Bioresource Technology 196 (2015) 78–87

Contents lists available at ScienceDirect

Bioresource Technology

journal homepage: www.elsevier.com/locate/biortech

Simulation of the ozone pretreatment of wheat straw

Sujala Bhattarai [a], Danny Bottenus [b], Cornelius F. Ivory [b,*], Allan Haiming Gao [a], Mahesh Bule [a], Manuel Garcia-Perez [a], Shulin Chen [a]

[a] Department of Biological Systems Engineering, Washington State University, Pullman 99164-6120, United States
[b] Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, P.O. Box 646515, Pullman, WA 99164-6515, United States

HIGHLIGHTS

- Two models for ozonolysis pretreatment of wheat straw were developed.
- First study that takes into account the residual lignin.
- Compared cuticle model with the existing general model for ozonolysis of biomass.
- Cuticle model better fit with experimental data.

ARTICLE INFO

Article history:
Received 22 April 2015
Received in revised form 2 July 2015
Accepted 3 July 2015
Available online 16 July 2015

Keywords:
Wheat straw
Ozone pretreatment
Mathematical modeling
Cuticle hypothesis

ABSTRACT

Wheat straw is a potential feedstock in biorefinery for sugar production. However, the cellulose, which is the major source of sugar, is protected by lignin. Ozonolysis deconstructs the lignin and makes cellulose accessible to enzymatic digestion. In this study, the change in lignin concentration with different ozonolysis times (0, 1, 2, 3, 5, 7, 10, 15, 20, 30, 60 min) was fit to two different kinetic models: one using the model developed by Garcia-Cubero et al. (2012) and another including an outer mass transfer barrier or "cuticle" region where ozone mass transport is reduced in proportion to the mass of unreacted insoluble lignin in the cuticle. The kinetic parameters of two mathematical models for predicting the soluble and insoluble lignin at different pretreatment time were determined. The results showed that parameters derived from the cuticle-based model provided a better fit to experimental results compared to a model without a cuticle layer.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Wheat straw is an agricultural byproduct of wheat that is annually produced in abundance around the world. The world's wheat production in 2014 was 716 Tg (USDA (2014). Assuming a residue/crop ratio of 1.3 (Talebnia et al., 2010), about 931 Tg of total wheat residue is annually produced. If 60% is used for ground cover to prevent soil erosion 559 Tg of wheat straw is available as waste. Wheat straw is composed of lignin (15–20%), celluloses (33–40%), and hemicelluloses (20–25%) (Talebnia et al., 2010). The lignin in the wheat straw is made up of monomer units such as p-hydroxy phenyl-guaiacyl-syringyl (H-G-S) lignin, and contains approximately 5, 49, and 46% of H, G, and S units, respectively (Lapierre et al., 1995). In order to utilize structural carbohydrates of the wheat straw in a biochemical biorefinery setting, a pretreatment process is necessary to disrupt the recalcitrant structure of mainly lignin. Pretreatment is known to increase the susceptibility of cellulose and hemicellulose to cellulolytic enzymes for the production of fermentable sugars. The main goal of pretreatment process is to increase the surface area and porosity of the substrate, reduce the crystallinity of the cellulose, degrade hemicellulose and lignin, and disrupt the heterogeneous structure of the cellulosic materials (Talebnia et al., 2010). The pretreatment processes are of four types: physical, physico-chemical, chemical, and biological. Physical pretreatment is based on size reduction of the wheat straw by means of milling, grinding, or chipping (Pedersen and Meyer, 2009). Liquid hot water (Petersen et al., 2009), steam explosion (Ballesteros et al., 2006), and ammonia fiber explosion (Sun and Cheng, 2002) are the physico-chemical pretreatment methods. The use of acids, alkalines, and oxidizing agents for the pretreatment of wheat straw is known as chemical pretreatment (Saha et al., 2005). The pretreatment by means of microorganisms such as white and soft rot fungi are types of biological pretreatment (Talebnia et al., 2010).

* Corresponding author. Tel.: +1 509 335 7716; fax: +1 509 335 4806.
E-mail address: cfivory@wsu.edu (C.F. Ivory).

http://dx.doi.org/10.1016/j.biortech.2015.07.022
0960-8524/© 2015 Elsevier Ltd. All rights reserved.

