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Climate-energy-water nexus in Brazilian oil refineries

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Abstract

Oil refineries are major CO₂ emitters and are usually located in water-stress sites. While some CO₂ mitigation options can reduce water withdrawals, others can increase it, and still others are neutral. By simulating two parametric models, one for all Brazilian refineries, and the other locally detailing the water balance of the country's largest refinery, this study aimed to quantify the impacts of CO₂ mitigation options on the water use of oil refineries. Findings show that, at 25 and 100 US\$/tCO₂, Brazilian refineries can abate CO₂ emissions by 10% and 26%, respectively, compared to current emissions. A relevant share of this abatement derives from the implementation of carbon capture facilities in fluid catalytic cracking and hydrogen generation units. However, these CC facilities offset the co-benefits of other CO₂ mitigation options that can reduce steam and cold water requirements in refineries. In fact, for the largest Brazilian oil refinery, the implementation of all mitigation measures had almost no effect on its water balance. This means that CO₂ abatement in refineries has no significant impact on water consumption (no negative trade-off). However, this also means that the water stress in oil refineries should be dealt with with measures not directly linked to CO₂ abatement (no significant co-benefits).

Keywords: Climate-energy-water nexus; oil refineries; Brazil.

1. Introduction

Two of the UN Sustainable Development Goals (SDGs) focus on achieving physical and economic access to energy and water in quantity and quality. SDG7 aims to provide affordable, secure, sustainable and modern energy for all; furthermore, SDG6 aims to provide available and sustainable management of water and sanitation for all (UN, 2016). Energy and water are key elements closely linked to all other sectors within an economy. They also interact closely in many aspects (BIGGS et al., 2015). In this way, achieving the goal of a natural resource will influence the fulfillment of the other goal. For instance, water is needed at all stages of energy

34 production, while water management, treatment and transportation require energy. Moreover,
35 global climate change can add a significant amount of uncertainty to these complex inter-
36 relations. Changes in climate variables, such as precipitation and temperature, can affect water
37 and energy resources, increasing their vulnerabilities. Also, the strategies to tackle climate
38 change by reducing (mitigating) greenhouse-gas (GHG) emissions can affect the water-energy
39 nexus (HOWELLS et al., 2013).

40 For instance, coal-fired thermoelectric plants need water resources, mainly for cooling
41 processes. For these plants, a promising GHG mitigation option could be the installation of
42 amine-based carbon capture (CC) systems (ROCHEDO and SZKLO, 2013). However, CC
43 would also increase both water withdrawal and consumption by the thermoelectric plant by
44 more than 100%, which may intensify its vulnerability and affect the water supply to other users
45 downstream from the power plant (ZHAI and RUBIN, 2011; MERSCHMANN et al., 2012). In
46 the case of the production of liquid biofuels, the nexus goes beyond the energy conversion
47 facility, which may also be affected by CO₂ mitigation options, and mostly refers to the biomass
48 production, which usually represents a significant share of water consumption (irrigation) in
49 countries such as Brazil (IEA, 2016). Interestingly enough, the increase of biomass productivity
50 arising from irrigation is an emblematic case of the tradeoff between GHG mitigation and water.

51 At the end, given all these complex and interconnected relationships, an integrated analysis is
52 needed to evaluate the nexus between energy-water under the challenges associated with climate
53 change (HOWELLS et al., 2013). In addition, each energy sector needs a proper analysis to
54 quantify this nexus. For this study, this analysis is performed at both country and local level. On
55 one hand, the country level provides the basic answer for the primary research question of this
56 study, which is: do CO₂ mitigation options affect the water consumption of an oil refinery
57 system (or even: what could the nexus be between the carbon mitigation cost curve and the
58 water consumption in refineries)? On the other hand, the detailed local level analysis, whose
59 focus is on a specific oil refinery, allows the answering of the secondary question of this study,
60 which is: do the impacts of climate mitigation options on water consumption affect the water
61 supply-demand balance of an oil refinery? Only local level analyses can solve this secondary
62 question, since it requires the proper evaluation of water sources (water supply) and sinks (water
63 users).

64 In fact, oil refining is an energy-intensive activity, whose greenhouse gas (GHG) emissions are
65 closely related to the combustion and chemical conversion of fossil fuels. The fuel combustion
66 in oil refineries is related to the generation of direct heat, process steam and even electricity, all
67 in stationary sources. The refineries' technological schemes are complex (GOMES et al., 2009;
68 COELHO and SZKLO, 2015), depending on the characteristics of the feedstocks, the units'

69 capacities, the production profile of the oil products (quantities and specifications), and the
 70 choice of technologies to be used (CASTELO BRANCO et al., 2011). For instance, refineries
 71 that process heavy crude oils to output light products present process schemes that use more
 72 final energy, and in turn emit more GHG (EPA, 2010). In addition, the more stringent the oil
 73 derivative specifications, the greater the energy and water consumption of the refining process,
 74 due to the need of severe hydro-treatment units, which use the hydrogen produced in units
 75 emitting CO₂ from the steam reforming of light hydrocarbons (SZKLO and SCHAEFFER,
 76 2007; CONCAWE, 2012; SUN et al., 2018). In 2012, oil refineries accounted for 2.7% of US,
 77 3.2% of European Union and 2.0% of Brazil CO₂ emissions (MCTI, 2013; PETROBRAS, 2013;
 78 EPA, 2014).

79 Nevertheless, the vast majority of the research associated with the nexus between energy and
 80 climate in oil refineries has focused on the trade-off between fuel specifications and CO₂
 81 emissions (CONCAWE, 2000; CHAN, 2006; SZKLO AND SCHAEFFER, 2007;
 82 JOHANSSON et al., 2012; CONCAWE, 2012). In the case of the nexus between energy and
 83 water, there are some studies on the relationship between water consumption and energy use in
 84 oil refineries (HIGHTOWER and PIERCE, 2008; IPIECA, 2010; HWANG and MOORE, 2011;
 85 PAN et al., 2012; MUGHEES and AL-AHMAD, 2014; SUN et al., 2018). Previous research
 86 has also focused on the implementation of CO₂ capture in oil refineries and its abatement cost,
 87 as ROCHEDO et al. (2016) have done, but it has failed to explore the water nexus with CO₂
 88 mitigation options in oil refineries.

89 At the end, few attempts have been made to quantify the relationship between climate (CO₂
 90 emission mitigation) and water-energy use in oil refineries. **Table 1** provides a brief summary
 91 of the opportunities for CO₂ abatement measures in oil refineries' processing units, and their
 92 likely impact on water consumption. It highlights the signs of the impacts that are quantified
 93 later in this study (positive and negative signs) through the use of simulation tools for all
 94 Brazilian refineries and for a specific refinery in detail.

95 **Table 1 – Qualitative Impacts on Water Consumption of CO₂ Mitigation Options in Oil Refineries**

Process Unit	Heat Integration	Reduce Boiler Blowdown/Water Treatment	Improved Maintenance/Steam Lines & Traps	Reduce Stand-by Boiler Requirements	Increase Steam Line Insulation	Recover Blowdown Steam	CC
ADU	-	-	-	-	-	-	-
VDU	-	-	-	-	-	-	-
CRU	-	-	-	-	-	-	-
HDT	-	-	-	-	-	-	-

RFCC	-	-		
FCC	-	-		+
DCU	-	-	-	
HGU				+

Note: The positive sign means that the measure has a positive impact on water consumption, ie it helps to reduce this consumption. On the other hand, the negative sign has a negative impact, indicating an increase in water consumption with the application of the measure.

