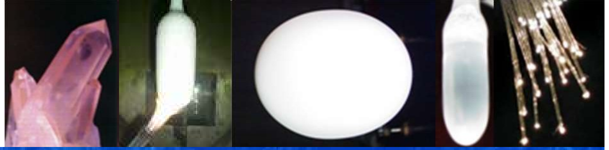


IECF 2021
The 2nd International Electronic Conference on Forests
Sustainable Forests: Ecology, Management, Products and Trade
01–15 SEPTEMBER 2021 | ONLINE

Supercritical Extraction of Essential Oils from Dry Clove: a Technical and Economic Viability Study of a Simulated Industrial Plant

Marco César Prado Soares [1,*], Paula Rocha Machado[2], Roger Eike Guinosa[2]

[1]School of Mechanical Engineering, University of Campinas, São Paulo , Brazil

[2]School of Chemical Engineering, University of Campinas, São Paulo, Brazil

1. Introduction

Supercritical Fluids

- Compound under conditions of temperature (T) and pressure (P) beyond its critical point (Tc, Pc).
- The liquid and vapor phases are, therefore, indistinguishable [1].

[1] Doane-Weideman, T.; Liescheskii, P. Analytical Supercritical Fluid Extraction for Food Applications. In *Oil Extraction and Analysis*; AOCS Publishing, 2004.

1. Introduction

Supercritical Fluid Extraction (SFE)

- SFE technology presents remarkable advantages over the traditional extraction techniques:
    - It allows the solvent to be easily removed by simply reducing the system's pressure or temperature.

1. Introduction

Supercritical Fluid Extraction (SFE)

- It is a green and eco-friendly methodology:
  - Results in enhanced energetic efficiency;
  - May proceed with minimal or even no amount of organic co-solvents;
  - Results in minimum quantities of residues [2].

[2] Mukhopadhyay, M. *Natural Extracts Using Supercritical Carbon Dioxide*; First Ed.; CRC Press: USA, 2000.

1. Introduction

Supercritical Fluid Extraction (SFE)

- Many industrial plants on Europe, USA and Japan already employ the SFE to separate compounds from: ***coffee, tea, and hop***.
- Compounds are extracted from solid matrices;
- The supercritical fluid is used to solubilize the desired materials while filling the vessel [3].

[3] Zacchi, P.; Pietsch, A.; Voges, S.; Ambrogi, A.; Eggers, R.; Jaeger, P. Concepts of phase separation in supercritical processing. *Chem. Eng. Process. Process Intensif.* **2006**, *45*, 728–733, doi:10.1016/j.cep.2006.03.006.

1. Introduction

Supercritical Fluid Extraction (SFE)

- The solvent flows inside the extractor, swelling its fixed bed and facilitating the mass transfer.
- In a second step, the pressure is reduced, with a consequent decrease of both the density of the solvent and of the solubility of the extracted compound.
  - It allows their easy separation. Finally, the solid residue (usually biomass) is removed from the extractor [4].
- Finally, the solid residue (usually biomass) is removed from the extractor [4].

[4] Brunner, G. *Gas extraction: An Introduction to Fundamentals of Supercritical Fluids ant the Application to Separation Processes.*; Steinkopff: Darmstadt, Germany, 1994.

1. Introduction

Solvent for Supercritical Fluid Extraction (SFE)

- One of the most used solvents for SFE is CO_2.
- That is because it presents:
  - Low toxicity and reactivity;
  - Is no inflammable;
  - Presents moderate Tc, Pc, and purchase costs; and
  - Results in no solvent residues in the equipment [5].

[5] Souza, A.T.; Corazza, M.L.; Cardozo-Filho, L.; Guirardello, R.; Meireles, M.A.A. Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO 2. *J. Chem. Eng. Data* **2004**, *49*, 352–356, doi:10.1021/je034190f.

1. Introduction

Clove Essential Oil

- A relevant compound which may be separated by SFE is the essential oil from clove (*Eugenia caryophyllata*).
- **It is mainly composed of**:
  - Eugenol (75.5% in mass);
  - Eugenyl acetate (11.0%);
  - trans-caryophyllene (12.1%); and
  - α-humulene (1.4%) [5].

1. Introduction

Clove Essential Oil

- Presents:
  - Antibacterial and antifungal activities;
  - May be used as antioxidant and anti-inflammatory;
  - May be used for asthma and allergy relief [5–7].

[6] Öztürk, A.; Özbek, H. The anti-inflammatory activity of Eugenia caryophyllata essential oil: An animal model of anti-inflammatory activity. *Eur. J. Gen. Med.* **2005**, *2*, 159–163.
[7] Lin, C.-H.; Lin, S.H.; Lin, C.-C.; Liu, Y.-C.; Chen, C.-J.; Chu, C.-L.; Huang, H.-C.; Lin, M.-K. Inhibitory effect of clove methanolic extract and eugenol on dendritic cell functions. *J. Funct. Foods* **2016**, *27*, 439–447, doi:10.1016/j.jff.2016.09.026.

1. Introduction

Clove Essential Oil

- In Brazil, clove is of particular economic importance:
  - Annual production estimated in **6000 ton/year**.
    - **5000 ton/year** destined to exportation [8].

[8] Vitaspice. O Cravo-da-Índia no Brasil. Graça Valença / Bahia – Brasil. Available online: http://www.vitaspice.com.br/bra/cravodaindia.asp (accessed on Oct 3, 2019).

1. Introduction

Clove Essential Oil Extraction Nowadays

- There are several studies analyzing the SFE of clove essential oil with CO_2 in laboratory [5,9–13].
- There is still a need for ***technical and economic feasibility studies covering large-scale extraction plants***.

[9] Hatami, T. *et al. J. Supercrit. Fluids* **2019**, *144*, 39–47, doi:10.1016/j.supflu.2018.10.003.
[10] Johner, J.C.F. *et al. Open Food Sci. J.* **2018**, *10*, 1–7, doi:10.2174/1874256401810010001.
[11] Ochoa, S. *et al. Food Bioprod. Process.* **2020**, *122*, 111–123, doi:10.1016/j.fbp.2020.04.007.
[12] Canabarro, N.I. *et al. J. Appl. Res. Med. Aromat. Plants* **2020**, *18*, 100261, doi:10.1016/j.jarmap.2020.100261.
[13] Viganó, J. *et al. J. Supercrit. Fluids* **2017**, *122*, 88–98, doi:10.1016/j.supflu.2016.12.006.

1. Introduction

Clove Essential Oil Extraction Nowadays

- **Pilot-scale SFE plants**: the minimum viable industries.
  - Typically employ extractors ranging from **2 to 100 L** [14].
- **Industrial plants**:
  - Work with average volumes of **400 L** [15].

[14] Capuzzo, A. *et al. Molecules* **2013**, *18*, 7194–7238, doi:10.3390/molecules18067194.
[15] Takeuchi, T.M. *et al. J. Supercrit. Fluids* **2008**, *43*, 447–459, doi:10.1016/j.supflu.2007.08.002.

1. Introduction

Proposal of This Work

- We used the ***SuperPro Designer 10 (Intelligen)*** to simulate an industrial production using **two 400 L-extractors**.

- We collected real purchase data from large-scale exporters of clove and its essential oil compounds; and from suppliers of pressurized CO_2 [16–21]. Then, we input these information in the simulator. for different clove's purchase costs.

[16] IndiaMART. Brown Whole Clove, Packaging Size: 5 Kg. Available online: https://www.indiamart.com/proddetail/clove-22530339073.html (accessed on Nov 1, 2020).
[17] IndiaMART. Katyani Exports Yellow Eugenol USP Extract Feed Grade, for Aromatherapy, Purity: 100% Pure And Natural. Available online: https://www.indiamart.com/proddetail/eugenol-usp-extract-feed-grade-3760659988.html (accessed on Oct 24, 2020).
[18] IndiaMART. Natural Aroma Liquid Eugenol Acetate. Available online: https://www.indiamart.com/proddetail/eugenol-acetate-8336104997.html?pos=1&kwd=eugenil+acetate (accessed on Oct 24, 2020).
[19] IndiaMART. Natural Aroma Liquid Caryophyllene Acetate, Packaging Type: Can,Barrel. Available online: https://www.indiamart.com/proddetail/caryophyllene-acetate-6309471897.html?pos=5&kwd=caryophyllene (accessed on Oct 24, 2020).
[20] IndiaMART. Alpha Humulene Available online: https://www.indiamart.com/proddetail/alpha-humulene-6309461933.html?pos=1&kwd=alpha+humolene (accessed on Oct 24, 2020).
[21] Made-in-China; Equipment, S.Y.S. 10L Seamless Steel Portable CO2 Carbon Dioxide Gas Cylinder. Available online: https://yacylinder.en.made-in-china.com/product/ISbJDRuVgjUp/China-10L-Seamless-Steel-Portable-CO2-Carbon-Dioxide-Gas-Cylinder.html (accessed on Nov 1, 2020).

1. Introduction

Proposal of This Work

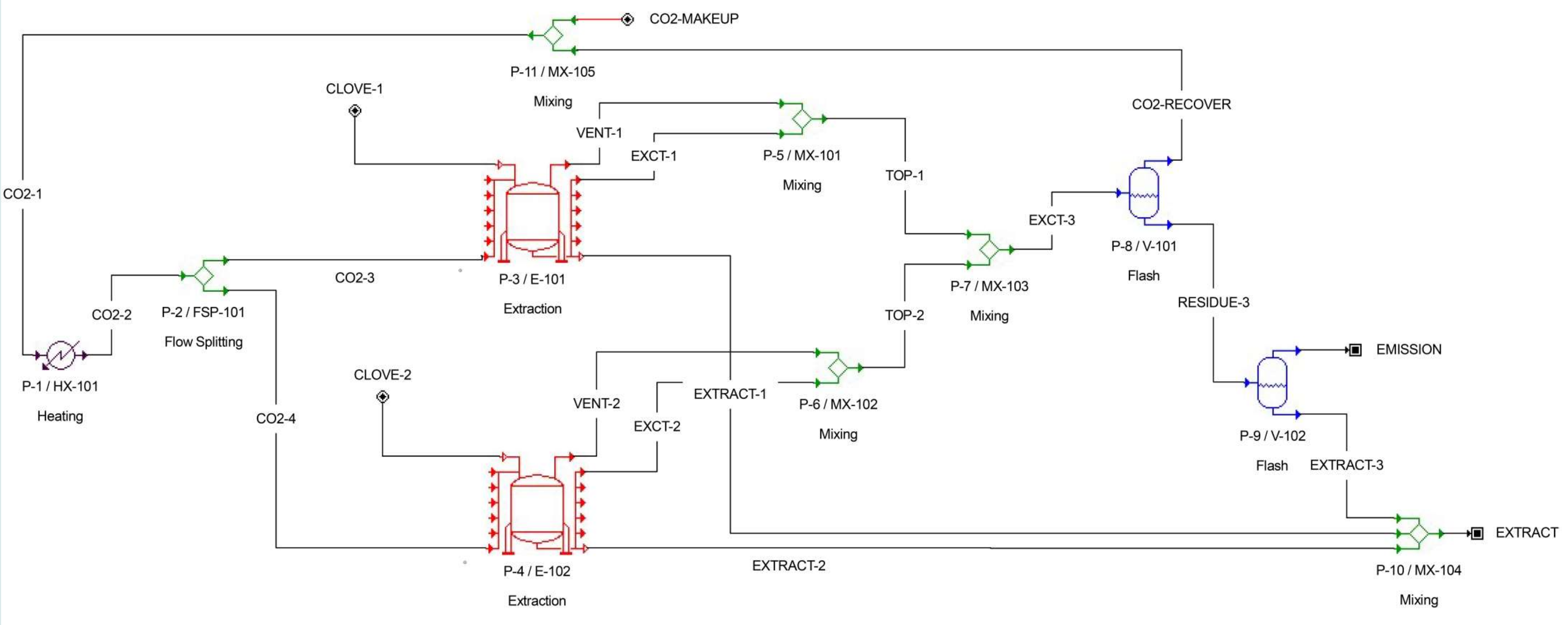
- Finally, we applied the ***Weighted Average Capital Cost (WACC)*** methodology [22] to ***perform the economic feasibility analysis***.

