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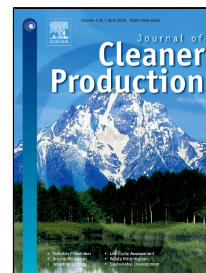
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1 **Multi-objective optimization of an industrial ethanol distillation system for vinasse**
2 **reduction – A case study**

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10

11 **Abstract**

12 The fluctuation in the price of oil and the positive consequences of fuels from renewable
13 sources (compared to fossil fuels) propel the expansion of biofuel global production. In this
14 work, the current distillation operation of an ethanol distillery is simulated and compared to
15 the use of indirect heating, evaluating the environmental and economic impacts associated with
16 vinasse fertirrigation by using an external automated tool. Results show that the replacement
17 proposed decreases approximately 15% of the amount of vinasse. Moreover, as the
18 modifications do not change the outlet flowrates, such revamping might be done without
19 additional operational changes that could affect the productivity. The environmental evaluation
20 presents positive results, showing that the new configuration may decrease all environmental
21 impacts categories assessed. From an economic perspective, the plant could also have higher
22 profits, presenting a payback period of 3.57 years. Finally, the new improved system is treated
23 as a multi-objective optimization problem and it is solved by using the weighted sum method
24 to obtain the Pareto frontier, providing the optimal solutions that trade-off economic and
25 environmental objectives.

26

27 **Keywords:** Simulation; Ethanol distillery; Waste reduction; Economic evaluation;
28 Environmental assessment; Sugarcane vinasse.

29

30 **Highlights**

- 31 • Ethanol distillation system using direct and indirect heating are compared.
- 32 • An automated evaluation tool integrates the simulation-optimization methodology.
- 33 • Vinasse impacts are treated as elementary flows.
- 34 • Environmental and economic aspects can be reduced simultaneously by using reboiler.
- 35 • Low investment costs leading to significant reduction in the environmental impacts.

36

37 **1. Introduction**

38

39 Sugarcane biofuel processing has been one of the most important and strategic sectors in the
40 Brazilian economy, being Brazil the world's largest sugarcane ethanol producer (UNICA and
41 APEX-BRASIL, 2017). However, the success of Brazilian distilleries depends on how they
42 overcome the new scientific challenges faced, mainly about process optimization, energy
43 integration, energy cogeneration, and sustainability (Amorim et al., 2011).

44

45 One of the main challenges is regarding the reduction of the sugarcane vinasse. This liquid
46 residue of the distillation process is rich in minerals and is commonly used to irrigate
47 sugarcane crops, known as fertirrigation; nevertheless, if produced in excess, it brings
48 environmental and economic problems. The direct application of vinasse to the soil may
49 cause salinization, leaching of metals present in the soil to groundwater (killing animals and
50 aquatic plants), changes in the soil quality due to unbalance of nutrients (mainly manganese),
51 alkalinity reduction, crop losses, increase of phytotoxicity, and unpleasant odor (Navarro et
52 al., 2000; Santana and Machado, 2008). Moreover, vinasse is an additional source of

53 greenhouse gases emissions to the atmosphere, especially N₂O and CH₄. Emissions might
54 result from aerobic and anaerobic decomposition of the organic matter contained in vinasse
55 that occurs during temporary storage, transportation, or after the application to the soil
56 (Carmo et al., 2012; Moraes et al., 2017; Oliveira et al., 2013). Other potential problems
57 related to vinasse storage in open ponds (which is the current scenario of the distillery
58 studied) are water pollution and insect proliferation (Dunkelberg et al. 2013). In Brazil,
59 fertirrigation frequently becomes an economic problem when the area to apply vinasse is not
60 available. This might happen when the crop belongs to the suppliers or it is located far away
61 from the industrial plant. Besides, Brazilian environmental legislation recently established
62 criteria and procedures for vinasse application to the soil. Such environmental technical
63 standard P4.231 (CETESB, 2015) defines the maximum dosage of vinasse to be used in the
64 fertirrigation, causing problems of surplus of vinasse stored in open ponds.

65
66 Although the use of vinasse is a topic widely investigated in literature, most of the researches
67 focuses on energy production, treatment before disposal, and yeast production (Christofoleti
68 et al., 2013; España-Gamboa et al., 2011; Leme and Seabra, 2017; Moraes et al., 2014; Pires
69 et al., 2016), but do not study the possibilities to improve economic and environmental
70 aspects by reducing the amount of vinasse produced. In order to achieve this objective, the
71 most promising options are concentration by evaporation and the use of indirect heating in
72 the distillation system. Concentration by evaporation reduces the volume of vinasse
73 considerably; however, the high energy demand, fast incrustation of evaporators, and
74 spontaneous crystallization are important limitations of this alternative (Christofoleti et al.,
75 2013; Gomes et al., 2011).

76

77 Thus, the objective of this work is simulate, analyze, and compare economic and
78 environmental aspects of a full-scale industrial system of an alcohol distillery operating with
79 direct and indirect heating using Aspen Hysys process simulator integrated to Matlab. The
80 models mimic the distillery of the *Cooperativa Agricola de Astorga Ltda* (COCAFE), which
81 is located in the Northwest of Parana State, (South of Brazil), processing around 180 t/h of
82 sugarcane juice and producing approximately 380 m³/day of hydrous ethanol.

83

84 **2. Problem Statement**

85

86 The problem addressed in this article can be formally stated as follows. Brazilian distilleries
87 are required to reduce their vinasse production in order comply with the recent environmental
88 technical standard, which in turn will meet RenovaBio purpose. RenovaBio is an initiative of
89 the Brazilian government whose objective is guarantee the expansion of biofuel production in
90 the country, based on environmental, economic, and financial sustainability, in harmony with
91 the Brazilian commitment at COP 21 (MME, 2017). Although many authors have been
92 proposing new design for ethanol plants in order to improve their sustainability (Leme and
93 Seabra, 2017; Macrelli et al., 2012; Moraes et al., 2015; Petersen et al., 2015), usually, the
94 capital costs are not feasible for Brazilian sugarcane industries, reducing the likelihood of
95 putting these improvement projects into practice. Therefore, the objective of this analysis is
96 to propose a low investment cost modification that leads to significant reductions in
97 economic expenses and environmental impacts.

98

99 **3. Case Study**

100

101 In this work, the Use of Reboiler (UR) and the Direct Steam Injection (DSI) are compared in
102 order to provide heat to the first distillation column of the COCAFE distillery. The UR and
103 the DSI alternatives are analyzed using two criteria to accomplish a fair comparison between
104 them. Firstly, the simulation is developed in Aspen Hysys to measure the production of
105 ethanol, flegma, and vinasse (the whole description of the process is available in the
106 Appendix A). Secondly, the information in the simulator is used to perform an economic and
107 environmental evaluation programmed in Matlab.

