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Sensitivity analysis and stochastic modelling of lignocellulosic feedstock pretreatment and hydrolysis

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ABSTRACT

Pretreatment and hydrolysis of lignocellulosic biomass are affected by several uncertainties, which must be systematically considered for a robust process design. In this work, stochastic simulations for expected uncertainties in feedstock composition, kinetic parameter values, and operational parameter values for these two steps were performed. The results indicated that these uncertainties significantly impacted the concentration profiles, which could also affect the optimal batch time. Global sensitivity analysis was then used to identify the critical uncertain parameters. In the feedstock components, cellulose and xylan fractions for acid pretreatment and cellulose fraction for enzymatic hydrolysis were important. Temperature was the most sensitive operating parameter for both acid pretreatment and hydrolysis. The activation energies for different reactions were ranked in terms of their impact on process output. The selected parameters were used to develop stochastic process models using Ito process and mean reverting process for feed composition and kinetic parameter uncertainty.

1. Introduction

Production of biomass-based renewable fuels such as ethanol from lignocellulosic biomass like agricultural residue, forestry residue, and dedicated energy crops have generated substantial interest in recent times (Hahn-Hägerdal et al., 2006). However, conversion of lignocellulosic biomass to ethanol is currently economically not feasible. While process development research continues at the interface of science and engineering, process design improvement and optimization is a potential avenue to achieve techno-economic feasibility and enable scale-up from pilot to commercial scale. It will lead to better material and energy efficiencies, higher yields, lower waste generation, and improved cost-efficiency. However, the presence of various uncertainties creates several challenges for process design and optimization.

A number of uncertainties influence the overall process of ethanol production from lignocellulosic feedstock (Kenney et al., 2013). From the viewpoint of the process operation, the uncertainties can be categorized into two types, namely internal and external. Internal uncertainty refers to the lack of process knowledge such as reaction mechanism, model structure, and the kinetic parameter values. On the other hand, external uncertainty captures the impact of market conditions that impact the process via flow rate, feedstock composition, product specification, prices, and supply of utilities. Following factors are of particular importance with respect to the biochemical processing of lignocellulosic biomass:

- **Variation in feedstock composition**: Various potential lignocellulosic feedstock alternatives such as forest residues, agricultural residues (corn stover, bagasse, and rice husk), municipal solid wastes, as well as dedicated energy crops such as *Jatropha curcas*, switchgrass, sorghum, and Miscanthus, are being proposed and evaluated (Sukumaran et al., 2010). The composition of each of these feedstock will vary from each other. The composition even for the same feedstock can vary significantly due to the impact of short-term weather fluctuations and site-specific production techniques. Templeton et al. (2009) quantified the significant variability in corn stover composition collected from different locations in the Midwestern US Hu et al. (2010) found that the composition varied for leaves, internodes, and nodes of switchgrass. Moreover, the composition will also depend on the harvest date and cultivation treatment. Ash content can also vary significantly as a result of a change in intrinsic biomass properties, such as plant type, maturity, and anatomical fraction collected (Tao et al., 2012; Kenney et al., 2013). For instance, the range of ash varied from 0.1% in woody biomass (such as debarked pinewood) to as high as 25% in the herbaceous crop (such as rice straw) (Tao et al., 2012).