- It allowed us to calculate the *main investment indicators* of the industrial SFE plant and to evaluate the *viability of the process for different clove's purchase costs*.

[22] Damodaran, A. *Damodaran On Valuation: Security Analysis for Investment and Corporate Finance*; 2nd Ed.; John Wiley & Sons, Inc., 2011.

2. Simulation and Technical-Economic Model

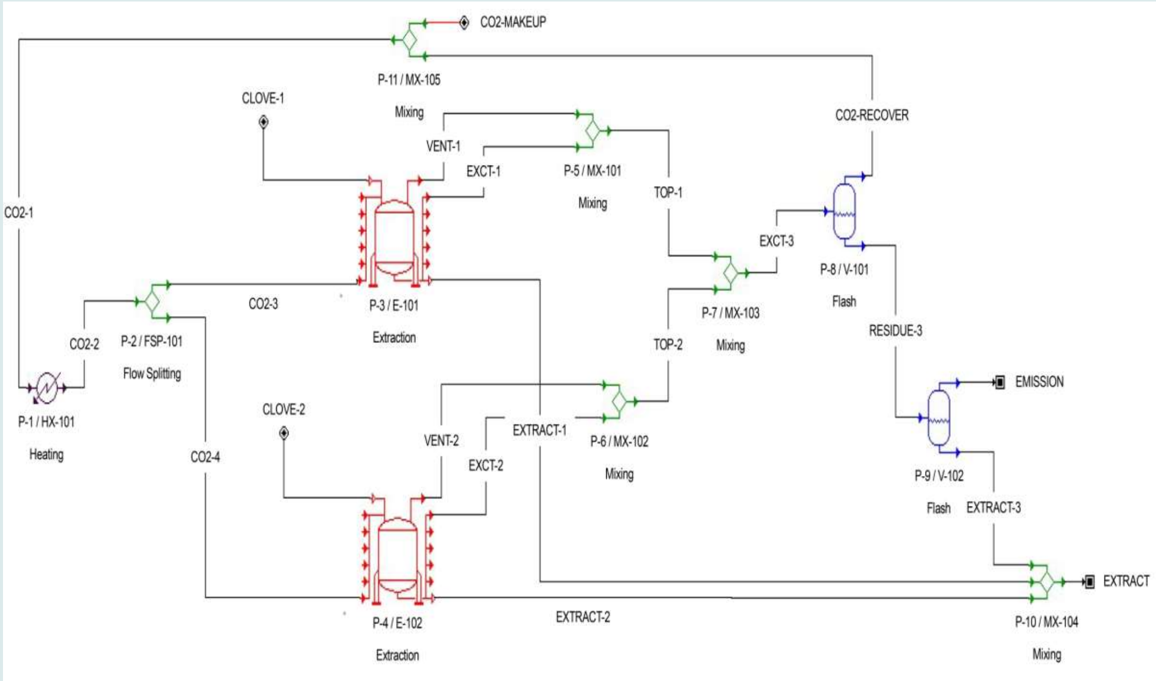
Simulation Model



2. Simulation and Technical-Economic Model

Simulation Model

- It basically consists of two 400 L-extractors that are charged with solid clove and then pressurized with CO_2.
- Two flash drums complete the system and allow the recovery of the oil compounds.



2. Simulation and Technical-Economic Model

Input Information

- Neither the oil compounds nor the solid clove are present in SuperPro Designer 10 database and must be manually input.
- Therefore, we firstly created each one of the clove oil's compounds and input their respective physicochemical data [5].

2. Simulation and Technical-Economic Model

Input Information: *Clove oil's physicochemical data [5,23-26]*

Component	Mass Fraction	Molar Mass (g/mol)	T_{crit} (K)	P_{crit} (bar)	V_{crit} (m^3/mol)	Z_{crit}	ω	$T_{melting}$ (K)	$T_{vaporization}$ (K)	Density (g/cm^3)	CAS Nº
Eugenol	0.755	164.2	763,2	33.42	500.9	2.64×10^5	0.65	264.0	525.2	1.07	97-53-0
Eugenyl Acetate	0.11	206.24	767.0	22.97	668.1	2.41×10^5	0.57	264.1	556.7	1.08	93-28-7
trans-Caryophyllene	0.121	204.36	714,7	18.98	701.3	2.24×10^5	0.48	264.2	536.2	0.90	87-44-5
α-Humulene	0.014	204.36	719.0	17.09	743.0	2.12×10^5	0,.45	264.2	440.2	0.89	67-53-98-6

[23] Merck. Eugenol Safety Data Sheet. Available online: https://www.merckmillipore.com/BR/pt/product/msds/MDA_CHEM-818455?Origin=PDP (accessed on Oct 10, 2020).
[24] Sigma-Aldrich. Eugenyl Acetate Safety Data Sheet. Available online: https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=BR&language=pt&productNumber=W246905&brand=ALDRICH&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fproduct%2Faldrich%2Fw246905%3Flang%3Dpt (accessed on Oct 10, 2020).
[25] Sigma-Aldrich. (−)-trans-Caryophyllene Safety Data Sheet. Available online: https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=BR&language=pt&productNumber=22075&brand=SIGMA&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fproduct%2Fsigma%2F22075%3Flang%3Dpt (accessed on Oct 10, 2020).
[26] Sigma-Aldrich. α-Humulene Safety Data Sheet. Available online: https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=BR&language=pt&productNumber=12448&brand=SIAL&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fsearch%3Fterm%3D6753-98-6%26interface%3DCAS%2520No.%26N%3D0%26mode%3Dpartialmax%26 (accessed on Oct 10, 2020).

2. Simulation and Technical-Economic Model

Input Information: *Clove oil's physicochemical data [5,23-26]*

Component	Cp (J/mol.K) [T in K]	Antoine Equation [P in mmHg and T in K]	ΔHv (J/mol)
Eugenol	46.763 + 0.4958T	log P = 5.08897 – (2463.351)/(T – 42.226)	$\Delta H_v = 40349(1 - T_r)^{0.2536}$
Eugenyl Acetate	41.9816 + (0.772)T - $(3\times10^{-4})T^2 + (7\times10^{-9})T^3$	log P = 5.36989 – (2782.976)/(T – 36.986)	$\Delta H_v = 40518(1 - T_r)^{0.2521}$
trans-Caryophyllene	314.194	log P = 3.30926 – (1443.925)/(T – 26.564)	$\Delta H_v = 37391(1 - T_r)^{0.2613}$
α-Humulene	313.282	log P = 3.29014 – (1459.619)/(T – 25.857)	$\Delta H_v = 38176(1 - T_r)^{0.2600}$

2. Simulation and Technical-Economic Model

Input Information

- Prior to registering a new compound, the software asks the user to select a "*default*" material from its database.

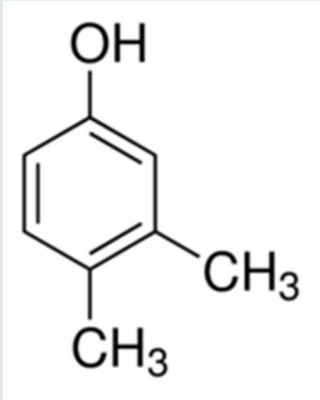
- This should be a compound with similar structure to the one being input because, ***if there is any information that is not known by the user, the software will automatically input the data from the default compound***.

2. Simulation and Technical-Economic Model

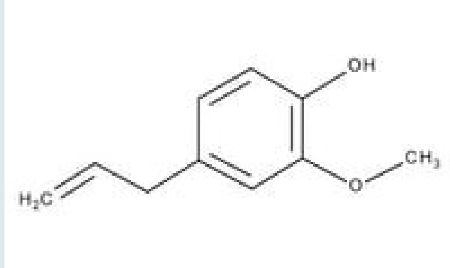
Input Information

- Then, we selected "***3,4-Xylenol***" as the ***default for eugenol and for eugenyl acetate***; and

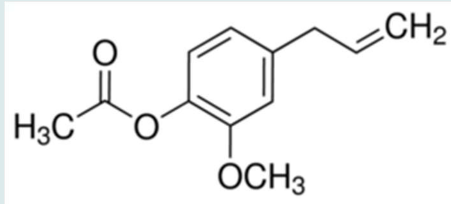
- Selected "***Fats***" (a general liquid compound from the database, which is the average obtained from fats gathered from different and non-homogeneous sources) ***for the other two compounds***.



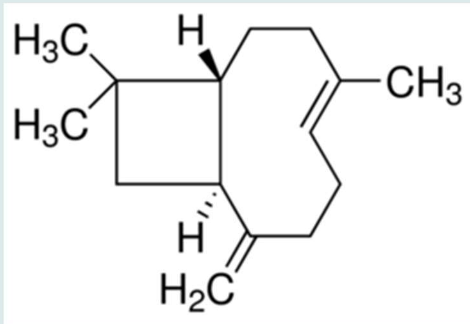
3,4-Xylenol



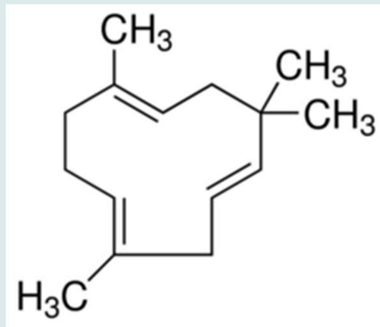
Eugenol



Eugenyl Acetate



trans-Caryophyllene



α-Humulene

2. Simulation and Technical-Economic Model

Input Information

- The software allows to **register selling and purchase costs**.
- We registered prices obtained from manufacturers that produce the compounds in large scale and for exportation:
    - 25.73 USD/kg (eugenol);
    - 32.51 USD/kg (eugenyl acetate);
    - 12.19 USD/kg (trans-caryophyllene);
    - 14.19 USD/kg (α-humulene) [17–20].

2. Simulation and Technical-Economic Model

Input Information

- We also registered mixtures:
- ***"Clove oil"***: mixture of the compounds of clove oil with the previously mentioned composition [5]:
  - 75.5 % (m/m) of Eugenol;
  - 11.0 % (m/m) of Eugenyl acetate;
  - 12.1 % (m/m) of trans-caryophyllene (12.1%);
  - 1.4% (m/m) of α-humulene.

