

## Supplementary material to

### MODELING AND SIMULATION OF THE BIOSURFACTANT PRODUCTION BY ENZYMATIC ROUTE USING XYLOSE AND OLEIC ACID AS REAGENTS

Ana Bárbara Moulin Cansian, Paulo Waldir Tardioli, Felipe Fernando Furlan, Ruy de Sousa Júnior\*

Federal University of São Carlos, Graduate Program in Chemical Engineering, Rod. Washington Luís, km 235 - CEP 13565-905, São Carlos, SP

*Chem. Ind. Chem. Eng. Q.* 28 (4) 265–276 (2022)

#### Appendix A

*Table A1. Remaining variables specified for the simulation*

Stream or Equipment	Variable	Name	Unit	Value
Stream 13	F	Molar flow of ethanol	kmol/h	0.52
Stream 13	T	Temperature	K	323.15
Stream 13	P	Pressure	atm	1
Tank 101	Conv	Conversion	dimensionless	0.90
Splitter after T 101	frac_sol	Fraction of solids in the liquid stream	dimensionless	0.99
Splitter after T 101	humidity	Fraction of liquid in the solid stream	dimensionless	0.10
Stream 18	F	Molar flow of water	kmol/h	0.30
Stream 18	T	Temperature	K	298.15
Stream 18	P	Pressure	atm	1
Cooler 102	Pdrop	Pressure loss	atm	0
Cooler 102	Outlet.T	Output temperature	K	323.15
Cooler 102	U	Global heat exchange coefficient	kW/m <sup>2</sup> /K	0.6945
Cooler 102	Lmtd	Logarithmic mean temperature difference	K	10
Tank 102	Conv(1)	Conversion of FFA precipitation	dimensionless	0.40
Tank 102	Conv(2)	Conversion of xylose ester precipitation	dimensionless	0.99
Tank 102	Conv(3)	Conversion of xylose solubilization	dimensionless	0.99
Splitter after T 102	frac_sol	Fraction of solids in the liquid stream	dimensionless	0.99
Splitter after T 102	humidity	Fraction of liquid in the solid stream	dimensionless	0.10
Stream 22	F	Molar flow of ethyl methyl ketone	kmol/h	0.60
Stream 22	T	Temperature	K	298.15
Stream 22	P	Pressure	atm	1
Tank 103	Conv	Conversion of FFA solubilization	dimensionless	0.90
Splitter after T 103	frac_sol	Fraction of solids in the liquid stream	dimensionless	0.99
Splitter after T 103	humidity	Fraction of liquid in the solid stream	dimensionless	0.10

