BIOREFINERY: A solution for a sustainable future

Part II. Analysis of two batch processes for the 1,3-propanediol production

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INTRODUCTION AND OBJECTIVE

Historically, 1,3-propanediol has been produced by chemical synthesis but its numerous disadvantages such as high pressure and temperature requirements and expensive catalysers have lead to a 1,3-propanediol production costs very high and demanding.

Alternative

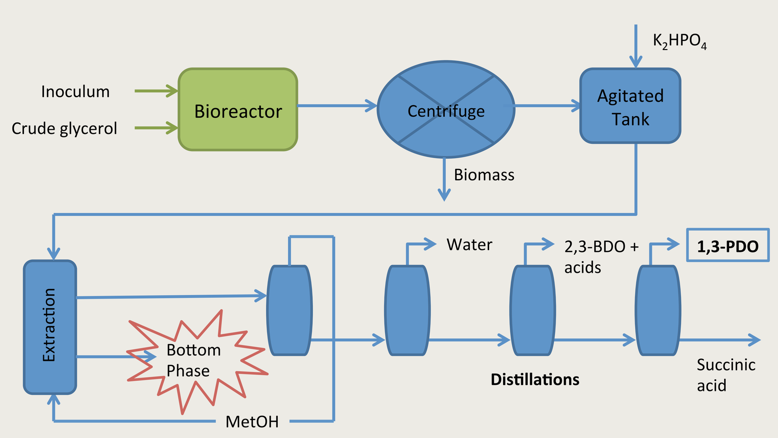
Microbial conversion of raw materials to 1,3-PDO

- ✓ Using crude glycerol from the biodiesel production.
- ✓ Bacterial strain Klebsiella pneumoniae.
- ✓ Analysing two different fed-batch processes.

Objective: develop two different fed-batch processes and compare them, taking into account not only its economic analysis but also especially its environmental impact. SuperPro designer was used as a simulation tool for the development of the two processes.:

PROCESS DESCRIPTION

SIMPLE PROCESS



Fermentation reaction

- ➡ Two 252 m^3 bioreactors.
- ➡ **Fed-batch** with an initial crude glycerol concentration of 40 g/L and after 15 h maintained at 15 g/L.
- ➡ Temperature at 37ºC
- ➡ pH fixed at 7 by addition of NH_4OH.
- ➡ Microareobic system 0,02 vvm.

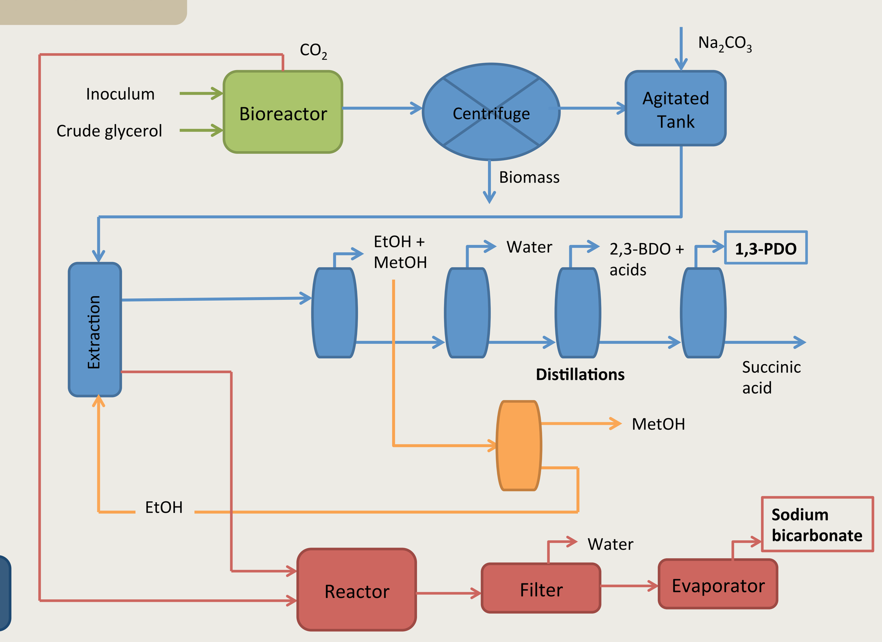
Aqueous two-phase system extraction

K_2HPO_4 / methanol — **Alcohol 24%** — **Salt 15%** — **Na_2CO_3 / ethanol**

The salt decreases the solubility of 1,3-PDO and achieve its dissolution in the alcohol, so can effective extract **1,3-PDO** from the fermentation broth.