ADU – atmospheric distillation unit; VDU – vacuum distillation unit; CRU – catalytic reforming unit; HDT – hydrotreatment unit; RFCC – resid fluid catalytic cracking; FCC – fluid catalytic cracking; DCU – delayed coking unit; HGU – hydrogen generation unit; CC: CO₂ capture

Source: WORREL and GALITSKY (2003); WORREL and GALITSKY (2005); CONCAWE (2008); BERGH, 2012; MORROW III et al. (2013)

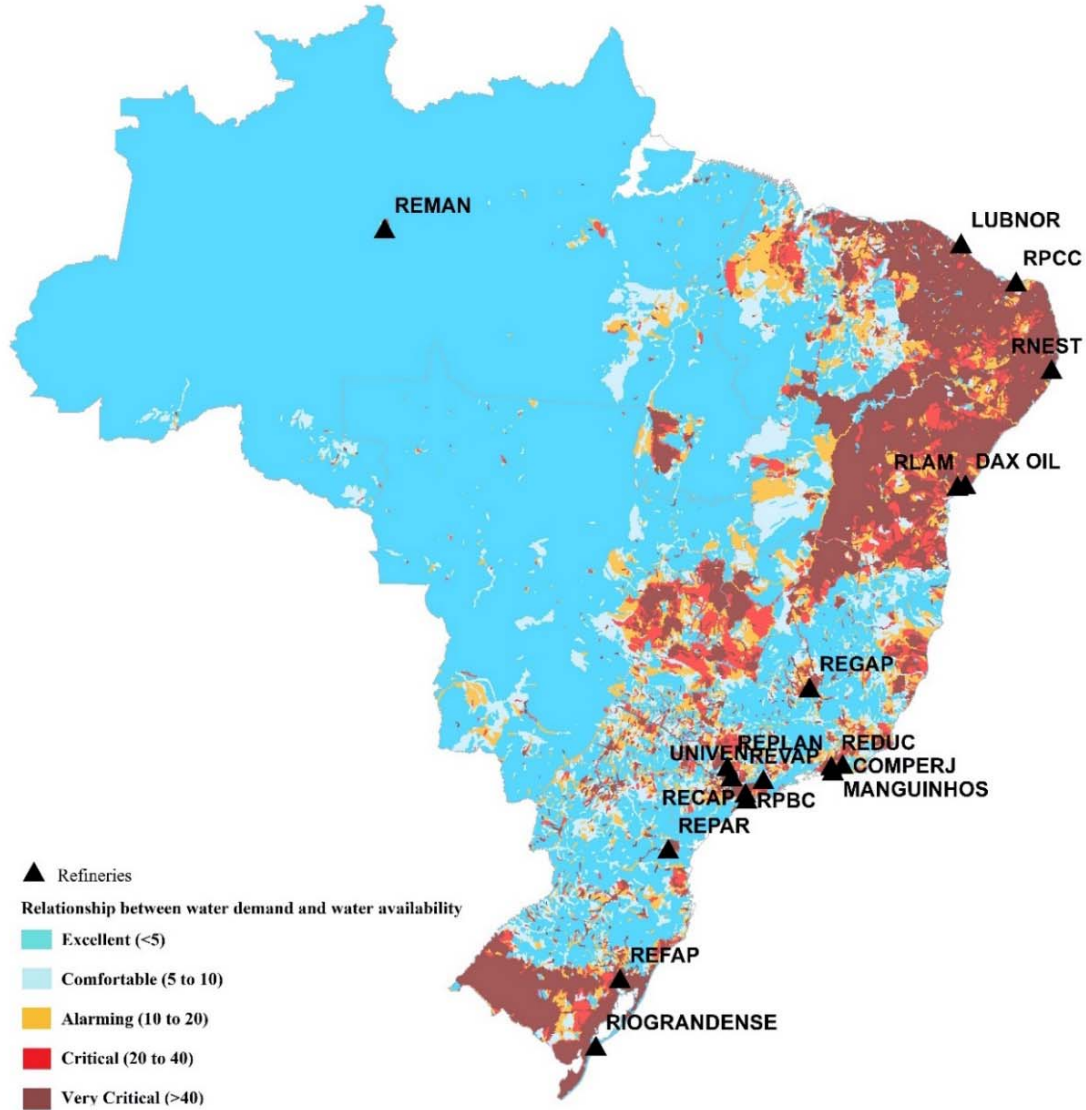
Regarding water use, oil refining requires considerable amounts of water, which vary significantly between refineries, depending on the process configuration (WU and CHIU, 2011; SUN et al., 2018), the petroleum specification (e.g., density, sulphur content, total acid number) (SUN et al., 2018), and the products’ requirements. Within this context, in Brazilian refineries, water requirements deserve attention due to the processing of heavy-to-medium crude oils, as well as to the increasingly stringent specifications of fuels that require the implementation of hydrotreatment units, associated with the water-intensive steam reforming process (CASTELO BRANCO et al., 2010; SZKLO, ULLER and BONFÁ, 2012; BARROS and SZKLO, 2015)¹.

In addition, in Brazil, water availability is not evenly distributed. While the northern region holds more than 80% of all water availability, the basins located in large urban centers, in the Brazilian southeast, for example, are currently facing low water availability coupled with high withdrawals. As shown in **Figure 1**, most Brazilian refineries are already dealing with water stress, measured in relation to the level of water criticality of watersheds. This index measures the ratio between water withdrawals for consumptive uses (irrigation, water supply, urban and industrial) and the water availability of each sub-basin expressed through the value of average flow with permanence of 95%. In fact, REPLAN, REVAP, RLAM and REDUC, which account

¹In 2018, the Brazilian oil refining industry consisted of 17 refineries in operation, with a total installed nominal capacity of 2.2 Mbb/day (ANP, 2018). Most Brazilian refineries were built before the 1980s with the objective of meeting the demand for gasoline and fuel oil in major urban centers (also close to Brazil’s coast). However, due to the increasing diesel demand after the 1980s (BORBA et al., 2017), as well as the ramp up of medium-to-heavy crude oil production in Brazilian offshore basins in the 1980s and 1990s (HALLACK et al., 2017), the refining schemes of existing refineries were altered to convert the heaviest fractions of crude into medium cuts – e.g., by adding delayed coking units and severe hydrotreatment processes (which remove nitrogen compounds, high sulfur compounds and aromatic rings) (SZKLO and SCHAEFFER, 2007; SZKLO et al., 2012).

121 for 54% of Brazil's refining capacity, are located in areas classified as having critical water
122 availability.

123



124

125

Figure 1 - Refineries locations and water criticality indicator of sub-basins in Brazil

126

Source: Based on ANA (2017)

127

128 To sum up, oil refineries are major CO₂ emitters and are usually located in sites with already
129 critical availability supply of water. This is the case for Brazil, but it can be seen worldwide
130 (OIL and GAS JOURNAL, 2018). Some CO₂ emission mitigation measures can positively or
131 negatively influence both withdrawal and water consumption at refineries. Within this context,
132 this study aims to quantify the extent to which these measures can impact refineries' water use.
133 First, by developing an energy, CO₂, H₂, water balance simulator for Brazilian oil refineries, and

134 applying it to different scenarios of CO₂ mitigation, this study evaluates the CO₂ mitigation-
135 energy-water nexus at the country level. Then, this study analyzes the water supply of the
136 hydrographic basin in which the largest Brazilian refinery, REPLAN, is located and how it
137 behaves over time. This detailed analysis, at a local level, not only quantifies the water
138 withdrawal impacts of CO₂ mitigation options, but also identifies whether or not these impacts
139 could be overcome by the current water supply of this specific refinery.

140 The next section presents the methodology used to carry out the analysis, as well as a brief
141 description of the simulation tools applied. Section 3 discusses the results obtained. Lastly, the
142 final remarks of the study, highlighting also its limitations, are presented.

143

144 **2. Methods**

145 **2.1. Methodological Procedure**

146

147 The methodological procedure applied by this study consisted of the following steps. The first
148 step is the definition of GHG mitigation measures in oil refineries, according to the scientific
149 literature and the experience of the authors regarding Brazil's oil refineries². Then, the study
150 simulates the baseline case for estimating the scenario without CO₂ mitigation, and simulates
151 the impacts of introducing CO₂ price scenarios into oil refineries, in terms of CO₂ emissions,
152 final energy use and water consumption. This provides the carbon mitigation cost curve, and
153 also helps to identify (quantify) the impacts of GHG mitigation options on the water
154 consumption for all Brazilian refineries. However, this step is not able to detail the water supply
155 balance at a local level. Therefore, using the mitigation cost curve for Brazilian refineries
156 (mentioned above), the proposed procedure includes a last step for detailing the case of the
157 largest Brazilian oil refinery, REPLAN. This step not only quantifies the water consumption
158 impacts of CO₂ mitigation options, but also identifies whether these impacts could be overcome
159 by the current water supply of REPLAN. In summary, the steps include:

- 160 1. To assess the CO₂ mitigation options focusing on the saving potential for the
161 consumption of fuels, steam, electricity and H₂.
- 162 2. To estimate the energy and mass balances for a baseline case, including final energy
163 consumption, CO₂ emissions and water requirements. This case does not consider the
164 application of CO₂ emission mitigation options (e.g., fuel switch, fuel saving and carbon
165 capture). This study applies an energy and mass balance simulator – the so-called

² See, for instance, GUEDES (2015).