2. Simulation and Technical-Economic Model

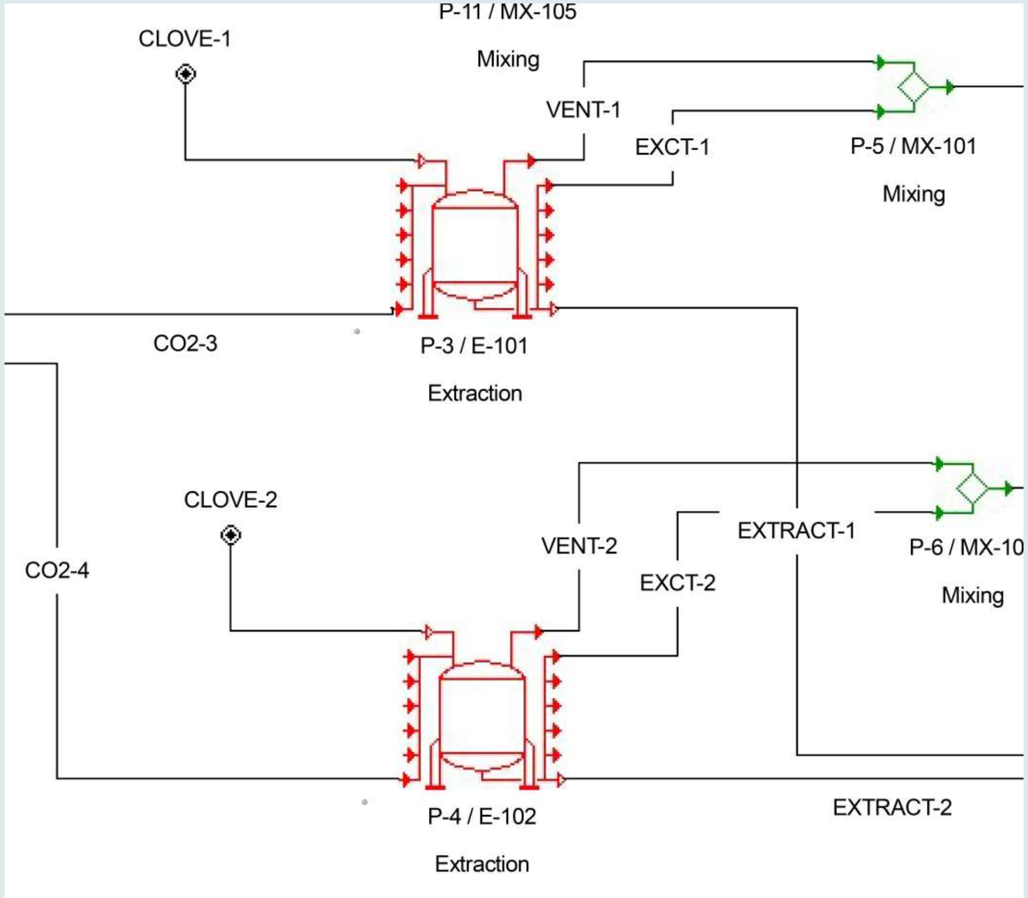
Input Information

- ***"Solid clove"***: mixture of "Biomass" and "clove oil".
- "***Biomass***": a solid compound from the database that represents the average information collected for different vegetable materials.
- Exportation manufactures' of dry solid clove guarantee an ***oil degree from 15 to 20% (m/m)***.
- Then, the average value of this range (**17.5%**) was took as the mass fraction of oil in this semi-solid mixture.
- The purchase cost was defined as **0.64 USD/kg of dry clove** [16].

2. Simulation and Technical-Economic Model

Simulation Model

- The software does not provide an equipment model for SFE.
- The extractor must also be created in the simulator from simpler equipment already present in its database.
- For this step, we created two extractors (E-101 and E-102) from batch stocking drums.



2. Simulation and Technical-Economic Model

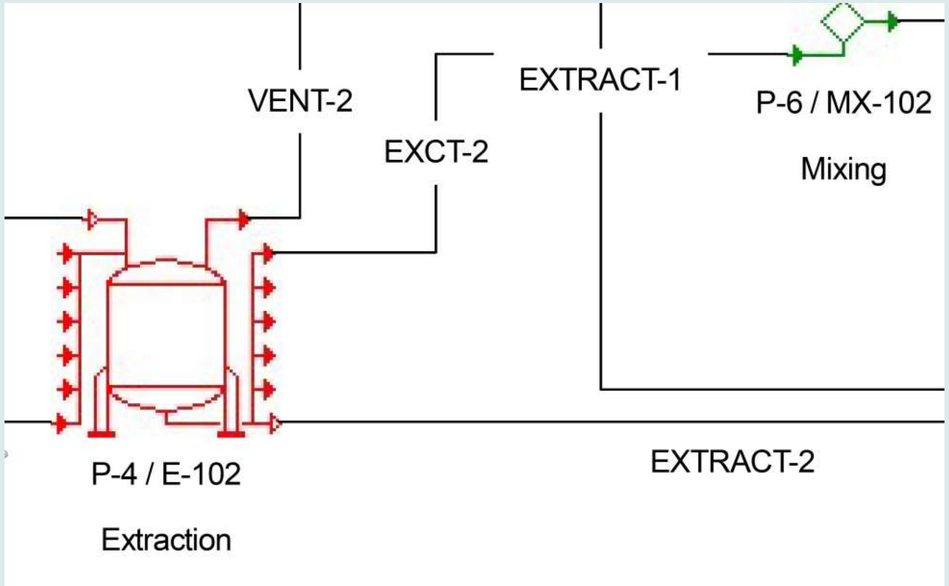
Simulation Model

- We added to the drums the following discrete unit operations, which together approximately represent the SFE:
  - Opening of the tank and charging with solid dry clove ("*Pull In*");
  - Transferring of CO_2 from the previous streamlines ("*Transfer In*");
  - Heating of the tank to the operating temperature ("*Heat*");
  - Pressurization with the supercritical fluid ("*Pressurize*");
  - SFE ("*Extract*");
  - and Discharging.

2. Simulation and Technical-Economic Model

Simulation Model

- *Discharging of the extractors*:
  - Light phase mainly composed of CO_2 and residual oil;
  - A heavy phase enriched in oil;
  - Solid biomass that sedimented.



The SFE cycle has **duration of 210 min and must proceed at 150 bar and 40 ˚C** [27].

[27] Zabot, G.L. *et al. J. Supercrit. Fluids* **2014**, *93*, 56–66, doi:10.1016/j.supflu.2013.10.001.

2. Simulation and Technical-Economic Model

Simulation Model

- Manufactures already provide the gas under **150 bar and at 15 ˚C**.
- The purchase from these suppliers eliminate the pressurization costs.
- For the **minimum purchase of 100 cylinders** (10L-cylinders, fabricated in accordance to ISO 9809-1:2019) the purchase cost is of **40 USD/cylinder** [21].

2. Simulation and Technical-Economic Model

Simulation Model

- Process parameters under 150 bar and 40 °C (*conditions for the SFE operation*):
  - Rate of mass of solvent per mass of solid feed (**S/F ratio**): must be equals or higher than 2, and **the ideal value is S/F = 6.6**.
  - Yield Y: ratio between the oil mass extracted and the maximum mass that could be extracted if infinitely high times and solvent amounts were given.
    - It is the extracted mass divided by the total amount of oil in the dry clove.
    - For S/F = 6.6, **Y = 90%** [27].

2. Simulation and Technical-Economic Model

Simulation Model

- Process parameters under 150 bar and 40 ˚C (*conditions for the SFE operation*):
  - For S/F = 6.6, the **maximum fraction of CO_2 that may remain dispersed on the heavy phase at the exit of the extractor is of 2.2% of the total gas mass.**
    - **Mass split to the bottom phase** to simulate the worst scenario conditions: 2.2% of CO_2 mass.
  - For pressures higher than 9 MPa, **only ~0.20% of the extracted oil mass remains in the light phase** at the exit of the extractor
    - **Mass split of oil to the upper phase**: 0.20% [15,23].

2. Simulation and Technical-Economic Model

Simulation Model

- To keep S/F = 6.6, we defined that the entrance of solid material in the 400 L-extractors should be directly proportional to what was empirically verified for a 1 L-process [27].

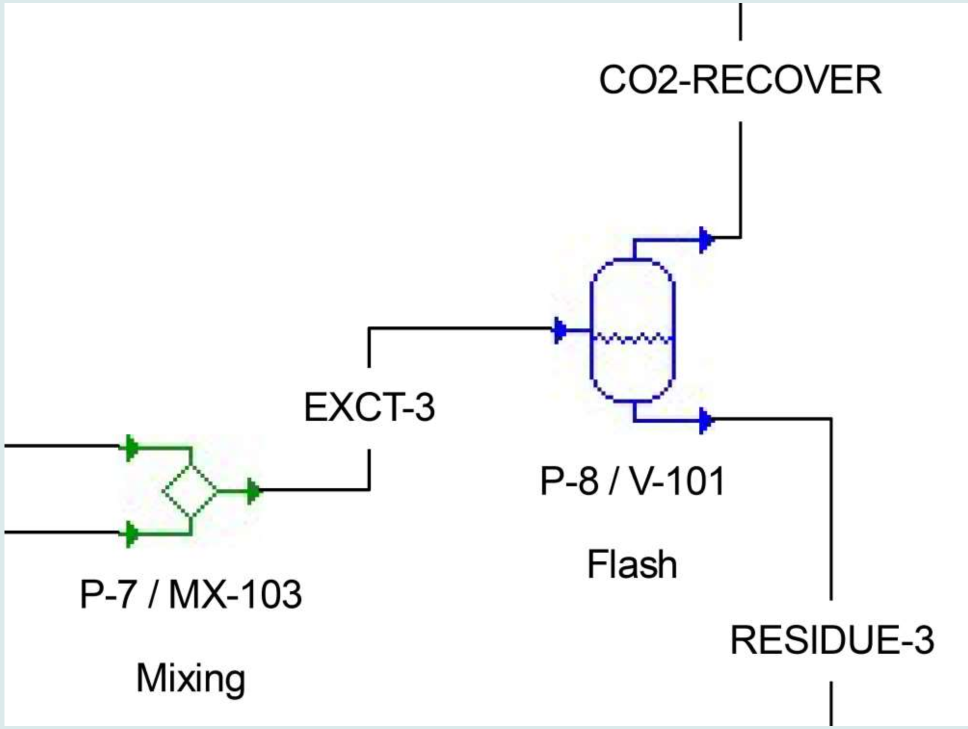
- Therefore, our extractors are charged with **228 kg of solid clove** and must be submitted to mass flows of 429.94 kg CO_2/h.

2. Simulation and Technical-Economic Model

Simulation Model

- After the extraction, the light phases are directed to an **adiabatic flash drum** for separating the CO_2 from the extracted compounds.

- At this stage, we put a pressure reducer to allow the vapor to reach the **pressure of 80.64 bar at 40 ˚C**.

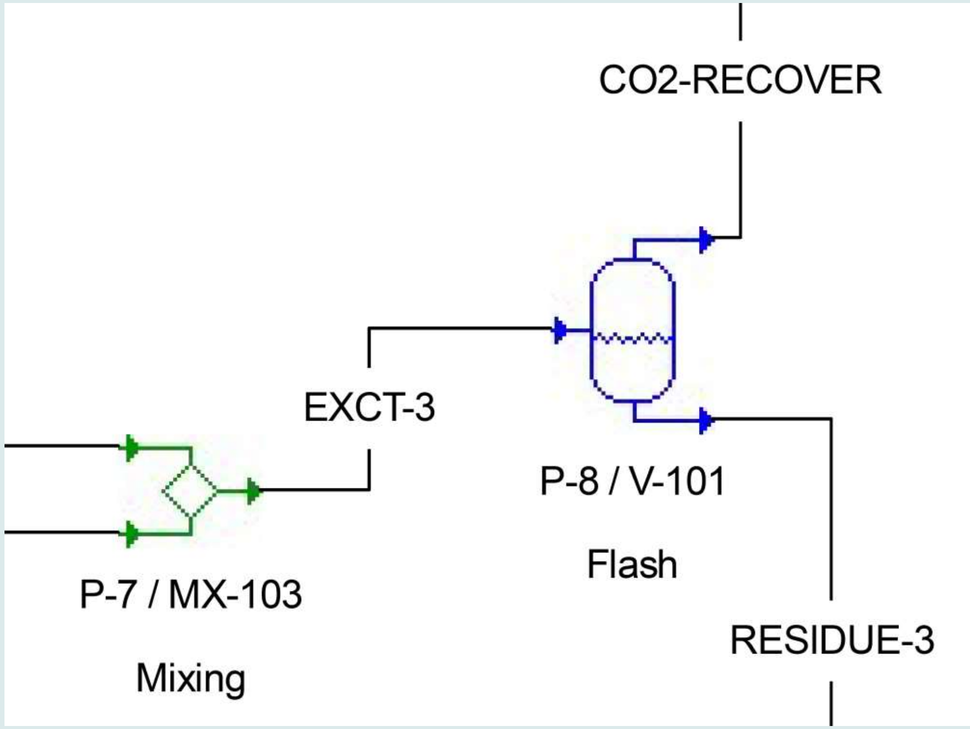


2. Simulation and Technical-Economic Model

Simulation Model

P = 80.64 bar, T = 40 ˚C.

