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Advanced control with parameter estimation of batch transesterification reactor

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ABSTRACT

The objective of this work is to enhance the economic performance of a batch transesterification reactor producing biodiesel by implementing advanced, model based control strategies. To achieve this goal, a dynamic model of the batch reactor system is first developed by considering reaction kinetics, mass balances and heat balances. The possible plant-model mismatch due to inaccurate or uncertain model parameter values can adversely affect model based control strategies. Therefore, an evolutionary algorithm to estimate the uncertain parameters is proposed. It is shown that the system is not observable with the available measurements, and hence a closed loop model predictive control cannot be implemented on a real system. Therefore, the productivity of the reactor is increased by first solving an open-loop optimal control problem. The objective function for this purpose optimizes the concentration of biodiesel, the batch time and the heating and cooling rates to the reactor. Subsequently, a closed-loop nonlinear model predictive control strategy is presented in order to take disturbances and model uncertainties into account. The controller, designed with a reduced model, tracks an offline determined set-point reactor temperature trajectory by manipulating the heating and cooling mass flows to the reactor. Several operational scenarios are simulated and the results are discussed in view of a real application. With the proposed optimization and control strategy and no parameter mismatch, a revenue of 2.76 \$ min^{-1} can be achieved from the batch reactor. Even with a minor parameter mismatch, the revenue is still 2.01 \$ min^{-1}. While these values are comparable to those reported in the literature, this work also accounts for the cost of energy. Moreover, this approach results in a control strategy that can be implemented on a real system with limited online measurements.

1. Introduction

Growing economies and the increasing need for mobility of people and goods result in a rising demand for energy resources. One of these energy resources in the transport sector is diesel fuel. Because petrodiesel is a limited commodity, biodiesel can be used as a renewable substitute [1]. Biodiesel can be produced from vegetable oils, such as soy bean oil or palm oil, waste cooking oil, animal fat, as well as algal oil. A drawback is the lack of cost competitiveness against conventional fuels [2]. Therefore, the existing process steps in the production of biodiesel have to be optimized to make biodiesel more cost competitive [3]. The transesterification of the triglyceride from oils using short chain alcohol in the presence of a catalyst is an essential part of the process. This reaction can be carried out in a continuous or batch reactor [4]. The batch process is often preferred because it is flexible and facilitates the operator to accommodate variations in feedstock type, composition as well as quantity, and to satisfy specific product requirements [5]. The initial capital and infrastructure investments are low [6]. Major drawbacks of the batch reactor are the intensive energy requirements [6] and the complexity of the system due to the highly nonlinear and time varying character of the batch process [7]. This behavior makes an advanced optimization and control strategy a necessity.

Literature shows burgeoning interest in advanced model based control of a transesterification reactor [5,8–16]. An approach to determine an optimal temperature trajectory for a batch reactor was presented in [5]. They formulated and solved an optimal control problem (OCP) to find a control law such that a certain optimality criterion was achieved. The study was extended by [13], and the productivity of the reactor under feedstock composition uncertainty was maximized. However, constraints were not directly taken into account. Furthermore, the OCP was solved

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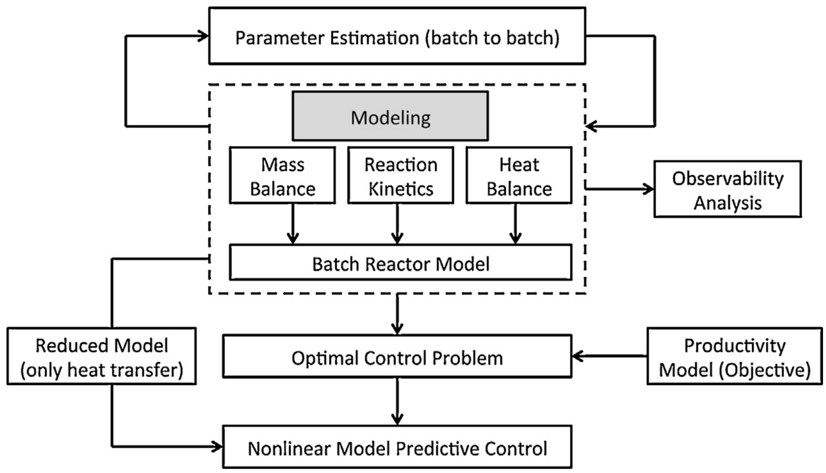