\* Email: ruy@ufscar.br

Table A2. Results for different process streams

Stream	Phase	Variable	Name	Unit	Value
Stream 5	Liquid	F	Molar flow	kmol/h	235
Stream 5	Solid	F	Molar flow	kmol/h	79.6
Stream 5	Liquid	Fw	Mass flow	kg/h	28596
Stream 5	Solid	Fw	Mass flow	kg/h	1818.05
Stream 5	All	P	Pressure	atm	1
Stream 5	All	T	Temperature	K	333.15
Stream 5	Liquid	zw(1)*	Composition	dimensionless	0.0525
Stream 5	Liquid	zw(2)*	Composition	dimensionless	0.4939
Stream 5	Liquid	zw(3)*	Composition	dimensionless	0
Stream 5	Liquid	zw(4)*	Composition	dimensionless	0.4536
Stream 5	Liquid	zw(5–7)*	Composition	dimensionless	0
Stream 5	Solid	zw(1)*	Composition	dimensionless	1
Stream 5	Solid	zw(2–4)*	Composition	dimensionless	0
Stream 6	Liquid	F	Molar flow	kmol/h	248.572
Stream 6	Solid	F	Molar flow	kmol/h	730.275
Stream 6	Liquid	Fw	Mass flow	kg/h	30247.2
Stream 6	Solid	Fw	Mass flow	kg/h	16679.3
Stream 6	All	T	Temperature	K	333.15
Stream 6	All	P	Pressure	atm	1
Stream 6	Liquid	zw(1)*	Composition	dimensionless	0.0505
Stream 6	Liquid	zw(2)*	Composition	dimensionless	0.4901
Stream 6	Liquid	zw(3)*	Composition	dimensionless	0.0056
Stream 6	Liquid	zw(4)*	Composition	dimensionless	0.4536
Stream 6	Liquid	zw(5–7)*	Composition	dimensionless	0
Stream 6	Solid	zw(1)*	Composition	dimensionless	1
Stream 6	Solid	zw(2–4)*	Composition	dimensionless	0
Stream 9, 10	Liquid	zw(1)*	Composition	dimensionless	0.0151
Stream 9, 10	Liquid	zw(2)*	Composition	dimensionless	0.4237
Stream 9, 10	Liquid	zw(3)*	Composition	dimensionless	0.1030
Stream 9, 10	Liquid	zw(4)*	Composition	dimensionless	0.4537
Stream 9, 10	Liquid	zw(5)*	Composition	dimensionless	0
Stream 9, 10	Liquid	zw(6)*	Composition	dimensionless	0.0045
Stream 9, 10	Liquid	zw(7)*	Composition	dimensionless	0
Stream 9, 10	Solid	zw(1)*	Composition	dimensionless	1
Stream 9, 10	Solid	zw(2–4)*	Composition	dimensionless	0
Tank 101	Liquid	F	Molar flow	kmol/h	231.434
Tank 101	Solid	F	Molar flow	kmol/h	9.8812
Tank 101	Liquid	Fw	Mass flow	kg/h	28045.2
Tank 101	Solid	Fw	Mass flow	kg/h	533.899
Tank 101	All	T	Temperature	K	323.15
Tank 101	All	P	Pressure	atm	1
Tank 101	Liquid	zw(1)*	Composition	dimensionless	0.0015
Tank 101	Liquid	zw(2)*	Composition	dimensionless	0.4291
Tank 101	Liquid	zw(3)*	Composition	dimensionless	0.1044
Tank 101	Liquid	zw(4)*	Composition	dimensionless	0.4595
Tank 101	Liquid	zw(5)*	Composition	dimensionless	0.0008
Tank 101	Liquid	zw(6)*	Composition	dimensionless	0.0045
Tank 101	Liquid	zw(7)*	Composition	dimensionless	0
Tank 101	Solid	zw(1)*	Composition	dimensionless	0.3011
Tank 101	Solid	zw(3–4)*	Composition	dimensionless	0
Tank 102	Liquid	F	Molar flow	kmol/h	207.265
Tank 102	Solid	F	Molar flow	kmol/h	24.0645
Tank 102	Liquid	Fw	Mass flow	kg/h	20298.1
Tank 102	Solid	Fw	Mass flow	kg/h	7697.17
Tank 102	All	T	Temperature	K	298.15
Tank 102	All	P	Pressure	atm	1
Tank 102	Liquid	zw(1)*	Composition	dimensionless	0.0023
Tank 102	Liquid	zw(2)*	Composition	dimensionless	0.3550

\* Component number: Liquids: 1-Xylose; 2-Oleic Acid; 3-Xylose Ester; 4-Tert-butanol, 5-Ethanol; 6-Water; 7-Ethyl Methyl Ketone. Solid: 1-Immobilized Lipase; 2-Xylose; 3-Oleic Acid; 4-Xylose Ester.

Table A2. Results for different process streams (continued)

Stream	Phase	Variable	Name	Unit	Value
Tank 102	Liquid	zw(3)*	Composition	dimensionless	0.0014
Tank 102	Liquid	zw(4)*	Composition	dimensionless	0.6336
Tank 102	Liquid	zw(5)*	Composition	dimensionless	0.0012
Tank 102	Liquid	zw(6)*	Composition	dimensionless	0.0065
Tank 102	Liquid	zw(7)*	Composition	dimensionless	0
Tank 102	Solid	zw(1)*	Composition	dimensionless	0.0002
Tank 102	Solid	zw(2)*	Composition	dimensionless	0
Tank 102	Solid	zw(3)*	Composition	dimensionless	0.6241
Tank 102	Solid	zw(4)*	Composition	dimensionless	0.3757
Tank 103	Liquid	F	Molar flow	kmol/h	24.3982
Tank 103	Solid	F	Molar flow	kmol/h	8.6713
Tank 103	Liquid	Fw	Mass flow	kg/h	5170.03
Tank 103	Solid	Fw	Mass flow	kg/h	3340.12
Tank 103	All	P	Pressure	atm	1
Tank 103	All	T	Temperature	K	298.15
Tank 103	Liquid	zw(1)*	Composition	dimensionless	0.0004
Tank 103	Liquid	zw(2)*	Composition	dimensionless	0.8860
Tank 103	Liquid	zw(3)*	Composition	dimensionless	0.0002
Tank 103	Liquid	zw(4)*	Composition	dimensionless	0.1037
Tank 103	Liquid	zw(5)*	Composition	dimensionless	0.0002
Tank 103	Liquid	zw(6)*	Composition	dimensionless	0.0011
Tank 103	Liquid	zw(7)*	Composition	dimensionless	0.0084
Tank 103	Solid	zw(1)*	Composition	dimensionless	0.0005
Tank 103	Solid	zw(2)*	Composition	dimensionless	0
Tank 103	Solid	zw(3)*	Composition	dimensionless	0.1423
Tank 103	Solid	zw(4)*	Composition	dimensionless	0.8571

