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Optimal control of dilute acid pretreatment and enzymatic hydrolysis for processing lignocellulosic feedstock

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ABSTRACT

Lignocellulosic feedstock is one of the potential renewable sources for producing ethanol for transportation. The process steps viz., acid pretreatment and enzymatic hydrolysis in bio-chemical process route are intended to produce fermentable sugars, which can be readily fermented for producing ethanol. However, the dilute acid pre-treatment and enzymatic hydrolysis process steps are found to be economically inefficient. The present work aims at optimizing these process steps for improving the process performance. Such optimization is expected to increase conversion, reduce energy or material requirement, thereby improving the economics. The kinetic models of acid pretreatment and enzymatic hydrolysis for lignocellulosic feedstock processing are adapted from literature. Subsequently, these kinetic models are augmented by associated mass and energy balances, to develop a batch reactor model and fed-batch reactor model for dilute acid pretreatment and enzymatic hydrolysis processes, respectively. Optimal control with Pontryagin's maximum principle has been implemented to determine the optimal time dependent profiles of heating and cooling fluid flow rates and operating temperatures for acid pretreatment and substrate feed rate profile for enzymatic hydrolysis to optimize the respective processes performance. Different objective functions such as maximizing concentration of desired product, minimizing the batch time, and maximizing profit have been considered. The simulation results yielded an increase of 6.7% and 8.8% in final concentration of desired product; 43% and 42.5% reduction in batch processing time for pretreatment and enzymatic hydrolysis processes, respectively. Finally, the simulation results have also provided optimal operating policies which have increased the profit of pretreatment by 124% and enzymatic hydrolysis by 150%, thereby improving the techno-economic feasibility for processing lignocellulosic feedstock.

1. Introduction

To overcome the current energy demand and future potential energy crisis due to the depleting fossil resources, research on alternative fuel sources has been ongoing for quite some time, especially for liquid transportation fuels [1,2]. Lignocellulosic feedstock such as wheat straw, corn stover, sugarcane bagasse, switchgrass, and rice husk, can be converted to ethanol as a gasoline replacement. They provide the additional benefit of avoiding the food vs fuel debate. However, the recalcitrant nature of this feedstock poses the challenge of technological bottlenecks and economic viability in the biochemical conversion of these feedstocks to produce ethanol [3,4]. Ethanol production from the lignocellulosic feedstock needs conditioning activities, which mainly include pretreatment and hydrolysis, to get sugars in monomeric forms. These sugars are then fermented to ethanol, followed by ethanol recovery and purification to comply with fuel grade specification [5]. The hydrolysis of cellulose to monosaccharides and its digestibility is hampered by the physio-chemical and structural factors. For this purpose, the pretreatment operation mainly focuses on disrupting the crystalline structure of the feedstock so that the proper enzyme accessibility during the hydrolysis is ensured. This maximal exposure of cellulose to enzyme results in minimum energy consumption and a maximum sugar recovery [6]. However, both these processes are not yet economically efficient, making lignocellulosic biofuels commercial non-viable. Model based optimization can identify desirable operating strategies to address this issue, which is the primary goal of this work. The processes of dilute acid pretreatment and enzymatic hydrolysis are optimized individually using the theory of optimal control. The novel contribution of this work is to investigate the optimization of pre-treatment and hydrolysis processes from an applied perspective, rather than emphasizing on new method to solve optimal control problems. It is expected that the results of these various optimal control studies