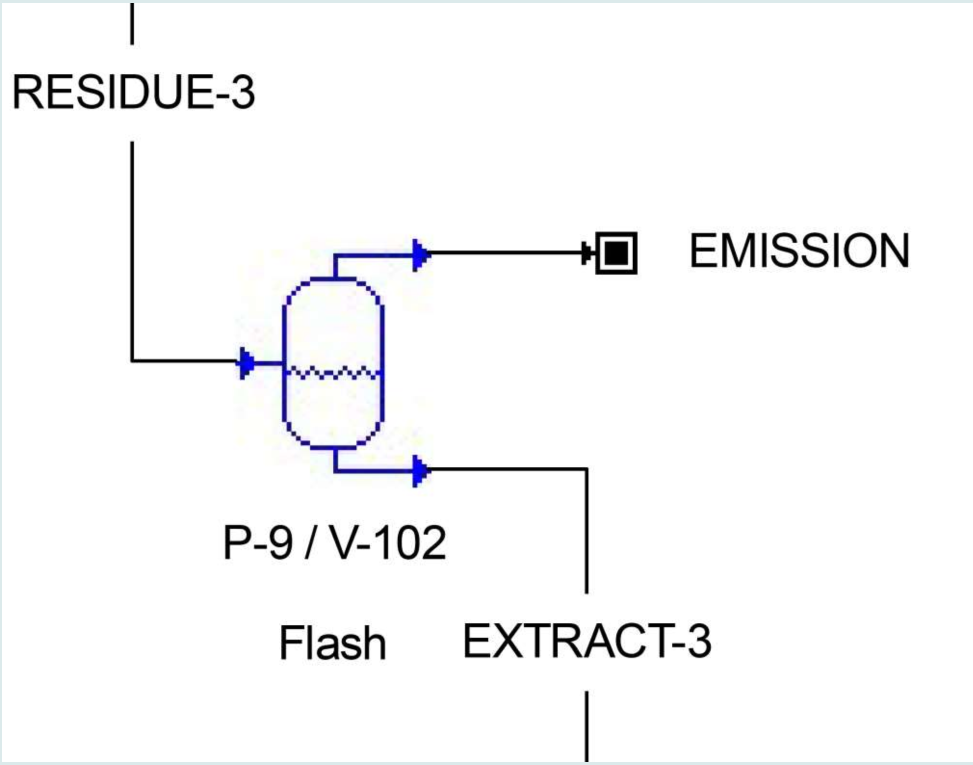
- Condition where a **vapor phase comprised of only CO_2** (molar fraction **y = 0.997 ≈ 1**) is present;
- It is in equilibrium with a liquid phase containing the molar fraction x = 0.6916 of CO_2 [5].



2. Simulation and Technical-Economic Model

Simulation Model

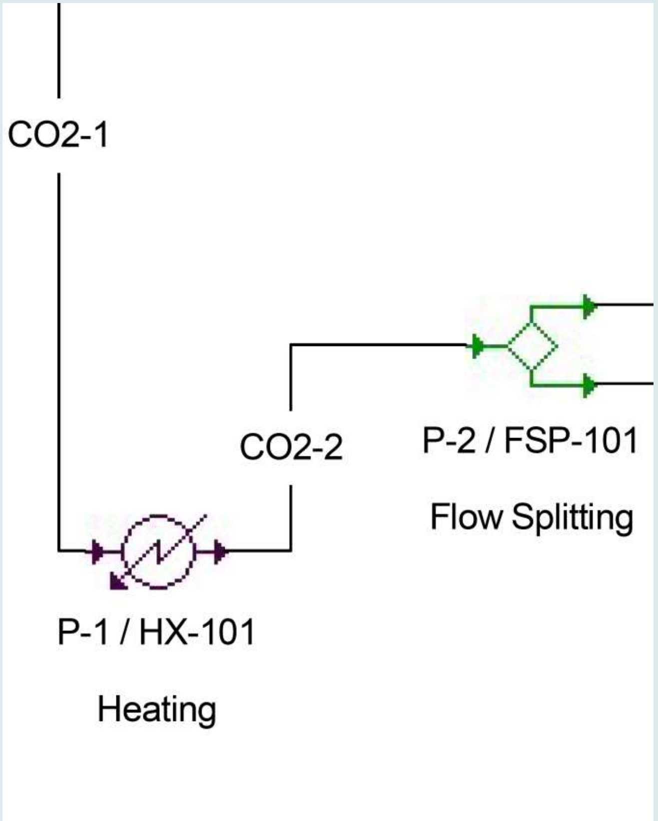
- We also created a **second adiabatic flash drum** under atmospheric pressure (**1.013 bar**).
- In this equipment, the **remaining gases are fully separated from the oil phase**.

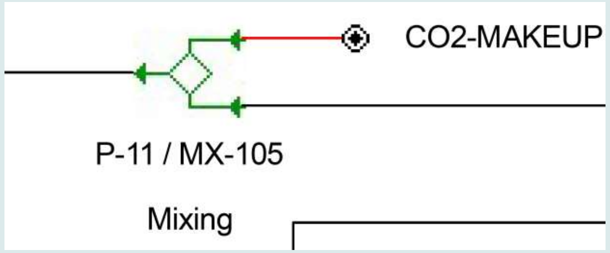


2. Simulation and Technical-Economic Model

Simulation Model

- A heat-exchanger guarantees the entrance of gases into the extractors **at 40 ˚C**.
- A CO_2 make-up entrance stream accounts for the gas losses in the flash drums.
- We limited the useful volume to **90% of the total volume** of each equipment.





2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- The plant costs estimates were performed according to ***Turton's method*** [28,29].
- This method based on correlations between the scaling costs and the dimensions of the equipment.
- Equation 1 is frequently applied: $$FC_2 = FC_1 \left(\frac{A_2}{A_1}\right)^n \quad (1)$$

[28] Pereira, C.G.; Prado, J.M.; Meireles, M.A.A. CHAPTER 12. Economic Evaluation of Natural Product Extraction Processes. In *RSC Green Chemistry*; 2013; pp. 442–471. ISBN 9781849736060. doi: 10.1039/9781849737579-00442
[29] Turton, R.; Bailie, R.C.; Whiting, Wallace B. Shaeiwitz, J.A.; Debangsu, B. *Analysis, Synthesis and Design of Chemical Processes*; 4th Ed.; Pearson, 2012.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

$$FC_2 = FC_1 \left(\frac{A_2}{A_1}\right)^n \quad (1)$$

- FC_i = fixed capital that must be expensed for acquiring a given equipment;
- A_i = capacity of the equipment in "i"-scale;
- n = cost exponent that ranges from 0.26 to 1.33 depending on the class of equipment.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

$$FC_2 = FC_1 \left(\frac{A_2}{A_1}\right)^n \quad (1)$$

- n represents the economy of scale of the plant.
- Many Chemical and Food Engineering equipment present n ≈ 0.6.
- Then, **n ≈ 0.6 is frequently applied to the estimation of plant scaling** (six-tenths rule) [29].

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- Plant's ***Direct Fixed Capital*** (**DFC**, also called ***Capital Expenditure***, **CAPEX**): estimated with basis on the ***Total Equipment Purchase Cost*** (**PC**).

- PC = sum of purchase costs of all equipment (estimated with Equation 1) with the ***costs related to equipment that are unlisted in the project***, but which are relevant to real plant operation.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- ***Cost of unlisted equipment***: estimated as 20% of the listed equipment costs.
- ***Project's Direct Cost*** (DC) = sum of PC costs with costs of:
  - Process piping (estimated as 35% of PC);
  - Instrumentation (40% of PC);
  - Insulation (3% of PC);
  - Electrical facilities (10% of PC);
  - Buildings (45% of PC);
  - Yard improvements (15% of PC);
  - Auxiliary facilities (40% of PC); and
  - Installation of listed and unlisted equipment (50% of PC).

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- ***Project's Indirect Costs*** (**IC**) = sum between:
  - Engineering costs (25% of DC);
  - Construction costs (35% of DC).
- ***Other Costs*** (**OC**) = sum of:
  - Contractor's fee costs (5% of the sum DC + IC); with
  - Project's contingency budget (10% of the sum DC + IC).

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- The DFC if finally calculated through **Equation 2**:

$$\mathrm{DFC} = \mathrm{CAPEX} = \mathrm{DC} + \mathrm{IC} + \mathrm{OC} \ (2)$$

- ***Facility-Dependent Costs*** (**FDC**) = sum of:
  - Maintenance;
  - Depreciation, and
  - Miscellaneous costs comprised of:
    - Insurance costs (estimated as 1% of DFC);
    - Local taxes (estimated as 2% of DFC); and
    - Factory expenses (5% of DFC).

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- **Other relevant estimated costs**:
- Laboratory quality control and quality assurance costs (15% of total costs related to the payment of factory operators);
- Additional electricity (15% of the calculated electricity cost); and
- Electrical power for unlisted equipment (5% of the calculated electricity cost) [29].

Operation Costs Estimations					
Facility					
Capital Investment Parameters					
FDC = (maintainance) + (Depreciation) + (Miscellaneous)					
Miscellaneous Costs					
Insurance	1	% DFC			
Local Taxes	2	% DFC			
Factory Expenses	5	% DFC			
Equipment Usage or Equipment Availability Rate					
FDC = SUM {(Equipment Rate) x (Equipment Hours)}					
Laboratory Quality Control and Quality Assurance Cost					
Estimated as	15	% of Total Labor Cost (TLC)			
Additional Electricity					
General Load					
Estimated as	15	% of Total per year			
Electrical Power for Unlisted Equipment					
Estimated as	5	% of Total per year			

Direct Fixed Capital (DFC) Estimations					
Estimated on Total Equipment Purchase Cost (PC)					
PC = (Listed Equipment Purchase Cost) + (Unlisted Equipment Purchase Cost)					
Unlisted Equipment Purchase Cost					
Estimated as	20	% Listed Equipment Purchase Cost			
Listed Equipment Purchase Cost					
Direct Fixed Capital (DFC) = Direct Cost (DC) + Indirect Cost (IC) + Other Cost (OC)					
Direct Cost (DC)					
Piping (A)	35	% of PC			
Instrumentation (B)	40	% of PC			
Insulation (C)	3	% of PC			
Electrical Facilities (D)	10	% of PC			
Buildings (E)	45	% of PC			
Yard Improvement (F)	15	% of PC			
Auxiliary Facilities (G)	40	% of PC			
Installation = (Installation of Listed Equipment) + (Installation of Unlisted Equipment)					
Listed Equipment Installation Cost					
Estimated as	50	% Listed Equipment PC			
Unlisted equipment installation cost					
Estimated as	50	% Unlisted Equipment PC			
DC = PC + Installation + A + B + C + D + E + F + G					
Indirect Costs (IC)					
Engineering (H)	25	% of DC			
Construction (I)	35	% of DC			
Other Costs (OC)					
Contractor's Fee	5	% (DC + IC)			
Contingency	10	% (DC + IC)			

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- Evaluation of investment feasibility: based on ***economic indicators***.
- ***Net Present Value*** (**NPV**): represents the real value of the general investment result after a defined period of time [22,30]:

$$\mathrm{NPV} = (\text{Value at the end of year n})/(1 + \mathrm{j})^{\mathrm{n}} \quad (3)$$

- Considered interval: project's lifetime = **40 years**.