\* Component number: Liquids: 1-Xylose; 2-Oleic Acid; 3-Xylose Ester; 4-Tert-butanol; 5-Ethanol; 6-Water; 7-Ethyl Methyl Ketone. Solid: 1-Immobilized Lipase; 2-Xylose; 3-Oleic Acid; 4-Xylose Ester.

## Appendix B

### Equipment Cost

According to [1], Eq. (B.1) can describe the equipment cost. The equipment has a minimum and maximum size specification to apply Eq. (B.1s). When necessary, a correction is made to consider the appropriate number of equipment units to match the total area or volume that satisfies the process specifications. The modular basic cost is calculated by Eq. B.2 (for Reactor and Filter) or Equation B.3 (for Exchangers and Process Vessels). Since Equations B.1, B.2, and B.3 were exposed in 2001 for the first time, it is necessary to correct the estimative for the present time (Equation B.4). Finally, it is also important to adapt the prediction to the equipment's location (Equation B.5).

$$\log_{10} C_P^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2 \quad (B.1)$$

$C_P^0$ : Equipment cost under standard conditions (carbon steel and atmospheric pressure);

$K_i$ : Specific constants for each equipment unit;

$A$ : Equipment cost attribute (area or volume).

$$C_{BM} = C_P^0 \cdot F_{BM} \quad (B.2)$$

$C_{BM}$ : Bare module equipment cost;

$F_{BM}$ : Bare module equipment cost factor.

$$C_{BM} = C_P^0 (B_1 + B_2) \quad (B.3)$$

$B_1$ : Bare module equipment cost factor 1;

$B_2$ : Bare module equipment cost factor 2.

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right) \quad (B.4)$$

$C_1$ : Cost of equipment at time 1;

$C_2$ : Cost of equipment at time 2;

$I_1$ : Price index (Marshall and Swift Equipment Cost Index (M&S)) at time 1;

$I_2$ : Price index at time 2.

For both price indexes, information from [2] was utilized.

$$C_B = C_{USGC} \cdot LF_B \quad (B.5)$$

$C_B$ : Equipment cost in Brazil;

$C_{USGC}$ : Equipment price in USA gulf coast;

$LF_B$ : Brazil location factor.

#### Esterification reactor (Jacketed agitated - carbon steel)

$$K_1 = 4.1052; \quad K_2 = -0.4680; \quad K_3 = -0.0005; \quad A_{\min} = 0.1m^3; \quad A_{\max} = 35m^3$$

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_p^0 = 4.1052 - 0.4680 \times \log_{10}(35) - 0.0005 \times [\log_{10}(35)]^2$$

$$C_p^0 = US\$2406.49$$

Each reactor has 35 m<sup>3</sup>, for A=1451.87 m<sup>3</sup>, we have 42 reactors:

$$C_p^0 = US\$2406.49 \times 42$$

$$C_p^0 = US\$101072.58$$

For bare module:

$$F_{BM} = 4.00; \quad C_p^0 = US\$101072.58;$$

$$C_{BM} = C_p^0 \cdot F_{BM}$$

$$C_{BM} = US\$101072.58 \times 4.00$$

$$C_{BM} = US\$404290.34$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$404290.34$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$404290.34 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$695868.93$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$695868.93; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$695868.93 \times 1.14$$

$$C_B = US\$793083.10$$

#### Filter (Gravity - carbon steel)

$$K_1 = 4.2756; \quad K_2 = -0.6480; \quad K_3 = 0.0714; \quad A_{\min} = 0.5m^2; \quad A_{\max} = 80m^2; \quad A = 39.74m^2$$

$$\log_{10} C_P^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_P^0 = 4.2756 - 0.6480 \times \log_{10}(39.74) + 0.0714 \times [\log_{10}(39.74)]^2$$

$$C_P^0 = US\$2641.71$$

For bare module:

$$F_{BM} = 1.65; \quad C_P^0 = US\$2641.71$$

$$C_{BM} = C_P^0 \cdot F_{BM}$$

$$C_{BM} = US\$2641.71 \times 1.65$$

$$C_{BM} = US\$4358.82$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$4358.82$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$4358.82 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$7500.49$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$7500.49; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$7500.49 \times 1.14$$

$$C_B = US\$8550.56$$

#### Heat exchanger 1 (Fixed tube - carbon steel)

$$K_1 = 4.3247; \quad K_2 = -0.3030; \quad K_3 = 0.1634; \quad A_{\min} = 10m^2; \quad A_{\max} = 1000m^2; \quad A = 25.74m^2$$

