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PRODUCTION OF 1,3-PROPANEDIOL FROM CRUDE GLYCEROL: BIOPROCESS DESIGN AND PROFITABILITY ANALYSIS

PRODUCCIÓN DE 1,3-PROPANODIOL A PARTIR DE GLICEROL CRUDO: DISEÑO DEL BIOPROCESO Y ANÁLISIS DE RENTABILIDAD

S. Espinel-Ríos[1,2], J.E. Ruiz-Espinoza[1]*

[1] *Facultad de Ingeniería Química, Universidad Autónoma de Yucatán. Periférico Norte km 33.5, Tablaje Catastral 13615, Col. Chuburná de Hidalgo Inn, 97203 Mérida, México.*

[2] *Current address: Bioprocess Engineering, Wageningen University and Research. Droevendaalsesteeg 1 Building 107 6708 PB Wageningen, Netherlands.*

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Abstract

Crude glycerol is the major byproduct of the biodiesel industry, and its low price due to its abundant market supply impacts negatively on this industry. The microbial production of 1,3-propanediol (1,3-PD) is a very promising way for valorizing glycerol. *Clostridium diolis* DSM 15410 converts glycerol into 1,3-PD and it is of industrial value due to its high fermentation yields and productivities. The aim of this study was to design a biotechnological process for the continuous production of 1,3-PD (> 99.0% purity) from crude glycerol using *C. diolis* DSM 15410 as biological system and evaluate the process economic profitability under different scenarios. Optimal fermentation parameters were considered for the analysis. The effects of the selling price of 1,3-PD ($2.3-$6/t), the purchase cost of crude glycerol ($100-$300/t) and the process throughput (100-1,000 kg 1,3-PD/h) on the process profitability were studied. The results showed that the process is economically profitable over a wide range of scenario combinations. This paper serves as a means for strategic decision making (e.g., go/no-go investment decisions) and further optimization of the 1,3-PD production process from crude glycerol.

Keywords: 1,3-propanediol, glycerol, modelling, simulation, economic analysis.

Resumen

El glicerol crudo es el mayor subproducto de la industria del biodiesel y, su bajo precio debido a su abundante oferta de mercado, impacta negativamente a esta industria. La producción microbiana de 1,3-propanodiol (1,3-PD) es un medio muy prometedor para la valorización del glicerol. *Clostridium diolis* DSM 15410 puede convertir glicerol en 1,3-PD y es de valor industrial dado sus altos rendimientos y productividades. El objetivo de este estudio fue el diseño de un proceso biotecnológico para la producción en continuo de 1,3-PD (> 99.0% pureza) a partir de glicerol crudo utilizando *C. diolis* DSM 15410 como sistema biológico, y la evaluación de la rentabilidad económica del proceso bajo diferentes escenarios. Condiciones óptimas de fermentación fueron consideradas para el análisis. Los efectos del precio de venta del 1,3-PD ($2.3-$6/t), precio de compra del glicerol crudo ($100-$300/t) y capacidad de producción (100-1,000 kg 1,3-PD/h) sobre la rentabilidad del proceso fueron estudiados. Los resultados mostraron que el proceso podría ser económicamente rentable sobre un rango amplio de combinaciones de escenarios. Este artículo sirve como un medio para la toma de decisiones estratégicas (p.ej., decisiones *go/no-go* de inversión) y para una futura optimización del proceso de producción de 1,3-PD a partir de glicerol crudo.

Palabras clave: 1,3-propanodiol, glicerol, modelamiento, simulación, análisis económico.

1 Introduction

Crude glycerol is the major waste byproduct of the biodiesel industry. About one part of glycerol is formed for every ten parts of biodiesel produced during the transesterification reaction of oils and fats (Ciriminna *et al*., 2014; Garlapati *et al*., 2016; Zavala *et al*., 2016). The increasing biodiesel production, greatly driven by the search for renewable and alternative fuels, has resulted in a market surplus of glycerol and a fall in its price (Yang *et al*., 2012). For example, the crude glycerol price was about 900-

* *Corresponding author. E-mail*: juan.ruiz@correo.uady.mx
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965 US$/t in 2013 (Rodrigues *et al*., 2017) and then dropped to 138 US$/t in 2017 (The Jacobsen, 2018). This issue has turned out to be a significant problem affecting the biodiesel business and economic viability (Quispe *et al*., 2013). Furthermore, the residual crude glycerol also represents a threat to sustainability as it cannot be directly disposed of in the environment (Garlapati *et al*., 2016).

