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Modelling the industrial production of vinegar in aerated-stirred fermentors in terms of process variables

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ABSTRACT

The production of vinegar in an aerated-stirred reactor was modelled using a hybrid approach. The growth rate was modelled according to the total biomass specific growth rate, $\mu_g v$, which represents the growth of an active biophase and the fraction of cells which are growing. A quadratic model based on the process variables, i.e. hydrostatic pressure, ethanol concentration, aeration, agitation and temperature, was developed for $\mu_g v$ and the substrate and product kinetics were related mechanistically to the growth rate, including the kinetics of acetoin and ethyl acetate production. This model was coupled with the models for oxygen transfer and gas–liquid transfer, reported in a previous study, and the prediction capacity of the system of equations was validated by simulating semi-continuous and continuous real processes developed in a pilot fermentor.

1. Introduction

Mechanistic and pseudo-empiric kinetic models have been widely applied to acetic fermentation (Bar et al., 1987; Caro et al., 1996; Gómez and Cantero, 1998; Ito et al., 1991; Mesa et al., 1986; Nanba et al., 1984; Ory et al., 1998; Park et al.,1991; Romero et al., 1994), based on the general scheme of reactions proposed by Sinclair and Kristiansen (1987). Most of the mathematical expressions for the specific growth rate have accounted for intracellular metabolism and divided the cells in terms of viability (Sinclair and Topiwala, 1970). An empirical model was also proposed using a different approach (Kruppa and Vortmeyer, 1999). These models could not satisfactorily explain the industrial process of vinegar production mainly because an inhibitory effect of acetic acid was considered (González-Sáiz et al., 2003). This inhibitory effect was not observed in industrial fermentation.

In a previous study (González-Sáiz et al., 2003), the authors proposed a new pseudo-empiric kinetic model. The parameters of the specific growth rate equation were optimised by a genetic algorithm applied to data obtained from fermentors in a vinegar manufacturing plant in La Rioja. The data were obtained in batch fermentors operating at constant temperature, oxygen supply, hydrodynamic conditions and initial concentration. The model assumed that the decrease in growth rate with time was due to ethanol consumption. However, it could only be applied to the standard process conditions prevailing in the industrial fermentor studied.

The effect of oxygen transfer has been studied in different biosystems (Çelik and Çalik, 2004; Elibol and Ozer, 2000; Tang and Zhong, 2003), but in acetic fermentation the effects of oxygen concentration have only been considered in the context of bacterial growth (Park et al., 1991; Romero et al., 1994). However, it is well known that a failure in oxygen supply can dramatically reduce cell population viability (Drysdale and Fleet, 1989; Muraoka et al., 1982). The effect of agitation and aeration has also been studied in the context of various biosystems (Croughan et al., 1987; El-Enshasy et al., 2006; Evans and Liu, 2003; Zuo et al., 2006), but not for acetic acid fermentation. A new model for acetic fermentation is required to explain the effects of oxygen transfer and hydrodynamic conditions on acetification rate.

Therefore, the main objective of this paper is the development of a global model for the industrial process of acetic fermentation. The kinetic model for cell growth, ethanol and oxygen consumption, and acetic acid production has been proposed on the basis of an hybrid approach, considering the results reported in a previous study (Garrido-Vidal et al., 2003), where the authors studied the effect of hydrostatic pressure, ethanol concentration, aeration, agitation and temperature, i.e. the process variables of an aerated-stirred fermentor on acetification rate. Hybrid models have been widely applied in several biosystems (Chen et al., 2000; Oliveira, 2004; Zorzetto et al., 2000). In these types of models, the structures