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_p^0 = 4.3247 - 0.3030 \times \log_{10}(25.74) + 0.1634 \times [\log_{10}(25.74)]^2$$

$$C_p^0 = US\$16688.67$$

For bare module:

$$B_1 = 1.63; \quad B_2 = 1.66; \quad C_p^0 = US\$16688.67$$

$$C_{BM} = C_p^0 (B_1 + B_2)$$

$$C_{BM} = US\$16688.67(1.63 + 1.66)$$

$$C_{BM} = US\$54905.71$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$54905.71$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$54905.71 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$94479.59$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$94479.59; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$94479.59 \times 1.14$$

$$C_B = US\$107706.73$$

#### Heat exchanger 2 (Fixed tube - carbon steel)

$$K_1 = 4.3247; \quad K_2 = -0.3030; \quad K_3 = 0.1634; \quad A_{\min} = 10m^2; \quad A_{\max} = 1000m^2; \quad A = 61.26m^2$$

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_p^0 = 4.3247 - 0.3030 \times \log_{10}(61.26) + 0.1634 \times [\log_{10}(61.26)]^2$$

$$C_p^0 = US\$20187.63$$

For bare module:

$$B_1 = 1.63; \quad B_2 = 1.66; \quad C_p^0 = US\$20187.63$$

$$C_{BM} = C_p^0 (B_1 + B_2)$$

$$C_{BM} = US\$20187.63(1.63 + 1.66)$$

$$C_{BM} = US\$66417.29$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$66417.29$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$66417.29 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$114288.26$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$114288.26; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$114288.26 \times 1.14$$

$$C_B = US\$130288.61$$

#### Process Vessel 1 (Horizontal - carbon steel)

$$K_1 = 3.5565; \quad K_2 = 0.3776; \quad K_3 = 0.0905; \quad A_{\min} = 0.1m^3; \quad A_{\max} = 628m^3; \quad A = 28.43m^3$$

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_p^0 = 3.5565 + 0.3776 \times \log_{10}(28.43) + 0.0905 \times [\log_{10}(28.43)]^2$$

$$C_p^0 = US\$19802.27$$

For bare module:

$$B_1 = 1.49; \quad B_2 = 1.52; \quad C_p^0 = US\$19802.27$$

$$C_{BM} = C_p^0 (B_1 + B_2)$$

$$C_{BM} = US\$19802.27(1.49 + 1.52)$$

$$C_{BM} = US\$59604.82$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$59604.82$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$59604.82 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$102565.64$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$102565.64; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$102565.64 \times 1.14$$

$$C_B = US\$116924.83$$

**Process Vessel 2 (Horizontal - carbon steel)**

$$K_1 = 3.5565; \quad K_2 = 0.3776; \quad K_3 = 0.0905; \quad A_{\min} = 0.1m^3; \quad A_{\max} = 628m^3; \quad A = 27.99m^3$$

$$\log_{10} C_P^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_P^0 = 3.5565 + 0.3776 \times \log_{10}(27.99) + 0.0905 \times [\log_{10}(27.99)]^2$$

$$C_P^0 = US\$19605.54$$

For bare module:

$$B_1 = 1.49; \quad B_2 = 1.52; \quad C_P^0 = US\$19605.54$$

$$C_{BM} = C_P^0 (B_1 + B_2)$$

$$C_{BM} = US\$19605.54(1.49 + 1.52)$$

$$C_{BM} = US\$59012.67$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$59012.67$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$59012.67 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$101546.68$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$101546.68; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$101546.68 \times 1.14$$

$$C_B = US\$115763.22$$

**Process Vessel 3 (Horizontal - carbon steel)**

$$K_1 = 3.5565; \quad K_2 = 0.3776; \quad K_3 = 0.0905; \quad A_{\min} = 0.1m^3; \quad A_{\max} = 628m^3; \quad A = 0.89m^3$$

