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A framework for model-based optimization of bioprocesses under uncertainty: Lignocellulosic ethanol production case

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ABSTRACT

This study presents the development and application of a systematic model-based framework for bioprocess optimization. The framework relies on the identification of sources of uncertainties via global sensitivity analysis, followed by the quantification of their impact on performance evaluation metrics via uncertainty analysis. Finally, stochastic programming is applied to drive the process development efforts forward subject to these uncertainties. The framework is evaluated on four different process configurations for cellulosic ethanol production including simultaneous saccharification and co-fermentation and separate hydrolysis and co-fermentation (SSCF and SHCF, respectively) technologies in different operation modes (continuous and continuous with recycle). The results showed that parameters related to pretreatment (e.g. activation energy of the reaction for glucose production, order of the reaction, etc.), hydrolysis (inhibition constant for xylose on conversion of cellulose and cellobiose, etc.) and co-fermentation (ethanol yield on xylose, inhibition constant on microbial growth, etc.), are the most significant sources of uncertainties affecting the unit production cost of ethanol with a standard deviation of up to 0.13 USD/gal-ethanol. Further stochastic optimization demonstrated the options for further reduction of the production costs with different processing configurations, reaching a reduction of up to 28% in the production cost in the SHCF configuration compared to the base case operation. Further, the framework evaluated here for uncertainties in the technical domain, can also be used to evaluate the impact of market uncertainties (feedstock prices, selling price of ethanol, etc.) and political uncertainties (such as subsidies) on the economic feasibility of lignocellulosic ethanol production.

1. Introduction

Process optimization is an important area within process systems engineering (PSE), actively used in the development, decision making, and subsequent improvement of chemical processes (e.g. for the design, synthesis and operation), aiming at maximizing the process performance while at the same time minimizing the processing costs (Grossmann & Guillén-Gonsálbez, 2010). Many mathematical programming techniques are applied in process optimization, such as nonlinear programming, mixed-integer non-linear programming, multi-objective optimization, quadratic programming, among others (Shapiro, Dentcheva, & Ruszczyński, 2009).

In reality the above-mentioned programming techniques can be further complicated by several sources of uncertainties that can be encountered in practice when solving optimization problems, where the variability of uncertain parameters is commonly neglected (Acevedo & Pistikopoulos, 1996; Grossmann & Guillén-Gonsálbez, 2010). The process optimization is a particularly challenging task in (bio)process development, notably in processes such as cellulosic bioethanol production because several processing configuration options are available and the plant operation is characterized by tight cost and yield margins. In addition, the uncertainties present in the system as a result of technological factors and, economical factors as well as the uncertainty in the mathematical model and parameters employed to perform the optimization task pose severe challenges. A number of publications concerning optimization under uncertainty are available, covering a range of topics, such as process synthesis, design and control under uncertainty (Acevedo & Pistikopoulos, 1996; Pintarič & Kravanja, 2008; Ricardez-Sandoval, Douglas, & Budman, 2011), planning under uncertainty (Hansen, Grunow, & Gani, 2011), uncertainty on scheduling (Wang & Rong, 2010), strategic and global supply chain networks (Verderame & Floudas, 2011; You & Grossmann, 2008), etc. Most of those publications, when addressing the uncertainty of the optimization problem, have focused on

