Bioresource Technology 204 (2016) 55–64

Contents lists available at ScienceDirect

Bioresource Technology

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

Techno-economic evaluation of a complete bioprocess for 2,3-butanediol production from renewable resources

Apostolis A. Koutinas [a], Bernardo Yepez [b], Nikolaos Kopsahelis [a], Denise M.G. Freire [b], Aline Machado de Castro [c], Seraphim Papanikolaou [a], Ioannis K. Kookos [d,*]

[a] Department of Food Science and Human Nutrition, Agricultural University of Athens, Iera Odos 75, 11855 Athens, Greece
[b] Biochemistry Department, Chemistry Institute, Federal University of Rio de Janeiro, Cidade Universitária, Centro de Tecnologia, Bloco A, Lab 549, Rio de Janeiro 21941-909, RJ, Brazil
[c] Biotechnology Division, Research and Development Center, PETROBRAS, Av. Horácio Macedo, 950. Ilha do Fundão, Rio de Janeiro 21941-915, Brazil
[d] Department of Chemical Engineering, University of Patras, Rio, 26504 Patras, Greece

HIGHLIGHTS

- Bioprocess design and costing for 2,3-butanediol production.
- Versatile downstream separation of 2,3-butanediol by reactive extraction.
- The composition of fermentation media affects the cost of 2,3-butanediol production.
- The prospects of bio-based 2,3-butanediol production is promising.

ARTICLE INFO

Article history:
Received 13 October 2015
Received in revised form 2 December 2015
Accepted 9 December 2015
Available online 17 December 2015

Keywords:
Bioprocess design
2,3-Butanediol
Fermentation
Minimum selling price
Sensitivity analysis

ABSTRACT

This study presents the techno-economic evaluation of 2,3-butanediol (BDO) production via fermentation using glycerol, sucrose and sugarcane molasses as carbon sources. Literature-cited experimental data were used to design the fermentation stage, whereas downstream separation of BDO was based on reactive extraction of BDO employing an aldehyde to convert BDO into an acetal that is immiscible with water. The selected downstream process can be used in all fermentations employed. Sensitivity analysis was carried out targeting the estimation of the minimum selling price (MSP) of BDO at different plant capacities and raw material purchase costs. In all cases, the MSP of BDO is higher than 1 $/kg that is considered as the target in order to characterize a fermentation product as platform chemical. The complex nutrient supplements, the raw material market price and the fermentation efficiency were identified as the major reasons for the relatively high MSP observed.

1. Introduction

2,3-Butanediol (BDO) could be employed as a platform intermediate for the production of numerous chemicals and fuel additives (Voloch et al., 1985). For instance, BDO could be used for the production of 1,3-butadiene with annual worldwide production capacity of around 10 million t. Winfield (1950) reported the dehydration of BDO over thorium oxide to methyl vinyl carbinol and 1,3-butadiene. A BDO to 1,3-butadiene conversion yield of 70% has been reported via esterification of BDO with a mixture of acetic and formic acids with subsequent pyrolysis of the diesters into 1,3-butadiene (Baek et al., 2014). BDO production via fermentation was initiated during the Second World War for the production of synthetic rubber. However, the lack of cost-competitiveness led to the establishment of petrochemical synthesis of 1,3-butadiene. Besides 1,3-butadiene, BDO could be converted into acetoin, diacetyl and various diesters with applications in food, pharmaceutical, cosmetic and polymer industries (Ji et al., 2011).

BDO production could be achieved by various bacterial strains belonging mainly in the genera *Klebsiella*, *Serratia*, *Bacillus*, *Paenibacillus* and *Enterobacter*. Wild-type bacterial strains produce BDO from various carbon sources including C5 and C6 sugars and disaccharides, such as sucrose and lactose. The hexose to BDO theoretical conversion yield is 0.5 kg/kg. One of the important advantages of fermentative BDO production is the high BDO concentrations and volumetric productivities achieved due to the lower inhibitory effect of high BDO concentrations than alcohols (e.g. ethanol, butanol) or various fermentation products (Magee

* Corresponding author: Department of Chemical Engineering, University of Patras, Rio, 26504 Patras, Greece. Tel.: +30 2610969567.
E-mail address: i.kookos@chemeng.upatras.gr (I.K. Kookos).

http://dx.doi.org/10.1016/j.biortech.2015.12.005
0960-8524/

and Kosaric, 1987; Zeng and Sabra, 2011). BDO production is achieved under anaerobic or oxygen limiting conditions and it usually coincides with the production of ethanol, acetoin and various organic acids (e.g. acetate, formate, lactate, succinate). This occurs due to NADH regeneration requirements.