Therefore, finding ways of converting this so-called crude glycerol into high-value-added products becomes essential. An example of this is the dehydration of glycerol into acrolein and allyl alcohol, which are both starting materials for the manufacturing of other compounds (Martínez-Rico, 2018). Another very promising option is to produce propanediols, especially 1,3-propanediol (1,3-PD) (Lee *et al*., 2015). This biodegradable specialty chemical has a large number of applications; it can be used as a material or intermediate for the production of polymers, fragrances, coatings, adhesives, laminates, solvents, detergents, medicines, personal care products, etc. (Kaur *et al*., 2012a; Lee *et al*., 2015).

1,3-PD can be both chemically and biologically produced. The first methodology is based on either the use of acrolein or ethylene oxide as starting material. However, some disadvantages of these chemical methods relate to the requirement of high pressures and temperatures, use of expensive catalysts, release of toxic intermediates, and dependence on non-renewable materials. The second option consists in the microbial production of 1,3-PD and, unlike the chemical method, (bio)reactions take place at mild temperature and pressure conditions. Moreover, the process can be fed on renewable feedstocks, it does not generate toxic byproducts, and it is generally regarded as a low-cost and environmentally friendly approach (Kaur *et al*., 2012a; Liu *et al*., 2010; Saxena *et al*., 2009).

In general, mathematical models and simulations contribute to a better understanding of processes, thereby facilitating their optimization and economic evaluation, as exemplified in the work of Anaya-Reza and López-Arenas (2018). In this study, a process for the continuous production of 1,3-PD from crude glycerol using *Clostridium diolis* DSM 15410 as biological system was designed and simulated to determine its profitability on an industrial scale.

2 Methodology

2.1 Modelling of the fermentation process

2.1.1 Selection of the biocatalyst

The fermentation step is critical for the viability of the overall design since it is there where the product is formed. Therefore, utmost care should be taken for selecting a high-performing biocatalyst with well-known kinetic parameters. By doing so, optimal conditions can be chosen when running the process and the outcome of the simulation will closely resemble reality.

It is well known that some species of *Clostridium* can convert glycerol to 1,3-PD under anaerobic conditions. In particular, non-pathogenic *Clostridium* ssp. are of industrial value due to their high fermentation yields and productivities, ability to tolerate high substrate concentrations, and relatively simple fermentation conditions (Leja *et al*., 2011; Xin *et al*., 2015).

Kaur *et al*. (2012b) developed a mathematical model for the substrate, product, and biomass specific rates describing the 1,3-PD fermentation by the non-pathogenic and obligate anaerobe *C. diolis* DSM 15410 growing on a statistically optimized medium. Due to its outstanding performance and the fact that this strain is well-characterized, it was selected as the biocatalyst for this study.

2.1.2 Mathematical model

Below, a system of differential equations describing the fermentation process in a continuous stirred tank bioreactor is presented. It is worth noting that Eq. 5 takes into account both substrate (glycerol) and product (1,3-PD) inhibition for the biomass specific growth rate, resulting in an overall more realistic and robust model. The model parameters used in the present study can be found in Table 1. The main assumptions were: a) the liquid flow in and out are equal; b) the liquid volume in the reactor remains constant in time; c) there is no product or biomass at the inflow; d) the bioreactor is ideally mixed; and e) glycerol is the only limiting nutrient, meaning that any other nutrient is present in excess.

Substrate balance:

$$\frac{dC_S}{dt} = D(C_{S\,in} - C_S) + q_S C_X;\ C_S(0) = C_{S\,in} \qquad (1)$$

Table 1. Summary of the kinetic parameters used in this study (Kaur *et al*., 2012b).

