MODELLING AND SIMULATION OF SEMI-BATCH POLYMERIZATION REACTOR FOR IMPROVED REACTANTS DOSING CONTROL

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Abstract

This paper presents a temperature model of an industrial, semi-batch, emulsion-polymerization reactor, which together with the already designed chemical reactions model is able to predict the temperature in the reactor as a result of varying operating conditions. The model was derived from the energy balance and validated on real-plant data. The model was used to analyse the influence of reactants dosing during the batch on the reactor temperature. The analysis shows that during the batch dosing of the two reactants, initiator and monomer, needs to be mutually balanced and adjusted to the current process situation, otherwise, the temperature in the reactor may become oscillatory and unstable towards the end of the batch because of the limited heat removal capacity of the condenser. To keep the reactor temperature in a narrow region also the control strategy was proposed that adjusts the monomer flow and initiator addition, using reactor temperature as a controlled variable. Simulation results show that the proposed reactants dosing control significantly reduces the variations in the reactor temperature and at the same time results in more uniform final batch results.

Keywords: emulsion polymerization, semi-batch industrial reactor, calorimetry model, gPROMS, control.

Presenting Author's biography

Nadja Hvala is employed as a researcher at Jožef Stefan Institute, Department of Systems and Control. Her research interests are modelling, simulation, control and optimization of chemical and biochemical processes. Some of the problems she was involved in are the following: pulp cooking, hydrolysis in TiO_2 production, polymerization. In the last ten years she is mainly involved in modelling and control of biological wastewater treatment processes.

1 Introduction

Emulsion polymerization is an important industrial process for the production of synthetic polymers, e.g., paints, adhesives, coatings and binders. Batch and semi-batch reactors are the most common reactors used in polymer engineering.

The production requirements typically addressed in polymerization reactors are the following:

- to achieve high monomer conversion,
- to reduce the total batch time,
- to achieve tight temperature control during the reaction.

The most often addressed control problem is the control of a reactor's temperature, which is needed because of the heat released in the exothermic reaction. Production requirements are to keep the temperature in a narrow region around the desired set-point (e.g. $\pm 1^{o}C$) to get the desired molecular weight and distribution of polymer particles, as well as to prevent the synthesis of an off-spec polymer at elevated temperatures.

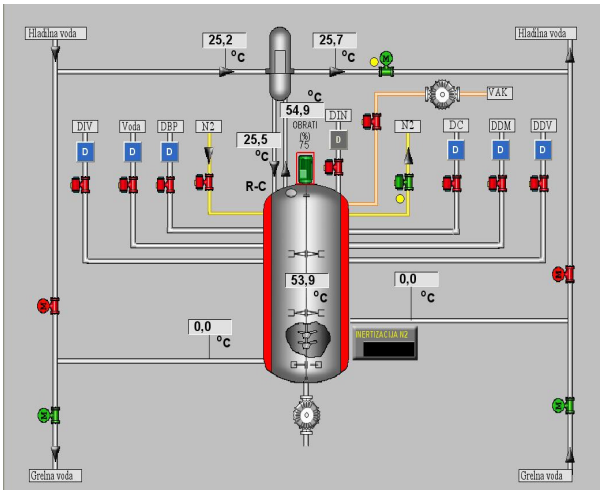
The temperature of the reactor is normally controlled by manipulating the temperature of the coolant, which is circulated through the cooling jacket, and various advanced control methods are used in these cases, e.g. feedforward control using an inverse reactor model [1], exact linearization [2], and nonlinear adaptive control based on differential geometric concepts [3]. However, much less often the cases are addressed, where the reaction heat is removed only by evaporative cooling. In such a case, the control of the temperature is only possible through the reactants dosing control.

In this study we present the design and validation of the reactor temperature model, derived from the energy balance, which together with the chemical reactions model [4] is used to optimize the process through reactants dosing control. The control approach is similar to the one presented in the recent paper [5], but differs in that in this case the feed rates of both reacting chemicals, the monomer and initiator, are used to control the reactor temperature.

This paper is organized as follows. In the next section we present the semi-batch polymerization process under study. The reactor temperature model derived from energy balance is presented in Section 3. Section 4 presents simulation analysis of initiator and monomer dosing, followed by the reactants dosing-control scheme proposed in Section 5. The obtained control results are shown in Section 6. The paper ends with the conclusions, where the main findings and directions for future work are described.

2 Process description

The process considered in the study is a semi-batch emulsion polymerization reactor in Mitol d.d. company, Slovenia (Fig. 1). The components involved in the reaction are water, monomer (vinyl acetate), initiator (potassium persulfate - KPS) and stabiliser (polyvinyl alcohol - PVOH). The reaction starts by the thermal decomposition of the initiator in the water phase, where free radicals are formed; these radicals then react with the monomer to form longer chains (oligomers). At a certain critical length oligomers precipitate and form particles, which are the target final product.



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