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Model-based plantwide optimization of large scale lignocellulosic bioethanol plants

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ABSTRACT

Second generation biorefineries transform lignocellulosic biomass into chemicals with higher added value following a conversion mechanism that consists of: pretreatment, enzymatic hydrolysis, fermentation and purification. The objective of this study is to identify the optimal operational point with respect to maximum economic profit of a large scale biorefinery plant using a systematic model-based plantwide optimization methodology. The following key process parameters are identified as decision variables: pretreatment temperature, enzyme dosage in enzymatic hydrolysis, and yeast loading per batch in fermentation. The plant is treated in an integrated manner taking into account the interactions and trade-offs between the conversion steps. A sensitivity and uncertainty analysis follows at the optimal solution considering both model and feed parameters. It is found that the optimal point is more sensitive to feedstock composition than to model parameters, and that the optimization supervisory layer as part of a plantwide automation system has the following benefits: (1) increases the economical profit, (2) flattens the objective function allowing a wider range of operation without negative impact on profit, and (3) reduces considerably the uncertainty on profit.

1. Introduction

Second generation lignocellulosic biorefineries reached commercial reality in 2012 [1], and several large scale plants are in operation nowadays including Beta Renewables, Abengoa Bioenergy, GranBio and POET-DSM [2]. Most biorefineries produce bioethanol, but the drop in oil price reduced the demand on the biofuel. However, plant upgrades for chemicals with higher-added values are pursued making biorefineries still competitive in an oil dependent environment [3].

This study deals with optimizing the daily operation of a large scale second generation biorefinery with a well established conversion route for bioethanol production. The biomass conversion route is typically the result of a previous techno-economic optimization assessment that took place at a design level before constructing the plant. In contrast, the focus of this contribution is to perform model-based optimization of the daily operation of a demonstration scale plant that has already been designed and built, which is a new scope as it addresses the operation optimization and not the design phase.

The latest developments in biorefinery technology show that integrating the facility with a nearby power plant following the Integrated Biomass Utilization System (IBUS) [4] has a major impact on cost efficiency. E.g. the Inbicon plant is integrated with Asnæsværket situated in Kalundborg Denmark and they are both owned by the same company, DONG Energy. The symbiosis between the biorefinery and the power plant allows the exchange of by-products for consumables, e.g. lignin bio-pellets for steam.

Modeling and simulation are used in this study as enabling technology to analyze plant performance as basis for an overall optimization. The objective of the optimization problem is to maximize the plant economical profit, considering prices for the most important consumables and end products of the process: biomass, enzymes, yeast and ethanol.

The conversion route from lignocellulosic material to products with higher added value consists of: pretreatment, enzymatic hydrolysis, fermentation, and purification [1,4]. Lignocellulosic biomass contains cellulose, hemicellulose (xylan and arabinan), lignin, ash, and other residues [5]. The scope of the pretreatment

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Nomenclature

β_k	the β coefficient in global sensitivity analysis
δ_k	non-dimeansional local differential sensitivity measure of cost function c with respect to parameter θ_k
$\dot{x}$	vector of state derivatives used in dynamic modelling
$\dot{x}_f$	vector of state derivatives used in fermentation dynamic model
$\mathbf{R}_F$	correlation matrix for fermentation model parameters
$\mathbf{R}_L$	correlation matrix for liquefaction model parameters
$\mathbf{R}_P$	correlation matrix for pretreatment model parameters
$\mathbf{R}$	correlation matrix for the entire integrated process
σ_y	standard deviation of the objective function
σ_{θ_k}	standard deviation of parameter θ_k
θ	the entire vector of model parameters. See Table 1 from the supplementary material for a full list of model parameters
θ_k	model parameter k. See Table 1 from the supplementary material for a full list of model parameters
θ_R	reduced set of model parameters after sensitivity analysis
$c(x, u)$	cost function as a relation of model states x and decision variables u. [unitcost]
C_b	feedstock composition in [g/kg]
c_f	cost of fermentation
c_o	value of cost function at the optimal solution
C_{AC_S}	acetyls concentration [g/kg]
C_{C_S}	cellulose concentration [g/kg]
c_{eh}	cost of enzymatic hydrolysis
C_{Eth}	concentration of ethanol [g/kg]
c_{ss_k}	cost value in steady-state when varying parameter k
E_H	5-HMF activation energy
$f(x, u)$	nonlinear process model of states x and inputs u formulated as equality constraints
F_b	feedstock flow rate [kg/h]
F_e	enzyme dosage [kg/h]
F_s	steam flow rate [kg/h]
$g(x, u)$	inequality constraints used as ranges for decision variables
$h(x_f, u_f)$	dynamic model for C5-C6 co-fermentation
K_2	cellulose to glucose reaction constant
M_y	yeast seed [kg]
M_{Eth}	mass of ethanol [kg]
P_b	feedstock price [unitcost/(kg/h)]
P_e	enzyme price [unitcost/(kg/h)]
P_s	steam price [unitcost/(kg/h)]
P_y	yeast price [unitcost/kg]
P_{MP_X}	ethanol inhibition on xylose uptake
$q_{Max_{Ac}}$	maximum acetate uptake rate
R_B	severity factor dependency
t_f	final time in fermentation [h]
T_{tr}	thermal reactor temperature [°C]
u	vector with all decision variables
u_f	input variables in fermentation
x_f	process states in fermentation
Y_{Cell_G}	biomass growth on glucose
Y_{Eth_G}	ethanol production from glucose uptake
Y_{Eth_X}	ethanol production from xylose uptake
z_i	initial guess for the optimization problem
z_o	optimal solution

