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Modeling and dynamic optimization of fuel-grade ethanol fermentation using fed-batch process

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ABSTRACT

This paper investigates optimization of operational strategies of an industrial ethanol fermentation process. One of the challenges associated with this type or process is that most of the measurements are only taken sporadically, thereby complicating process monitoring and optimization. The one exception to this rule involves temperature measurements, which are readily available. However, an existing model of the plant investigated in this paper does not include an energy balance and, accordingly, the temperature measurements cannot be used to estimate model parameters. This paper addresses these deficiencies and proposes modifications to an existing ethanol fermentation model. The proposed changes include the derivation of an energy balance, modification of the reaction kinetics to include additional inhibition terms, and also estimation of model parameters from industrial data. The new model is validated against plant data and then used for optimization of the process operations. It is shown that modifications of the input profiles for the cooling rate and the glucoamylase addition can lead to an approximately 10% increase in ethanol yield. These are promising results, even though these findings will ultimately need to be validated during real plant operations.

1. Introduction

Fuel-grade ethanol can be produced from plants such as maize, sugar cane, or sweet sorghum. Producing bioethanol has one potential advantage in that the amount of greenhouses gases absorbed during the growing process can reduce the gases produced during the combustion process. Furthermore, ethanol can be used as a substitute for fuel additives (Lin & Tanaka, 2006).

As the world's largest biofuel producer, the U.S. is producing approximately 57 billion liters of ethanol in 2012, and the production is estimated to reach 136 billion liters in 2022 (Walker, 2012). Most of the fuel-grade ethanol in the U.S. is produced from maize-based plants, and more than 90% of the plants make use of the dry mill process, where the whole grain is processed in four steps: milling, liquification, simultaneous saccharification and fermentation (SSF), and distillation (RFA. Accelerating Industry Innovation, 2012). Simultaneous saccharification and fermentation is the most important step in the production process. In this process, dextrin is broken down into fermentable dextrose by glucoamylase, and dextrose is converted into ethanol by yeast, e.g., *S. cerevisiae*. The theoretical maximum yield of ethanol from maize starch is 0.364 (kg ethanol/kg dry corn) (Patzek, 2006), which translates to an ethanol concentration of over 160 (g/l) after SFF in the batch fermenter. Currently, the most advanced commercial plants claim to produce approximately 150 (g/l) of ethanol after SSF, however, the average yield from these plants using traditional techniques is less than 140 (g/l). Improving the operations of the SSF process based on current facilities is undoubtedly the most economic approach to increase ethanol yield, but optimization of SSF operations requires a good understanding of the process, usually represented by data and models.

Models of the SSF process consist of dynamic balances of components such as the concentrations of yeast, dextrose, ethanol, and other substances. A variety of models of different complexity have been developed, ranging from relatively simple models (Fogler, 2005), to quite detailed ones (De Andres-Toro et al., 1998; Lee, Kim, & Rhee, 1992; Ochoa, Yoo, Repke, Wozny, & Yang, 2008). The main differences in the complexity of the models results from

- Addition of intermediate steps in the saccharification process;
- Use of more appropriate kinetics reflecting yeast growth rate, substrate inhibition, and product inhibition;
- Study of the temperature influence on enzyme and yeast activity.

The early work of adding intermediate steps in the saccharification process was done by Lee et al. A kinetic model with a

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Nomenclature

F_{Prop}	Flowrate from the propagation tank (l/h)
F^0_{Prop}	Designed flowrate from the propagation tank (l/h)
t_{start}	Time point that the enzyme starts to flow into the fermenter (h)
t_{drop}	Time point that the enzyme stops flowing into the fermenter (h)
F_{Slurry}	Flowrate from the liquification tank (l/h)
F^0_{Slurry}	Designed flowrate from the liquification tank (l/h)
V	Liquid volume in the fermenter (l)
V_{full}	Volume of the fermenter (l)
V_{GA}	Volume of the glucoamylase in the fermenter (l)
F_{GA}	Flowrate of glucoamylase (l/h)
y_{GA}	Concentration of glucoamylase in the fermenter (g/l)
ρ_{GA}	Density of glucoamylase (g/l)
y_{Dex}	Concentration of dextrin in the fermenter (g/l)
y^{IN}_{Dex}	Concentration of dextrin from liquification tank (g/l)
$y_{dextrose}$	Concentration of dextrose in the fermenter (g/l)
y_{active}	Concentration of active yeast in the fermenter (g/l)
y_{lag}	Concentration of lag yeast in the fermenter (g/l)
y^0_{lag}	Concentration of lag yeast from propagation tank (g/l)
y_{EtOH}	Concentration of ethanol in the fermenter (g/l)
y^0_{EtOH}	Concentration of ethanol from liquification tank (g/l)
T	Temperature inside the fermenter (°F)
T_{ref}	Reference temperature used to calculate internal energy (°F)
H_{feed}	Internal energy from the slurry flow and yeast flow (Btu/h)
H_{cool}	Heat taken away by cooling facility (Btu/h)
F_{cool}	Flowrate of cooling water (gal/h)
ρ	Density of the liquid in the fermenter (g/l)
C_P	Heat capacity of the liquid in the fermenter (Btu/°F/l)
r_{GA}	Dextrin→dextrose conversion rate (h^{-1})
μ_a	Dextrose→ethanol conversion rate (h^{-1})
μ^{max}_a	Maximum dextrose→ethanol conversion rate (h^{-1})
μ_{lag}	Lag yeast→active yeast conversion rate (h^{-1})
μ^{max}_{lag}	Maximum lag yeast→active yeast conversion rate (h^{-1})
μ_s	Dextrose consumption rate (h^{-1})
μ^{max}_s	Maximum dextrose consumption rate (h^{-1})
μ_x	Active yeast growth rate (h^{-1})
μ^{max}_x	Maximum active yeast growth rate (h^{-1})
r_d	Active yeast death rate (h^{-1})
f_a	Ethanol inhibition factor