108

109 After the distillation process, which is the first process inside the system boundary analyzed
110 (Fig. A.1), the pumping station sends the stored vinasse from open ponds to the lorry, being
111 transported at relatively long distance and then applied to the soil, by broadcaster. The
112 characteristics of this transportation step to perform the economic and environmental analysis
113 are: (i) lorry capacity of 60 m³; (ii) average distance for the vinasse fertirrigation from the
114 sugarcane processing facility to the sugarcane crop of 90 km; (iii) vinasse dosage of 150
115 m³·ha⁻¹ and (iv) cost of fertirrigation per ton of vinasse = \$ 0.75 (Santos et al., 2015;
116 Zorzenoni et al., 2014). It is important to highlight that as the rest of the activities
117 (evaporation and fermentation processes) are common for DSI and UR, all the evaluations are
118 executed only inside the boundary system, which covers the distillation and fertirrigation
119 processes.

120

121 Finally, for the best configuration found in the second step, a multi-objective optimization is
122 performed in order to obtain a set of alternative solutions representing the optimal trade-off
123 between the economic and environmental aspects.

124

125 *3.1 Comparative study of the process alternatives*

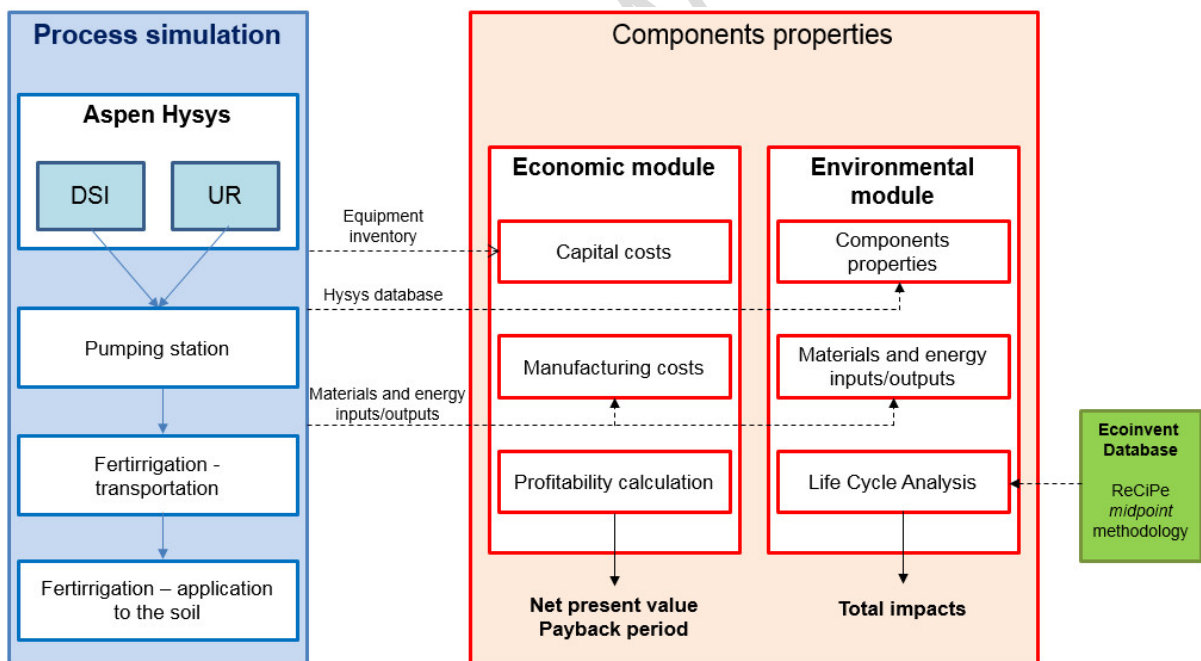
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127 A comparative study is performed by setting the mass flow of the stream $VI-A$ to zero $\text{kg}\cdot\text{h}^{-1}$
 128 and removing the adjust block $ADJ-1$ (Fig. A.1). Thus, the variation of vinasse, flegma, and
 129 ethanol mass flow are calculated when the direct heating is replaced by indirect heating.

130

131 The evaluation tool programmed in Matlab includes independent modules for the economic
 132 and environmental impact assessment based on the material and energy balance and the
 133 equipment inventory retrieved from Aspen Hysys simulation used to obtain a rigorous model
 134 of the plant. The approach uses a dynamic link, known as Component Object Module (COM)
 135 technology, to connect and send the results to Matlab. Fig. 1 summarizes the procedure
 136 followed. Detailed information about the automated tool can be found in Torres et al (2011).

137



138

139 Figure 1. Flow diagram of the automated procedure for the environmental and economic
 140 evaluation based on process modeling.

141

142 *3.1.1 Economic module*

143

144 The following section is a brief description of the economic methodology used in this work
145 taken from Turton et al. (2012). The capital cost estimation is based on the inventory of the
146 equipment and their design parameters directly retrieved from the simulation, which in turn
147 are fixed based on the operational parameters of the COCAFE plant. The direct
148 manufacturing costs include the following material and energy streams: product streams,
149 utilities, emissions, and waste streams. Usually, the fuel used to supply the energy to produce
150 steam in the boiler is one of the major operating expenses; however, as the ethanol distillery
151 uses its own sugarcane bagasse as a fuel, the prices of low (LP), medium (MP) and high-
152 pressure (HP) steam are computed considering the estimated savings avoiding the cost of
153 burning natural gas in the boiler. The waste treatment cost is due to the cost of vinasse
154 discharge based on its transportation and application to the soil. All the sugarcane vinasse
155 produced is considered to be used in the fertirrigation. The operating labor cost is estimated
156 based on the number of operators required per equipment unit per shift. Then the fixed costs
157 and general expenses can be calculated applying factors to the values previously computed to
158 obtain a final manufacturing cost, which are calculated from capital cost investment
159 regarding Brazil conditions: annual interest rate of 12.65% for the capital investment (BCB,
160 2016), and an equipment life span of 20 years.

161

162 The economic indicators to evaluate the profitability of the process alternatives are the Net
163 Present Value (NPV) and the discounted payback period. The initial cost is the difference of
164 the total investment costs (\$) between DSI and UR and the cash flow is the difference of total
165 manufacturing costs (\$/yr) of DSI and UR alternatives.

166

167 *3.2.2 Environmental module*

168

169 The environmental impact is quantified using Life Cycle Assessment (LCA) principles. The
170 damage factors are taken from Ecoinvent v3.01 database using attributional approach (Swiss
171 Centre for Life Cycle Inventories, 2014). In order to perform the environmental assessment
172 of vinasse for the UR alternative, the new quantity of fixed solids is estimated based on the
173 average chemical composition of fixed solids of vinasse from sugacarne (21500 mg·L⁻¹)
174 measured by Prada et al. (1998) and the density of 1.143 g·mL⁻¹ (Camargo et al., 2009).