Sodium bicarbonate

IMPROVED PROCESS



Using Na_2CO_3 for the extraction allows to use the bottom phase of the extraction together with the CO_2 emitted during fermentation to produce sodium bicarbonate, which can be sold as a revenue.

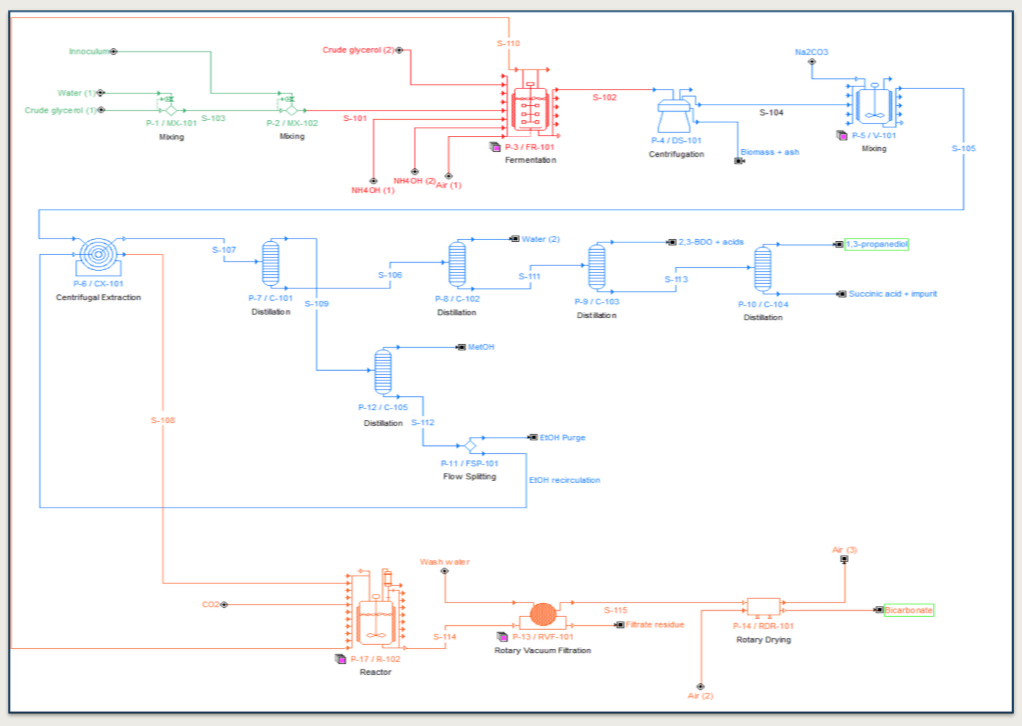


Figure 1 – Improved process flux diagram designed with SuperPro Designer. All flows and equipment have been characterized in detail.

ECONOMIC ANALYSIS

SIMPLE PROCESS

PDO selling price: **60 $/kg**

Total investment ($)	**70.789.000**
Annual operating cost ($)	**51.956.000**
Revenues ($/yr)	**243.652.000**
Unit production cost ($/kg)	**12,8**
Unit production revenue ($/kg)	**60,05**
Gross margin	**79 %**
Return on investment	**171 %**
Payback time	**0,58 yr**
NPV (7% interest) ($)	**729.459.000**

The process seems to be economically feasible because the **unit production cost is lower than the unit production revenue.** But there are two critical points that lead to increase drastically the **annual operating cost:**

- ➡ **Raw materials cost, due to the high amount of K_2HPO_4 that is needed for the extraction.**
- ➡ **Waste treatment cost, due to the high cost of the treatment that needs to be applied on the solid bottom phase of the extraction.**

NOT an ECO-FRIENDLY PROCESS

IMPROVED PROCESS

Depending on the selling price, the **economic feasibility** of the process varies from an unfeasible process to a short payback time process:

- ➡ **3 $/kg PDO** corresponds to a market based on PTT production.
- ➡ **60 $/kg PDO** corresponds to pharmaceutical and cosmetics market.

➡ In both cases, the **product is exactly the same**, and its high purity makes the process costs extremely high.