Fig. 1. Overview of the structure of this work.

before the operation of the reactor, and therefore the approach was an open-loop control strategy, where the output of the controlled process was not considered. Consequently, deviations between the desired and actual states occurring during the process cannot be corrected and disturbances cannot be compensated. A method to overcome these drawbacks of open-loop control was presented by [14]. In this work, the economic performance of a semi-batch reactor for the production of biodiesel was optimized by using a nonlinear model predictive control (NMPC) strategy. In each time step, all states were estimated from measurements, and the optimal methanol feed flow rate and the optimal heat duty were computed. However, the heat exchange between the reactor and the jacket was not further investigated in their work. Moreover, the observability of the system was not examined. It is doubtful that there is enough online information available on real plants to estimate all states, which is necessary for the NMPC strategy. The literature review, therefore, shows that although there have been some studies exploring advanced control of the transesterification reaction, they are limited in terms of their applicability to an actual reactor. The objective of this paper is to address this research gap.

This work provides a comprehensive and realizable strategy to optimize and control a batch transesterification reactor. This is achieved by first using optimal control theory to develop an open-loop control strategy using reactor temperature as the control variable. An objective function representing the productivity of the batch reactor is used for this purpose. Subsequently, this optimal reactor temperature trajectory is tracked by using nonlinear model predictive control (NMPC). The NMPC problem is solved using a reduced model of the batch reactor that considers only the heat balance. The advantage of such an approach is that online measurements for all the state variables of the reduced model are available and hence the model is completely observable. This property enables the proposed approach to be implemented on a real batch reactor. Since model parameter values may change over time or may not be known accurately, a batch to batch parameter estimation using evolutionary algorithm is proposed, which uses offline measurements available at the end of the batch. An overview of the structure of this work is given in Fig. 1.

This paper is organized as follows: The next section describes the theoretical foundation of this work. This includes the development of the batch reactor model, discussion on the measurements and observability, description of the evolutionary algorithm for parameter estimation, and the formulation of the advanced control problems. Section 3 describes the simulation results of this work, including those for batch to batch parameter estimation as well as the optimal control and NMPC application. The approach is evaluated with respect to its applicability to a real batch reactor. Finally, Section 4 summarizes the main aspects of this contribution and gives an outlook for further research.

2. Materials and methods

In order to optimize and control the batch transesterification reactor, a realistic model of the process that describes the relationships among its inputs and outputs is needed. With the help of the model, the system is analyzed and different optimization and control strategies are evaluated.

2.1. Transesterification reaction model

Commonly, biodiesel (E) is made by the transesterification reaction between lipids and short chain alcohol such as methanol or ethanol to produce fatty acid esters. The lipids can be derived from animal fats or plants, such as soy, palm and rapeseed. Even the oily part of algae can be extracted and used for biodiesel production. The reaction is driven by a base or acid catalyst. Typically, the reaction is carried out with vegetable oil, methanol and an homogenous alkaline catalyst [17]. Thereby, free fatty acid methyl esters (FAME) are formed from triglyceride (TG) and methanol (A). Three consecutive and reversible reactions occur and the intermediates diglyceride (DG) and monoglyceride (MG) as well as the byproduct glycerol (GL) emerge. These equilibrium reactions can be described by the following equations:

$$\mathrm{TG} + \mathrm{CH_3OH} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathrm{DG} + R_1\mathrm{COOCH_3} \tag{1}$$

$$\mathrm{DG} + \mathrm{CH_3OH} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} \mathrm{MG} + R_2\mathrm{COOCH_3} \tag{2}$$

$$\mathrm{MG} + \mathrm{CH_3OH} \underset{k_6}{\overset{k_5}{\rightleftharpoons}} \mathrm{GL} + R_3\mathrm{COOCH_3} \tag{3}$$

where R_1, R_2 and R_3 are long-chain hydrocarbons, also called fatty acid chains [18]. The reaction rate constant k_i is dependent on the temperature and can be expressed by the Arrhenius equation:

$$k_i(T_R) = k_{0,i}\exp\left(-\frac{E_{a,i}}{RT_R}\right) \quad \mathit{for}\ i = 1, \ldots, 6, \tag{4}$$

where $k_{0,i}$ stands for the respective pre-exponential factor, $E_{a,i}$ stands for the respective activation energy, R represents the universal gas constant and T_R represents the reactor temperature. The state equations of the concentrations can be obtained by a mass