Parameter (unit)	Value
$\mu_{\max}$ (h^{-1})	0.65
K_S (g/L)	12.8
$Y_{XS}^{\max}$ (g/g)	0.067
m_S (g/g/h)	0.23
K_1 (g/g)	7.3
K_2 (g/g)	0.15
C_{Sm} (g/L)	98.3
C_{Pm} (g/L)	65.2
a (-)	1.12
b (-)	1

Biomass balance:

$$\frac{dC_X}{dt} = -DC_X + \mu C_X; C_X(0) > 0 \quad (2)$$

Product balance:

$$\frac{dC_P}{dt} = -DC_P + q_P C_X; C_P(0) = 0 \quad (3)$$

Volumetric productivities:

$$r_i = q_i C_X \quad (4)$$

Biomass specific growth rate (Kaur *et al*., 2012b):

$$\mu = \mu_{\max}\left(\frac{C_S}{C_S + K_S}\right)\left[1 - \left(\frac{C_S}{C_{Sm}}\right)^a\right]\left[1 - \left(\frac{C_P}{C_{Pm}}\right)^b\right] \quad (5)$$

Substrate specific consumption rate (Kaur *et al*., 2012b):

$$q_S = -\left(\frac{1}{Y_{XS}^{\max}}\mu + m_S\right) \quad (6)$$

1,3-PD specific production rate (Kaur *et al*., 2012b):

$$q_P = K_1\mu + K_2 \quad (7)$$

2.1.3 Selection of the optimal operating conditions

Since product toxicity has been regarded as a bottleneck in the production of 1,3-PD, the fermentation process was modelled in a continuous way. In this manner, one can circumvent the product inhibition issue while achieving a long-term and highly efficient process (Kaur *et al*., 2012b; Xin *et al*., 2015). Aiming at selecting the optimal dilution rate and incoming substrate concentration, a response surface methodology (central composite design) was developed with Minitab 17. The upper and lower limits for C_{Sin} were 98.3 and 54.15 g/L, corresponding to the critical substrate concentration and the optimal substrate concentration in a batch process found by Kaur *et al*. (2012b), respectively. On the other hand, the upper and lower limits for the dilution rate were 0.85 times $\mu_{\max}$ (to prevent wash-out scenarios) and 0.05 (minimum growth scenario). Mathcad 15 was used in parallel to numerically simulate and solve the mathematical model described above, making use of the internal function Odesolve which returns the solution of ordinary differential equations. The resulting steady-state values were the input for the response surface experimental design. Note that the 1,3-PD volumetric productivity (r_p) was the response to be optimized.

2.1.4 Obtention of the process reaction

Based on the previous optimization routine, the molar stoichiometry of the overall growth plus product reaction was determined solving a linear system of equations of the elemental balances. It is well-known that *C. diolis* DSM 15410 produces acetic ($C_2H_4O_2$) and butyric acid ($C_4H_8O_2$) as by-products when grown on glycerol ($C_3H_8O_3$). Because of a lack of mathematical models for the specific production rates of these compounds, their yields on 1,3-PD ($C_3H_8O_2$) were estimated from literature data (Xin *et al*., 2015) and assumed to be constant. Ammonium sulfate was chosen as the nitrogen source for the fermentation as it was the one present in the optimized medium developed by Kaur *et al*. (2012b). Below, the generalized process reaction normalized to 1 mol 1,3-PD is presented.

$$\begin{aligned}\frac{q_S}{q_p}C_3H_8O_3 + \frac{q_N}{q_p}NH_3 \rightarrow C_3H_8O_2 \\ + \frac{\mu}{q_p}CH_1.8O_{0.5}N_{0.2} + \frac{q_{ButAc}}{q_p}C_4H_8O_2 \\ + \frac{q_{AcAc}}{q_p}C_2H_4O_2 + \frac{q_C}{q_p}CO_2 + \frac{q_W}{q_p}H_2O\end{aligned} \quad (8)$$

For the sake of simplicity during the simulation, only uncharged molecules were considered for the stoichiometry. However, be aware that at the pH at which the fermentation takes place NH_3 will occur as NH_4^+ and both butyric and acetic acid will be present in their carboxylate forms (butyrate and acetate, respectively). The simulated culture conditions were 33 °C and pH 7 (Kaur *et al*., 2012b), and the addition of acid/base to control the pH was implicitly assumed. Finally, the fermentation residence time was calculated as the inverse of the selected dilution rate.