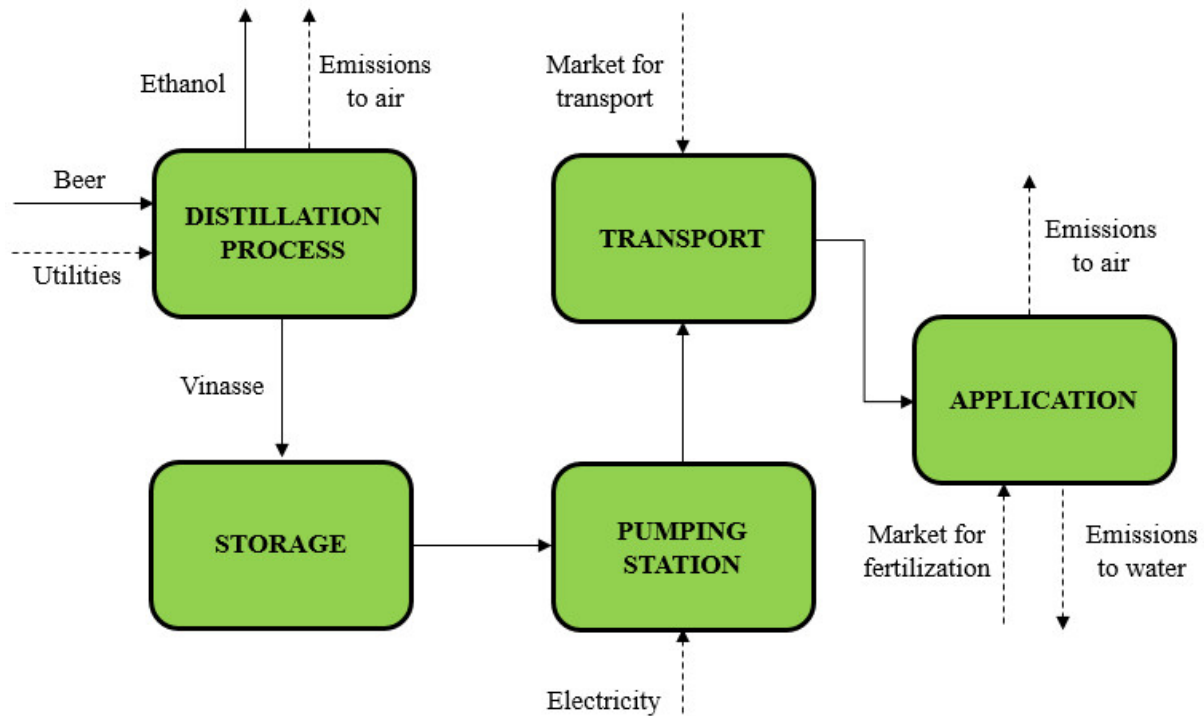
175

176 The ReCiPe *midpoint* impact assessment methodology is selected using the hierarchist
177 perspective, which includes eighteen impacts categories: agricultural land occupation (ALO),
178 climate change (CC), fossil depletion (FD), freshwater ecotoxicity (FET), freshwater
179 eutrophication (FE), human toxicity (HT), ionizing radiation (IR), marine ecotoxicity (MET),
180 marine eutrophication (ME), metal depletion (MD), natural land transformation (NLT), ozone
181 depletion (OD), particulate matter formation (PMF), photochemical oxidant formation (POF),
182 terrestrial acidification (TA), terrestrial ecotoxicity (TET), urban land occupation (ULO), and
183 water depletion (WD).

184

185 The functional unit selected is 1 kg of hydrous ethanol produced. All the thermal and electric
186 energy required for the production process is produced in combined heat and power units
187 using bagasse as a fuel, which means that sugarcane processing facilities are self-sufficient on
188 energy consumption (the same approach was used by Cavalett et al. (2013)). The materials
189 and energy inputs and outputs related to the distillation process are retrieved from the
190 validated process simulation. The scenario scheme for LCA evaluation is illustrated in Fig. 2.
191 The dashed lines show the input for the Life Cycle Impact Assessment (LCIA).

192



193

194 Figure 2. Scenario scheme for the LCA evaluation.

195

196 Emissions from vinasse are treated as elementary flows. The ReCiPe methodology provides
 197 information about the impact of the nutrients (*i.e.*, N-based, P₂O₅ and K₂O contained in the
 198 vinasse from sugarcane when applied to the soil); however, no emissions are considered.

199 Thus, the data of N contained in the dry mass of vinasse ($4.73 \cdot 10^3$ kg N/ kg dry mass) and
 200 P₂O₅ ($2.22 \cdot 10^3$ kg P₂O₅/ kg dry mass) are used to estimate the quantity of emissions to the air
 201 and to the underground water according to Table 1.

202

203 Table 1. Emission factors resulting from mineral fertilization.

Released substances	Ratio	Emission	Reference
CO ₂	3.64 kg CO ₂ /kg N	air	IPCC (2006)
N ₂ O	0.05 kg N ₂ O/kg N	air	Crutzen et al. (2008)
NO _x	0.053 kg NO _x /kg N	air	Renouf et al. (2008)

NH ₃	0.026 kg NH ₃ /kg N	air	Renouf et al. (2008)
NO ₃ ⁻	0.065 kg NO ₃ ⁻ /kg N	water	Renouf et al. (2008)
PO ₄ ³⁻	0.128 kg PO ₄ ³⁻ /kg N	water	Bloesch et al. (1997)
C ₂ H ₆ O	-	air	Retrieved from Aspen Hysys

204

205 **4. Mathematical description and solution method**

206

207 In mathematical terms, the synthesis of chemical processes, treated as a multi-objective
 208 optimization of mixed integer nonlinear programming (moMINLP) problem, that accounts
 209 for economic and environmental aspects, has been applied successfully, providing important
 210 contributions (Gao and You, 2017; García-Montoya et al., 2016). In this paper, a systematic
 211 methodology for design and modeling of chemical processes that relies on the combined use
 212 of simulation and optimization techniques is applied. More precisely, the design task is
 213 solved by a simulation-optimization method presented by Brunet et al. (2012) that exploits
 214 the complementary strengths of optimization tools (*i.e.*, nonlinear programming (NLP)) and
 215 commercial process simulators (*i.e.*, Aspen Hysys).

216

217 An external NLP solver in Matlab is employed for searching the values of the design and
 218 operating variables that minimize the total cost and the environmental impacts of the process.
 219 As NLP solver, the “*fminsearchbnd*” function is used, which combines “*fminsearch*” and
 220 “*fminbnd*” well adapted for an objective function type “smooth nonlinear” with constraints.
 221 The termination criterion applied is defined according to the upper and lower bounds of each
 222 variable (*i.e.*, the algorithm stops when the vectors of upper and lower bounds for all
 223 variables are evaluated and detect a global minimum in the range). Since Matlab function
 224 “*fminsearch*” minimizes a given objective function, the objective function must be changed

225 to pose the problem as a moMINLP one. To accomplish this task, it is necessary to obtain
 226 gradient information with respect to the objective function and constraints, presented
 227 hereafter.