[30] Williams, J.; Bettner, M.; Carcello, J. *Financial & Managerial Accounting*; 19th Ed.; McGraw-Hill, 2021; ISBN 9781260247930.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

$$\text{NPV} = (\text{Value at the end of year n})/(1+\text{j})^{\text{n}} \quad (3)$$

- j = the ***rate of return*** or ***discount rate***: the minimum interest rate that makes one investment attractive;
- n = number of periods, in years.
- A higher NPV implies a better investment;
- It directly represents the ***wealth generated at the end of the analyzed period*** [29,30].

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

$$\mathrm{NPV} = (\mathrm{Value\ at\ the\ end\ of\ year\ n})/(1+\mathrm{j})^{\mathrm{n}} \quad (3)$$

- For the sake of the evaluation, we estimated a **depreciation rate of 20% per year**;
- The depreciation was **linearly adjusted** to the basic cash flow;
- The rate of return was defined as the **Brazil's basic interest rate, 2.30% per year** [29,31].

[31] BACEN. *Ata da 231ª Reunião do Comitê de Política Monetária (Copom) do Banco Central do Brasil, Junho de 2020*; Brasília, DF, Brasil, 2020.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- Economic analysis: performed in accordance to the ***Weighted Average Capital Cost*** (**WACC**) methodology for evaluating the ***annual free cash flow*** (**FCF**) of the plant.
- **WACC**: consists on evaluating the ***contribution of the debt costs*** (interest on the amount) and the ***return demanded by the shareholders*** for performing an investment (capital cost) [22].
- A given investment will be considered ***feasible if it results in a return superior than the debt and capital costs***.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- ***Operational Expenditure*** (**OPEX**) of the project: considered constant and equals to the sum of costs of:
  - Acquisition of raw materials;
  - Labor costs;
  - Utilities costs (*cooling water, water steam, and electricity costs*); and
  - Laboratory quality control and quality assurance costs [29].

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- ***Plant construction period*** = **30 months**;
- ***Plant start-up period*** = **4 months**.
- These periods are the **standard values** of the SuperPro Designer 10 database.
- **Operational profits**: obtained only after the initial 34 months, but;
- We considered that the ***OPEX is incident from the first year***.

Project Operation		Reference
Project Lifetime (years)	40	
Plant Construction Period (months)	30	Software Standard (Database)
Plant Start-up Period (months)	4	
Total Working Days (per year)	330	
Cost of Operational Labor (COL)	Industrial Scale (400 L - Extractor)	
Wage (with benefits, administration, supervision and supplies) (USD/h)	14.93	[9,10,12]
Workers per shift	3	[9–11]
Total Wage per year (USD/year)	1673956.00	
Cost of Utilities (CUT)		
Electricity (USD/kWh)	0.25	[9–13]
Cooling Water (USD/ton)	0.78	
Water Steam (USD/ton)	16.80	

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- "***Earnings Before Interest, Taxes, Depreciation and Amortization***" (**EBITDA**): considers the net revenue discounted of the value expended on the production, stocking and commercialization.

- It allows the comparison of the project with competitors from different countries, *even when they are submitted to different tax regimes*.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- WACC methodology **discounts the depreciation effects from the EBITDA**.
- It is of *particular importance for Chemical and Food Industries*.
- That is because the **equipment costs represent a high percent of the total plant cost in these sectors**.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- **Only cash flow expenses are considered for the discount of income tax** on the cash flow;
- It reduces the total amount of interest paid.
- The discount of the income tax results in the **operating profits after taxes**.

2. Simulation and Technical-Economic Model

Technical and Economic Evaluation

- Some companies may receive tax benefits to obtain better competition conditions [22].
- We applied a **standard income tax rate of 34% per year with no benefits**.
- The **annual net working capital** necessary: considered constant and estimated as **5% of the initial fixed capital investment** [29].

3. Simulation Results and Economic Feasibility Analysis

Simulation

- The simulation results indicated that **virtually all of the CO_2 may be recycled**;
- It leads to an almost null annual cost related to the purchase of this raw material.
- This is **only an ideal situation**, and the stocking of this gas is necessary for different reasons.

STREAM DETAILS - COMPONENT FLOWRATES (kg/h)				
COMPONENT	**CO2-2**	**CO2-3**	**CO2-4**	**CLOVE-1**
a-Humulene	0.00	0.00	0.00	0.13
Biomass	0.00	0.00	0.00	50.11
Carb. Dioxide	206361.60	103189.39	103189.39	0.00
Caryophyllene	0.00	0.00	0.00	1.13
Eugenol	0.00	0.00	0.00	7.07
Eugenyl acetate	0.00	0.00	0.00	1.03
Nitrogen	0.00	0.00	0.00	0.00
Oxygen	0.00	0.00	0.00	0.00
TOTAL (kg/h)	**206361.60**	**103189.39**	**103189.39**	**59.48**
TOTAL (L/h)	**1513945.83**	**757035.92**	**757035.92**	**56.69**
COMPONENT	**VENT-1**	**EXCT-1**	**EXTRACT-1**	**TOP-1**
a-Humulene	0.00	0.00	0.13	0.00
Biomass	0.00	0.00	50.11	0.00
Carb. Dioxide	103180.80	0.00	0.00	103180.80
Caryophyllene	0.00	0.00	1.13	0.00
Eugenol	0.00	0.00	7.07	0.00
Eugenyl acetate	0.00	0.00	1.03	0.00
Nitrogen	0.06	0.00	0.00	0.06
Oxygen	0.02	0.00	0.00	0.02
TOTAL (kg/h)	**103180.88**	**0.00**	**59.48**	**103180.88**
TOTAL (L/h)	**756759.40**	**0.00**	**56.69**	**756735.23**

COMPONENT	CLOVE-2	VENT-2	EXCT-2	EXTRACT-2
a-Humulene	0.13	0.00	0.00	0.13
Biomass	50.11	0.00	0.00	50.11
Carb. Dioxide	0.00	103180.80	0.00	0.00
Caryophyllene	1.13	0.00	0.00	1.13
Eugenol	7.07	0.00	0.00	7.07
Eugenyl acetate	1.03	0.00	0.00	1.03
Nitrogen	0.00	0.06	0.00	0.00
Oxygen	0.00	0.02	0.00	0.00
TOTAL (kg/h)	**59.48**	**103180.88**	**0.00**	**59.48**
TOTAL (L/h)	**56.66**	**756759.40**	**0.00**	**56.69**
COMPONENT	**TOP-2**	**EXCT-3**	**CO2-RECOVER**	**RESIDUE-3**
a-Humulene	0.00	0.00	0.00	0.00
Biomass	0.00	0.00	0.00	0.00
Carb. Dioxide	103180.80	206361.60	206361.60	0.00
Caryophyllene	0.00	0.00	0.00	0.00
Eugenol	0.00	0.00	0.00	0.00
Eugenyl acetate	0.00	0.00	0.00	0.00
Nitrogen	0.06	0.11	0.00	0.11
Oxygen	0.02	0.03	0.00	0.03
TOTAL (kg/h)	**103180.88**	**206361.76**	**206361.60**	**0.15**
TOTAL (L/h)	**756735.23**	**1513518.81**	**1513674.19**	**0.15**

COMPONENT	CO2-MAKE UP	CO2-1	EMISSION	EXTRACT-3	EXTRACT
a-Humulene	0.00	0.00	0.00	0.00	0.26
Biomass	0.00	206361.60	0.00	0.00	100.22
Carb. Dioxide	0.00	0.00	0.00	0.00	0.00
Caryophyllene	0.00	0.00	0.00	0.00	2.27
Eugenol	0.00	0.00	0.00	0.00	14.15
Eugenyl acetate	0.00	0.00	0.00	0.00	2.06
Nitrogen	0.00	0.00	0.11	0.00	0.00
Oxygen	0.00	0.00	0.03	0.00	0.00
TOTAL (kg/h)	**0.00**	**206361.60**	**0.15**	**0.00**	**118.96**
TOTAL (L/h)	**0.00**	**1513722.53**	**166.40**	**0.00**	**113.39**

Component	Selling Price (USD)	Basis of Cost	Output (kg/year)	Output (%)
a-Humulene	14.90	kg	2077.41	0.22
Biomass	0	kg	793749.29	84.14
Caryophyllene	12.19	kg	17954.75	1.90
Eugenol	25.73	kg	112031.71	11.88
Eugenyl acetate	32.51	kg	16322.50	1.73
Nitrogen	0	kg	902.54	0.10
Oxygen	0	kg	273.99	0.03

3. Simulation Results and Economic Feasibility Analysis

Simulation

- Firstly: our hypothesis was that the gas was **supplied in cylinders already under the pressure of 150 bar** [21].

- This supply condition is **necessary for eliminating the costs of purchasing and operating a compressor**.

3. Simulation Results and Economic Feasibility Analysis

Simulation

- It is also necessary to have **stocked gas for moments of:**
  - Stopping;
  - Maintenance; and
  - Start-up of the plant; as well as for
  - Compensating **losses from non-idealities** not covered by the project.

3. Simulation Results and Economic Feasibility Analysis

Simulation

- We considered that the **annual cost correspondent to the acquisition of CO_2** corresponds to the **minimum purchase allowed by the suppliers**;
- It is the purchase of **100 cylinders of 10 L under 150 bar**.
- It corresponds to a cost of **4,000 USD/year** [21].

3. Simulation Results and Economic Feasibility Analysis

Simulation

- The following Tables show the process equipment and the correspondent dimensions, fabrication materials, and costs estimated by the simulator.

- These estimates were performed for equipment fabricated in ***carbon steel*** (**CS**), or in ***stainless steel SS316*** (the case of the two extractors).

Quantity	Name	Type	Useful Size (Capacity)		Material of Construction	Purchase Cost (USD/Unit)
1	HX-101	Heat Exchanger (Plate and Frame)	0,02	m²	CS	8,000.00
1	FSP-101	Flow Splitter	206378.78	kg/h	CS	0.00
1	V-101	Flash Drum	~0.00	L	CS	0.00
1	MX-103	Mixer	206361.76	kg/h	CS	0.00
1	V-102	Flash Drum	0.03	L	CS	0.00
1	MX-101	Mixer	103180.88	kg/h	CS	0.00
1	E-101	Vertical-On-Legs Tank	241.47	L	SS316	19,000.00
1	E-102	Vertical-On-Legs Tank	241.47	L	SS316	19,000.00
1	MX-102	Mixer	103180.88	kg/h	CS	0.00
1	MX-104	Mixer	118.96	kg/h	CS	0.00
1	MX-105	Mixer	206361.60	kg/h	CS	0.00

ITEMIZED EQUIPMENT LIST		
HX-101 (Heat Exchanger)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Heat Exchanger)	7,500.00	USD/unit
Heat exchanger type	Plate and Frame	
Heat Transfer Area	0.02	m^2

FSP-101 (Flow Splitter)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Flow Splitter)	0.00	USD/unit
Rated Throughput	206378.78	kg/h

V-101 (Flash Drum)			
Number of Units		1	
Number of Standby Units		0	
Number of Staggered Units		0	
Installation Factor		0.50	
Maintenance Factor		0.10	
Cost Allocation Factor		1.00	
Usage Rate		100.00	USD/equipment-hour
Availability Rate		100.00	USD/h
Material of Construction		Carbon Steel (CS)	
Purchase Cost Purchase Cost (system model for Flash Drum)		0.00	USD/unit
Max Volume		2000.00	L
Min Working/Vessel Volume		0.00	%
Max Working/Vessel Volume		90.00	%
Volume		0.00	L
Height		0.02	m
Design Pressure		1.52	bar
Vessel is constructed according to ASME standards			
Diameter		0.01	m

MX-103 (Mixer)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Flow Splitter)	0.00	USD/unit
Rated Throughput	206361.76	kg/h