High BDO concentrations (up to 152 kg/m^3) and productivities (up to 4.2 kg m^{-3} h^{-1}) have been produced by risk group 2 bacteria such as *Klebsiella pneumoniae* and *Serratia marcescens* H30 using pure carbon sources (Ma et al., 2009; Zhang et al., 2010a,b). Risk group 1 bacteria such as *Bacillus licheniformis* DSM 8785 have also been used for the production of high BDO concentrations (144.7 kg/m^3) with relatively high productivity (1.14 kg m^{-3} h^{-1}) (Jurchescu et al., 2013). Crude renewable resources, such as corncob molasses, sugarcane molasses, crude glycerol, seaweed hydrolysate, raw inulin extract from Jerusalem artichoke tubers and lignocellulosic hydrolysates, have also led to high BDO concentrations (up to 118 kg/m^3) and productivities (up to 2.7 kg m^{-3} h^{-1}) (Afschar et al., 1991; Gao et al., 2010; Petrov and Petrova, 2010; Wang et al., 2010; Metsoviti et al., 2012; Jung et al., 2013; Suman et al., 2013; Huang et al., 2013; Moo-Young et al., 2013; Lixiang et al., 2014).

The main fermentation parameters that should be optimized in order to maximize BDO production are nutrient requirements, aeration at different fermentation stages and pH. High dissolved oxygen concentrations favors bacterial growth, whereas low dissolved oxygen concentrations and low pH conditions favors BDO synthesis (Celinska and Grajek, 2009). Low pH conditions may trigger BDO synthesis, but prolonging the exposure at low pH conditions will inhibit bacterial growth. Therefore, optimization of aeration, agitation and pH is necessary in order to optimize BDO production by different microorganisms.

The fermentation efficiency of BDO production indicates that industrial implementation is feasible. However, this should be assessed via techno-economic evaluation in order to identify the stages that contribute the highest expenditure. This study focuses on the techno-economic evaluation of BDO production using literature-cited data based on sucrose, sugarcane molasses and glycerol consumption as carbon sources (Table 1). These feedstocks are produced in significant quantities in Brazil and there is an interest in their utilization for fermentative production of chemical building blocks, such as BDO. The particular literature-cited publications were selected because, to the best of our knowledge, the fermentation efficiencies reported for these specific feedstocks, regarding productivity, final BDO concentration and carbon source to BDO conversion yield, were among the highest found in the literature. Process flowsheets have been developed for each fermentation feedstock. The downstream separation and purification of BDO was based on the process developed by Li et al. (2013) and Hao et al. (2006). Sensitivity analysis has been carried out in order to evaluate the effect of crucial parameters on the production cost of BDO. To the best of our knowledge, this is the first study that focuses on the evaluation of BDO production using crude renewable resources and a novel downstream separation strategy based on reactive extraction.

2. Methods

2.1. Description of the design strategy

The determination of the cost of manufacture of BDO was based on the estimation of the total capital investment and operating costs of process flowsheets using a preliminary economic analysis approach. A total production capacity of 10,000 t/y and an annual plant operation of 8300 h/y were assumed. The software used to develop the bioprocess design simulations was UniSim (Honeywell).

Table 1
Summary of experimental data on BDO production from renewable raw materials.

Raw material	Molecular formula	Mode of operation	Micro-organism	Temperature (°C)	Fermentation time t_F (h)	Productivity p_V (kg m^{-3} h^{-1})	Yield (kg/kg)	Major byproduct	By-product concentration (kg/m^3)	Aeration (vvm)	Agitation (rpm)
Glycerol[a]	$C_3H_8O_3$	Fed-batch	*Klebsiella pneumoniae*	37	96	0.57	0.35	1,3-Propanediol	17.2	1.1–2.2	200
Sucrose[b]	$C_{12}H_{22}O_{11}$	Fed-batch	*Serratia marcescens* H30	30	42	3.33	0.414	Acetoin	6.65	Adjusted to achieve RQ = 1.8–2	
Molasses[c]	$C_6H_{12}O_6$[d]	Fed-batch	*Enterobacter aerogenes*	37	36	2.74	0.366	Acetoin and ethanol	6.81 3.51	1.5	280

[a] Yeast extract (2 kg/m^3) and various minerals are used as nutrient supplements.
[b] Yeast extract (33.36 kg/m^3) and various minerals are used as nutrient supplements.
[c] Yeast extract (5 kg/m^3), casamino acids (10 kg/m^3) and various minerals are used as nutrient supplements.
[d] Equivalent to glucose and fructose (a total content of 57.02% of total sugars with 87 kg/m^3 fructose, 81 kg/m^3 glucose, and 387 kg/m^3 sucrose).