166 “CAESAR – Carbon and Energy Strategy for Refineries” tool, which is briefly
167 described here, and better described in the Supplementary Material.

168 3. To run CAESAR with CO₂ emission prices³ of 25, 50, 100 and 200 US\$/tCO₂. In this
169 case, the CO₂ emissions mitigation options are selected according to their marginal
170 abatement cost – that is, technological options with costs lower than or equal to the
171 exogenously established CO₂ price are automatically selected by the simulation tool,
172 allowing the construction of a CO₂ average abatement cost curve for all Brazilian oil
173 refineries. The Supplementary Material provides the basic equation associated with the
174 estimation of the abatement cost.

175 4. To develop a case study for REPLAN, the largest Brazilian refinery in terms of
176 processing capacity, thus quantifying the water stress in detail, or locally. This allows
177 investigating whether mitigation measures that were selected in step 3 can be adopted in
178 cases where a greater water withdrawal is required. This case study is performed using
179 the software tool Water Evaluation and Planning – WEAP (see section 2.2. and
180 Supplementary Material).

181

182 **2.2. CAESAR tool – Carbon and Energy Strategy Analysis for** 183 **Refineries**

184

185 The tool used for evaluating all Brazilian refineries, without detailing the water supply-demand
186 balance at a local level, is the simulator CAESAR – Carbon and Energy Strategy Analysis for
187 Refineries. It was originally developed by TOLMASQUIM and SZKLO (2000), later being
188 used by the Brazilian Government in its Long-Term Energy Plan 2030 (EPE, 2007). Finally, it
189 was updated by GUEDES (2015) and by VÁSQUEZ-ARROYO (2018) and MAGALAR (2018)
190 for incorporating water balances.

191 The simulation is performed within Excel (visual basic), and relies on refining schemes,
192 including the following units’ energy and mass balances: atmospheric distillation, vacuum
193 distillation, alkylation, atmospheric residue delayed coking, vacuum residue delayed coking,
194 propane desasphalter, catalytic reformer, fluid catalytic cracker, hydrocracker, residue fluid
195 catalytic cracker, hydrotreaters (naphtha, diesel, kerosene and instable products),
196 hydrotreatment of finished gasoline, lube unit, and hydrogen generation unit. The processing
197 units’ capacities are determined, as well as the processed feedstocks, specific utilities
198 consumption (steam, fuel and hydrogen) and specific water consumption. The outputs of the
199 tool consist of the final energy consumption, CO₂ emissions, oil product output, and refineries’
200 water consumption and withdrawal.

³ They represent an established price to be paid for a given amount of CO₂ emitted.

201 Therefore, CAESAR is a bottom-up model mostly based on the simulation of the mass (water,
202 H₂) and energy balances of Brazilian oil refineries. It has an additional feature for optimizing
203 the energy consumption aimed at minimizing the cost of operation of oil refineries. The model
204 also includes a list of CO₂ mitigation options, which are detailed according to the processing
205 units in which they can be implemented, their potential for saving fuel and/or electricity, their
206 investment, operation and maintenance costs, and their penetration rates. In total, 204 options of
207 technologies are available in CAESAR (see Supplementary Material for detailed data).

208 For the carbon price scenarios, CO₂ emission prices were exogenously introduced into the
209 simulator, which also affected the optimization problem that finds the least-cost fuel mix of
210 refineries. Prices of 25, 50, 100 and 200 US\$/tCO₂ were considered, thus building five different
211 scenarios for the current configuration of Brazilian oil refineries. As 204 CO₂ emission
212 mitigation options are available in the simulator, their abatement costs range from negative
213 values, which represent “non-regret” measures, to values above 100 US\$/tCO₂. The highest cost
214 measures would hardly come into effect without economic incentives or more robust
215 technological learning.

216 Therefore, depending on the CO₂ emission price applied, the tool automatically selects different
217 GHG mitigation options from the set list available, affecting the final energy use, CO₂ emissions
218 and water consumption. The Supplementary Material includes the basic data of the model and a
219 description of how to run it.

220

221 **2.3. WEAP**

222

223 Before using the tool WEAP, REPLAN mass and energy balances were simulated in the above-
224 described tool, CAESAR. This aimed to quantify the impacts of CO₂ emission mitigation
225 options on the water required by REPLAN. Then, the results of water withdrawals obtained in
226 CAESAR were inserted as input into the WEAP tool. This is a tool for integrated water
227 resources management (IWRM) developed by the Stockholm Environmental Institute (SEI).
228 WEAP integrates physical hydrological processes with water withdrawal management and
229 infrastructure, as well as environmental and economic aspects of water planning. Its simulations
230 are based on scenarios that can be analyzed according to different trends in hydrology, water use
231 and demand, demography, technology, operating rules and water management policies
232 (SIEBER and PURKEY, 2015).

233 The WEAP analysis consists of, firstly, configuring the time horizon, catchment areas, system
234 components and configuration of the problem to be evaluated. Then, the model is used to

235 simulate alternative scenarios to assess the impact of different water supply and demand
236 management options, as well as evaluate the water availability within a region of study.

237 The model simulates the use of water in hydrological basins by using a linear programming
238 algorithm, which aims to maximize the water delivered to demand sites, according to a set of
239 priorities defined by the user. When water is limited, the algorithm is formulated to
240 progressively constrain water allocation to the lowest priority demand sites. More details of the
241 model can be found in SIEBER and PURKEY, 2015. See the Supplementary Material for
242 further details on how WEAP is calibrated and used by this study.

243

244 **2.4. Input Data**

245

246 **2.4.1. Brazilian Case Study in CAESAR**

247

248 The analysis performed by this study was based on the current Brazilian oil refinery system,
249 thus, no greenfield refinery was constructed in the simulation. The mass and energy balances
250 rely on the breakdown in processing units, which have specific characteristics. The capacity of
251 these units is shown in **Table 2**. The average utilization factor of the atmospheric distillation
252 unit was set as 70%, following MME (2018).

253

254

Table 2 - Brazilian Process Unit Capacities as of December 2017

Unit	Capacity (barrels/d)
ADU	2,138,000
VDU	804,740
FCC	378,729
RFCC	123,158
ALK	6,290
DCU	115,319
CRU	2,386
HDS G	3,054
HDT N	10,528
HDT Q	28,125
HDT D	200,041
HDT I	11,698
LUB	20,009
HGU	126

255

256

257

258

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ADU – atmospheric distillation unit; VDU – vacuum distillation unit; ; FCC – fluid catalytic cracking; RFCC – resid
fluid catalytic cracking; ALK – alkylation unit; DCU – delayed coking unit; CRU – catalytic reforming unit; HDS G– gasoline
hydrodesulphurization unit; HDT N – naphtha hydrotreatment unit; HDT Q – kerosene hydrotreatment unit; HDT D – diesel
hydrotreatment unit; HDT I – severe hydrotreatment unit; LUB – lubricants unit; HGU – hydrogen generation unit (in this case, the
capacity is given in MMcfd)

262 **Table 3** shows the estimates for Brazilian refineries' typical utility consumption (negative
 263 values mean a net production of the utility by the unit). Although there are variations in the
 264 specific energy consumption of utilities for the same unit, depending on the supplier of the
 265 technology, local characteristics or even different design considerations, the values adopted in
 266 CAESAR seek to represent a typical Brazilian unit.