V-102 (Flash Drum)			
Number of Units		1	
Number of Standby Units		0	
Number of Staggered Units		0	
Installation Factor		0.50	
Maintenance Factor		0.10	
Cost Allocation Factor		1.00	
Usage Rate		100.00	USD/equipment-hour
Availability Rate		100.00	USD/h
Material of Construction		Carbon Steel (CS)	
Purchase Cost Purchase Cost (system model for Flash Drum)		0.00	USD/unit
Max Volume		2000.00	L
Min Working/Vessel Volume		0.00	%
Max Working/Vessel Volume		90.00	%
Volume		0.03	L
Height		0.08	m
Design Pressure		1.52	bar
Vessel is constructed according to ASME standards			
Diameter		0.02	m

E-101 (Vertical-On-Legs Tank)			
Number of Units		1	
Number of Standby Units		0	
Number of Staggered Units		0	
Installation Factor		0.40	
Maintenance Factor		0.10	
Cost Allocation Factor		1.00	
Usage Rate		100.00	USD/equipment-hour
Availability Rate		100.00	USD/h
Material of Construction		Stainless Steel SS316	
Purchase Cost Purchase Cost (system model for Flash Drum)		19,000.00	USD/unit
Max Volume		400.00	L
Min Working/Vessel Volume		0.00	%
Max Working/Vessel Volume		90.00	%
Volume		241.47	L
Height		1.40	m
Design Pressure		1.52	bar
Vessel is constructed according to ASME standards			
Diameter		0.47	m

E-102 (Vertical-On-Legs Tank)			
Number of Units		1	
Number of Standby Units		0	
Number of Staggered Units		0	
Installation Factor		0.40	
Maintenance Factor		0.10	
Cost Allocation Factor		1.00	
Usage Rate		100.00	USD/equipment-hour
Availability Rate		100.00	USD/h
Material of Construction		Stainless Steel SS316	
Purchase Cost Purchase Cost (system model for Flash Drum)		19,000.00	USD/unit
Max Volume		400.00	L
Min Working/Vessel Volume		0.00	%
Max Working/Vessel Volume		90.00	%
Volume		241.47	L
Height		1.40	m
Design Pressure		1.52	bar
Vessel is constructed according to ASME standards			
Diameter		0.47	m

MX-101 (Mixer)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Flow Splitter)	0.00	USD/unit
Rated Throughput	103180.88	kg/h

MX-102 (Mixer)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Flow Splitter)	0.00	USD/unit
Rated Throughput	103180.88	kg/h

MX-104 (Mixer)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Flow Splitter)	0.00	USD/unit
Rated Throughput	118.96	kg/h

MX-105 (Mixer)		
Number of Units	1	
Number of Standby Units	0	
Number of Staggered Units	0	
Installation Factor	0.50	
Maintenance Factor	0.10	
Cost Allocation Factor	1.00	
Usage Rate	100.00	USD/equipment-hour
Availability Rate	100.00	USD/h
Material of Construction	Carbon Steel (CS)	
Purchase Cost (system model for Flow Splitter)	0.00	USD/unit
Rated Throughput	206361.60	kg/h

3. Simulation Results and Economic Feasibility Analysis

Simulation

- A remarkable conclusion regarding the results is that the **useful volumes of the extractors are substantially lower than the projected target-value** (400 L).

3. Simulation Results and Economic Feasibility Analysis

Simulation

- It is caused by the fact that the **solid material actually forms a fixed bed inside the tank**.
- It results in a substantial reduction of the volume available for the fluid.
- The fluid volume depends on the porosity and on permeability of the fixed bed [27].

3. Simulation Results and Economic Feasibility Analysis

Simulation

- Then, once we did not programmed the simulator to account for this feature, but only:
  - Used the optimized value of S/F = 6.6 (which already takes in account the effects of the bed);
  - Manually defined the volume as 400 L; and
  - Input both the information regarding the split of materials through the phases (equilibrium information), and the time for completing the extraction cycle (210 min);
- The software calculated a low value volume actually used.

3. Simulation Results and Economic Feasibility Analysis

Simulation

- The next tables, in their turn, summarize the **general project costs and earns** calculated through Equations 1 and 2 when using the previously mentioned hypotheses.

Fixed Capital Estimate Summary			
Total Plant Direct Cost (TPDC) (physical cost)			
1	Equipment Purchase Cost	57,000.00	USD
2	Installation	25,000.00	USD
3	Process Piping	20,000.00	USD
4	Instrumentation	23,000.00	USD
5	Insulation	2,000.00	USD
6	Electrical	6,000.00	USD
7	Buildings	26,000.00	USD
8	Yard Improvement	9,000.00	USD
9	Auxiliary Facilities	23,000.00	USD
TPDC		**188,000.00**	**USD**

Fixed Capital Estimate Summary			
Total Plant Indirect Cost (TPIC)			
10	Engineering	47,000.00	USD
11	Construction	66,000.00	USD
TPIC		113,000.00	USD
Total Plant Cost (TPC = TPDC + TPIC)			
TPC		302,000.00	USD
Contractor's Fee & Contingency (CFC)			
12	Contractor's Fee	15,000.00	USD
13	Contingency	30,000.00	USD
CFC = 12 + 13		45,000.00	USD
Direct Fixed Capital Cost (DFC = TPC + CFC)			
DFC = CAPEX		**347,000.00**	**USD**

Annual Operating Cost				
Cost Item		Cost		%
1	Raw Materials	607,233.00	USD/year	23.37
2	Labor-Dependent	1,674,000.00	USD/year	64.43
3	Facility-Dependent	65,000.00	USD/year	2.50
4	Laboratory/QC/QA	251,000.00	USD/year	9.66
5	Utilities	1,000.00	USD/year	0.04
OPEX		**2,598,233.00**	**USD/year**	**100.00**

Direct Fixed Capital Cost (DFC = TPC+CFC)					
DFC				**347,000.00**	**USD**
LABOR COST - PROCESS SUMMARY - 1 Operator					
Labor Type	Unit Cost (USD/h)	Annual Amount (h)	Annual Cost (USD)		
Operator	**14.93**	**40,006.00**	**597,165.00**		
LABOR COST - PROCESS SUMMARY - 3 Operators					
Labor Type	Unit Cost (USD/h)	Annual Amount (h)	Annual Cost (USD)		
Operator	**14.93**	**112,143.00**	**1,673,956.00**		
MATERIALS COST - PROCESS SUMMARY					
Bulk Material	Unit Cost (USD/kg)	Annual Amount (kg)	Annual Cost (USD)	%	OBS
Carb. Dioxide	-	-	**4,000.00**	0.66	**Fixed**
SOLID CLOVE	0.64	942552.00	**603,233.28**	99.34	
TOTAL			**607,233.28**	100.00	

TOTAL SELLING (USD/year)		**3,663,042.18**	
ANNUAL OPERATING COST			
Cost Item		Cost	
1	Raw Materials	607,233.28	USD/year
2	Labor-Dependent	1,674,000.00	USD/year
3	Facility-Dependent	65,000.00	USD/year
4	Laboratory/QC/QA	251,000.00	USD/year
5	Utilities	1,000.00	USD/year
TOTAL COSTS		**2,598,233.28**	**USD/year**

3. Simulation Results and Economic Feasibility Analysis

Simulation

- The results indicate that **64.43% of the OPEX correspond to labor-dependent costs**.
- It was obtained for the hypothesis that the plant must **work with three operators**.

3. Simulation Results and Economic Feasibility Analysis

Simulation

- Then, this plant has a great potential of **economic gains by extra-investing in automation**.
  - We estimated that the labor-dependent costs would ***drop to ~597,200.00 USD/year if there was only one operator*** directly working in the plant
- It would represent a **reduction of ~41.4% of the annual operating costs**.

3. Simulation Results and Economic Feasibility Analysis

Simulation

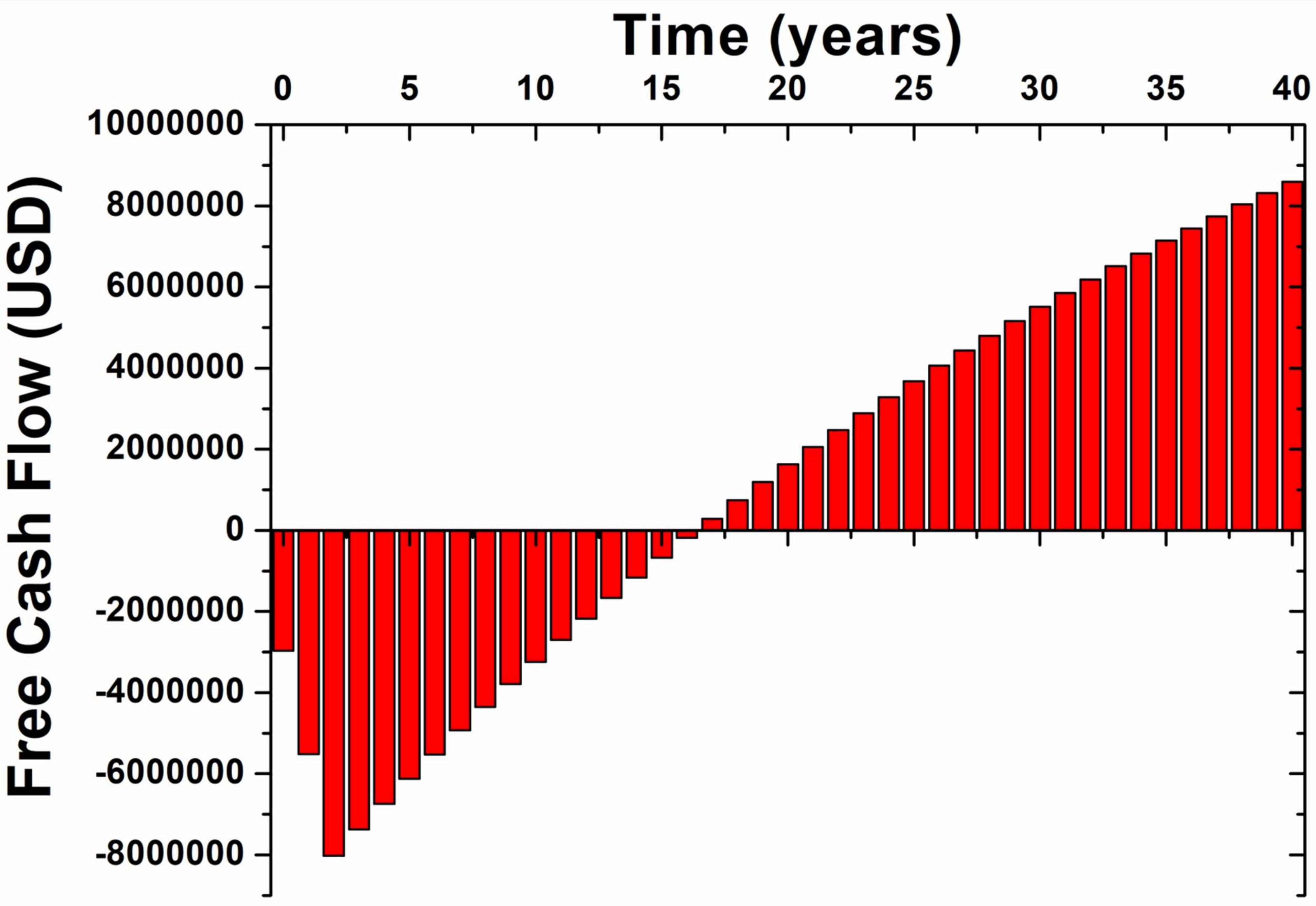
- The simulation also showed that the operation of this plant **requires very low amounts of utilities**.
- It shows how eco-friendly is the supercritical fluid extraction process.
- It is also a consequence of choosing a CO_2 supplier **which already sells the gas in a pressure adequate for the SFE operation**.