228

229 4.1 Economic objective function: total annualized cost

230

231 The total annualized cost (TAC) accounts for the annual capital cost (CF) and operating costs
 232 (CO).

$$TAC = CF + CO \quad (1)$$

233 The CF includes only the cost to purchase and install the reboiler on the column (C_R). The
 234 Guthrie's correlation for economic assessment is adopted for carbon steel kettle reboilers up
 235 to 1000 m² of area (Turton et al. 2012) using the most recent Chemical Engineering Plant
 236 Cost Index for the year analyzed (Chemical Engineering, 2016).

237

$$C_R = C_p^0 \cdot F_{bm} \cdot F_p \quad (2)$$

238

239 where C_p^0 is the purchased cost of the kettle reboiler for the required area, F_{bm} is the bare
 240 module factor and F_p is the pressure variation calculated according to Eq. (3) taken from
 241 Turton et al. (2012):

242

$$\log_{10} C_p^0 = K_1 + K_2 \cdot \log_{10}(A_r) + K_3 \cdot [\log_{10}(A_r)]^2 \quad (3)$$

243

244 The area of the reboiler (A_r) is calculated from the logarithmic mean temperature difference (
 245 ΔT_{lm}), the overall heat transfer coefficient (U_r) and the heat duty (Q_r) as follows:

246

$$A_r = \left(\frac{Q_r}{U_r \cdot \Delta T_{lm}} \right) \quad (4)$$

247

248 The equipment cost is multiplied by the capital recovery factor (crf), which is a function of
 249 the interest rate (i) and the plant life cycle (parameter t).

250

$$CF = C_R \cdot crf \quad (5)$$

$$crf = \left(\frac{i(1+i)^t}{(1+i)^t - 1} \right) \quad (6)$$

251

252 The operating costs are calculated in order to obtain a final manufacturing. Then, aiming at
 253 optimize the best configuration, the considered factors are electricity demand (E), steam
 254 production (SP), cooling water energy (CW), raw materials (RM), waste management (WM),
 255 and general operating costs (c). For the economic optimization, the total operating cost is thus
 256 the sum of all factors mentioned.

257

$$CO = \sum_{m \in M} (E_m \cdot c_E + SP_m \cdot c_{SP} + CW_m \cdot c_{CW} + RM_m \cdot c_{RM} + WM_m \cdot c_{WM} + c_o) \cdot \tau \quad (7)$$

258

259 The operational costs for each equipment unit m are calculated by multiplying each factor by
 260 its respective price (\$/unit) then by the total annual operating time (τ) as shown in Eq. 7. The

261 parameters c_E , c_{SP} , c_{CW} , c_{RM} , c_{WM} and c_o (\$/unity) are the direct costs for electricity, steam
 262 production, cooling water, raw materials, waste management, and general operations,
 263 respectively (Quaglia et al., 2012). The process simulator provides E_m , SP_m , CW_m , RM_m , and
 264 WM_m .

265

266 *4.2 Environmental objective function and assumptions*

267

268 The LCIA phase translates the Life Cycle Inventory (LCI) data into the corresponding
 269 environmental impacts. The damage in a given category (DMA_d) is determined from the life
 270 cycle inventory entries (LCI_b) and the corresponding set of damage factors (df_{bd}).

271

$$DMA_d = df_{bd} \cdot LCI_b \quad \forall d \in D \quad (8)$$

272

273 The optimization is performed in terms of climate change, similar to the work of Zhang et al.
 274 (2014). It is important to highlight that the focus of ReCiPe methodology for climate change
 275 impact category is on the marginal effect of adding a relatively small amount of CO₂ or other
 276 greenhouse gases, and not the impact of all emissions (Goedkoop et al., 2009).

277

278 *4.3 Solution method: multi-objective optimization*

279

280 One of the main advantages of the approach adopted is that it facilitates the work
 281 implemented as it allows optimizing chemical process models and associated thermodynamic
 282 packages that are already provided by the simulator without having to define the
 283 aforementioned equations in an explicit way. To solve the moMINLP problem, the design
 284 variables are fixed to the optimal value obtained in the latest iteration of the algorithm.

285

286 The original problem is first solved by optimizing each single scalar objective separately. The
 287 weighted sum method is used to obtain the Pareto frontier, providing a practical and easy-to-
 288 use approach for multi-objective optimization and is useful as such (Marler and Arora, 2010).
 289 A key issue in the algorithm is that the process simulator must converge at each time the
 290 solver sends a set of values of the design variables. Otherwise, the overall procedure may fail
 291 and the solver must automatically go to the next iteration. To ensure this, the NLP is modified
 292 to disregard infeasible solutions by adding slack variables and an exact penalty vector to the
 293 objective function. This approach ensures that the solution found is at least locally optimally,
 294 as opposed to other meta-heuristic approaches that do not present this property (Brunet et al.,
 295 2012). Hence, the modified NLP takes the following form:

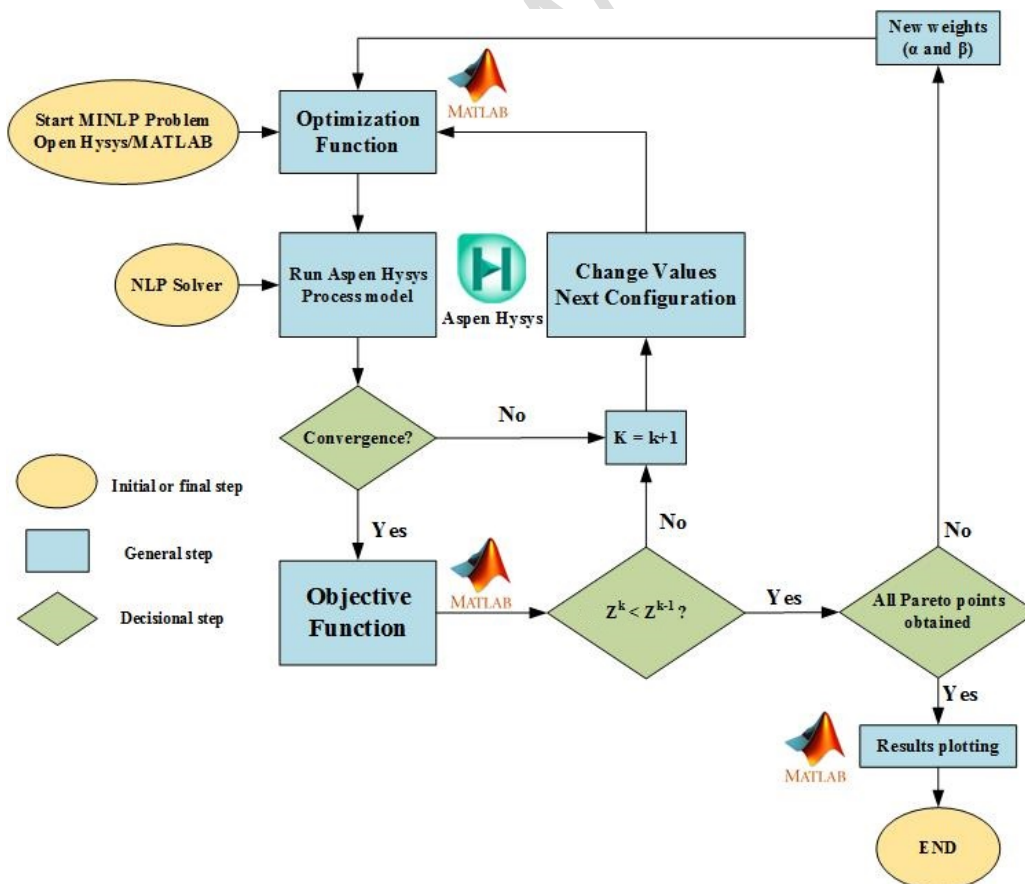
296

$$\begin{aligned}
 (MA) \quad & \min_{x_D} \quad z = \alpha \cdot f_1(x, u, x_D) + \beta \cdot f_2(x, u, x_D) + \prod (s_1 + s_2 + s_3) \\
 s.t. \quad & \alpha = 1 - \beta \\
 & h_I(x, u, x_D) = 0 \\
 & h_E(x, u, x_D) + s_1 - s_2 = 0 \\
 & g_E(x, u, x_D) \leq s_3 \\
 & s_1 \geq 0; s_2 \geq 0; s_3 \geq 0
 \end{aligned} \tag{9}$$

297

298 In model (MA), f_1 is the economic objective function, f_2 denotes the LCA metrics,
 299 whereas \prod is a penalty parameter vector, and s_1 , s_2 , and s_3 are vectors of positive slack
 300 variables. As observed, α is the economic cost weight and β is the environmental impact
 301 weight. Both, α and β vary from zero to one, thus giving rise to different results to obtain a
 302 Pareto curve where all values are optimal. Functions h_I are implicit equations solved by the

303 process simulator (*e.g.*, energy and mass balances), whereas h_E and g_E are explicit external
 304 equality and inequality constraints (*i.e.*, temperature of fermenter and vinasse to storage,
 305 ethanol composition, ethanol volume flow). The continuous design variables are given by x_D ,
 306 whereas x denotes the remaining process variables calculated by the simulator, and u
 307 represents fixed parameters not modified during the calculations. Note that x_D includes only
 308 continuous variables (*e.g.*, heat flow, pressures, temperatures, flow rates). The task to decide
 309 among different alternatives is performed by the decision makers, according to their
 310 preferences. Function accuracy is 0.001 for the normalized function against 1.0 for the cost
 311 and environmental optimization, considering the same variables tolerance between each
 312 optimization. A termination criterion that works well in practice is to stop when the pre-
 313 defined number of Pareto points is generated. Fig. 3 outlines the methodology containing the
 314 algorithm process used in mathematical programming.



315

316

Fig. 3. Algorithm of the proposed methodology.

317

318 **5. Results and discussions**

319

320 *5.1 Comparison of alternatives*

321

322 The evaporation process was successfully integrated into the distillation process by inserting
 323 the fermentation and ethanol recovery processes in Aspen Hysys, which can be seen in
 324 Appendix A. The table 2 presents the comparative study between DSI and UR. There is a
 325 significant decrease of the vinasse produced (15.59%). Decreasing the amount of this by-
 326 product means that the environmental and economic problems associated are also minimized.
 327 In addition, the production of flegma has a marginal variation and the ethanol remains
 328 constant (achieving the desired composition), which is assured by the specifications of the
 329 distillation columns during the simulation step. This study shows that, at industrial level, the
 330 replacement proposed can be implemented without any effect on the ethanol productivity.
 331 Moreover, there is a reduction of 24.32% in the quantity of energy used to cool the vinasse
 332 before storage and a lower energy consumption by the reboiler (around 83%) when compared
 333 to the heat flow of the steam used to heat the distillation column in the current configuration.

334

335 Table 2. Comparison between DSI and UR alternatives.

	DSI	UR	Variation (%)
Vinasse (kg·h ⁻¹)	1.86E+05	1.57E+05	-15.59
Flegma (kg·h ⁻¹)	3.17E+04	3.18E+04	0.32
Ethanol (kg·h ⁻¹)	1.62E+04	1.62E+04	0
Cooling energy (kJ·h ⁻¹)	3.29E+7	2.49E+7	-24.32
Reboiler energy (kJ·h ⁻¹)	0	6.55E+7	-

V1-A energy (kJ·h ⁻¹)	3.90E+8	0	-
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336

337 One of the advantages of this new configuration is related to the fact that the steam used in
 338 the reboiler returns to the process, giving rise to an additional alternative to perform the heat
 339 integration as well as reducing the operating cost of the plant when eliminating steam
 340 injection. These results are in line with the findings of Silva et al. (2017), who demonstrated
 341 that the use of reboilers over others cases (direct steam injection and distillation with
 342 mechanical vapor recompression) may contribute to the development of green sugarcane
 343 distillery processes as well as being an attractive from an economic perspective.

344

345 *5.2 Economic assessment*

346

347 Table 3. Capital and operating costs for the process alternatives

	DSI	UR	Variation (%)
<i>Capital investment costs (\$)</i>			
Heat exchangers (including reboilers)	274,749	350,636	27.62
<i>Manufacturing cost (\$/yr)</i>			
Waste treatment	1,261,237	1,170,296	-7.21
Utilities			
- Electricity	151,880	151,880	0
- Steam (LP/MP/HP)	158,863	41,050	-74.16
- Cooling water	198,915	178,829	-10.10
Operating labor	331,695	331,690	0
General expenses ^a	538,631	739,660	37.32
<i>Total</i>	2,641,221	2,613,405	-1.05

348 ^a It includes maintenance, repairs, operating supplies, depreciation, local taxes, insurances,
349 plant overhead costs, and administration costs (Turton et al., 2012).

350

351 As expected, Table 3 shows that the capital investment costs of the UR are higher than DSI
352 (more than 27%) due to the need to purchase and installation of the reboiler, which is the
353 main difference between these two configurations. Contrarily, the cost of waste treatment (the
354 most expensive cost inside the system boundary) is lower when direct steam injection is
355 replaced by the use of reboiler (7.21% lower) due to the reduction of more than 15% in the
356 vinasse production (as shown in Table 2).

