Sensitivity analysis and stochastic modelling of lignocellulosic feedstock pretreatment and hydrolysis

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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 reversion process for feed composition and kinetic parameter uncertainty.

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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<sub>i</sub>**: Feedstock components of the <i>i</i>th reaction scheme (i = 1, 2, 3, ..., 7)
- **R<sub>i</sub>**: Desired products of the <i>i</i>th reaction scheme (i = 1, 2, 3, ..., 7)
- **S<sub>i</sub>**: Degradation products of the <i>i</i>th reaction scheme (i = 1, 2, 3, ..., 7)
- **C**: Cellulose
- **X**: Xylan
- **a**: Arabinan
- **g**: Glucuronic acid
- **f**: Furfural
- **l**: Lignin
- **[C<sub>j</sub>]<sub>i</sub>**: Concentration of feedstock of the <i>j</i>th component (g/g of dry bagasse) (i = c, g, l)
- **[C<sub>j</sub>]<sub>i</sub>**: Concentration of desired product of the <i>j</i>th component (g/g of dry bagasse) (i = c, g, l)
- **[C<sub>j</sub>]<sub>i</sub>**: Concentration of degradation product of the <i>j</i>th component (g/g of dry bagasse) (i = c, g, l)
- **[C<sub>Ak</sub>]<sub>i</sub>**: Concentration of feedstock of the <i>k</i>th component (g/g of dry bagasse) (i = k = x, a)
- **[C<sub>Rk</sub>]<sub>i</sub>**: Concentration of desired product of the <i>k</i>th component (g/g of dry bagasse) (i = k = x, a)
- **[C<sub>Sf</sub>]<sub>i</sub>**: Concentration of degradation product of the <i>k</i>th component (g/g of dry bagasse) (i = k = x, a)
- **[C<sub>Sf</sub>]<sub>i</sub>**: Concentration of furfural from xylan and arabinan (g/g of dry bagasse)
- **k<sub>j1</sub>**: Rate constant for the first reaction of the <i>j</i>th component (i = c, g, l)
- **k<sub>j2</sub>**: Rate constant for the second reaction of the <i>j</i>th component (i = c, g, l)
- **k<sub>k1</sub>**: Rate constant for the first reaction of the <i>k</i>th component (i = k = x, a)
- **k<sub>k2</sub>**: Rate constant for the second reaction of the <i>k</i>th component (i = k = x, a)
- **k<sub>1f</sub>**: Rate constant for furfural formation from xylan and arabinan
- **k<sub>2f</sub>**: Rate constant for degradation product from furfural
- **k<sub>1i</sub>**: Rate constant for the first reaction of the <i>i</i>th reaction scheme (i = 1, 2, 3, ..., 7)
- **k<sub>2i</sub>**: Rate constant for the second reaction of the <i>i</i>th reaction scheme (i = 1, 2, 3, ..., 7)
- **A<sub>mi</sub>**: Pre-exponential factor of the <i>m</i>th parameter for reaction (i = 1, 2, 3, ..., 7; m = 1, 2)
- **E<sub>mi</sub>**: Activation energy of the <i>m</i>th parameter for reaction (i = 1, 2, 3, ..., 7; m = 1, 2)
- **n<sub>rmi</sub>**: Order of the <i>m</i>th step for reaction with respect to acid concentration (i = 1, 2, 3, ..., 7; m = 1, 2)
- **C<sub>acid</sub>**: Acid concentration (wt% of liquid)
- **Φ**: Ratio of solid bagasse material to liquid (g/g<sup>-1</sup>)
- **E<sub>B</sub>**: Bound concentration of enzyme (g/kg) (i = 1, 2)
- **E<sub>f</sub>**: Free concentration of enzyme (g/kg) (i = 1, 2)
- **K<sub>ad</sub>**: Dissociation constant for enzyme adsorption (g protein/g cellulose) (i = 1, 2)
- **E<sub>max</sub>**: Maximum mass of enzyme that can adsorb onto a unit mass of substrate (g protein/g cellulose)
- **r<sub>1</sub>**: Rate equations for cellulose to cellulbiose
- **r<sub>2</sub>**: Rate equations for cellulbiose to glucose
- **r<sub>3</sub>**: Rate equations for cellulose to glucose
- **k<sub>ir</sub>**: Reaction rate constant (kg/g/h) (i = 1, 2, 3)

**G**: Concentration (g/kg) of glucose
**G<sub>2</sub>**: Concentration (g/kg) of cellobiose
**S**: Concentration (g/kg) of substrate (cellulose)
**X**: Concentration (g/kg) of xyllose
**K<sub>1G</sub>**: Inhibition constants for glucose (g/kg) (i = 1, 2, 3)
**K<sub>2G</sub>**: Inhibition constants for cellobiose (g/kg) (i = 1, 2)
**K<sub>1X</sub>**: Inhibition constants for xylose (g/kg) (i = 1, 2, 3)
**K<sub>3M</sub>**: Substrate (cellobiose) saturation constant (g/kg)
**x**: State vector
**u**: Parameter vector
**r**: Perturbation vector, r = [−0.2 −0.1 0.1 0.2]
**σ**: Uncertain variable
**d<sub>z</sub>**: Increment in wiener process and defined as, σ<sub>i</sub>√Δt
**e<sub>1</sub>**: White noise at each time instant
**Δt**: Time progression step length
**C<sub>p</sub>**: State variable of the <i>p</i>th component (i = 1, 2, 3, ..., 17)
**Ψ<sub>p</sub>**: Variance parameter for the <i>p</i>th component (i = 1, 2, 3, ..., 17)
**f<sub>p</sub>**: RHS terms of state equations of deterministic model (i = 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 (Ul-Islam 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 (Sukumar 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.
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