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Nomenclature

A_i	Feedstock components of i^{th} reaction scheme (i = 1,2,3,. . .,7)
R_i	Desired products of i^{th} reaction scheme (i = 1,2,3,. . .,7)
S_i	Degradation products of i^{th} reaction scheme (i = 1,2,3,. . .,7)
c	Cellulose
x	Xylan
a	Arabinan
g	Glucuronic acid
f	Furfural
l	Lignin
$[C_{Aj}]$	Concentration of feedstock of j^{th} component (g/g of dry bagasse) (j = c, g, l)
$[C_{Rj}]$	Concentration of desired product of j^{th} component (g/g of dry bagasse) (j = c, g, l)
$[C_{Sj}]$	Concentration of degradation product of j^{th} component (g/g of dry bagasse) (j = c, g, l)
$[C_{Ak}]$	Concentration of feedstock of k^{th} component (g/g of dry bagasse) (k = x, a)
$[C_{Rk}]$	Concentration of desired product of k^{th} component (g/g of dry bagasse) (k = x, a)
$[C_{Sk}]$	Concentration of degradation product of k^{th} component (g/g of dry bagasse) (k = x, a)
$[C_{Rf}]$	Concentration of furfural from xylan and arabinan (g/g of dry bagasse)
$[C_{Sf}]$	Concentration of degradation product from furfural (g/g of dry bagasse)
k_{1j}	Rate constant for first reaction of j^{th} component (j = c, g, l)
k_{2j}	Rate constant for second reaction of j^{th} component (j = c, g, l)
k_{1k}	Rate constant for first reaction of k^{th} component (k = x, a)
k_{2k}	Rate constant for second reaction of k^{th} component (k = x, a)
k_{1f}	Rate constant for furfural formation from xylan and arabinan
k_{2f}	Rate constant for degradation product from furfural
k_{1i}	Rate constant for first reaction of i^{th} reaction scheme (i = 1,2,3,. . .,7)
k_{2i}	Rate constant for second reaction of i^{th} reaction scheme (i = 1,2,3,. . .,7)
A_{mi}	Pre-exponential factor of m^{th} parameter for reaction i (s^{-1}) (i = 1,2,3,. . .,7; m = 1,2)
E_{mi}	Activation energy of m^{th} parameter for i^{th} reaction (KJ/mol) (i = 1,2,3,. . .,7; m = 1,2)
n_{mi}	Order of m^{th} step for i^{th} reaction with respect to acid concentration (i = 1,2,3,. . .,7; m = 1,2)
C_{acid}	Acid concentration (wt% of liquid)
Φ	Ratio of solid bagasse material to liquid ($g.g^{-1}$)
E_{iB}	Bound concentration of enzyme (g/kg) (i = 1,2)
E_{iF}	Free concentration of enzyme (g/kg) (i = 1,2)
Ki_{ad}	Dissociation constant for enzyme adsorption (g protein/g cellulose) (i = 1,2)
E_{max}	Maximum mass of enzyme that can adsorb onto a unit mass of substrate (g protein/g cellulose)
r_1	Rate equations for cellulose to cellobiose,
r_2	Rate equations for cellulose to glucose
r_3	Rate equations for cellobiose to glucose
k_{ir}	Reaction rate constant (kg/g.h) (i = 1,2,3)
G	Concentration (g/kg) of glucose
G_2	Concentration (g/kg) of cellobiose
S	Concentration (g/kg) of substrate (cellulose)
X	Concentration (g/kg) of xylose
K_{iIG}	Inhibition constants for glucose (g/kg) (i = 1,2,3)
K_{iIG2}	Inhibition constants for cellobiose (g/kg) (i = 1,2)
K_{iIX}	Inhibition constants for xylose (g/kg) (i = 1,2,3)
K_{3M}	Substrate (cellobiose) saturation constant (g/kg)
$\mathbf{x}$	State vector
$\mathbf{u}$	Parameter vector
r	Perturbation vector, r = [−0.2 −0.1 0.1 0.2]
x	Uncertain variable
dz	Increment in wiener process and defined as, $\varepsilon_t\sqrt{\Delta t}$
ε_t	White noise at each time instant
Δt	Time progression step length
C_p	State variable of p^{th} component (p = 1,2,3,. . .,17)
Ψ_p	Variance parameter for p^{th} component (p = 1,2,3,. . .,17)
f_p	RHS terms of state equations of deterministic model (p = 1,2,3,. . .,17)
K	Uncertain model parameter
μ	Expectation of the uncertain parameter range
ξ	Reversion parameter

- **Variation in particle morphology and moisture**: Particle morphology is affected by operation parameters such as milling speed, screening as well as material feed rate, particle size, and moisture content (Miao et al., 2011). This influences the variability during the handling and feeding system of feedstock. Other than particle morphology, the performance of the biomass feeding and handling system also depends upon the particle size, sphericity, moisture content, temperature, bulk density, and history of the material. Moisture content varies considerably among biomass types, geographic and weather condition, and water availability (Kenney et al., 2013).
- **Lack of process knowledge**: Novel pretreatment and hydrolysis methods for biomass processing are being developed (Huber et al., 2006). The performance parameters of these processes such as kinetic constants, conversion efficiency, and yield are known only at laboratory or pilot scale. Moreover, the kinetic parameters are often determined using pure components, such as microcrystalline cellulose, in laboratory experiments. The actual process will, however, involve the presence of multiple components which may lead to interactions and inhibitory effects and consequent changes in the kinetic parameters for a realistic process. Thus, values of kinetic parameters for a commercial scale process need to be estimated, which can be considered as an important source of uncertainty (Ulas and Diwekar, 2004).
- **Biomass mixing and standardization**: Biomass has very low energy and bulk density. Therefore, multiple sources of biomass may need to be processed together in a single facility to reach the required processing capacity. This is especially true for countries such as India where land availability is limited (Sukumaran et al., 2010). Hess et al. (2009) have proposed mixing of feedstock to improve supply efficiency. However, the compositional variability of different feedstock, and different mixing ratios will impact the input biomass quality to the biorefinery.
- **Seasonal availability and dynamic fluctuations**: The biomass feedstock is available on a seasonal basis, and therefore the feedstock available for processing may vary. Although storage of biomass is possible to ensure a relatively steady supply, short-term dynamic fluctuations in the supply quantity and quality are still expected.