Biochemical Engineering Journal 93 (2015) 179–195

Contents lists available at ScienceDirect

Biochemical Engineering Journal

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

Regular article

Modeling and simulation of direct production of acetic acid from cheese whey in a multi-stage membrane-integrated bioreactor

Jayato Nayak[a], Madhubonti Pal[b], Parimal Pal[a,*]

[a] Environment and Membrane Technology Laboratory, Department of Chemical Engineering, National Institute of Technology Durgapur, Durgapur 713209, India

[b] Department of Chemistry, Presidency University, Kolkata, India

ARTICLE INFO

Article history:
Received 15 July 2014
Received in revised form
14 September 2014
Accepted 4 October 2014
Available online 12 October 2014

Keywords:
Acetic acid
Membrane bioreactor
Growth kinetics
Transport
Bio separations
Modeling

ABSTRACT

Modeling and simulation of direct and continuous production of acetic acid in a two-stage membrane-integrated hybrid reactor system was done. The total production and purification scheme involved fermentation of a cheap, renewable carbon source (cheese whey) under non-neutralizing regime in a membrane-integrated new reactor with provisions of downstream separation and recycle of microbial cells and unconverted carbon source from product acetic acid by microfiltration and nano-filtration membranes. The model attempts to capture the major governing parameters like dilution rate, cross flow rate, recycling of materials, pH along with fermentation kinetics under substrate-product inhibitions and all the associated transport phenomena of the components through micro and nanofiltration membranes. The system produced 98.6% pure acetic acid at a flux of 75 L/(m^2 h) with yield of 0.98 g/g and productivity of 4.1 g/(L h). Performance of the model is well reflected in low relative error (<0.05), high Willmott *d*-index ($d > 0.97$) and high overall correlation coefficient ($R^2 > 0.98$).

1. Introduction

Industrial houses involved in chemical and biochemical production of commodities around the world are desperately seeking replacement of their existing manufacturing schemes by green and economically attractive technologies for sustainable business. Emergence of varieties of new membranes has greatly facilitated development of such sustainable technologies in chemical and biochemical production processes. Direct production of acetic acid in membrane-integrated hybrid reactor system represents one such possible sustainable technology [1]. In transferring such a technology to production field, scale up confidence is absolutely essential and to this effect, modeling and simulation studies along with economic analysis are necessary. Studies on these aspects are very scanty. Moreover, reported experimental studies mostly concentrate on production of acetic acid using finished raw materials rather than a renewable or low cost waste material as carbon source [2,3] and this results in higher production cost. Most of the investigated production schemes produce salts of the acid in pH-controlled regime instead of direct production of the acid, thereby, necessitating further treatments with acids and alkalis to regenerate acetic acid. Such production schemes are thus never eco-friendly ones. Product purity and also productivity are often compromised in such schemes. Membranes have been used for effective removal of microbes [4] from fermentation broth. But in majority of the cases, it is a single stage membrane separation process using mostly microfiltration membranes in hollow fiber modules [4,5] for downstream processing of fermentation broth. Recycling of unconverted carbon source and high purity of the product can't be ensured in such a system. Reported other modeling studies[6–9] in some cases considered pervaporation in acid separation and concentration and are often based on batch production process using glucose as carbon source. Though kinetics have been covered in some of these studies, transport has not received attention in modeling and these processes lead to production of salt of the acid instead of direct acid. Some modeling studies used model acetate solution instead of real fermentation broth. Though attempts have been made in using membranes for cell separation and product purification, no complete membrane-integrated scheme for separation and recycling of microbial cells and unconverted carbon source with simultaneous recovery of highly pure product has been considered in early modeling and simulation studies. To fill the

* Corresponding author. Tel.: +91 9434469750; fax: +91 3432754078.
E-mail addresses: parimalpal2000@yahoo.com, ppal.nitdgp@gmail.com (P. Pal).