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Nomenclature

$\Delta H_{r,j}$	heat of reaction for jth reaction, [J/g]
$\dot{p}(t)$	differential costate vector at time t
$\dot{R}(t)$	differential influence functions vector at time t
$\dot{x}(t)$	differential state vector at time t
$p(t)$	costate vector at time t
$R(t)$	influence functions vector at time t
$u(t)$	control vector at time t
$x(t)$	state vector at time t
$\mathcal{H}$	Hamiltonian
$\mathcal{J}$	objective functional
$\mathcal{L}$	Lagrangian
$\mathcal{S}$	terminal cost function
$\mathcal{V}$	integral cost
A	pre-exponential factor, [s^{-1}]
a	heat transfer area, [m^2]
C_a	acid concentration, [w/w]
C_i	mass concentration of ith species,[kg/m^3]
c_i	concentration of ith species, [g/g]
$c_{p,i}$	specific heat, [J/kg K]
$D(t)$	dilution rate at time t, [h^{-1}]
E	activation energy,[J/mol]
E_{1B}	bound concentration of CBH and EG, [g/kg]
E_{2B}	bound concentration of β-glucosidase, [g/kg]
$E_B(t)$	bound enzyme concentration at time t, [g/kg]
$E_F(t)$	free enzyme concentration at time t, [g/kg]
E_{max}	maximum mass of enzyme that can adsorb onto a unit mass of cellulose, [g protein/g cellulose]
$E_T(t)$	total enzyme concentration at time t, [g/kg]
E_i	enzyme concentration, [g/kg]
$F(t)$	substrate flow rate at time t, [l/h]
G	glucose concentration, [g/kg]
G_2	cellobiose concentration, [g/kg]
K_{3M}	cellobiose saturation constant, [g/kg]
K_{iIG_2}	inhibition constant for cellobiose, [g/kg]
K_{iIG}	inhibition constant for glucose, [g/kg]
K_{iX}	inhibition constant for xylose, [g/kg]
k_{ij}	rate constant of jth component in ith reaction, [s^{-1}]
m_b	mass of the dry biomass, [g]
n_{ij}	order of ith reaction for jth polymer species
R	universal gas constant, [J/mol K]
R_s	cellulose reactivity
r_i	reaction rate of ith reaction
S	cellulose concentration, [g/kg]
T	temperature, [K]
T_c	temperature of cold fluid, [K]
T_h	temperature of hot fluid, [K]
$T_j(t)$	jacket temperature at time t, [K]
$T_r(t)$	reactor temperature at time t, [K]
U	over all heat transfer coefficient, [kW/m^2K]
$V(t)$	volume of fed-batch reactor at time t, [l]
v_j	volume of the reactor jacket, [m^3]
V_r	volume of the reaction mixture in batch reactor, [m^3]
X	xylose concentration, [g/kg]
α	constant relating cellulose reactivity with degree of hydrolysis
γ	multiplier
ν	stoichiometric coefficient
ϕ	biomass loading, $\left[\frac{kg\ of\ biomass}{kg\ of\ liquid}\right]$
ρ	density, [kg/m^3]
g	state function
$m_c(t)$	mass flow rate of cold fluid at time t, [kg/min]
$m_h(t)$	mass flow rate of hot fluid at time t, [kg/min]
BC	base case
BG	β-glucosidase
CBH	cellobiohydrolase
EG	endoglucanase
GHG	greenhouse gases
HMF	hydroxy methyl furfural
INR	Indian rupee
LC	lignocellulose
MCP	maximum concentration problem
MPP	maximum profit problem
MTP	minimum time problem
OCP	optimal control problem
PI	performance index
TPBVP	two point boundary value problem

would provide guidelines to practitioners to maximize the profit from these processes. Furthermore, the solution time issues are not considered since the optimal control problems are solved offline to generate open loop control profiles. Therefore, well established methods to solve the optimal control problems are used.

The article is organized as follows. Section 2 describes the process for converting lignocellulosic feedstock to fermentable sugars through acid pretreatment and enzymatic hydrolysis. Modeling of batch and fed-batch reaction systems for pretreatment and enzymatic hydrolysis processes, respectively, is explained in Section 3. The various optimization problem formulations are reported in Section 4. Finally the simulation results and conclusions obtained by solving these optimization problems are discussed in Sections 5 and 6, respectively.

2. Process description

The biochemical route for the production of ethanol from lignocellulosic biomass consists of following steps viz. pre-treatment, enzymatic hydrolysis, fermentation and separation. Among these, pre-treatment and enzymatic hydrolysis are most challenging from a techno-economic perspective. The major objective of the pretreatment is to disrupt the structural matrix of lignocellulose to enhance cellulose accessibility for enzyme in subsequent enzymatic hydrolysis step. A variety of pre-treatment techniques have been explored [7,4]. However, dilute acid pretreatment has been found to be more favorable from an economics and environmental impacts standpoint [8,9]. In dilute acid pretreatment, xylan (major fraction in hemicellulose) is hydrolyzed into xylose. It also leads to the conversion of lignin into acid soluble lignin [5]. Both these reactions lead to the disruption of the lignocellulose structure and enhance cellulose accessibility for enzyme hydrolysis. Pretreatment has an important role in downstream processing steps and even has a significant share of about 17% of the total operating cost [10].

The pretreated feedstock consists of cellulose, which can be converted to fermentable sugars like glucose by enzymes. Enzymatic process, although considered to be slow, results in minimum degradation products formation [4]. However, it typically accounts for about 20% of the total operating cost [10], mainly due to the high enzyme loading. This demands improving this specific process step for overall economic feasibility [11]. One such possibility is minimizing the energy requirement in the downstream separation processes (like distillation) by having a high ethanol concentration in the fermentation broth, which in turn requires a higher concentration of fermentable sugars in the hydrolyzate [12]. This higher sugars concentration in the hydrolyzate can be achieved in