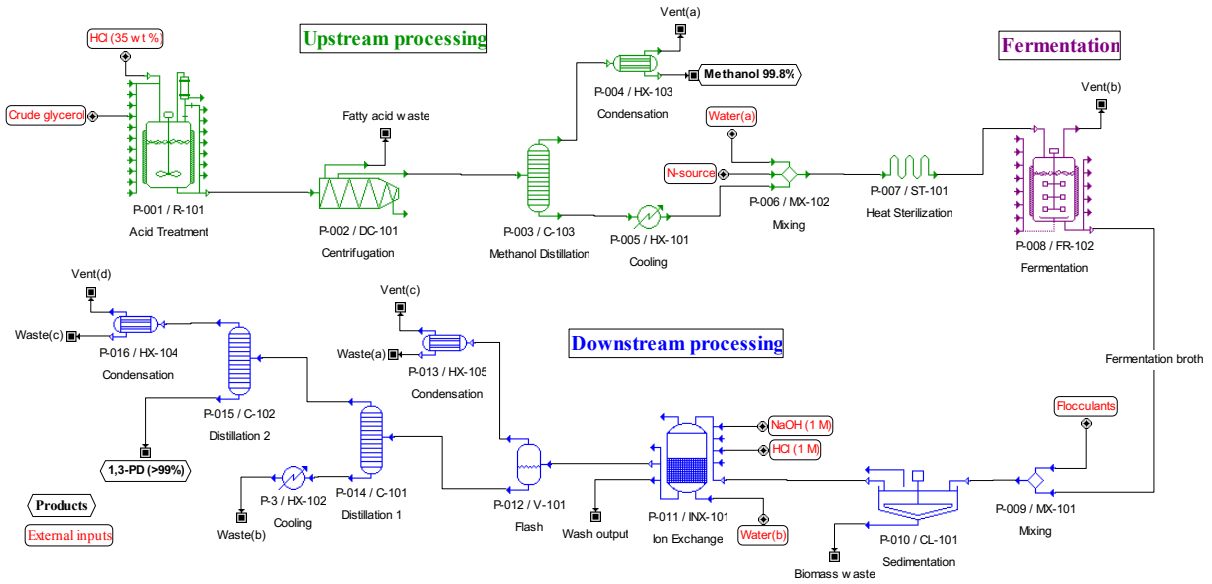

Fig. 1. Process flow diagram for the 1,3-PD production from crude glycerol by *C. diolis* DSM 15410.

2.2 *Design of the upstream processing*

For this study, a typical composition of crude glycerol obtained from the biodiesel industry was assumed to be as follows (wt %) (Posada *et al*., 2013): methanol 32.59%, glycerol 60.05%, $NaOCH_3$ 2.62%, fats 1.94%, and ash 2.8%. The first step in the purification of the crude glycerol stream was an acid treatment (pH 3.5) with HCl (35 wt %) aiming at converting any remaining soaps to free fatty acids which can then be removed by centrifugation. In the same unit operation, sodium methoxide reacts with HCl forming methanol and sodium chloride (Haas *et al*., 2006; Hájek and Skopal, 2010).

Additionally, a distillation process was added to recover methanol (light phase) as a by-product which could be reused by the biodiesel industry in the transesterification of fatty acids (Haas *et al*., 2006). Bear in mind that the methanol fraction was considered as an income during the future economic analysis. Then, the glycerol stream (heavy phase) was mixed with the nitrogen source and water to achieve the desired incoming concentrations to the bioreactor. Prior to feeding the medium to the bioreactor, a heat sterilization step was considered.

2.3 *Design of the downstream processing*

The target of the downstream process design was a 1,3-PD purity higher or equal to 99.0% so that it could be sold at a competitive price. To do so, a flocculation step was included to remove the cellular debris and soluble proteins from the fermentation broth by using an optimal combination of chitosan (150 ppm) and polyacrylamide (70 ppm) (Hao *et al*., 2006). Then, an ion exchange column was set to serve two main purposes: a) remove all the inorganic salt impurities and ashes, and b) remove both butyrate and acetate organic salts (Murali *et al*., 2017). Finally, an evaporation step was included to concentrate the stream followed by two distillation columns. The first distillation column was set to remove molecules having a boiling point greater than that of 1,3-PD, while the aim of the second column was to remove molecules with a lower boiling point than that of 1,3-PD.

2.4 *Bioprocess simulation and techno-economic analysis*

The simulation and techno-economic analysis were carried out using the software SuperPro Designer 9.0 (Intelligent, Inc.). All unit operations described above were placed in sequence and connected through streamlines. The process flow diagram can be seen in Fig. 1. Based on a certain process throughput, and after setting all the necessary input data, the software was employed to solve and calculate the corresponding mass and energy balances, equipment sizing, and process economics.