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Nomenclature

$A^{PT}_{1,Xy}$ pre-exponential factor for xylose production, h^{-1}
$A^{PT}_{2,Xy}$ pre-exponential factor for xylose degradation, h^{-1}
$A^{PT}_{1,A}$ pre-exponential factor for arabinose production, h^{-1}
$A^{PT}_{2,A}$ pre-exponential factor for arabinose degradation, h^{-1}
$A^{PT}_{1,G}$ pre-exponential factor for glucose production, h^{-1}
$A^{PT}_{2,G}$ pre-exponential factor for glucose degradation, h^{-1}
$A^{PT}_{1,F}$ pre-exponential factor for furfural production, h^{-1}
$A^{PT}_{2,F}$ pre-exponential factor for furfural degradation, h^{-1}
$A^{PT}_{1,ASL}$ pre-exponential factor for reaction to produce ASL, h^{-1}
$A^{PT}_{2,ASL}$ pre-exponential factor for reaction to consume ASL, h^{-1}
$A^{PT}_{3,ASL}$ pre-exponential factor for reversible reaction to produce ASL, h^{-1}
b_i regression coefficients in the fitted linear multivariate model
C_{Acid} acid concentration, %(wt/v)
C_{An} arabinan concentration, g/kg
C_{Ash} ash concentration, g/kg
C_{ASL} acid-soluble lignin concentration, g/kg
C_{Ln} lignin concentration, g/kg
C_{Xn} xylan concentration, g/kg
C_{Gn} glucan (cellulose) concentration, g/kg
CI confidence interval
C_{OC} other compounds concentration, g/kg
c^T constant vector of economic information, USD/kg
$c^T \mathbf{x}$ deterministic term of the stochastic optimization cost function, USD/gal-ethanol
C_{yeast} yeast concentration, g/kg
SHCF with double recycle separate hydrolysis and co-fermentation working in continuous and recycle for both unit operations
SHCF with single recycle separate hydrolysis and co-fermentation working in continuous and recycle for in the enzymatic hydrolysis and continuous regime in the co-fermentation reactor
DLB1.0 dynamic lignocellulosic bioethanol model version 1.0
E_a activation energy for enzyme 1, cal/mol
$E_{a,\beta G}$ activation energy for enzyme 2, cal/mol
$Ea^{PT}_{1,Xy}$ activation energy reaction to produce xylose, J/mol
$Ea^{PT}_{2,Xy}$ activation energy for xylose degradation, J/mol
$Ea^{PT}_{1,A}$ activation energy reaction to produce arabinose, J/mol
$Ea^{PT}_{2,A}$ activation energy reaction for arabinose degradation, J/mol
$Ea^{PT}_{1,G}$ activation energy reaction to produce glucose, J/mol
$Ea^{PT}_{2,G}$ activation energy reaction for glucose degradation, J/mol
$Ea^{PT}_{1,F}$ activation energy reaction to produce furfural, J/mol
$Ea^{PT}_{2,F}$ activation energy reaction for furfural degradation, J/mol
$Ea^{PT}_{1,ASL}$ activation energy reaction to produce ASL, J/mol
$Ea^{PT}_{2,ASL}$ activation energy reaction for ASL degradation, J/mol
$Ea^{PT}_{3,ASL}$ activation energy for reversible reaction to produce ASL, J/mol
EL_1 enzyme loading of exo-β-1,4-cellobiohydrolase + endo-β-1,4-glucanase, mg-enzyme/g-cellulose
EL_2 enzyme loading of β-glucosidase, mg-enzyme/g-cellulose
$E_{1\,max}$ maximum mass of enzyme 1 that can be adsorbed onto a unit mass of substrate, g-protein/g-substrate
$E_{2\,max}$ maximum mass of enzyme 2 that can be adsorbed onto a unit mass of substrate, g-protein/g-substrate
$Et_{max,G}$ ethanol concentration above which cells do not grow in glucose fermentation, 95.40 for $Et \le 95.4$ g/L, 129.90 for 95.4 g/L < $Et \le 129.9$ g/L
$Et_{max,Xy}$ ethanol concentration above which cells do not grow in xylose fermentation, g/L
$Et'_{max,G}$ ethanol concentration above which cells do not produce ethanol in glucose fermentation, 103 for $Et \le 103$ g/L, 136.40 for 103 g/L < $Et \le 136.4$ g/L
$Et_{max,Xy}$ ethanol concentration above which cells do not produce ethanol in xylose fermentation, g/L
$\mathbf{E}_s[f(x,\theta_i)]$ expected value of the stochastic optimization cost function
$f(x,(\theta_i))$ uncertain term of the stochastic optimization cost function, USD/gal-ethanol
g set of inequality constrains
h vector of equality constrains
K_{1ad} dissociation constant for enzyme 1, g-protein/g-substrate
K_{2ad} dissociation constant for enzyme 2, g-protein/g-substrate
$k_{1\,ad,Eq}$ rate of adsorption in equilibrium for enzyme 1
$k_{2\,ad,Eq}$ rate of adsorption in equilibrium for enzyme 2
$k^{EH}_{1,G}$ reaction rate constant for glucose 1 in the enzymatic hydrolysis, g/(mg h)
$k^{EH}_{2,G}$ reaction rate constant for glucose 2 in the enzymatic hydrolysis, h^{-1}
k^{EH}_{G2} reaction rate constant for cellobiose formation in the enzymatic hydrolysis, g/(mg h)
$K^{EH}_{1\,IEt}$ inhibition constant for ethanol 1 in the SSCF unit, g/kg
$K^{EH}_{1\,IG}$ inhibition constant for glucose 1, g/kg
$K^{EH}_{2\,IG}$ inhibition constant for glucose 2, g/kg
$K^{EH}_{3\,IG}$ inhibition constant for glucose 3, g/kg
$K^{EH}_{1\,IG2}$ inhibition constant for cellobiose 1, g/kg
$K^{EH}_{2\,IG2}$ inhibition constant for cellobiose 2, g/kg
$K^{EH}_{1\,IXy}$ inhibition constant for xylose 1, g/kg
$K^{EH}_{2\,IXy}$ inhibition constant for xylose 2, g/kg
$K^{EH}_{3\,IXy}$ inhibition constant for xylose 3, g/kg
$K^{CF}_{1\,G}$ Monod constant, for growth on glucose, g/L
$K^{CF}_{2\,Xy}$ Monod constant, for growth on xylose, g/L
$K'^{CF}_{5\,IG}$ inhibition constant, for product formation from glucose, g/L
$K'^{CF}_{6\,IXy}$ inhibition constant, for product formation from xylose, g/L
$K'^{CF}_{5\,G}$ Monod constant, for product formation from glucose, g/L
$K'^{CF}_{6\,Xy}$ Monod constant, for product formation from xylose, g/L