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Nomenclature

A	acetic acid concentration in the bioreactor and in the effluent stream, g L^{-1}
AMC	acethyl methy carbinol (acetoin) concentration in the bioreactor and in the effluent stream, g L^{-1}
$C^*_{i,L}$	concentration of component i in liquid phase before mass transfer, g L^{-1}
C_i	concentration of component i in fermentation medium and effluent stream
C_{if}	concentration of component i in the feed stream
$C_{O_2,L}$	concentration of oxygen in liquid phase, g L^{-1}
$C^*_{O_2,L}$	concentration of oxygen in oxygen-saturated liquid phase, in equilibrium with partial oxygen pressure in the oxygen-saturated gas phase, g L^{-1}
D	dilution rate, h^{-1}
F_1	volumetric flow rate of filtered vinegar stream, L h^{-1}
F_2	volumetric flow rate of purged vinegar stream, L h^{-1}
F_V	volumetric flow rate of vinegar effluent stream, L h^{-1}
F_W	volumetric flow rate of feed wine, L h^{-1}
E	ethanol concentration in the bioreactor and in the effluent stream, g L^{-1}
EA	ethyl acetate concentration in the bioreactor and in the effluent stream, g L^{-1}
$k_{A,G}a$	volumetric acetic acid transfer coefficient in gas-side interphase, h^{-1}
$k_{AMC,G}a$	volumetric acetoin transfer coefficient in gas-side interphase, h^{-1}
$k_{E,G}a$	volumetric ethanol transfer coefficient in gas-side interphase, h^{-1}
$k_{EA,G}a$	volumetric ethyl acetate transfer coefficient in gas-side interphase, h^{-1}
$k_{i,G}a$	volumetric component i transfer coefficient in gas-side interphase, h^{-1}
k_La	volumetric oxygen transfer coefficient in liquid-side interphase, h^{-1}
$k_{W,G}a$	volumetric component i transfer coefficient in gas-side interphase, h^{-1}
$LGTR_i$	liquid–gas transfer rate for component i, g L^{-1} h^{-1}
N	impeller rotation speed, rpm or s^{-1}
$O_{2(o)}$	oxygen effluent stream, g L^{-1} h^{-1}
$O_{2(i)}$	oxygen feed stream, g L^{-1} h^{-1}
OTR	oxygen transfer rate, g L^{-1} h^{-1}
OUR	oxygen uptake rate, g L^{-1} h^{-1}
P	pressure in fermentation medium, atm
P_g	aerated mechanical power input, w
R	recycling rate
r_A	acetic acid production rate due to the fermentation process, g L^{-1} h^{-1}
r^2A	adjusted correlation rate
r_{AMC}	acethyl methy carbinol (acetoin) formation rate due to the fermentation process, g L^{-1} h^{-1}
r_{EA}	ethyl acetate formation rate due to the fermentation process, g L^{-1} h^{-1}
r_E	ethanol consumption rate due to the fermentation process, g L^{-1} h^{-1}
r_i	rate of production or consumption of component i within the fermentor, g L^{-1} h^{-1}
r_{O_2}	oxygen consumption rate due to the fermentation process, g L^{-1} h^{-1}
r_{X_t}	cell growth rate due to the fermentation process, g L^{-1} h^{-1}
SM	suspended matter concentration in the bioreactor and in the effluent stream, gDW L^{-1}
SM_f	suspended matter concentration in the feed stream, gDW L^{-1}
t	fermentation time, h
T_L	liquid-phase temperature, °C
V_c	volume of wine charged, L
V_d	volume of vinegar discharged, L
V_L	liquid-phase volume, dm^3 or m^3
vvm	air-flow rate divided by the reactor working volume, h^{-1}
X_t	total biomass concentration in the bioreactor and in the effluent stream, gDW L^{-1}
X	factors of the quadratic model
$Y'_{A/E}$	acetic acid/ethanol yield factor, g acetic acid/g ethanol
$Y_{A/E}$	acetic acid/ethanol stoichiometric coefficient, 1.30 g acetic acid/g ethanol
$Y'_{AMC/X}$	acetoin/biomass yield factor, g acetoin/g biomass
$Y'_{A/O}$	acetic acid/oxygen yield factor, g acetic acid/g oxygen
$Y_{EA/A}$	ethyl acetate/acetic acid stoichiometric coefficient, 1.47 g ethyl acetate/g acetic acid
$Y_{EA/E}$	ethyl acetate/ethanol stoichiometric coefficient, 1.91 g ethyl acetate/g ethanol
$Y'_{EA/X}$	ethyl acetate/biomass yield factor, g ethyl acetate/g biomass
$Y_{E/O}$	ethanol/oxygen stoichiometric coefficient, 1.44 g ethanol/g oxygen
$Y'_{E/O}$	ethanol/oxygen yield factor, g ethanol/g oxygen
$Y'_{X/E}$	biomass/ethanol yield factor, g biomass/g ethanol
$Y'_{X/O}$	biomass/oxygen yield factor, g biomass/g oxygen
X_t	total biomass concentration, gDW L^{-1}
Greek symbols	
$\mu_g v$	total biomass specific growth rate, h^{-1}
μ_g	overall specific growth rate, h^{-1}
μ_S	superficial air velocity through the liquid medium, m s^{-1}
v	viability factor

including conservation laws such as material and/or energy balance equations are combined with non-parametric models for the specific growth rate, such as artificial neural networks. These types of models require several sets of data for validation and their predictive ability is unreliable under extrapolation conditions, so they are usually applied to well-established processes where data is readily available or for batch-to-batch iterative optimisation (Teixeira et al., 2006). Therefore, empirical models with secondary order polynomials have been widely applied to study the effect of variables on cell growth and optimisation of bioprocesses (Henriques et al., 2006; Nikerel et al., 2006; Rita et al., 2003).

Another new feature of this research has been the inclusion of a kinetic model of ethyl acetate and acetoin production. The global model was coupled with a model for k_La and gas–liquid transfer, reported in a previous study (González-Sáiz et al., 2008), which enables dissolved oxygen concentration and the impact of gas–liquid transfer on the concentration of the compounds to be predicted. The predictive ability of the global model was demonstrated by simulating an exhaustive set of fermentation processes developed in a pilot fermentor. This validation was undertaken for all important operating configurations of industrial fermentors, i.e. continuous fermentor, continuous fermentor with cell recycling and semi-continuous fermentor. The broad applicability range of the global model developed in this study has not been reported in literature on mechanistic acetic fermentation models.