Table 2. Summary and assumptions for the total capital and operating cost calculations.

Total capital cost		Total operating cost	
1. Direct cost (DC)	DC = PC + installation + A + B + C + D + E + F + G	Materials and consumables	Calculated from mass balances
Total purchase equipment cost (PC)	Listed equipment purchase cost + unlisted equipment purchase cost[*1]	Maintenance	6% of DFC
Installation	Installation cost of listed equipment + unlisted equipment[*2]	Depreciation	10% of DFC
A. Piping	0.30 x PC	Insurance	1% of DFC
B. Instrumentation	0.20 x PC	Local taxes	2% of DFC
C. Insulation	0.01 x PC	Factory expenses	5% of DFC
D. Electrical facilities	0.10 x PC	Labor	Labor rate = (Basic rate) x (1 + Benefits + Supervision + Supplies + Administration)
E. Buildings	0.10 x PC	Labor basic rate	$2.18/h
F. Yard improvement	0.05 x PC	Benefits factor	0.40
G. Auxiliary facilities	0.20 x PC	Supervision factor	0.20
2. Indirect cost (IC)	IC = H + I	Supplies factor	0.10
H. Engineering	0.20 x DC	Administration factor	0.60
I. Construction	0.30 x DC	Work time devoted to process-related activities	70%
3. Other cost (OC)		Laboratory costs	15% of labor cost
Contractor's fee	0.03 x (DC + IC)	Waste treatment cost	$0.20/m^3
Contingency	0.07 x (DC + IC)	Utilities	Electricity and heat transfer agents
4. Direct fixed capital (DFC)	DFC = DC + IC + OC	Electricity unit cost	$0.08/kW-h
5. Working capital	30 days of labor, raw materials, utilities, waste treatment	Chilled water unit cost	$0.04/t
6. Start-up and validation cost	5% of DFC	Cooling water unit cost	$0.05/t
		Steam unit cost	$12/t
		Steam (High P) unit cost	$20/t

[*1] 10% of listed equipment.
[*2] 25 % of installation listed equipment.

Table 3. Initial economic evaluation parameters inspired on a Mexican scenario.

Parameter	Value
Year of analysis	2018
Year construction starts	2018
Construction period	30 months
Startup period	4 months
Project lifetime	15 years
Annual inflation	4%
Income taxes	30%
Currency	US Dollar ($)[*1]
Annual operating time	330 days

[*1] To make the results more readable to an international audience.

2.4.1 *Economic configuration*

In Table 2, the assumptions made for all capital and operating cost calculations are shown. The total capital cost corresponds to the sum of all fixed costs related to carrying out the project, while the total operating cost includes all the costs related to producing the product. Note that SuperPro Designer uses a range of multipliers to calculate these costs. For more detailed information about this methodology, please refer to Petrides (2013). A summary of the most relevant economic evaluation parameters used for the simulation is presented in Table 3.

2.4.2 *Profitability analysis*

The effects of the crude glycerol purchase price, 1,3-PD selling price and process throughput on the economics of the process were evaluated. A response surface methodology (Box-Behnken) was developed using Minitab 17. The lower and upper limits for the 1,3-PD cost were chosen based on two extreme-scenarios ($2.3 and $6/t) found in the bulk chemical market (Alibaba Group, 2018). Regarding the crude glycerol cost, arbitrary limit values ($100 and $300/t) were selected considering that the average crude glycerol cost in 2017 was $138/t (The Jacobsen, 2018). Finally, the process throughput ranged from 100 to 1,000 kg 1,3-PD/h. The optimization criterion was the return on investment (%ROI) which is calculated as the net profit divided by the investment cost (total capital cost). Thus, the ROI is a good way to determine the efficiency of investing on a project and can be easily translated into the payback time (ROI^{-1}). The higher the ROI, the shorter the payback time and the most profitable the investment is.

Finally, in order to identify possible process bottlenecks, an analysis of the operating costs was

performed based on the mass and energy balances. The base scenario to evaluate was selected from the profitability study.