series of Michaelis–Menten equations has been proposed by introducing a degree of polymerization (Lee et al., 1992). This approach has subsequently been incorporated into several other models to provide a more detailed description of the saccharification process (Murthy, Johnston, Rausch, Tumbleson, & Singh, 2012). The kinetics of SSF have also been extensively studied: the growth rate of yeast and the conversion rate between different substances are usually expressed by a Monod equation, while Moser and Tessier growth laws have alternatively been used to provide better agreement with experimental data at the beginning or end of fermentation. Also, several different types of equations have been used to account for substrate and product inhibition in various models (Mulchandani & Luong, 1989).

The operating temperature has been found to have a significant impact on the process. Ethanol fermentation is an exothermic process and temperature changes will significantly affect enzyme and yeast activity. This influence of the temperature on enzyme and yeast activity is usually expressed using Arrhenius-type equations such as those presented by Carvalheiro et al. (Banat, Nigam, Singh, Marchant, & McHale, 1998; Phisalaphong, Srirattana, & Tanthapanichakoon, 2006). Due to this temperature dependence, glucoamylase has an optimum activity at 140 °F in the saccharification process, while the optimal temperature for yeast growth and ethanol fermentation is in the range of 84–94 °F. These competing optimal process temperatures for the SSF process highlight the complexity of selecting an optimal temperature profile over the course of a batch. It should be noted that most commercial plants hold the temperature constant between 86 and 90 °F.

One significant challenge for the use of SSF models in commercial plants is the lack of data, since lag yeast, active yeast, and dead yeast cannot be measured independently (dye or counting numbers using a microscope have proven to be unreliable for this system). In addition, fed-batch fermenters are operated as a "black box". Dextrose and ethanol concentrations can be measured only every few hours and other intermediate substances are difficult to measure. Due to this lack of data, it is non-trivial to accurately estimate model parameters from plant data, i.e., a model may fit existing data well, but it is not possible to determine if the parameters are within a reasonable range as the models are overparameterized. The one process variable that is measured often in commercial plants is the process temperature, however, an energy balance is required if these temperature data are to be used for parameter estimation or monitoring of any quantity other than just the temperature. Unfortunately, none of the existing models for SSF include an energy-balance equation as SSF is a complex process and energy balances require a significant number of parameters and relationships to describe the thermo-physical properties. This paper addresses the above-mentioned challenges by

- Expanding an existing model to also include an energy-balance equation with new parameters that are to be estimated from available data;
- Establishing the relationship between cooling water flowrate, temperature, and active yeast concentration, so that temperature data can be used to estimate unknown parameters arising from balance equations other than the energy balance;
- Computing optimal input profiles for a fermenter used for ethanol fermentation by using the developed model and a simultaneous approach for solving the dynamic optimization problem.

The authors believe that this combination of a model, which is based upon industrial plant data, with the determination of an optimal input profile for the manipulated variables during a batch is of interest to practitioners and researchers alike. The paper is structured as follows: preliminaries about the process, the model, and dynamic optimization are presented in Section 2. Section 3 discusses the presented model in detail, including the estimated parameters. The optimization problem for determining optimal input profiles is formulated and solved in Sections 4 and 5 presents the conclusions.

2. Preliminaries

2.1. Description of industrial ethanol fermentation

Fuel-grade ethanol is produced in one of two ways, using either the wet mill or dry mill process. Wet milling involves