357

358 Regarding the profitability analysis, with a discount rate of 12.65% and a span time of 20
359 years, the projected cash flows are worth \$153,071, which is greater than the initial cost. The
360 resulting positive NPV of the project is \$77,184 and the discounted payback period is equal
361 to 3.57 years, indicating a high profitability. These results indicate that pursuing the UR
362 alternative is the best economic option.

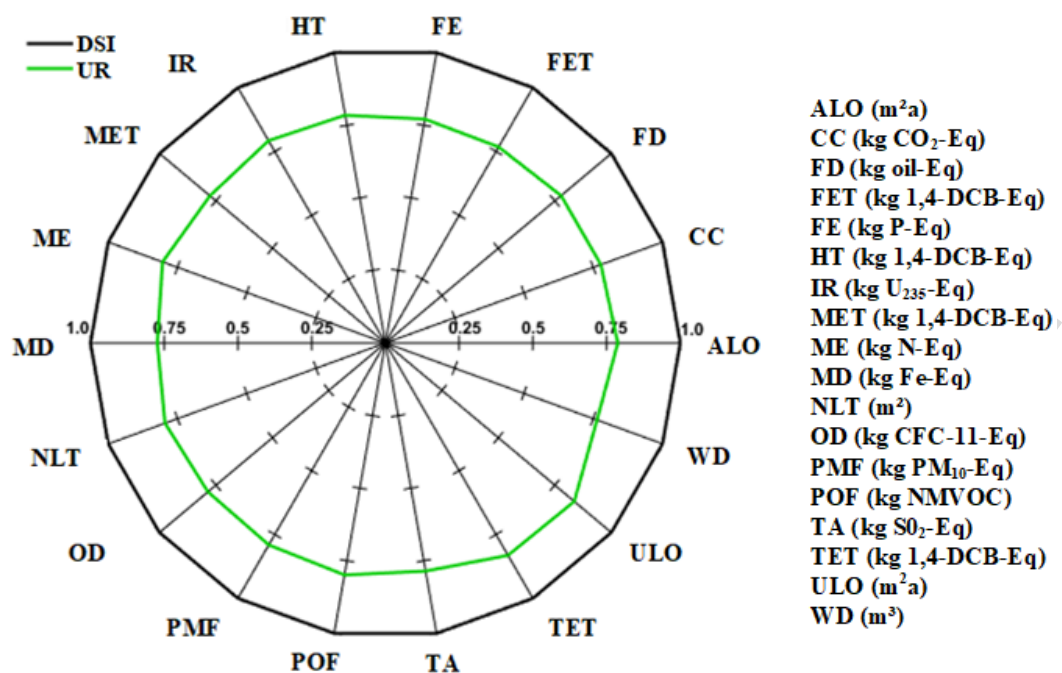
363

364 *5.3 Environmental assessment*

365

366 The impacts of each category are calculated following the ReCiPe *midpoint* methodology, the
367 values obtained are normalized by the impacts of the current configuration (Fig. 4).

368



369

370 Figure 4. Comparison of the normalized impacts for the DSI and UR process
 371 alternatives.

372

373 The UR configuration presented lower impacts in all categories when compared to the DSI
 374 and the most significant reductions are related to water depletion (reduction of 23.62%) and
 375 freshwater ecotoxicity (reduction of 23.20%), mainly caused by the reduction of the quantity
 376 of water used to cool the vinasse up to the suitable temperature (49 °C) to be stored in open
 377 ponds. Depending on the area, extracting water may cause very significant damages to
 378 ecosystems and human health. Although the distillery studied is located in the South of
 379 Brazil, 10.8% of the sugarcane crops are located in the Northeast region (CONAB, 2016),
 380 where are commonly drier areas, worsening their impacts. Besides, the reduction of
 381 freshwater ecotoxicity, regarded to the toxic effects of chemicals on an ecosystem, may avoid
 382 biodiversity loss, contributing to build a more sustainable distillery.

383

384 It is worth to highlight that emissions from vinasse storage is not considered due the lack of
 385 information on Ecoinvent database. However, a recent study (Moraes et al., 2017) assessed

386 GHG emissions in experiments simulating the vinasse management system and concluded
387 that CH₄ emission from untreated vinasse was measured from the day 7 of storage (this
388 seven-day lag phase is probably due to a low initial pH) equivalent to 43.8 kg CO_{2eq}·kg⁻¹ C-
389 vinasse during 21 days. Such result indicates that a lower amount of vinasse produced would
390 also reduce CH₄ emissions to the atmosphere in case the distillery needs to storage it for more
391 than 7 days. In the current case studied, considering a concentration of C-vinasse of 1,337.60
392 mg·L (information provided by COCAFE distillery), vinasse volume flow of 186.6 m³·h
393 (retrieved from the simulation), and a period of storage of 21 days, vinasse would emit a
394 quantity of 10.927 kg CO_{eq}·kg⁻¹ C-vinasse to the atmosphere.

395

396 All of these environmental results are related to a specific distillery in Brazil with materials
397 and energy inputs fixed, but if the same technology is used, results can be extrapolated to
398 other plants. The COCAFE distillery usually has a stable crops, which means that the input
399 parameters vary slightly. However, for many distilleries this is not the case. For these plants,
400 it is also important to include in this investigation a sensitivity analysis varying some inputs
401 parameters (*e.g.*, clarified juice mass flow, distance traveled for vinasse application) in order
402 to better fit the results.