Table 3 - Process Units' Utilities Specific Energy Consumption

Unit	HP Steam	MP Steam	LP Steam	Electricity	Fuel	Coke	H ₂ Consumption	H ₂ Production	BFW	CW
	kg/bbl	kg/bbl	kg/bbl	kWh/bbl	MJ/bbl	MJ/bbl	m ³ /bbl	m ³ /bbl	m ³ /bbl	m ³ /bbl
ADU	0.00	11.00	0.00	0.60	127.00	0.00	0.00	0.00	0.02	0.35
VDU	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.35
FCC	-16.00	20.00	-3.60	8.80	0.00	368.00	0.00	0.00	0.07	1.00
RFC C	-18.00	0.00	0.00	1.00	0.00	368.00	0.00	0.00	0.07	1.00
ALQ	0.00	90.00	0.00	9.00	0.00	0.00	0.00	0.00	0.05	7.00
CRU	-15.60	0.00	0.00	10.00	382.00	0.00	-48.00	0.00	0.02	1.74
DCU	0.00	-18.40	0.00	3.60	126.00	0.00	0.00	0.00	0.06	2.03
HDS G	3.00	0.00	0.00	2.00	105.00	0.00	4.00	0.00	0.04	0.96
HDT N	3.00	0.00	0.00	2.00	105.00	0.00	7.00	0.00	0.01	0.19
HDT Q	4.00	0.00	0.00	3.00	158.00	0.00	7.00	0.00	0.18	0.49
HDT D	4.00	0.00	0.00	3.00	158.00	0.00	7.00	0.00	0.04	0.73
HDT I	5.00	0.00	0.00	6.00	211.00	0.00	17.00	0.00	0.05	0.71
LUB	0.00	1.60	5.60	1.60	135.00	0.00	0.00	0.00	0.05	1.00
HGU	0.00	0.00	0.00	0.00	2.55	0.00	0.00	0.16	0.00	0.00

269 HP – high pressure; MP – medium pressure; LP – low pressure; BFW – boiler feed water; CW – cooling
 270 water

271 Source: Based on HYDROCARBON PROCESSING (2008); MEYERS (2004); GARY AND
 272 HANDWERK (2001); STANISLAUS et al. (2010)

274 For Brazilian oil refineries, as of 2017, coefficients of water withdrawals per process unit were
 275 determined, as indicated in **Table 4**. The coefficients consist of low-pressure steam (LP Steam),
 276 medium-pressure steam (MP Steam) and high-pressure steam (HP Steam), related to the process
 277 units. The water balance also includes the water consumed in the cooling system (CW – cooling
 278 water) and the volume of demineralized water used in the boiler (BFW – boiler feed water) per
 279 barrel of oil processed. **Figure 2** shows the basic water balance applied in the simulation tool.

280

281

Table 4 - Water Use Coefficients per Process Unit

	CW (m ³ /bbl)	BFW (m ³ /bbl)	LP Steam (kg/bbl)	MP Steam (kg/bbl)	HP Steam (kg/bbl)
ADU	0.3	0.02	-	11.0	-
VDU	0.3	0.05	-	-	-
FCC	1.0	0.07	3.6	20.0	16.0
RFCC	1.0	0.07	-	-	18.0
ALQ	7.0	0.05	-	90.0	-
CRU	1.7	0.02	-	-	15.6
DCU	2.0	0.06	-	18.4	-
HDS G	1.0	0.04	-	-	3.0
HDT N	0.2	0.01	-	-	3.0
HDT Q	0.5	0.18	-	-	4.0
HDT D	0.7	0.04	-	-	4.0
HDT I	0.7	0.05	-	-	5.0
LUB	1.0	0.05	-	-	-
HGU	-	-	-	-	-

282

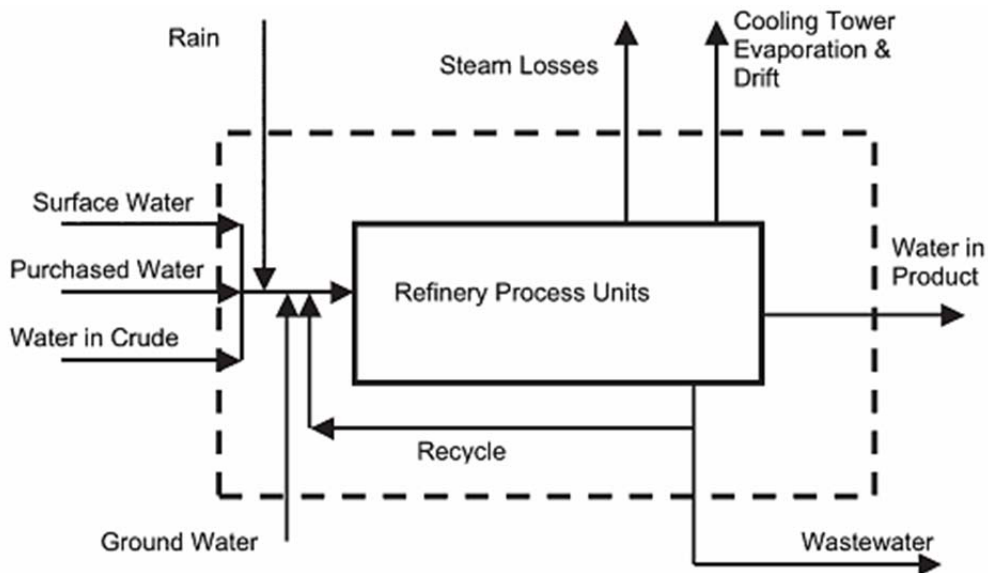
HP – high pressure; MP – medium pressure; LP – low pressure; BFW – boiler feed water; CW – cooling
283 water

283

284

Source: VÁSQUEZ ARROYO et al. (2016)

285



286

287

Figure 2 - Water balance in CAESAR

288

Source: Based on IPIECA (2010)

289

290 After obtaining the steam demand, CW and BFW, parameters were adopted to estimate the
291 water consumed by the refinery, based on ANZE (2013). They are composed of the make-up
292 water used in the cooling towers, the make-up water for the boilers and the water used by the
293 processes (water incorporated into products, for instance, in the production of H₂, because of
294 steam reforming and water gas shift, during chemical reactions). A value of 1.7% was
295 considered for the cooling system's total circulating water, according to typical Brazilian oil
296 refineries' concentration ratios (MAGALAR, 2018). For the boiler water make-up, a value of
297 49.7% was applied to the sum of the amount of water used in the boilers (BFW) and the total
298 amount of steam consumed in process units. Steam consumed is defined as lost steam that did
299 not return as condensate. For this, a value of 33% of all generated steam was used (VÁSQUEZ
300 ARROYO et al., 2016). Equation (1) summarizes these assumptions and the water balance.

301

$$302 \quad Demand = (0.017 \times \sum_i CW_i) + \{0.497 \times \sum_i BFW_i + [0.33 \times \sum_i Steam_i]\} \quad (1)$$

303

304 Where "CW_i" represents the cooling system's circulating water of each process unit "i";
305 "BFW_i" is the amount of water used in boilers of each process unit "i"; "Steam_i" is steam
306 consumed in each process unit "i".

307

308 **2.4.2. REPLAN Case Study in WEAP**

309

310 REPLAN is the largest Brazilian refinery in terms of processing capacity (66 thousand m³/day)
311 (ANP, 2018). This refinery is located in Paulínia in the state of São Paulo and is placed in the
312 Piracicaba, Capivari and Jundiá River Basin (PCJ), which is classified as "critical" in relation
313 to water availability (MAGALAR, 2018).

314 In this study, the water availability of Jaguari basin was calculated by simulating a water
315 balance between the inflows and outflows of its drainage area over time. The Jaguari River
316 basin was chosen due to the catchment point of REPLAN being located in this river. In addition,
317 the basin of the Camanduacaia, Ribeirão do Pinhal rivers was integrated into the case study
318 because these rivers are tributaries of the Jaguari River.

319 The water balance method chosen by this study was the simplified coefficient Method - Rainfall
320 Runoff, in which water requirements are calculated based on evapotranspiration and
321 precipitation data. Twenty-six rainfall stations were evaluated within the three catchment areas:
322 Jaguari River catchment and its tributary rivers, Camanduacaia and Pinhal. The data loaded after

323 treatment of the missing data and outliers was the monthly average rainfall. In order to use the
324 mean value of evapotranspiration for each catchment area, the monthly average of all
325 municipalities in each area was calculated. For more details of data, see Supplementary
326 Material.