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

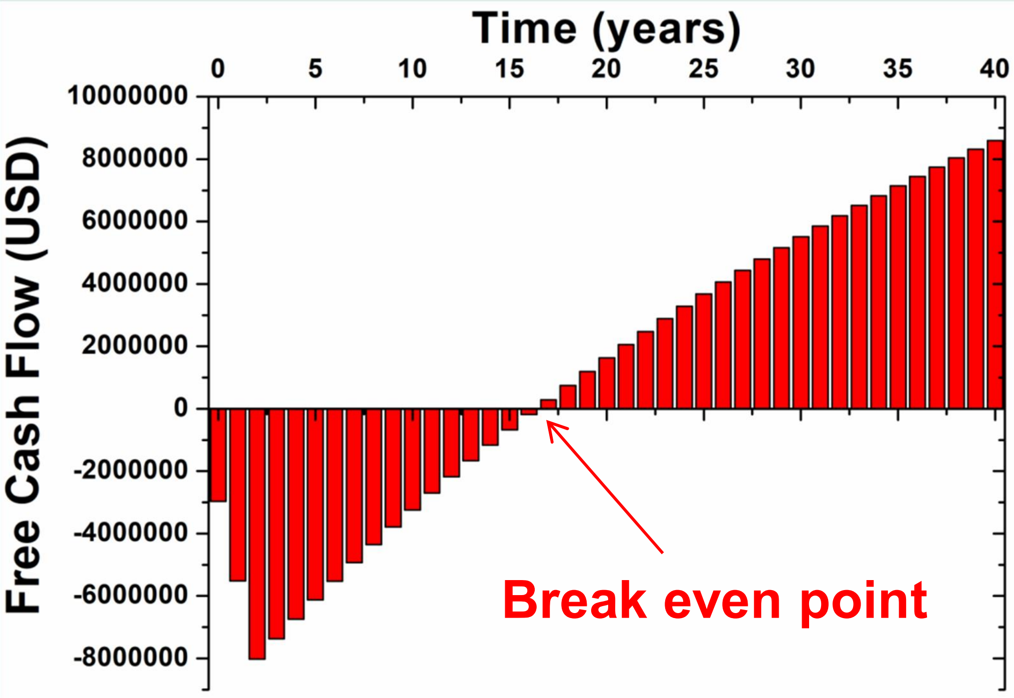
- The following Figure and Table show the **free cash flow** (**FCF**) of the plant project and the **main economic indicators** calculated through WACC methodology.

Free Cash Flow (FCF) of the Plant



Economic Indicators	
Investment (CAPEX) (USD)	347,000.00
Earns (USD/year)	3,663,042.18
OPEX (USD/year)	2,598,233.00
EBTIDA (USD/year)	1,064,809.18
Depreciation Rate (per year, linear)	20.00%
Net Working Capital (NWC) (USD/year)	17,350.00
Income Tax	34.00%
Operational Profits (after taxes, USD/year)	691,323.06
Net Present Value (NPV) (USD)	8,598,312.83
Discount Rate (per year)	2.30%
Internal Rate of Return (IRR) (per year)	7.29%
Discounted Payback Period (years)	18.67
Break Even Point (years)	17.00

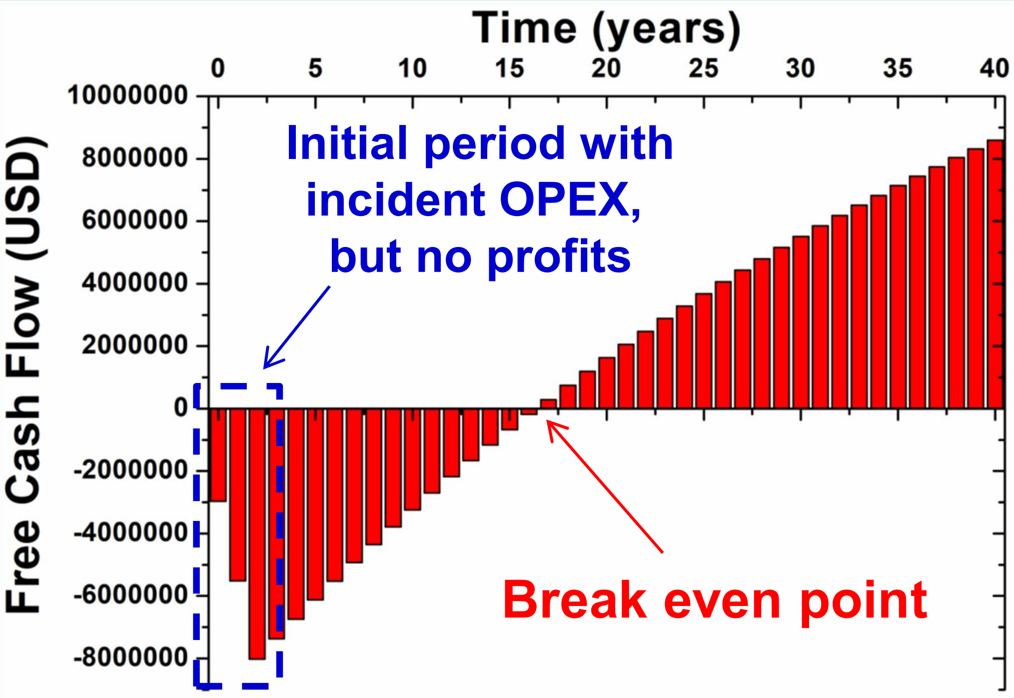
3. Simulation Results and Economic Feasibility Analysis



- **Payback period:** the time necessary for the investment to pay itself;
- **Break even point:** when the free cash flow reaches zero [22,30].

We may notice in this figure that the **payback period is slightly superior than the break even point**: 18.67 years for the payback, against 17 years for the break even.

3. Simulation Results and Economic Feasibility Analysis



- The difference between the break even point and the payback period is a consequence of **defining an initial period for construction and start-up of the plant where we considered that the OPEX was already present,** but in which there were no earns.

This initial period with costs but no earns may be observed on the FCF as **growing negative bars on the three first years**.

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

- The operation is *not only attractive for its green-approach*.
- The payback period (**18.67 years**) ***is lower than half of the lifetime of the project*** (**total of 40 years**).

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

- The operational profits after taxes are substantial (691,323.06 USD/year).
- The consequence is a **high internal rate of return (IRR) of 7.29% per year**.

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

- The IRR is of great importance when analyzing the viability of an investment.
- It is the **discount rate that a cash flow must present to equal the NPV to zero**.
- Then, **greater differences between the IRR and the minimum rate of return make an investment more attractive** [22,30].
- We considered the minimum rate of return equals to 2.30% (basic interest rate in Brazil) [31].

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

- The net present value also confirms that the investment in this supercritical fluid extraction **plant has an outstanding capacity of generating wealth**.

- The initial fixed capital investment of 347,000 USD is **converted into a NPV of ~8,600,000.00 USD** after the project lifetime.

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

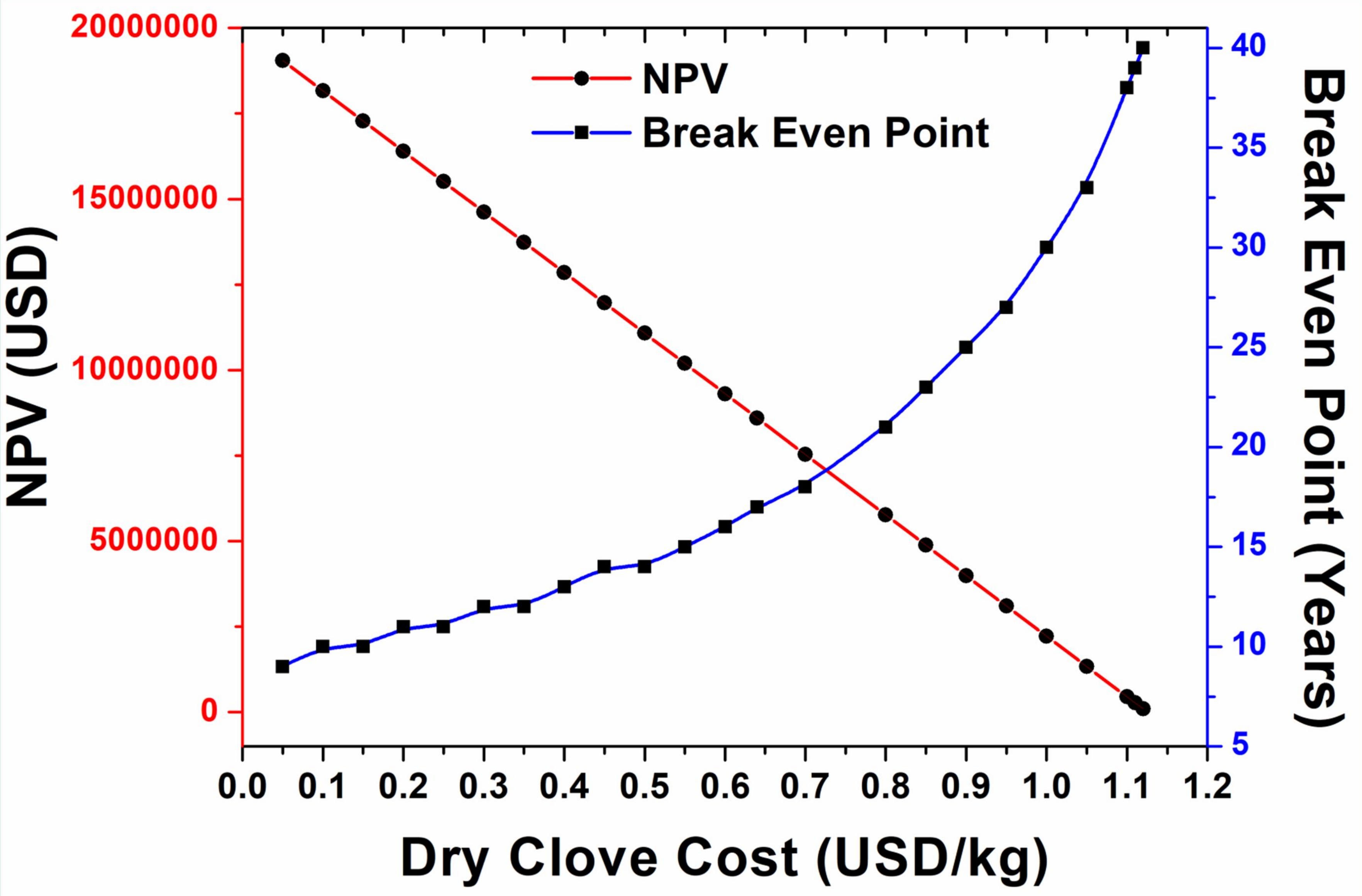
- Finally, it is important to verify the **effect of different purchase prices on the economic indicators**.
- This process is based on an ***agricultural commodity*** (clove).
- This class of products may be **highly influenced by oscillations of the international markets** and the consequent variations of the purchase costs [22,29,30].