403

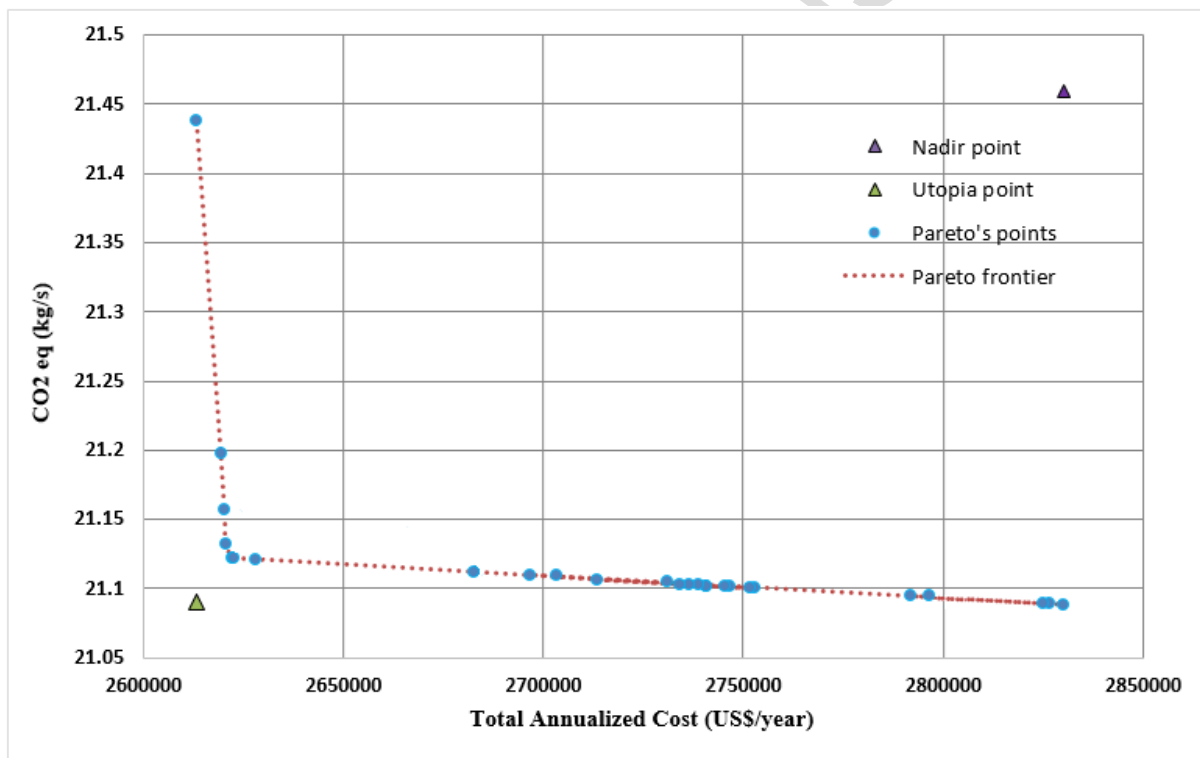
404 The application of LCA to evaluate the environmental impacts caused by vinasse does not
405 allow a complete analysis because there are uncertainties about the lixiviation and
406 volatilization of the vinasse applied to the soil. Furthermore, the information related to the
407 impacts of the vinasse application in literature are limited and does not include any
408 uncertainty parameters (Rocha et al., 2010).

409

410 *5.4 The Pareto frontier*

411

412 The individual analysis showed that low investment costs can lead to significant reduction in
 413 the environmental impacts. Finally, the multi-objective optimization is applied to the UR
 414 configuration, which presented the best results for both economic and environmental
 415 assessment. All the points are Pareto frontiers, but during the optimizations, many suboptimal
 416 points were obtained and those ones dominated were removed from the analysis. This occurs
 417 in non-linear problems when the solver is trapped in a local minimum or maximum, which is
 418 a common problem in complex models. The results of Pareto frontier are shown in Figure 5.
 419



420

421 Figure 5. Pareto set of solutions for the climate change *versus* Total Annualized Cost.

422

423 Two different parts are identified in the Pareto curves. In the first part, from the left to the
 424 right, the impact is decreased by using less electricity and slightly increasing the flegmass
 425 and vinasse volume flows. In the second part, the flegmass and vinasse volume flows are

426 virtually identical for all configurations. More electricity power and more cooling water are
 427 used to compensate the temperature and pressure modifications concerning the clarified juice
 428 and the wash water used in the absorber column. In this case, CO₂ stream purged from the
 429 process was taken into account.

430

431 From Figure 5, it can also be seen that the set of individual optimums $f^U =$
 432 $[f_1^*(x_1^*); f_2^*(x_2^*)] = [2,613,411; 21.09]$ represents the Utopia point (impossible to reach),
 433 while the set of maximum values (non-optimums) $f^N = [f_1^N(x_1^N); f_2^N(x_2^N)] =$
 434 $[2,830,242; 21.44]$ indicates the Nadir point. Thus, the optimum considered is the nearest
 435 point to the Utopia point (knee point = $[2,621,739.13; 21.13]$), which represents the feasible
 436 optimum cost and optimum environmental impact. The knee point compared to the current
 437 plant operation presented a reduction of 25.9% in CO₂_{eq} and 24.5% in the total annualized
 438 costs. The results are detailed in Table 4.

439

440 Table 4. Comparison between the current operation and the optimum results obtained.

Description	Current Plant Operation	Optimal TAC Solution	Optimal Environmental Solution
<i>Capital investment costs (US\$)</i>			
Heat exchangers (including reboilers)	274,749	350,636	350,636
<i>Manufacturing costs (US\$/year)</i>			
Waste treatment	1,401,499	1,170,297	1,179,277
Utilities			
- Electricity	151,880	151,880	151,880

- Steam (LP/MP/HP)	850,249	41,050	219,960
- Cooling water	198,915	178,829	178,829
Operating labor	331,695	331,695	331,690
Other manufacturing costs	538,631	739,660	739,660
Total Manufacturing cost	3,472,869	2,613,411	2,801,296
<i>Environmental impact</i>			
CO ₂ eq (kg/s)	28.52	21.46	21.09

441

442 **6. Conclusions**

443

444 The case study showed the use of reboilers in the distillation process, when compared
 445 to direct steam injection, presented a reduction of 15.59% in the quantity of vinasse produced
 446 with a marginal effect on ethanol flow. In this way, the environmental and economic impacts
 447 caused by vinasse are minimized, while the quality and productivity of the plant are
 448 maintained.

449 Replacing direct by indirect heating, the economic assessment presents a high
 450 profitability with a positive NPV of the project of U\$77,184 and a discounted payback period
 451 of 3.57 years. This high profitability is mainly due to reduction of the vinasse quantity.
 452 Furthermore, the environmental evaluation revealed that all the impacts of the proposed
 453 configuration (use of reboiler) are lower when compared to the direct steam injection. In this
 454 scenario, the categories terrestrial ecotoxicity and urban land occupation presented the most
 455 significant reductions (more than 14%).

456 For the improved scenario proposed, an operational ethanol distillation system using
 457 an external optimizer (Matlab) was optimized considering simultaneously the cost and the
 458 environmental impacts. The knee point of the Pareto frontier indicates that the CO₂ eq and
 459 total annualized cost might both be reduced in more than 24%.

460 In short, this work demonstrates that a validated process simulation automatically
461 integrated to a mathematical programming is a powerful tool to evaluate the performance of a
462 wide range of industrial processes. It can find the best configuration among a set of
463 alternatives as well as the viability of revamping projects. Therefore, this work must
464 contribute for future works of interest of this area.

465

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467

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471 availability to develop this research.

472

473 **Appendix A. COCAFE industrial process description and Hysys model operating with** 474 **direct steam injection.**

475

476 Here follows the description of the COCAFE process simulation and it is illustrated in
477 the Fig. A.1. All the input data were provided by the distillery, unless otherwise stated. The
478 NRTL model is selected based on Marquini et al. (2007) who compared results obtained from
479 simulations of ethanol distillation columns using different thermodynamic models and find it
480 the most suitable one.