3 Results and discussions

3.1 Fermentation process

3.1.1 Design values for $C_{S\,in}$ and D

When analyzing the response r_P from the central composite design, the following regression equation ($R^2 = 0.91$) was obtained:

$$r_P = 44.0 - 0.494C_{S\,in} - 85.5D + 0.00475C_{S\,in}^2 + 151.5D^2 - 0.755C_{S\,in}D \quad (9)$$

The 2D contour plot of the response r_P is presented in Fig. 2 which is a graphical representation of Eq. 9. By analyzing the graph, it is very clear that the maximum predicted response is achieved when $C_{S\,in}$ is kept at its maximum level (98.3 g/L) and D is set to its minimum level (0.05 h^{-1}). This was corroborated with the response optimizer tool of Minitab, in which the target was to maximize r_P. Moreover, it is worth noting that there is some kind of "optimal region" at dilution rate values below 0.1 h^{-1}, covering all the different incoming substrate concentrations. However, as the goal is to produce as much product as possible, the higher $C_{S\,in}$, the better. Therefore, the numerical optimal values found by Minitab were considered for the design of the fermentation process. The Mathcad simulation at these optimal conditions is presented in Fig. 3. In addition, a summary of the steady-state values of the most relevant fermentation parameters is presented in Table 4. These values should describe the performance of the continuous bioreactor if ideal mixing conditions are assumed. Therefore, they were used to validate or double-check the bioprocess simulation with SuperPro Designer during the profitability analysis.

3.1.2 Fermentation stoichiometry

By fixing the dilution rate at 0.05 h^{-1}, the fermentation stoichiometry was determined:

$$1.566C_3H_8O_3 + 0.101NH_3 \rightarrow C_3H_8O_2 + 0.504CH_1.8O_0.5N_0.2 + 0.098C_4H_8O_2 + 0.232C_2H_4O_2 + 0.34CO_2 + 1.108H_2O \ [\Delta H_r^0 = -71.0kJ/mol1,3-PD] \quad (10)$$

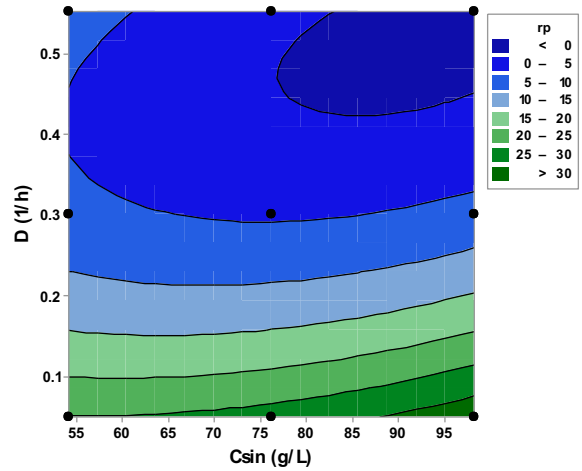

Fig. 2. Contour plot for the 1,3-PD productivity (r_P) varying the dilution rate (D) and the incoming substrate concentration ($C_{S\,in}$).

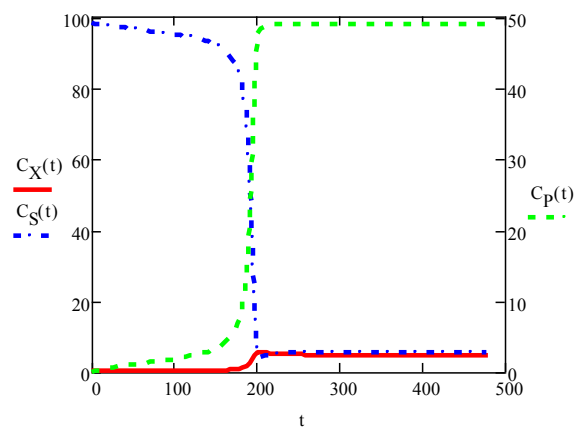

Fig. 3. Mathcad simulation of the optimal scenario for the fermentation process (D = 0.05 h^{-1} and $C_{S\,in}$ = 98.3 g/L). Concentrations and time are given in g/L and h, respectively.

From the stoichiometry, it becomes evident that one potential way of increasing the product yield is by redirecting the carbon flux towards 1,3-PD production (reductive reactions), thereby avoiding byproduct formation (oxidative reactions). Recently, genetic and metabolic engineering approaches have focused on either knocking-out or overexpressing certain genes involved in the 1,3-PD metabolism with promising results (Yang *et al.*, 2018). Therefore, in combination with process engineering studies like the one here presented, it is hoped that these efforts can contribute to the goal of obtaining a technically viable process in the short- to medium-term.

