validated for the methyl methacrylate monomer where a simplified model was identified.

1. Introduction

Controlling chemical processes is essential in order to ensure process safety and the desired product quality. Polymerization processes are concerned with advanced process control since they are exothermic, rapid, and sensitive to impurities and the process model is nonlinear. Additionally, the process usually has constraints on the inputs and the states.

One of the main polymer properties is the molecular weight or molecular weight distribution. This property is related to the final product characteristics, such as its viscosity and mechanical and thermal properties. However, online monitoring of the polymer molecular weight by hardware sensors is not feasible. Techniques such as gel permeation chromatography (GPC) are inefficient for online analyzes since they necessitate sample preparation and long analysis time. For this reason, it will be important for process control to have an online estimate of this property.

These objectives were treated in the literature by different ways. Open loop control and batch to batch optimization were the main methods employed to control the polymer quality and to minimize the process time (see for instance, Sayer et al. [16], Fonteix et al. [6], Lima et al.[15]). However, due to unpredictable changes in the process dynamics or raw materials, online control that uses online measurements or estimations is necessary. Concerning online feedback control, Kozub and MacGregor [13] employed internal model control to track the copolymer molecular weight and composition while minimizing the process time in emulsion polymerization reactors. The extended Kalman filter was used for state estimation and the whole scheme was studied only in simulation. Gesthuisen et al. [9] presented a simulation study of the simultaneous control of the heat produced by the reaction and the polymer molecular weight. A decentralized PI linear controller was combined to a Kalman Filter to manipulate the flowrates of monomer and chain transfer agent. Echevarria et al. [4] studied the polymer molecular weight control in emulsion polymerization by manipulating the flowrates of monomer and chain transfer agent. An online optimization algorithm was employed for this objective and the controller was validated experimentally. The use of a chain transfer agent allows controlling the polymer molecular weight on a range of usually much smaller molecular weights.

Besides controlling the polymer properties, it is important in polymerization processes to optimize the process productivity. The process productivity is a function of the reaction operating conditions: the reactor temperature and the different concentrations which are affected by the flowrates of monomer, initiator and surfactant in the case of emulsion polymerization. Many works considered controlling the process productivity by manipulating only the flowrate of monomer Arzamendi and Asua [2], Vicente et al. [20]. Sheibat-Othman and Othman [18] were the first to manipulate both the monomer flowrate and the jacket temperature to

* Corresponding author. Tel.: +33 04 72 43 18 50; fax: +33 04 72 43 16 99.
E-mail address: nida.othman@lagep.univ-lyon1.fr (N. Sheibat-Othman).

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