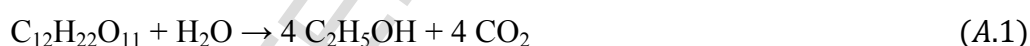
481 The sugarcane industry model is simulated from the validated evaporation process.

482 The evaporation system is made based on Foust et al. (1980) who described an evaporator as
483 a heat exchanger capable of raising the solution temperature up to the boiling point and a
484 flash to separate both phases. Using this concept, Jorge et al. (2010) successfully simulated
485 the COCAFE evaporation system using Aspen Hysys, where each of the three evaporators

486 was represented by the combination of multitubular heat exchangers and flash tanks. Thus,
487 the first combination of this simulation mimics the evaporation first effect, producing the
488 bleeding (the quantity produced is determined by the spreadsheets *Evaporation Rate 1* and
489 *Evaporation Rate 2-3*), a steam used for other operations (mainly distillation) and to provide
490 heat for the evaporation second effect. There is also a heater (*Heater1*) between the first and
491 second effect that simulates the need of medium pressure steam when the first effect energy
492 cannot provide the heat required by the second effect. The input and output of the evaporation
493 system are clarified juice and concentrated juice, which contains 13.0% w/w and 19.1% w/w
494 of sucrose, respectively.

495 The concentrated juice is cooled to 33°C and then sent to the fermentation system
496 which is composed by a fermentation reactor and an absorption column. In this work, the
497 reaction used the global stoichiometry (Eq. 1) of two reactions, one for fermentation and the
498 second one for conversion of fructose and glucose to ethanol, with a 91.0% conversion,
499 retrieved according to historical plant data.

500



501

502 As CO₂ gas leaving the fermenter carries away some ethanol, this stream is treated in
503 the absorption column, where ethanol is recovered using water. The gaseous stream leaving
504 the absorber contains negligible amount of ethanol and is vented to the atmosphere. The
505 liquid stream is recycled to the fermenter.

506 The liquid stream leaving the fermenter (*Beer*) is a dilute ethanol solution containing
507 (w/w) 7.49% of ethanol, 86.70% of water, and 5.81% of other components such as aldehyde,
508 acids, yeasts, sugars, minerals, CO₂, and SO₂. This stream is pumped to the first distillation
509 column (*A1*), exchanging heat in *HE4* and *Heater2* to reach the appropriate feed temperature.

510 The *AI* column has 26 equilibrium stages, a total condenser and is fed in stage #25. The
511 bottom product of this column is vinasse (exchanging heat in *HE4*) while *Flegma* is obtained
512 as side vapor stream (stage #22), which is a stream rich in ethanol ($\approx 30\text{-}40\%$ v/v) that enters
513 the second distillation column (*BI*) in stage #16, operated with 59 equilibrium stages and
514 total reflux. The bottom product of the second column is *Flegmass*, also a by-product but less
515 harmful than vinasse as it is almost composed by water. Finally, the ethanol is withdrawn as
516 lateral extraction (#57) of the second distillation column with $93.2 \pm 0,6\%$ w/w.

517 All the heating of the distillation columns is provided by direct steam injection, which
518 is the bleeding stream that goes through an expander (*K-100*) to adjust its pressure. In this
519 model, the exclusive heating by direct steam injection is ensured by setting the reboilers heat
520 flow of the streams *Energy2* and *Energy4* to zero, using the operation adjusts *ADJ-1* and
521 *ADJ-2*, respectively. This adaptation was successful performed by Jorge et al. (2015) who
522 developed a model of an industrial column system of ethanol distillation heated by direct
523 injection of vapor, and validated the model prediction with plant data.

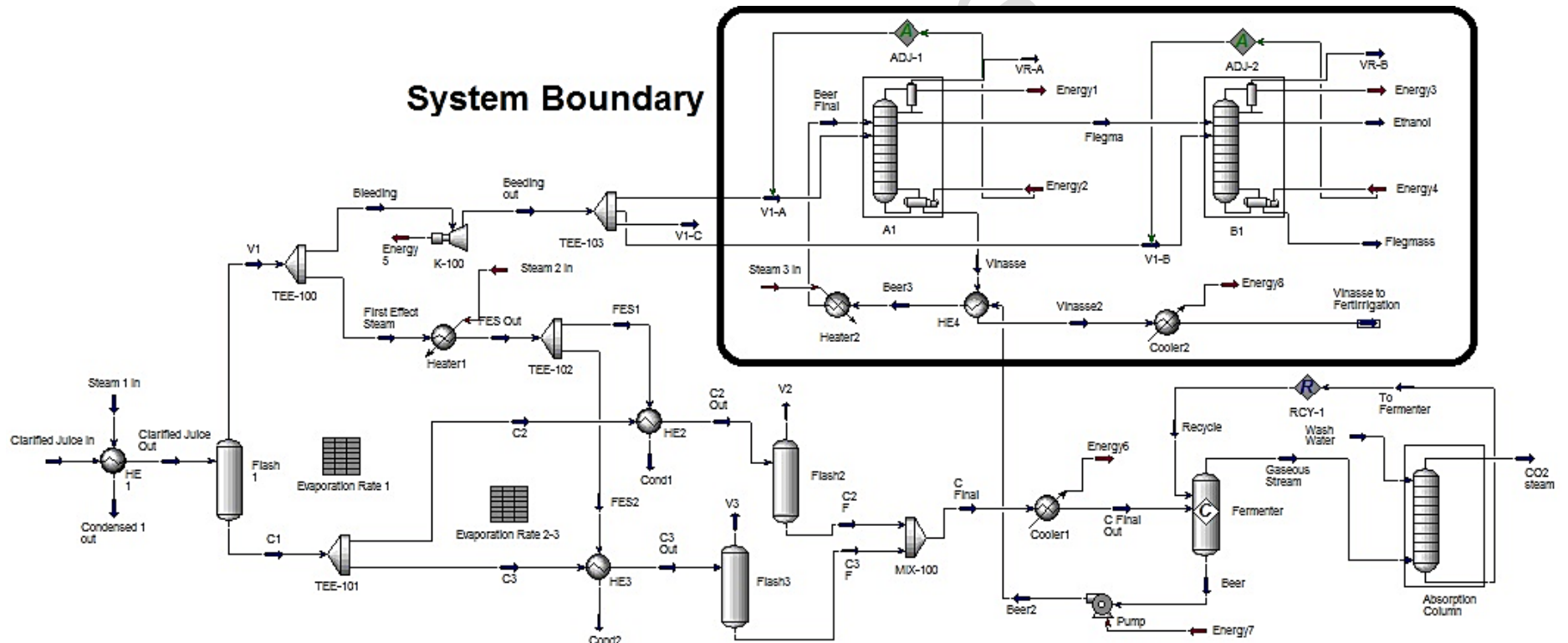
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529

530

531 Fig. A.1. COCAFE Aspen Hysys model operating with direct steam injection.

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