3. Simulation Results and Economic Feasibility Analysis

Economic Feasibility Analysis

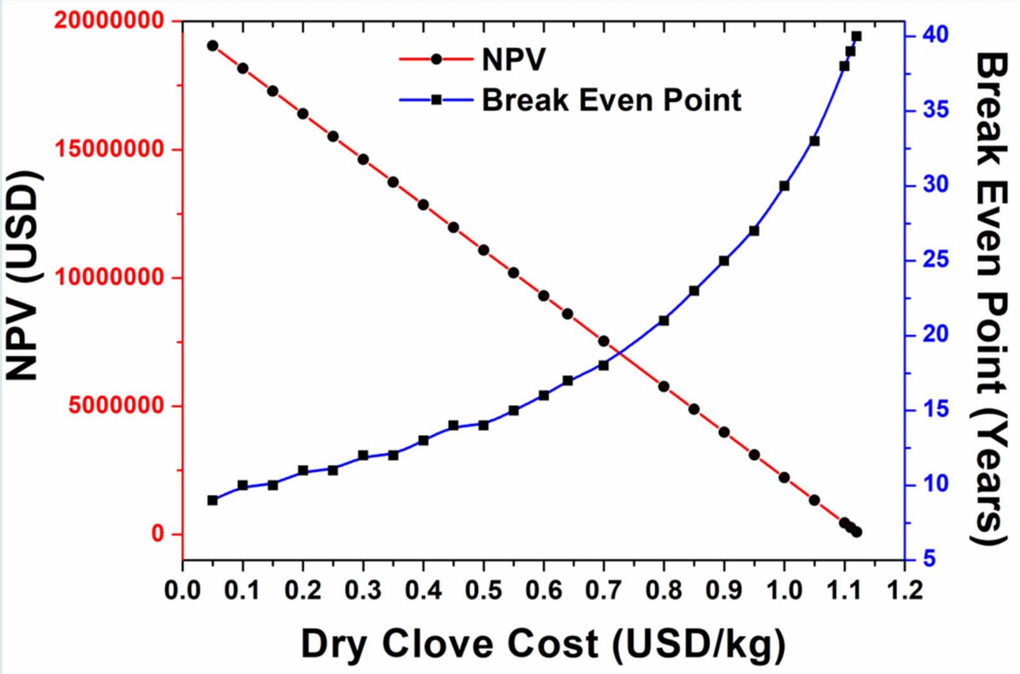
- We calculated the **NPVs and the correspondent break even points** for purchase costs of dry clove ranging from **0.05 to 1.12 USD/kg**.

NPVs and break even points for different purchase costs of dry clove.



3. Simulation Results and Economic Feasibility Analysis

- The **break even point increases linearly until the cost of 0.70 USD/kg of clove**, when its rate of grown suffers a substantial enhancement.

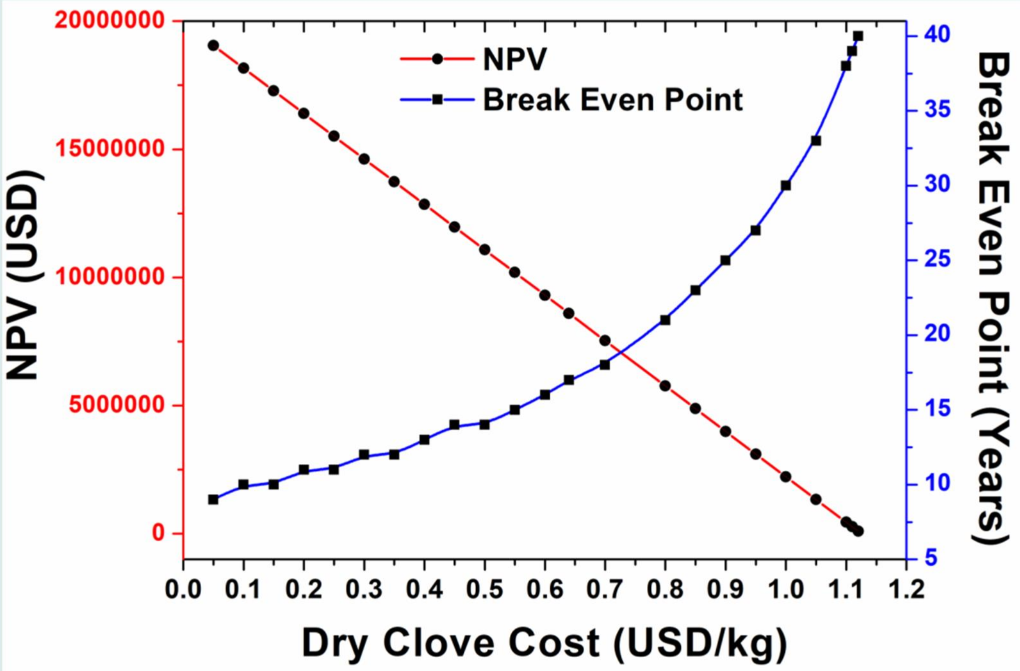


The results show a **linear decrease of the NPV** as the clove's price rises:

NPV (in USD) = -1,771,750,000,000.00 x (**clove's purchase cost, in USD/kg**) + 1,993,750,000,000.00, **adjusted $R^2 \approx 1$**.

3. Simulation Results and Economic Feasibility Analysis

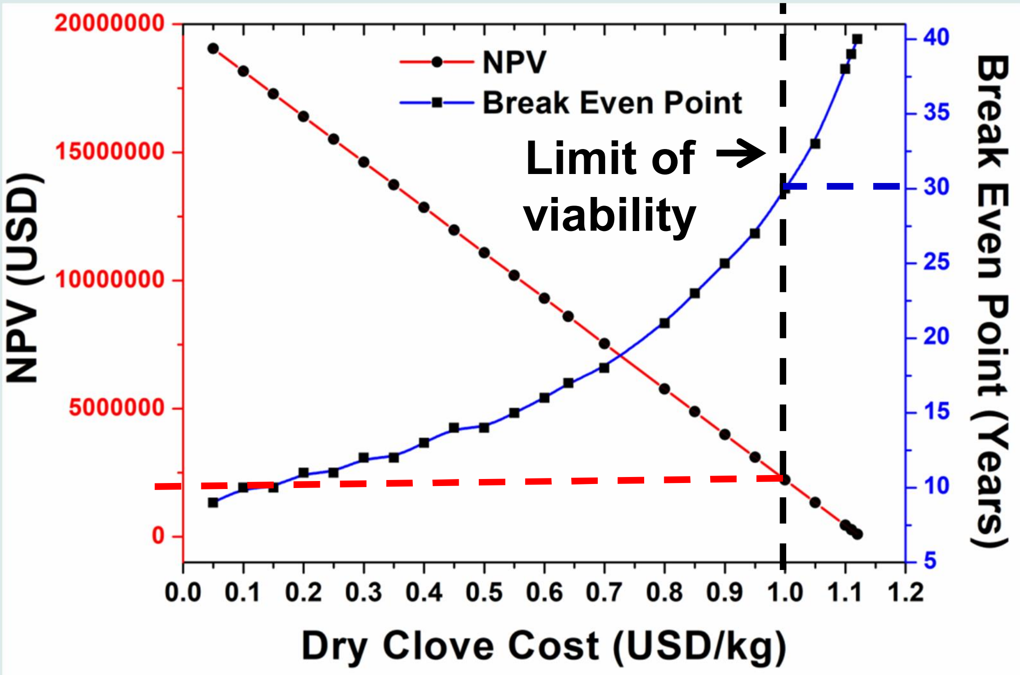
- If we define that the process is viable:
  - if the **NPV is higher than the CAPEX investment**.
    - i.e., the **operating effectively generates wealth**;



- and if the **break even point is not superior than 75% of the project's lifetime.** if the **NPV is higher than the CAPEX investment**.
  - This is a limit situation where the *FCF is negative over 30 years and it is positive only during the last 10 years* of the projected lifetime.

3. Simulation Results and Economic Feasibility Analysis

- Using these viability criteria:
- The process is viable **for clove costs until 1.00 USD/kg**.
- That means that the process is still viable even **if there are increases of until 56.25% of the raw materials' purchase cost**.



In this limit situation of 1.00 USD/kg of clove, **the NPV after the project's lifetime is of 2,220,018.89 USD**, with a **break even point at 30 years**.

4. Conclusions

- Both the economic analysis and the simulations verified that the investment in an **industrial plant for the supercritical extraction of the clove's essential oil compounds with CO_2** is very attractive.

4. Conclusions

- This oil presents many relevant **food and biomedical applications**, including: antibacterial and antifungal activities; and use as antioxidant, anti-inflammatory, and for asthma and allergy relief [5–7].

- Besides that, clove and its essential oil also play a **great role in Brazil's exportations** [8].

4. Conclusions

- The SFE is not only a green-process which:
  - Does not rely on organic solvents;
  - Results in low and harmless emissions; and
  - Consumes a low amount of raw materials and utilities;
- but it also presents excellent economic indicators that show that it is a very attractive investment.

4. Conclusions

- The required capital expenditure of 347,000 USD is converted into a **NPV of 8,600,000** after the project lifetime period (40 years), with:

- A payback time of **18.67 years**; and

- An internal rate of return of **7.29% per year**.

4. Conclusions

- Moreover, the process is still viable even **if clove's purchase cost is increased by up to 56.25%**, reaching 1.00 USD/kg.

4. Conclusions

- Enormous amounts of biomass (**793,749.29 kg/year**) are produced as residues of the process.

- This is not a problem, though.

4. Conclusions

- Experimental studies with three other species that also belong to the same family as clove (*Myrtaceae* family) and which are present in Brazilian flora reported **an average heat of combustion of 18.25 MJ/kg for the dry biomasses** [32,33].

- Typically, **25% of this energy is effectively available** [34].

[32] Vale, A.T. do; Felfili, J.M. *Rev. Árvore* **2005**, *29*, 661–669, doi:10.1590/S0100-67622005000500001.
[33] Yu, D. *et al. Powder Technol.* **2016**, 294, 463–471, doi:10.1016/j.powtec.2016.03.016.
[34] Al-Hamamre, Z. *et al. Renew. Sustain. Energy Rev.* **2017**, *67*, 295–314, doi:10.1016/j.rser.2016.09.035.

4. Conclusions

- Therefore, the produced biomass represents a potential for the generation of **3.62×10^6 MJ/year**.

4. Conclusions

- Such high amount of energy could be used to
  - Generate water steam:
    - for use on the heat exchanger or,
    - for the generation of electricity in turbines; or

4. Conclusions

- Could be even converted into more flexible energy sources like:
  - gaseous and liquid fuels through **thermochemical processes**:
    - combustion, pyrolysis, or gasification;
  - or through biochemical routes:
    - anaerobic or aerobic digestion, and liquid-phase fermentation [32,34].
- The converted energy would be **to reduce the OPEX of the plant** (through the reduction of the utilities purchases) or as a **new source of revenue**.

4. Conclusions

- In fact, there is a growing market for the acquisition of wood pellets and for their use as energy source.

- Since the introduction of the **Renewable Heat Incentive** by the United Kingdom (UK) government in 2011, this country started to develop a **biomass boiler market** that reached:

  - ~16,500 commercial and industrial systems (systems with capacity above 200 kW), and

  - 12,700 domestic boilers at the end of 2019.

4. Conclusions

- Now, there are already at least **two high power generators** installed in UK which rely on the use of wood pellets as raw material:
  - the Drax generator, in North Yorkshire (three **645 MW** biomass-processing units);
  - and the Czech-Slovak Lynemouth plant, in northeast England (**396 MW**).
- On the other hand, the **UK manufacturers can produce only 300,000 ton of pellets/year**.

4. Conclusions

- Therefore, this country presents an enormous and increasing market for these pellets:
  - in April 2020, the **UK imported 896,000 tons of wood pellets**, an **increase of 39.3%** in relation to the 643,000 tons imported in April 2019.
  - From these importations registered in April 2020, only **44,000 ton came from Brazil**;
  - The highest suppliers were **USA (475,000 ton), Canada (202,000 ton), and the Baltic countries (127,000 ton)**; and there were also substantial contributions from Russia (32,000 ton) and Portugal (12,000 ton) [35,36].

[35] Aldridge, J. UK wood pellet imports hit record April high Available online: https://www.argusmedia.com/en/news/2118063-uk-wood-pellet-imports-hit-record-april-high (accessed on Nov 23, 2020).
[36] Harrison, N. UK Wood Pellet Market: Past, Present and Future Available online: http://biomassmagazine.com/articles/16876/uk-wood-pellet-market-past-present-and-future (accessed on Nov 23, 2020).

4. Conclusions

- These data indicate that **there is not a single supplier that dominates the whole international market**, representing an opportunity for the **entrance of new players.**

Thank you for your attention!

Questions?

marcosoares.feq@gmail.com

Funding: São Paulo Research Foundation (FAPESP) Grant 2019/22554-4.