327 The water outputs considered in this study are the projected demands for public supply,
328 industry, irrigation and for animal husbandry. These demands were identified and projected to
329 the year 2040 to assess the extent to which water availability changes as a function of the
330 multiple uses of water within the PCJ basin and whether the REPLAN could be impacted.

331 The demand for water for urban supply was calculated using a coefficient of water demand per
332 inhabitant per day that was adjusted to account for the water losses in distribution. The same
333 coefficient was used for the projection of water demand for future public supply. The method
334 used for the estimation of the population of each city is described in the Supplementary
335 Material.

336 Water consumption for animal husbandry was calculated from data on the number of animals
337 per city and then calculated the product of the effective number of herds by a per capita
338 coefficient of daily water consumption known as equivalent cattle for water demand. In order to
339 estimate the industrial demand, the volume of water granted by industry in the water agency
340 was consulted.

341 The demand for irrigation is calculated by multiplying the area under cultivation by the
342 difference between the water requirement of the crop and the precipitation occurring over the
343 cultivated area. For this, it is necessary to know the water demand of each crop, which is
344 calculated from the reference evapotranspiration and crop coefficient.

345 After all climatic parameters, data on land use and water demands are inserted into the model,
346 the observed values of the fluvioimetric stations are compared with the flow data modeled by
347 WEAP. From the observed and simulated flow data, two calibration indices are calculated, the
348 Nash-Sutcliffe efficiency index and the BIAS index.

349 To evaluate the water availability of the REPLAN catchment area, a minimum ecological flow
350 was defined. The minimum flows most commonly used in Brazil are $Q_{7,10}$ ⁴ or Q_{95} ⁵, depending
351 on the state where the drainage area is located. According to the water resources committee of
352 the PCJ (CBH-PCJ, 2000), areas considered critical are those in which the total water demand
353 exceeds 50% of the minimum availability $Q_{7,10}$. In addition, the water resources policy in the
354 state of Sao Paulo determines that the volume of water withdrawal in the industrial sector

⁴ Lowest flow on seven consecutive days for 10-year return period.

⁵ Flow with 95% of permanence over a period.

355 should be reduced if the flow of the Jaguari River reaches the minimum flow established in
356 specific gauge stations. Therefore, in the water balance simulation done by this study, the
357 analysis tried to find out if periods of restriction of water for REPLAN could happen.

358 **3. Results**

359

360 **3.1. Baseline Scenario for all Brazilian Refineries**

361

362 The total consumption of utilities and fuels in existing Brazilian refineries is shown in **Table 5**.
363 Negative values indicate exports or utility surpluses, while positive values indicate consumption
364 of utilities.

365

366

Table 5 - Utilities Consumption

HP Steam (kt/year)	-752,5
MP Steam (kt/year)	7,340.4
LP Steam (kt/year)	-375.9
Electricity (GWh/year)	12,162.7
Fuel (TJ/year)	284,018.2
Coke (TJ/year)	58,952.6
H₂ (M Nm³/year)	6,116.5

367

HP – high pressure; MP – medium pressure; LP – low pressure

368

369 From the utilities consumption, it was possible to determine the fuel consumption. The refinery
370 fuels include natural gas, refinery gas, fuel oil, naphtha and petcoke. Electricity purchased from
371 the grid was also accounted for, either from those refineries that do not have cogeneration or
372 from the excess demand in relation to the capacity of cogeneration units. Natural gas is used for
373 producing hydrogen in HGUs, electricity in cogeneration units, and steam in boilers and direct
374 heating in process units. Refinery gas and fuel oil were accounted for direct heating in process
375 units. In general, leftover refinery gas was directed toward flare emissions accounting.
376 Furthermore, a 100% flare combustion efficiency was assumed to be conservative on the GHG
377 emission estimates. Finally, the consumption of petcoke was accounted for in FCC and RFCC
378 units. **Table 6** shows the estimation of the final energy consumption for the existing Brazilian
379 refineries.

380

381

Table 6 - Final Energy Consumption - Baseline (PJ/year)

Natural Gas	367.8
-------------	-------

Refinery Gas	84.4
Fuel oil	85.4
Coke	59.0
TOTAL	596.6
Grid Electricity (GWh/year)	7,252.7

382

383 As such, the water requirement of the existing Brazilian refineries is detailed in **Table 7**. The
384 water intensity of 108.2 m³/bbl is compatible with the figures found in VANELLI (2004) for
385 REVAP – Refinaria Henrique Lage; PETROBRAS (2005) and NOGUEIRA (2007) for
386 REPLAN – Refinaria de Paulínia; SCHOR (2006) for REDUC – Refinaria Duque de Caixas;
387 and CETESB (2011) for RPBC – Refinaria Presidente Bernardes.

388

389

Table 7 - Water Requirements - Baseline

BFW (t/h)	8,809.2
CW (t/h)	118,486.2
Steam (t/h)	3,720.4
Condensed Steam (t/h)	2,492.7
BFW spent (t/h)	10,036.9
BFW Make-up (%)	49.7
BFW Make-up (t/h)	4,988.4
CW Make-up (%)	1.7
CW Make-up (t/h)	2,014.3
Consumption (t/h)	1,610.5
Withdrawal (t/h)	7,002.6
Consumption (m ³ /bbl)	24.9
Withdrawal (m ³ /bbl)	108.2
Consumption (km ³ /year)	14107.9
Withdrawal (km ³ /year)	61351.7

390

BFW – Boiler feed water; CW – Cooling water

391

392 It was also possible to estimate the CO₂ emissions of Brazilian refineries as of 2017, through the
393 multiplication of the emission factors reported by IPCC (2006) of the respective fuels used by
394 Brazilian refineries (**Table 8**). For electricity's CO₂ emissions, the average Brazilian grid
395 emission factor for 2017 was considered, equal to 92.7 tCO₂/GWh (MCTIC, 2018).

396

397

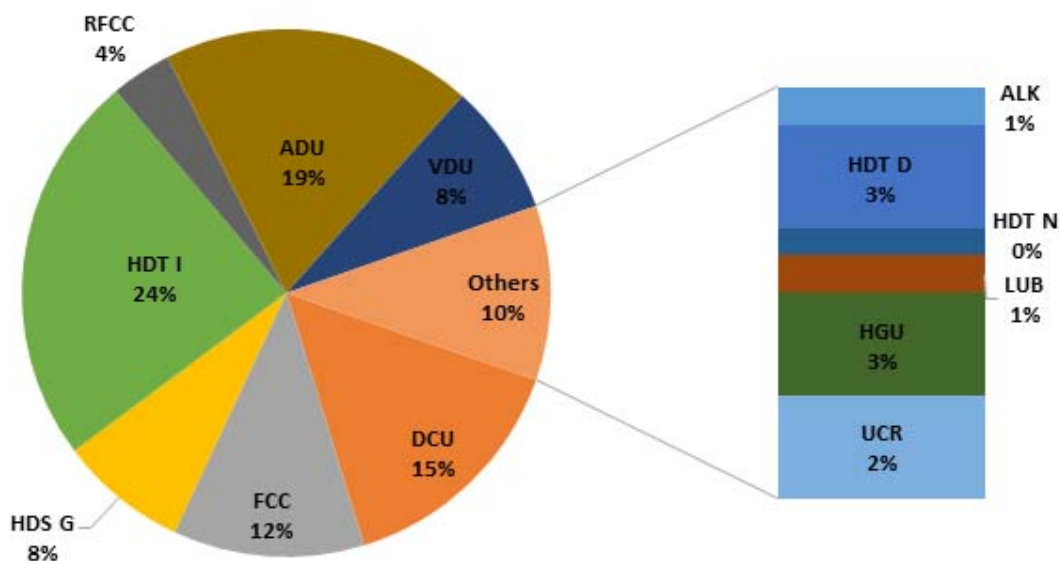
Table 8 - CO₂ Emissions (MtCO₂/year) - Baseline

Natural Gas	20.6
Refinery Gas	4.9
Fuel Oil	6.6
Coke	5.7
Grid Electricity	0.4

398

399 By dividing the total emissions by the processed feed, this study estimated an emission intensity
 400 of 0.4 tCO₂/t oil, which is compatible with the 2012 data presented by the Brazilian oil company
 401 that owns most of the country's refineries (PETROBRAS, 2013)⁶. Just for comparison,
 402 worldwide several works in the literature present CO₂ emission intensities of oil refineries
 403 hovering between 0.1 and 0.4 tCO₂/t of oil processed, with an average of 0.22 (CONCAWE,
 404 2008; IEAGHG, 2008; STRAELEN et al., 2010; DNV, 2010). For example, the US has an
 405 average emission of 0.33 tCO₂/t of processed oil, while the European Union has an average
 406 value of 0.27 (EPA, 2014).