$$\log_{10} C_P^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2$$

$$\log_{10} C_P^0 = 3.5565 + 0.3776 \times \log_{10}(0.89) + 0.0905 \times [\log_{10}(0.89)]^2$$

$$C_P^0 = US\$3448.29$$



For bare module:

$$B_1 = 1.49; \quad B_2 = 1.52; \quad C_p^0 = US\$3448.29$$

$$C_{BM} = C_p^0(B_1 + B_2)$$

$$C_{BM} = US\$3448.29(1.49 + 1.52)$$

$$C_{BM} = US\$10379.34$$

For time effect:

$$I_1 = 1262; \quad I_2 = 2171.6; \quad C_1 = US\$10379.34$$

$$C_2 = C_1 \left( \frac{I_2}{I_1} \right)$$

$$C_2 = US\$10379.34 \left( \frac{2171.6}{1262} \right)$$

$$C_2 = US\$17860.37$$

For location purposes: (USA - BRA):

$$C_{USGC} = US\$17860.37; \quad LF_B = 1.14$$

$$C_B = C_{USGC} \cdot LF_B$$

$$C_B = US\$17860.37 \times 1.14$$

$$C_B = US\$20360.82$$

#### Plant installation cost (CAPEX - capital investments)

The work [1] describes the cost of installing the plant as in Equation B.6:

$$C_{TM} = 1.18 \times \sum_{i=1}^n C_{BM,i} \quad (B.6)$$

$C_{TM}$  : Plant total cost;

$C_{BM,i}$  : Equipment - i price (already corrected for time and location).

$$\sum_{i=1}^n C_{BM,i} = US\$1292677.87$$

$$C_{TM} = 1.18 \times \sum_{i=1}^n C_{BM,i}$$

$$C_{TM} = 1.18 \times US\$1292677.87$$

$$C_{TM} = US\$1525359.90$$

#### NPV (Net present value) calculation

NPV is calculated according to Equation B.7, according to [3]:

$$NPV(X) = \sum_{j=1}^N \frac{CF(X)}{(1+r)^j} - CAPEX(X) \quad (B.7)$$

$NPV(X)$  : Net present value as a function of process variables;

$CF(X)$  : Cash flow as a function of process variables;

$r$  : Minimum acceptable rate of return;

$N$  : Project lifetime;

$CAPEX(X)$  : Capital investments as a function of process variables.

$$r = 0.11; \quad N = 25 \text{ years} \quad [4]$$

$$NPV(X) = 0$$

NPV = 0 indicates that the project has obtained the stipulated minimum rate of return. Therefore, the NPV was zeroed to get the product's value (US\$ 72.37/kg), which makes the process profitable.

### Raw material costs

Table B.1 shows all the calculations about the raw material.

Table B.1. Raw material cost (per hour and per year)

Component	kg/h	R\$/kg	US\$/kg	R\$/h	US\$/h	
Xylose	1501.32	126.2 <sup>a</sup>	21.94	189466.58	32944.41	
Enzyme	9.66 <sup>+</sup>	3048 <sup>b</sup>	529.99	29436.00	5118.33	
Tert-butanol	259.43 <sup>+</sup>	131.51 <sup>c</sup>	22.87	34117.60	5932.36	
Ethanol	0.4791 <sup>+</sup>	21.47 <sup>d</sup>	3.73	10.287	1.79	
Ethyl Methyl Ketone	0.1081 <sup>+</sup>	161.74 <sup>e</sup>	28.12	17.48	3.04	
Oleic Acid	14123.3	78.57 <sup>f</sup>	13.66	1109693.52	192953.27	US\$/year
Output product	3306.72	416.22 <sup>g</sup>	72.37	1376305.80	239311.75	1.034 x 10 <sup>9</sup>
Total without product				1362741.49	236953.19	1.024 10 <sup>9</sup>

+The calculation for the enzyme was performed considering its concentration in the immobilized support such as proposed by [5] (0.53% of enzyme w/w); \*It was regarded as a partial recovery of these reagents (for tert-butanol, ethanol and ethyl methyl ketone). Thus, it was adopted 2% from original simulation flows (for tert-butanol, ethanol, and ethyl methyl ketone), being 1% associated with recuperation costs and other 1% with separation inefficiencies; <sup>a, e</sup> [6]; <sup>b</sup> [7]; <sup>c</sup> [8]; <sup>d, f</sup> [9]; <sup>g</sup> the value of the product obtained in the analysis (NPV=0).