process is to open the biomatrix, relocate lignin and partially hydrolyze the hemicellulose such that cellulose would become more accessible to the downstream process of enzymatic hydrolysis [6]. During pretreatment, inhibitors such as organic acids, furfural, and 5-Hydroxymethylfurfural (5-HMF) are also created due to sugar degradation. Organic acids change the pH of medium, but can be automatically neutralized by a pH controller for ensuring optimal enzymatic conditions [7]. Furfural, 5-HMF, and acetate are fermentation inhibitors [8], while the remaining hemicellulose fraction leads to xylooligomers and xylose formation in the enzymatic hydrolysis process, which strongly inhibit the enzymatic activity [9].

There are trade-offs between the conversion steps. Too little biomass pretreatment would reduce the exposed cellulose to enzymes, and also increases the amount of hemicellulose for enzymatic hydrolysis, which would eventually decrease the glucose yield due to xylose and xylooligomers inhibition. On the other hand, too much biomass pretreatment would increase the amount of fermentation inhibitors leading to a lower ethanol yield.

Most existing studies focus on operational optimization conducting small scale experiments in the laboratory for finding the best pretreatment conditions such that ethanol yield is maximized [10–13]. The traditional focus is on one unit at a time (pretreatment versus enzymatic hydrolysis versus fermentation) but the entire process is rarely considered although the biomass conversion steps are inherently dependent and integrated. The single step methods are suboptimal from an economic point of view as they do not focus on overall process economics. Furthermore, in existing studies, the enzymatic hydrolysis and fermentation processes are usually conducted following a fixed recipe, i.e. no correction action or feedback is taken to counteract the effects of inhibitors. For example, one could increase the enzyme dosage when xylooligomers and xylose inhibit glucose production, or adjust the yeast seed in fermentation to compensate for inhibitors.

Therefore the focus of this paper is on systematic methods and tools to facilitate the further process optimization and daily operation of second generation bioethanol plants. The paper shows how overall optimization can be achieved and how sensitivity and uncertainty can be assessed with respect to feedstock composition and kinetic parameters. A Monte Carlo technique with Latin Hypercube Sampling and correlation control is used for the uncertainty analysis following the methodology from [14,15].

This paper is structured as follows: the methods section revises the methodology for building the optimization layer for plantwide operation, along with the theoretical part of the sensitivity and uncertainty analysis. The results and discussion follow where the profit curve, costs, and optimal solutions are presented along with their uncertainty bounds. The paper concludes with a summary of all important findings.

2. Methods

2.1. Second generation bioethanol plant

Fig. 1 illustrates a generic large scale second generation biorefinery concept for bioethanol production. The pretreatment process consists of a continuous thermal reactor and a separation press, which were modeled and analyzed in [16,17]. The thermal reactor is equipped with temperature control for adjusting the reaction temperature T_{tr} [18]. When hemicellulose is hydrolyzed, it produces xylose and arabinose (C5 sugars). After separation, the liquid part containing the C5 sugars is directly pumped into fermentation reactors, bypassing the enzymatic hydrolysis reactors. Cellulose can also be degraded in the pretreatment process,