407 Finally, concerning the relationship between CO₂ emissions and water withdrawals, the
 408 estimative for the baseline scenario is 0.62 tCO₂/m³. **Figure 3** and **Figure 4** present, for this
 409 scenario, the most representative units in terms of water consumption and CO₂ emissions,
 410 respectively.



411

⁶ Equal to 0.45 tCO₂/ t of oil processed in 2012. Of course, this intensity may vary slightly among years given the focus of the ADU campaign (in our study we focused on diesel), the possible maintenance of downstream units, which can affect the utilization factor of oil refineries (we used the ADU average utilization factor of 2017, equal to 70%), and the crudes processed in the refineries. In our study, we have considered the ramp-up of a lighter and sweeter feed that has been made available in Brazil in the last five years, from pre-salt fields. That is why we run the model with 4% of the feed from paraffinic oils from Saudi Arabia; 2% from ultra-light African crudes; 32% from Brazilian heavy crudes, and the remaining 62% from medium-to-slightly light Brazilian crudes, mostly from pre-salt fields. Therefore, the feedstock blend has become lighter than it was in 2012.

412

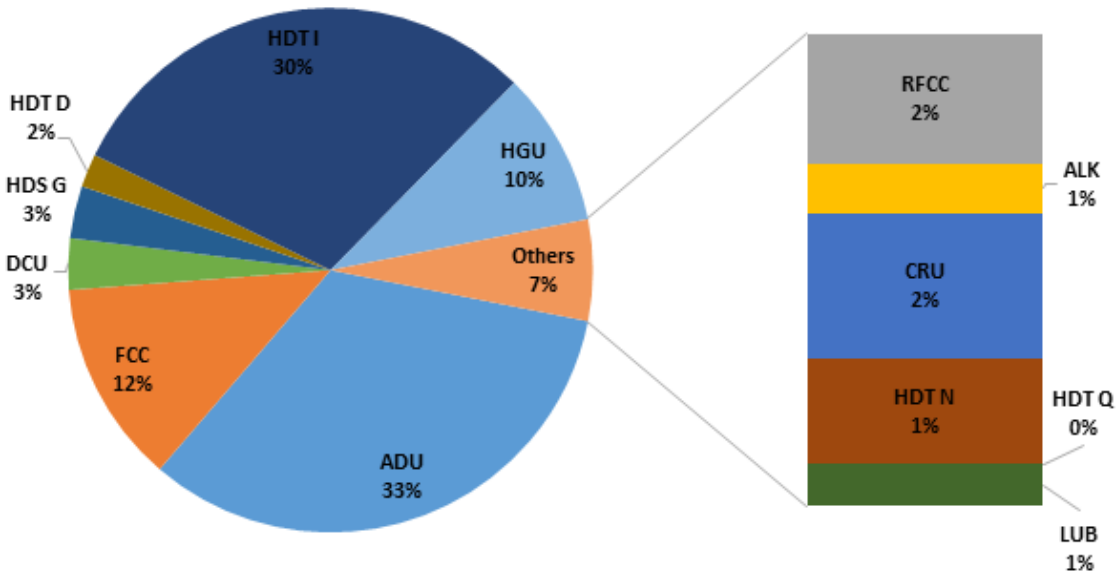
Figure 3 - Water consumption per processing unit in the baseline scenario

413

ADU – atmospheric distillation unit; VDU – vacuum distillation unit; ; FCC – fluid catalytic cracking; RFCC – resid fluid catalytic cracking; ALK – alkylation unit; DCU – delayed coking unit; CRU – catalytic reforming unit; HDS G – gasoline hydrodesulphurization unit; HDT N – naphtha hydrotreatment unit; HDT Q – kerosene hydrotreatment unit; HDT D – diesel hydrotreatment unit; HDT I – severe hydrotreatment unit; LUB – lubricants unit; HGU – hydrogen generation unit

417

418



419

420

Figure 4 - CO₂ emissions per processing unit in the baseline scenario

421

ADU – atmospheric distillation unit; VDU – vacuum distillation unit; ; FCC – fluid catalytic cracking; RFCC – resid fluid catalytic cracking; ALK – alkylation unit; DCU – delayed coking unit; CRU – catalytic reforming unit; HDS G – gasoline hydrodesulphurization unit; HDT N – naphtha hydrotreatment unit; HDT Q – kerosene hydrotreatment unit; HDT D – diesel hydrotreatment unit; HDT I – severe hydrotreatment unit; LUB – lubricants unit; HGU – hydrogen generation unit

425

426

According to SZKLO and SCHAEFFER (2007), most CO₂ emissions from Brazilian refineries come from burning fuels. Interestingly, the fuel consumption of refineries in absolute terms concentrates on few processes, which are not the most energy intensive (in terms of energy consumption per barrel) but process large volumes of feedstock. Typically, atmospheric and vacuum distillation units account for 35-40% of a refinery's final energy use (API, 2000) because any barrel of oil entering a refinery passes through the topping separation units. This explains their share of CO₂ emissions. Also, for global refining, between 16% and 20% of the total are non-energy emissions associated with the chemical reactions of hydrogen production and cracking of the FCC (SZKLO AND SCHAEFFER, 2007). This average figure agrees with our findings for Brazil. Finally, severe hydrotreatment (for unstable and unfinished distillates) results in both higher water consumption and CO₂ emissions due to the severity (temperature

436

437 higher than 450°C, H₂ partial pressure up to 21 MPa, and low liquid hourly space velocity⁷ and
 438 hydrogen pressure) under which reactions must happen (GARY et al, 2007; STANISLAU et al,
 439 2010).

440

441 3.2. CO₂ Price Scenarios for all Brazilian Refineries

442

443 As described above, four CO₂ price scenarios were simulated in CAESAR. According to the
 444 levelized cost of mitigation options on the database of the tool, different options were selected
 445 for each scenario. Moreover, the fuel mix also changed to minimize operational costs
 446 considering the CO₂ prices (and the emission factors of each possible fuel to be used). **Table 9**
 447 summarizes the results for different CO₂ prices, and **Figure 5** shows CO₂ emissions and water
 448 requirements for different CO₂ emission prices scenarios.