### Labor costs

The following equation can be used to estimate the number of shift operators in a chemical plant [3]:

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (B.8)$$

$N_{OL}$  : Number of shift operators;

$P$  : Number of steps involving solids;

$N_{np}$  : It is given by the sum of equipment units.

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5}$$

$P = 2$  (Two steps involve solids: enzymes in the reactor and purification step)

$$N_{np} = 48 \text{ (number of equipment units)}$$

$$N_{OL} = (6.29 + 31.7(2)^2 + 0.23 \times 48)^{0.5}$$

$$N_{OL} = 12.005 \approx 12 \text{ workers/turn}$$

In three turns: 36 workers

In Brazil, the average salary of an employee who has completed high school is around R\$1658.19, with a 37% tax [B.10]. Considering the exchange rate of 5.7511 US\$/R\$ and the period of one year, it is possible to calculate the operating cost [11]. See Table B.2.

Table B.2. Raw material cost (per hour and per year)

NOL	12.005 = 12	workers/per turn
12h (3 turns)	36	workers
Salary	1658.19	R\$/month
Taxes	0.37	%
Taxes	1658.19 x 0.37 = 613.53	R\$/month
Worker cost per month	1658.19 + 613.53 = 2271.72	R\$/month
Worker cost per month	2271.72 / 5.7511 = 395.01	US\$/month
Total (per month)	395.01 x 36 = 14220.22	US\$/month
Total (per year)	14220.22 x 12 = 511928.07	US\$/year

### Utility costs

Table B.3 and Table B.4 present all the information and calculations about the utility costs.

Table B.3. Utility costs with information and calculation

	Heat (kWh)	US\$/MWh [12]		Total Heat (MWh)
Cold utility	-604.13	5.26	12h per day/ 30 days per month	604.13 x 12 x 30/1000 = -217.49
Hot utility	137.58	10.1		137.58 x 12 x 30/1000 = 49.53

Table B.4. Total utility costs

Heat (MWh)	Total US\$/month
-217.49	217.49 x 5.26 = 1143.98
49.53	49.53 x 10.1 = 500.24
Total	US\$ 1644.22/month
Total	US\$ 19730.66/year

### Total operating costs

According to [3], the operating supervision costs are about 5% of operating labor costs, and the maintenance costs are about 5% of capital costs. See Table B.5.

Table B.5. Total operating costs with calculations

Operating labor cost	US\$ 511928.07/year
Capital cost (Plant installation cost)	US\$ 1525359.90/25 years
Operating supervision costs	511928.07 x 0.05 = US\$ 25596.40/year
Maintenance costs	1525359.90 x 0.05 = US\$ 76267.99/year

## REFERENCES

- [1] R. Turton, R. C. Bailie, W. B. Whiting, J. A. Shaeiwitz, United States, 3 (2009).
- [2] Y. Camaraza-Medina, A. A. Sánchez-Escalona, Y. Retirado-Mediaceja, O. F. García-Morales. Heat and technology.38-2 (2020) 425–431.
- [3] M. Peters, K. Timmerhaus, R. West. New York (2002).
- [4] A. A. Longati, A. R. A. Lino, R. C. Giordano, F. F. Furlan, A. J. G. Cruz, A. Bioresour. Technol. 263 (2018) 1–9.
- [5] V. Vescovi, J.B.C. Santos, P.W. Tardioli, Biocatal. Biotransform. 35 (2017) 298–305.
- [6] Synth. <<https://www.lojasynth.com/reagentes-analiticosmaterias-primas/reagentes-analiticosmaterias-primas/xilose-d-extra-pura?parceiro=2827>> [accessed 01 November 2021].
- [7] Glasslab. <<https://www.glasslab.com.br/reagentes-e-meios/alcool-butilico-terc-3-butanol-pa-1?parceiro=6858>> [accessed 01 November 2021].
- [8] Neon. <<https://www.neoncomercial.com.br/#produtos>> [accessed 01 November 2021].
- [9] Sigma Aldrich. <<https://www.sigmaaldrich.com/catalog/substance/2butanone72117893311?lang=pt&region=BR>> [accessed 01 November 2021].
- [10] CAGED, 2018. Cadastro Geral de Empregados e Desempregados. Governo Federal do Brasil.
- [11] BCB. Banco central do Brasil: cotação de moedas.
- [12] C. M. Oliveira, L. V. Pavao, M. A. S. S. Ravagnani, A. J. G. Cruz, C. B. B. Costa, Appl. Energy. 213 (2018) 520–539.