http://dx.doi.org/10.1016/j.bej.2014.10.002
1369-703X/

Nomenclature

A_k	porosity of the membrane
B_c	cell bleeding ratio
$c_{w,i}$	concentration of any ion i (mol/m^3) on membrane wall
$c_{w,i,\mathrm{av}}$	average concentration of any ion i (mol/m^3) on membrane wall
$C_{p,i}$	concentration of any ion i (mol/m^3) in permeate solution
$C_{B,\mathrm{Ac}}$	bulk concentration of acetate (mol/m^3)
C_{fnf}	bulk feed concentration of uncharged solute (mol/m^3)
C_{Pnf}	uncharged solute permeate concentration (mol/m^3)
C	average concentration of uncharged solute concentration within pore (mol/m^3)
D_s	uncharged solute pore diffusion coefficient (m^2/h)
D_i	hindered diffusivity of ion i (m^2/s)
$D_{B,\mathrm{i}}$	bulk diffusivity of ion i (m^2/s)
F	Faraday constant
F_R	flow rate through which cell has been recycled back to fermenter (cm^3/s)
F_o	output flow rate of fermentation broth from fermenter (cm^3/s)
H_i	hindrance factor for convection of ion i
H_{US}	uncharged solute hindrance factor for convection
J_a	uncharged solute flux (pore area basis) (mol/m^2 s)
J_v	volumetric flux of uncharged solute (L/(m^2 h))
J_{Ac}	solute flux of acetate (mol/m^2/s)
J_{MF}	the solvent flux in permeate stream of microfiltration (L/(m^2 h))
k	Boltzmann constant, 1.38066×10^{-23} J/K
k_d	cell death rate constant (h^{-1})
$K_{D,i}$	hindrance factor for diffusion of ion i
K_i	substrate inhibition constant for growth of biomass (g/L)
$K_{i\mathrm{Act}}$	substrate inhibition constant for acetic acid production (g/L)
$K_{s\mathrm{Act}}$	substrate limitation constant for acetic acid production (g/L)
$K_{i\mathrm{Lac}}$	substrate inhibition constant for sugar consumption (g/L)
$K_{s\mathrm{Lac}}$	substrate limitation constant for sugar consumption (g/L)
k_m	Mass transfer coefficient of acetate ion (m/s)
K_s	substrate limitation constant for growth of biomass (g/L)
$S_{\mathrm{Lct,ct}}$	Lactose concentration in fermenter during continuous production (g/L)
S_{Lac}	Lactose concentration (g/L)
$S_{\mathrm{Lac,ct}}$	substrate concentration in fermenter during continuous production (g/L)
$S_{R,\mathrm{Lac}}$	substrate concentration in membrane cell recycle stream (g/L)
$q_{\mathrm{Act,max}}$	maximum specific acetic acid production rate (g/g h)
$q_{\mathrm{Act,net}}$	maximum specific acetic acid production rate during continuous process (g/g h)
$q_{\mathrm{Lac,max}}$	maximum specific lactose utilization rate (g/g h) during substrate consumption
Pe_i	Peclet number (dimensionless)
P_{Act}	acetic acid concentration (g/L)
$P_{\mathrm{Act,ct}}$	product concentration in fermenter during continuous process (g/L)
P_m	product inhibition constant for growth of biomass (g/L)
r_{mp}	effective pore radius (nm)
$r_{s,i}$	solute radius of ion i (nm)
$R_{j,\mathrm{Act}}$	rejection of acetic acid (%)
R	universal gas constant (J/mol/K)
R_m	membrane resistance (m^{-1})
R_f	membrane fouling resistance (m^{-1})
R_c	cake resistance (m^{-1})
T	absolute temperature (K)
t	fermentation time (h)
V	radially averaged solution velocity (m/s)
V_f	working volume of the fermenter (cm^3)
V_s	uncharged solute partial molar volume (m^3/mol)
x	membrane thickness (m)
X	biomass concentration (g/L)
X_{Cm}	Effective charge membrane density (mol/m^3)
X_{ct}	biomass concentration in fermenter during continuous production (g/L)
Y_{AL}	product yield on sugar consumption
Y_{xL}	biomass yield on sugar consumption
z_i	valence of ion i
Δp_a	applied pressure difference (kg/cm^2)
ΔP_{eff}	effective pressure difference, (kg/cm^2)