	3 $/kg PDO	60 $/kg PDO
Total investment ($)	91.531.000	
Annual operating cost ($)	27.789.000	
Revenues ($/yr)	19.029.000	233.911.000
Unit production cost ($/kg)	7,37	
Unit production revenue ($/kg)	5,05	62,05
Gross margin	- 46 %	88 %
Return on investment	- 0,62 %	144 %
Payback time	N/A	0,7 yr
NPV (7% interest) ($)	- 91.879.000	847.787.000

Feasible process

Although the main goal of this process is to produce 1,3-PDO, two other revenues are produced during the process:

- ➡ Methanol, separated from ethanol (0,3 $(kg).
- ➡ Sodium bicarbonate (0,25 $/kg).

PDO SELLING PRICE DETERMINES THE PLANT FEASIBILITY, WHICH RESULTS TO BE FEASIBLE WHEN PDO IS SOLD AT 60 $/kg

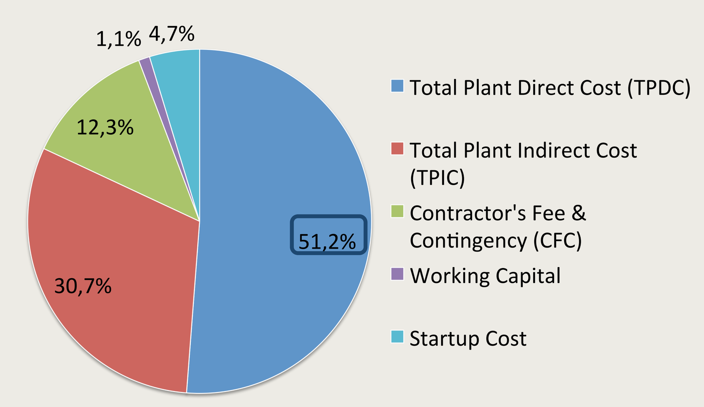


Figure 2 – Total investment.

A **31%** of the TPDC corresponds to the **equipment cost**, due to the extremely high operation equipment volume.

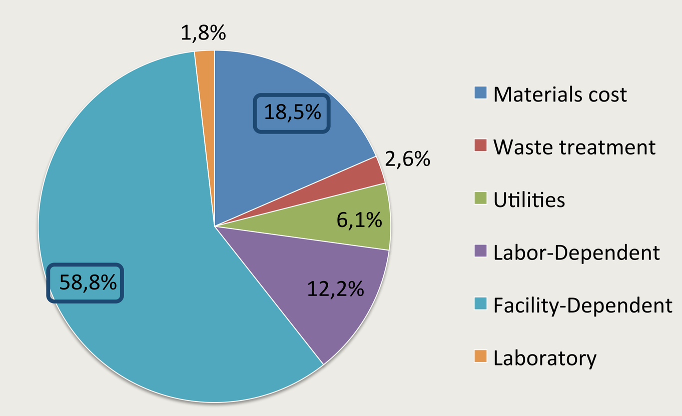
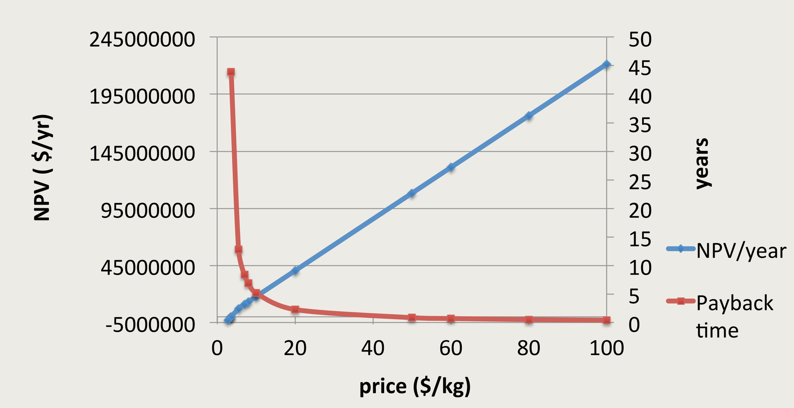


Figure 3 – Annual operating cost. .

A **18,5%** of the AOC corresponds to the **materials cost**, being the most important the salt used in the extraction (Na_2CO_3), which represents a 60% of the total material cost, followed by the crude glycerol used as a substrate.