Table 4. Steady state fermentation parameters under optimal D and $C_{S\,in}$ values.

Parameter	Steady-state values
C_S (g/L)	5.7
C_X (g/L)	4.9
C_P (g/L)	49
r_X (g/L/h)	0.23
r_S (g/g/L)	-4.63
r_P (g/g/L)	36.07

3.2 Techno-economic analysis

3.2.1 Profitability analysis

When analyzing the Box-Behnken experimental results, the following regression equation (R^2 = 0.98) was obtained:

$$\%ROI = -41.9+11.81A-0.009B+0.0179C-0.793A^2 -0.000088B^2-0.000032C^2+0.0043AB+0.01049AC -0.000033BC \quad (11)$$

where A: Selling price of 1,3-PD ($/t); B: Crude glycerol purchase price ($/t); C: Process throughput (kg 1,3-PD/h).

In Figs. 4-5, the 2D contour plots describing the equation above are presented. They show how the return on investment is affected by changes on two of the variables while keeping a third one constant. The hold values were set as the average of the upper and lower limits of each factor. This type of analysis is a valuable tool for engineers since it facilitates the strategic planning and decision-making process, giving information on the profitability of the process under several scenarios. As expected, the best scenario was that one in which both the 1,3-PD selling price and the process throughput were maximal, and the cost of crude glycerol was minimal. Most importantly, if we consider a value of ROI above or equal to 17-20 % (payback time of around 5-6 years) as a "profitable investment", then there was a wide range of scenarios in which the process was attractive from an economic point of view. This range was even wider if only positive values of ROI were sought.

At the selected hold values, positive ROI figures were found at a selling price of 1,3-PD ≥ $4.0/t, crude glycerol purchase price $100-300/t and process throughput ≥~ 220 kg 1,3-PD/h. Although the analysis is limited by the range of the evaluated parameters, it is worth noting that the ROI remains positive even at very high crude glycerol purchase costs (up to $300/t).

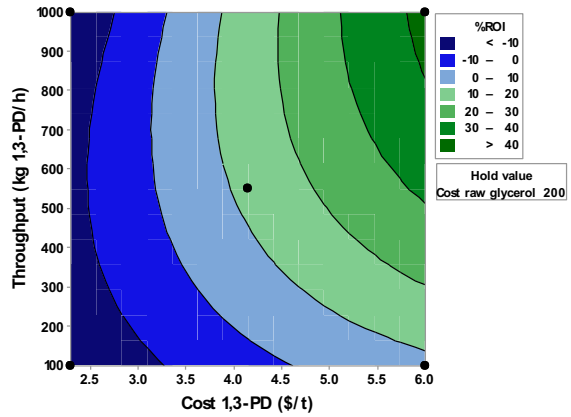

Fig. 4. Contour plot for the %ROI varying the process throughput and the selling price of 1,3-PD.

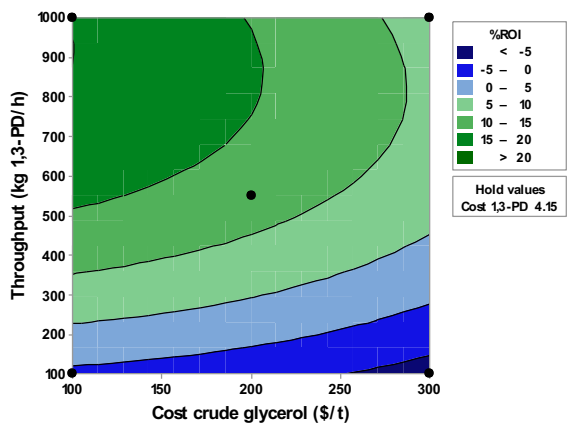

Fig. 5. Contour plot for the %ROI varying the process throughput and the crude glycerol purchase price.

This is relevant considering that the glycerol price is greatly affected by policymaking (e.g., incentives to the biodiesel industry) and the price of crude oil, which are both volatile by nature (Pagliaro, 2017).