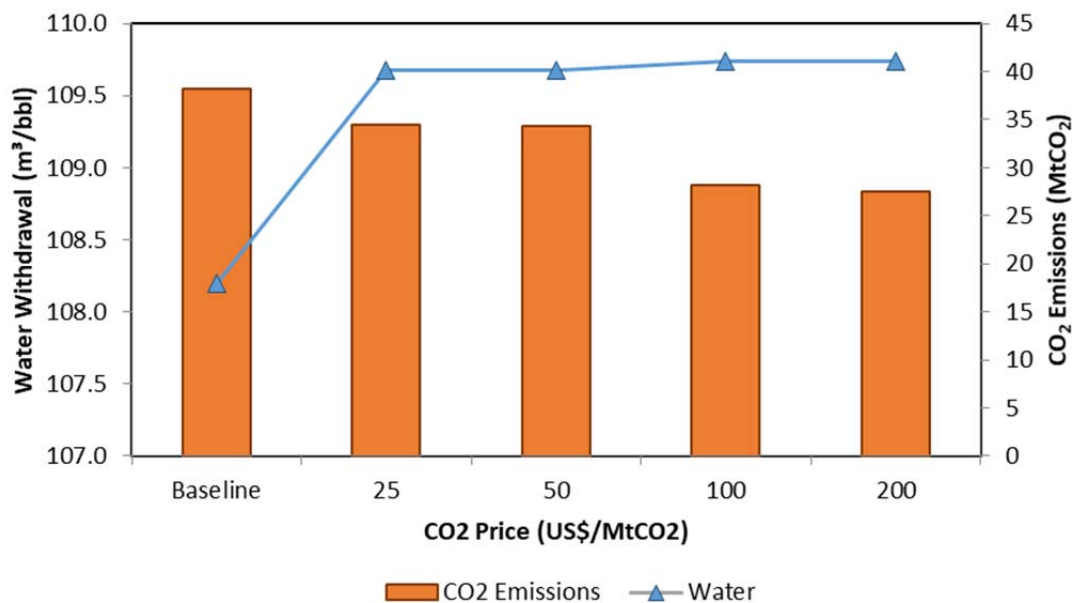
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Table 9 – Summary of Results

Final Energy Use (PJ/year)	CO ₂ Emission Price (US\$/tCO ₂)				
	Baseline	25	50	100	200
Natural Gas	367.84	367.84	367.84	367.84	367.84
Refinery Gas	84.39	84.39	84.39	84.39	84.39
Fuel oil	85.26	78.76	78.22	71.32	62.05
Coke	58.95	58.95	58.95	58.95	58.95
TOTAL	596.40	589.94	589.40	582.50	573.23
Grid Electricity (GWh/year)	7252.71	7393.02	7199.61	7772.97	7643.62
Water requirements					
Consumption (km ³ /year)	14107.86	14143.04	14143.04	14154.36	14154.36
Withdrawal (km ³ /year)	61351.69	62191.48	62191.48	62228.12	62228.12
CO₂ emissions (MtCO₂/year)	38.20	34.43	34.38	28.18	27.46

450

⁷ This is expressed in m³ of fresh feed per m³ of catalyst per hour. The inverse of LHSV is generally called residence time (STANISLAU et al, 2010).



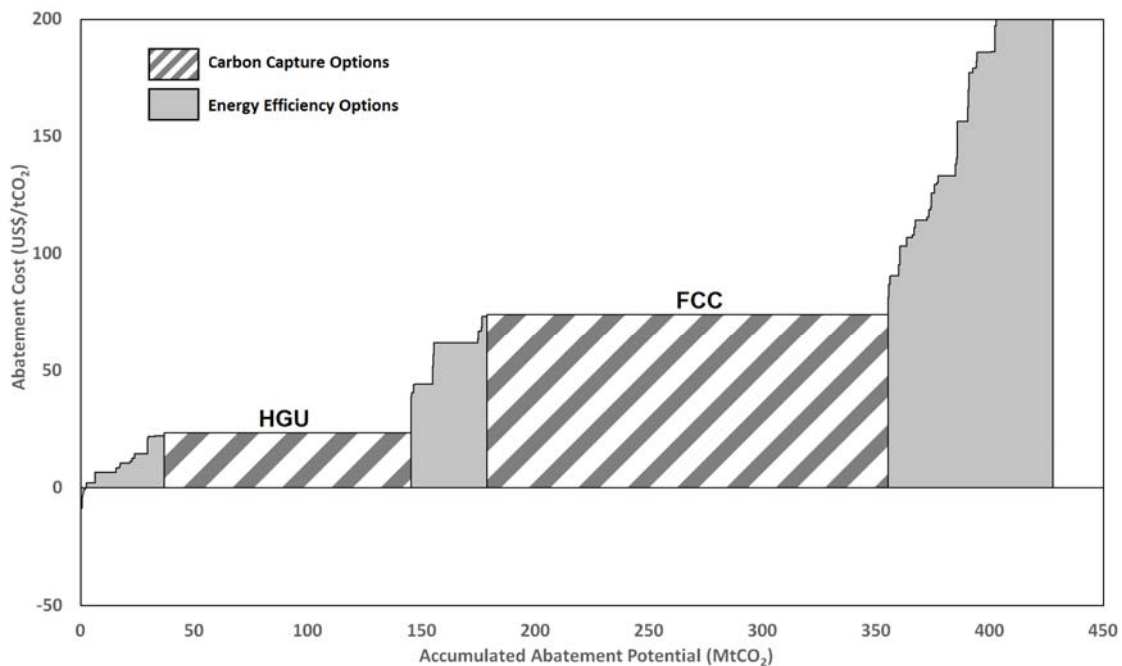
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452

Figure 5 - Water withdrawal versus CO₂ emissions

453

454 The most significant CO₂ emission abatement occurs at 25 and 100 US\$/tCO₂, 10% and 26%,
 455 respectively, compared to the baseline. This is explained by the total abatement potential of the
 456 technologies found in the cost ranges 0-25 US\$/tCO₂ and 50-100 US\$/tCO₂, equal to 143.5 and
 457 205.7 MtCO₂ (see Supplementary Material). In respect to water requirements, a slight change of
 458 less than 1% occurs between the baseline scenario and 25 US\$/tCO₂ scenario. In other
 459 scenarios, the water withdrawals remain practically stable, with a small change, less than 0.5%
 460 in the 100US\$/tCO₂ scenario. To better illustrate the relationship between the abatement costs
 461 and the accumulated abatement potential, the abatement cost curve (**Figure 6**) was produced,
 462 including the 204 technologies considered in the study.



463

464

465

Figure 6 - Abatement cost curve for Brazilian refineries
 Note: HGU – Hydrogen generation unit; FCC – Fluidized catalytic cracking.

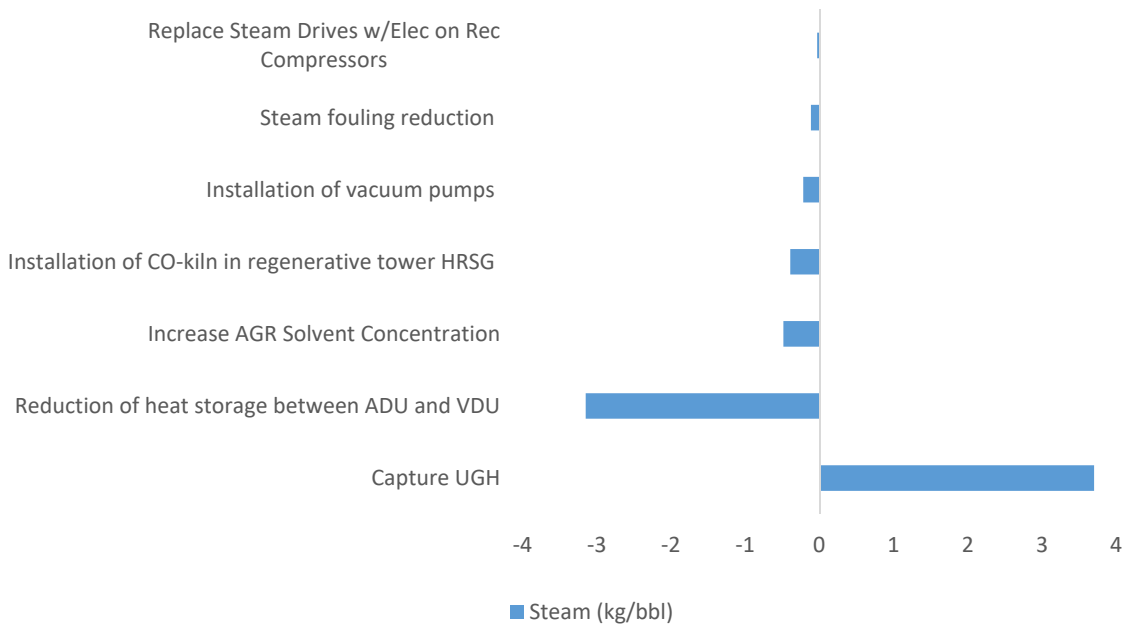
466

467 The graph performs a static analysis of the accumulated abatement potential of the mitigation
 468 options. For instance, it demonstrates that at a cost of \$200/tCO₂, it would be possible to
 469 implement a series of measures that have a cumulative abatement potential of 423.78 MtCO₂.
 470 The two striped areas marked on the graph represent the CC technologies, while the gray-
 471 colored areas represent the other mitigation options. The first one, with an accumulated
 472 abatement potential of 145.5 MtCO₂, refers to the HGU capture with SMR/MDEA, while the
 473 second one, with 355.3 MtCO₂ of accumulated abatement potential, represents the FCC capture
 474 with Oxyfiring. These carbon capture technologies represent 65.7% of the total accumulated
 475 abatement cost, given the cracking pattern of Brazilian refineries and the recent regulations that
 476 tightened diesel and gasoline specifications in the country.