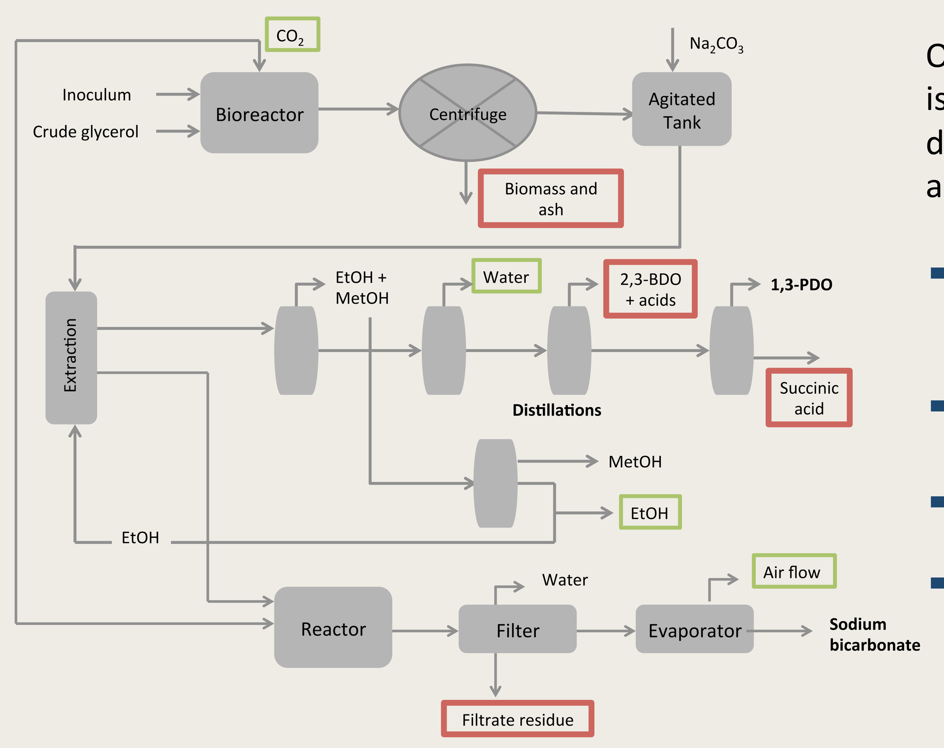
Return on investment is negative when PDO is sold at 3 $/kg. This is due to the unit production revenue is lower than the unit production cost.

When PDO is sold at 60 $/kg, the inversion is quickly recovered and the benefit is high. This situation leads to a consideration of the PDO selling price. According to figure 3, the minimum optimal selling price is 20 $/kg since the payback time has decreased dramatically and NPV is positive.

ENVIRONMENTAL ANALYSIS

IMPROVED PROCESS

To describe the impact that the process may cause to the environment, it is necessary to identify the process outputs and whether they are formed by toxic compounds or not:



Toxic compounds — Non toxic compounds

Once the harmless outflows have been identified, it is necessary to describe its composition in order to decide which waste treatment process is going to be applied:

- ➡ Biomass and ash: anaerobic digestion, due to its TOC and COD values.
- ➡ 2,3 – BDO and acids; ➡ Succinic acid and impurities — Neutralization treatment and anaerobic digestion.
- ➡ Filtrate residue: wastewater treatment plant.

CONCLUSIONS

Two processes for the production of highly pure 1,3-propanediol using crude glycerol as a substrate have been described. A *Klebsiella pneumoniae* strain has been used as a catalyser in both reactions, leading to a product/substrate yield of 50%:

- ➡ Simple process: the bottom phase from the extraction is a solid waste with a difficult an expensive treatment, so that leads to a low feasible and no eco-friendly process.
- ➡ Improved process: - NO CO_2 emissions; - Low waste treatment cost — 3 REVENUES, ECO-FRIENDLY

What is next ?

There are some options to consider in order to improve the production process designed:

- ➡ Using a genetically modified *Klebsiella* strain that could tolerate even better the substrate.
- ➡ Operating in continuous reaction mode in order to decrease the reactor volume.
- ➡ Purification of 2,3-butanediol and lactic acid, obtained as a fermentation products.

SELECTED REFERENCES

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