3.2.2 Operating cost breakdown

For the following analysis, an arbitrary scenario was chosen trying to avoid being too optimistic or pessimistic: $ 4.5/t 1,3-PD; $ 138/t crude glycerol; 500 kg 1,3-PD/h. The executive summary of such project is presented in Table 5. Overall, the payback time would be around 5.7 years, requiring a total investment close to $25.3 million. The annual operating cost breakdown can be seen in Fig. 6. In an ideal situation, most of the operating costs should be well-distributed among the different items. However, in this case almost 45% of the operating expenditures corresponded to the utilities, meaning that the process is relatively high-

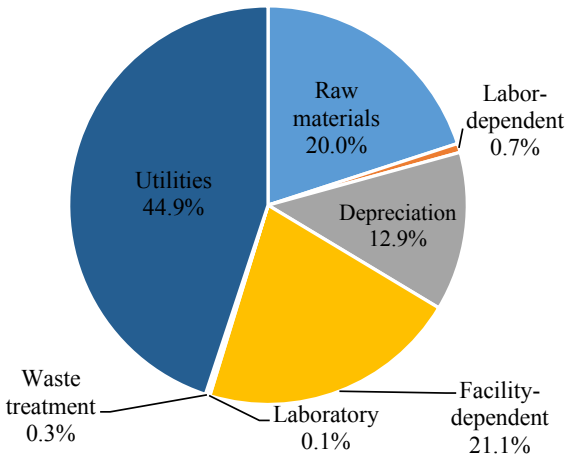

Fig. 6. Annual operating cost breakdown.

Table 5. Executive summary of the project at 500 kg 1,3-PD/h; $ 4.5/t 1,3-PD; $ 138/t crude glycerol.

Item	Value
Total capital investment	$25,335,159
Annual operating costs	$15,426,790
Main annual revenues	$17,820,000
Other annual revenues*1	$1,130,954
Unit production cost	$3.90/kg 1,3-PD
Unit production revenue	$4.79/kg 1,3-PD
Gross margin	18.60%
ROI	1.58%
Payback time	5.69 years
IRR (after taxes)	25.23%
Net present value (NPV) (at 7.0 % interest)	$6,756,514

*1 Revenue due to the methanol produced during the purification of crude glycerol.

energy intensive. This can be explained by the fact that the design included several distillation and other heat-consuming processes like evaporation and heat sterilization. Therefore, finding alternative unit operations or fermentation methodologies could result in a more cost-efficient process. For example, the production of 1,3-PD using immobilized cells could allow the reuse of the biocatalyst, yielding more biological stability, a simplified downstream processing, and a decrease in bioreactor volumes (Loureiro-Pinto *et al.*, 2017). Another plausible alternative could be to use non-sterile raw glycerol in the fermentation, lowering the intensity of the upstream processing (Kaeding *et al.*, 2015).

Conclusions

In this paper, a feasibility analysis of the production of 1,3-PD (> 99.0% purity) from crude glycerol by *C. diolis* DSM 15410 was performed based on optimal fermentation parameters. Different scenarios concerning the selling price of 1,3-PD, the purchase cost of crude glycerol and the throughput were evaluated in terms of their effect on the profitability of the process. The results showed that the process design hereby presented was profitable over a wide range of scenarios. Finally, this study contributes with a mathematical model for the 1,3-PD productivity in a continuous fermentation and offers economic models for strategic decision making (e.g., go and no-go investment decisions) and further optimization of the process.

Nomenclature

D	dilution rate, h^{-1}
C_i	concentration of component i (S: glycerol, P: 1,3-PD, X: biomass), g_i/L
dC_i/dt	rate of reaction of component i, g_i/L/h
q_i	specific production/consumption rate of i, g_i/g_X/h
μ	biomass specific growth rate ($\mu = qX$), h^{-1}
μ_{max}	maximum biomass specific growth rate, h^{-1}
r_i	volumetric productivity of component i, g_i/L/h
K_S	saturation constant for substrate, g_S/L
$C_{S\,in}$	inlet substrate concentration, g_S/L
$C_{S\,m}$	critical substrate concentration, g_S/L
$C_{P\,m}$	critical product concentration, g_P/L
K_1	growth associated contribution for 1,3-PD production, g_P/g_X
K_2	non-growth associated contribution for 1,3-PD production, g_P/g_X/h
m_S	maintenance energy constant, g_S/g_X/h
Y_{XS}^{max}	maximum yield of biomass on substrate, g_X/g_S
a,b	model constants, dimensionless

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