Nomenclature

CI_i	confidence intervals
c_{ii}	*i*th diagonal element of covariance matrix
Cov	covariance matrix
DF	degree of freedom
Do_3	diffusion coefficient, m^2/s
d_p	diameter of particle, m
iLg	insoluble lignin, kg_iLg/kg_{Straw}
iLg_c	insoluble lignin in cuticle, kg_iLg/kg_{Straw}
$iLg_{c,o}$	initial insoluble lignin in cuticle, kg_iLg/kg_{Straw}
$iLg_{c,Model,i}$	predicted insoluble cuticle lignin, kg_iLg/kg_{Straw}
$iLg_{Exp,i}$	experimental insoluble lignin, kg_iLg/kg_{Straw}
$iLg_{Model,i}$	predicted insoluble lignin, kg_iLg/kg_{Straw}
iLg_s	insoluble lignin of solid, kg_iLg/kg_{Straw}
J	Jacobian matrix
k_1	reaction rate, $kg_{Straw}/kg\_iLg/min$
k_2	reaction rate, $kg_{Straw}/kg\_sLg/min$
$K_{O,CS}a_p$	mass transfer coefficient between cuticle and the interior solid, *1/min*
$K_{O,GC}a_p$	mass transfer coefficient between gas phase and the cuticle, *1/min*
$K_{O,S}a_p$	mass transfer coefficient between gas phase and solid phase, *1/min*
K	condition number
$O_{3,C}$	ozone in the cuticle, $kg\_O_{3,S}/kg_{Straw}$
$O_{3,G}$	ozone in the gas phase, $kg\_O_{3,G}/kg_{Straw}$
$O_{3,S}$	ozone in the solid phase, $kg\_O_{3,S}/kg_{Straw}$
θ_i	best fit parameter
P	pressure, pa
P	products
PI	prediction interval
R_1	reaction kinetics, kg_{Straw}. kg_sLg/min
R_1	reaction kinetics, kg_{Straw}. kg_sLg/min
$R_{1,C}$	reaction kinetics, kg_{Straw}. kg_sLg/min
$R_{2,C}$	reaction kinetics, kg_{Straw}. kg_sLg/min
$R_{1,S}$	reaction kinetics, kg_{Straw}. kg_sLg/min
$R_{2,S}$	reaction kinetics, kg_{Straw}. kg_sLg/min
SE	standard error
sLg	soluble lignin, kg_sLg/kg_{Straw}
sLg_c	soluble lignin in cuticle, kg_sLg/kg_{Straw}
$sLg_{c,Model,i}$	predicted soluble cuticle lignin, kg_sLg/kg_{Straw}
$sLg_{c,Exp,i}$	experimental soluble lignin, kg_sLg/kg_{Straw}
$sLg_{Model,i}$	predicted soluble lignin, kg_sLg/kg_{Straw}
sLg_s	soluble lignin of solid, kg_sLg/kg_{Straw}
T	time, min
$t_{\alpha/2,Df}$	student's t inverse cumulative distribution
U	velocity, m/sec
V_s	voluble of solid, m^3
W_s	weight of solid, kg
Z	distance, m

Greek

α_1, α_4	stoichiometric, dimensionless
α_2	stoichiometric, $kg\_iLg/kg\_O_{3,S}$
α_3	stoichiometric, $kg\_sLg/kg\_O_{3,S}$
α_5	stoichiometric, $kg\_sLg/kg\_O_{3,S}$
ε	void fraction, dimensionless
ρ_S, ρ	density of solid, kg/m^3
λ_c	cuticle lignin fraction, dimensionless
μ	dynamic viscosity, pa sec
κ_{br}	permeability, m^2
λ_{max}	largest eigen value
λ_{min}	smallest eigen value
β_F	Forchheimer drag coefficient, kg/m^4
ϕ	sphericity, dimensionless
Δ	square root of machine precision
A	confidence interval

Ozone pretreatment uses ozone as an oxidizing agent. Ozone is a very powerful oxidizing species with an oxidation potential of 2.07 eV (Mandavgane and Yenkie, 2011). There are many advantages of the ozone pretreatment process compared to other pretreatment techniques. For instance, ozone causes minimal degradation of cellulose and hemicelluloses due to the considerably higher reaction rate of ozone with substituted aromatic molecules such as lignin. The ozonation process also does not produce toxic compounds and can be performed at room temperature and pressure, which reduces the capital and energy costs (Neely, 1984). In addition, earlier studies demonstrated efficiency of ozone pretreatment to improve sugar release during enzymatic hydrolysis (Bule et al., 2013; García-Cubero et al., 2009; Wu et al., 2013).

The majority of studies involving the ozonation pretreatment of lignocellulose required a relatively long residence time in the reactor, typically 60 min or greater. As a result, utilizing ozone as a sole pretreatment process for lignocellulose can be unpractical. The study demonstrating ozonolysis of wheat straw and rye straw which increased sugar yield from 29% and 16% (untreated) to 88.6% and 57% (ozone treated), respectively (untreated) (García-Cubero et al., 2009) required 2.5 h of ozone exposure. Also, the ozonolysis of sugarcane bagasse showed an increase in glucose yield from 6.64% (untreated) to 52.44% (ozone treated) after 120 min of ozone pretreatment (Travaini et al., 2013). In contrast, the ozonolysis (for 120 min) of energy grasses showed a lower sugar yield compared to untreated energy grasses after enzymatic hydrolysis (Panneerselvam et al., 2013). These observations suggest that the applicability of ozone pretreatment depends upon the biomass characteristics. In order to make ozone pretreatment economically feasible, its optimization either through better elucidation of the ozone interaction with lignin or through the reduction of the overall pretreatment time is urgently needed.

Although many studies have been conducted on the ozonolysis process, mathematical models explicitly predicting ozone lignin degradation phenomena are rare. García-Cubero et al. (2012) introduced a model to characterize the effects of ozonation on the insoluble and soluble lignin (MBachu and Manley, 1981) content of biomass. However, the model presented by García-Cubero et al. (2012) did not take into account the residual lignin that remained unaffected by the ozone. In contrast, their model predicts that prolonged ozone exposure removes lignin completely which contradicts experimental results where lignin concentration reaches a plateau.

Several attempts have been made in the development of numerical models for the ozone lignin interaction process. The kinetic model proposed by Binder et al. (1980) showed that the ozone lignin interaction has two different kinetic behaviors: a falling rate phase followed by a constant rate phase, however, only the falling rate period was addressed in their model. MBachu and Manley (1981) suggested that lignin degradation follows first-order kinetics, and they derived the first order reaction equation of lignin degradation of ozone treated spruce periodate and spruce cuoxam lignin as follows:

Download English Version:

https://daneshyari.com/en/article/7074075

Download Persian Version:

https://daneshyari.com/article/7074075

Daneshyari.com