477 In the end, the findings of this study show that the co-benefits of GHG abatement measures that
 478 also reduce steam consumption (e.g., reduction of heat storage between ADU and VDU, steam
 479 fouling reduction in ADU, installation of vacuum pumps to replace steam injectors in ADU,
 480 increase AGR solvent concentration in HDS G, replace steam drive for electric in HDT N, and
 481 installation of CO-kiln in regenerative tower HRSG in FCC), which were chosen⁸ by our

⁸ Steam fouling reduction in ADU and vacuum pumps to replace steam injectors in ADU are installed at 25 US\$/tCO₂. Increase AGR solvent concentration in HDS G is chosen at 50 US\$/tCO₂. Replace steam drive for electric in HDT N is chosen at 100 US\$/tCO₂. CO-kiln in regenerative tower HRSG in FCC is installed at 200 US\$/tCO₂ tax.

482 simulations, were offset by the water consumption increase related to CC options, especially in
 483 HGU. In summary, at a national level and on average, CO₂ mitigation impacts on water use by
 484 oil refineries in Brazil are neutral. **Figure 7** illustrates how steam consumption reduction from
 485 some mitigation measures is overcome by the increase required with CC implementation.



486

487

Figure 7 – Steam requirements impacts of CO₂ mitigation options

488

489 **3.3. Case Study: REPLAN**

490

491 At a local level, for the largest Brazilian oil refinery, the water balance undertaken showed that,
 492 although there was no unmet water demand at the REPLAN's catchment point, the conflict
 493 between the multiple water users in the basin should intensify. This is due to the trend in the
 494 river flow being progressively closer to the critical threshold of 50% of the minimum
 495 availability (Q_{7,10}). In addition, it was observed that the point of flow observation at Jaguari
 496 River faces instants when the flow must be restricted. This means that REPLAN may sometimes
 497 suffer impacts on its operation due to a 30% reduction in the volume of water it receives from
 498 the Jaguari River.

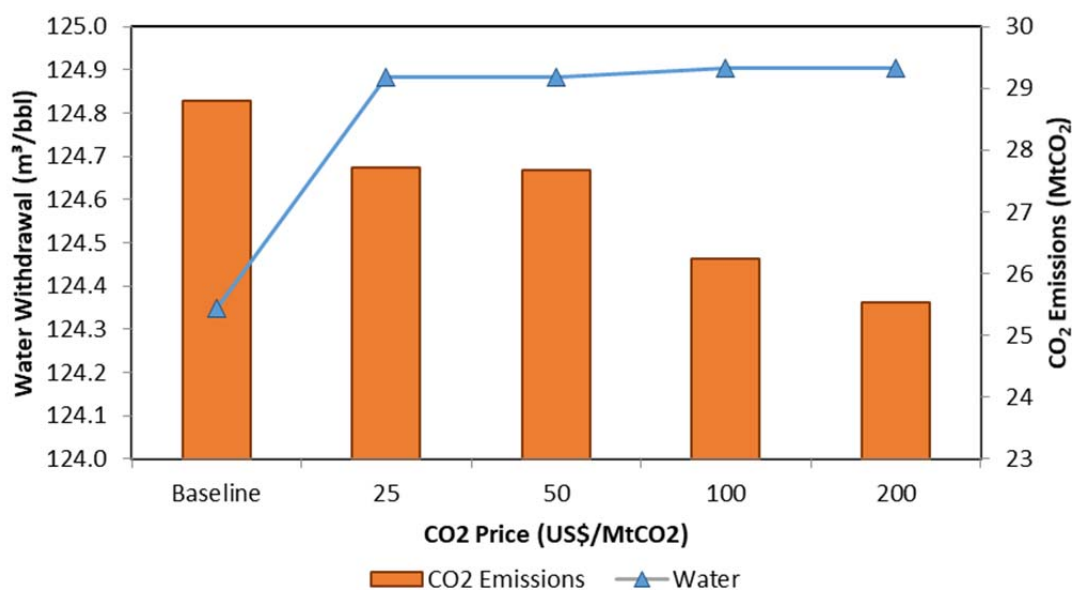


Figure 8 - Water withdrawal versus CO₂ abatement in REPLAN

499

500

501

502 **Figure 8** shows an increase in water withdrawal in all scenarios. Although some mitigation
 503 measures reduce steam consumption, in the refinery's overall water balance, this reduction is
 504 offset by the increase in the demand for boiler feed water and for cooling. Mitigation measures
 505 costing up to US\$ 25/MtCO₂ were the ones that most demanded water due to the increase in
 506 boiler feed water need, which was 1.4% more than in the baseline scenario. In addition, the
 507 slight increase that occurred between scenarios US\$ 50/MtCO₂ and 100 was due to the
 508 implementation of CC, which increased the demand for cooling water.

509 Nevertheless, as a final balance, a reduction of less than 1% was obtained when implementing
 510 all CO₂ mitigation measures in REPLAN. This means that, contrary to what happens in other
 511 energy sectors (ZHAI and RUBIN, 2011; MERSCHMANN et al., 2012), the implementation of
 512 CO₂ abatement in oil refineries has no significant impact on water consumption (no negative
 513 trade-off). However, this also means that the water stress in oil refineries should be dealt with
 514 measures not directly linked to CO₂ abatement (no significant co-benefits). This is valid both at
 515 local and country levels.

516

4. Final Remarks

517

518

519 This study developed an energy, CO₂, H₂, water balance simulator for Brazilian oil refineries,
 520 and applied it to different scenarios of CO₂ mitigation (at 25, 50, 100 and 200 US\$/tCO₂)
 521 aiming at investigating the climate-energy-water nexus. A Baseline scenario, i.e., a scenario

522 without CO₂ prices was also elaborated. Results for both scenarios included final energy
523 consumption, CO₂ emissions and water requirements. The most significant reductions in CO₂
524 emissions were due to the implementation of the carbon capture. However, this option offsets
525 the co-benefits of CO₂ abatement measures that reduced the water requirements of Brazilian oil
526 refineries, especially those already located in areas under water supply stress, such as the largest
527 refinery in Brazil (REPLAN), whose water balance with carbon mitigation options was detailed
528 in this study.

529 Nevertheless, as this study focused on the impacts of CO₂ mitigation options on water
530 requirements, it was not able to follow the reverse path of the nexus: from climate to water
531 availability. This means that climate change can affect the water availability to oil refineries
532 (water supply, instead of water demand side). Hence, future studies could focus on this issue,
533 also including the analysis of alternatives to regularize river flows to deal with climate impacts
534 on water supply. Another idea could be optimizing refineries for minimizing water consumption
535 (or withdrawals).

536 It is also worth noting that this study tried to validate the findings of the tools used by
537 comparing them to real data from Brazil. However, an important issue for the simulation tool is
538 to calibrate the feedstock blend to be run, and the focus of the refinery operation. As of today,
539 although the Brazilian refinery system, on average, focuses on diesel optimization (e.g. when
540 establishing the distillation cuts), single refineries can present a different feature (e.g. focusing
541 on lube oils or petrochemicals). Similarly, the yearly focus of the average refinery operation on
542 diesel does not mean that this is valid for all days of the year.

543 Finally, although the 204 CO₂ mitigation options considered by this study represent an extensive
544 list of measures, there are always new possibilities to be assessed. For example, some studies
545 have evaluated the use of renewable energy sources to supply the energy demand (PINSKE et
546 al., 2012) and the hydrogen consumption (SILVA, 2017) of oil refineries.

547

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549

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553

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