

## Climate-Energy-Water Nexus in Brazilian Oil Refineries

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## RECHERCHE

CLIMATE-ENERGY-WATER NEXUS IN BRAZILIAN OIL REFINERIES

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## 1 Climate-energy-water nexus in Brazilian oil refineries

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## 8 Abstract

9 Oil refineries are major  $CO_2$  emitters and are usually located in water-stress sites. While some 10  $CO_2$  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 11 12 locally detailing the water balance of the country's largest refinery, this study aimed to quantify 13 the impacts of  $CO_2$  mitigation options on the water use of oil refineries. Findings show that, at 14 25 and 100 US\$/tCO2, Brazilian refineries can abate CO2 emissions by 10% and 26%, 15 respectively, compared to current emissions. A relevant share of this abatement derives from the 16 implementation of carbon capture facilities in fluid catalytic cracking and hydrogen generation 17 units. However, these CC facilities offset the co-benefits of other  $CO_2$  mitigation options that 18 can reduce steam and cold water requirements in refineries. In fact, for the largest Brazilian oil 19 refinery, the implementation of all mitigation measures had almost no effect on its water 20 balance. This means that  $CO_2$  abatement in refineries has no significant impact on water 21 consumption (no negative trade-off). However, this also means that the water stress in oil 22 refineries should be dealt with with measures not directly linked to CO<sub>2</sub> abatement (no 23 significant co-benefits).

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

25

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

For instance, coal-fired thermoelectric plants need water resources, mainly for cooling 40 processes. For these plants, a promising GHG mitigation option could be the installation of 41 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 more than 100%, which may intensify its vulnerability and affect the water supply to other users 44 45 downstream from the power plant (ZHAI and RUBIN, 2011; MERSCHMANN et al., 2012). In the case of the production of liquid biofuels, the nexus goes beyond the energy conversion 46 47 facility, which may also be affected by  $CO_2$  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 arising from irrigation is an emblematic case of the tradeoff between GHG mitigation and water. 50

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 study, which is: do  $CO_2$  mitigation options affect the water consumption of an oil refinery 56 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).

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

capacities, the production profile of the oil products (quantities and specifications), and the 69 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 final energy, and in turn emit more GHG (EPA, 2010). In addition, the more stringent the oil 72 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 CO<sub>2</sub> 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 CO<sub>2</sub> emissions (MCTI, 2013; PETROBRAS, 2013; 78 EPA, 2014).

79 Nevertheless, the vast majority of the research associated with the nexus between energy and climate in oil refineries has focused on the trade-off between fuel specifications and  $CO_2$ 80 emissions (CONCAWE, 2000; CHAN, 2006; SZKLO AND SCHAEFFER, 2007; 81 JOHANSSON et al., 2012; CONCAWE, 2012). In the case of the nexus between energy and 82 83 water, there are some studies on the relationship between water consumption and energy use in oil refineries (HIGHTOWER and PIERCE, 2008; IPIECA, 2010; HWANG and MOORE, 2011; 84 PAN et al., 2012; MUGHEES and AL-AHMAD, 2014; SUN et al., 2018). Previous research 85 has also focused on the implementation of CO<sub>2</sub> capture in oil refineries and its abatement cost, 86 as ROCHEDO et al. (2016) have done, but it has failed to explore the water nexus with  $CO_2$ 87 88 mitigation options in oil refineries.

At the end, few attempts have been made to quantify the relationship between climate ( $CO_2$ emission mitigation) and water-energy use in oil refineries. **Table 1** provides a brief summary of the opportunities for  $CO_2$  abatement measures in oil refineries' processing units, and their likely impact on water consumption. It highlights the signs of the impacts that are quantified later in this study (positive and negative signs) through the use of simulation tools for all Brazilian refineries and for a specific refinery in detail.

 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	-	-	-	-	-	-	

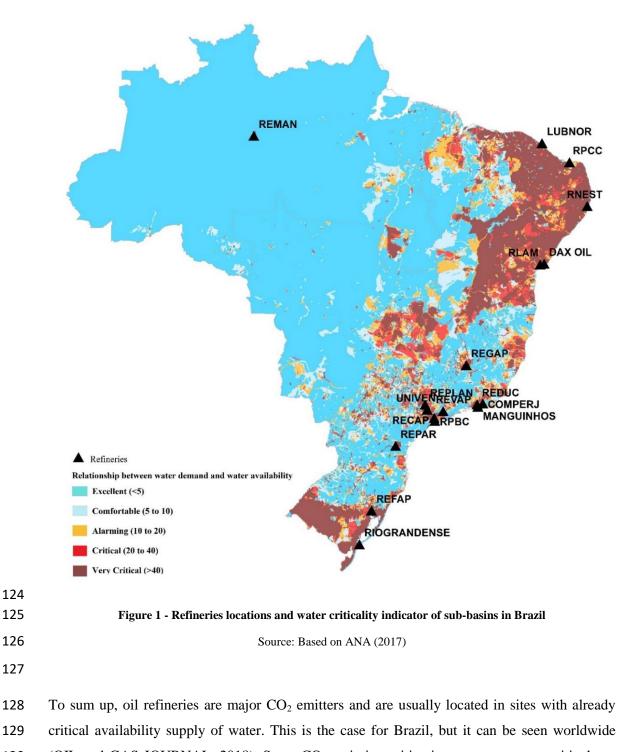
	RFCC	-	-			
	FCC	-	-			+
	DCU	-	-		-	
	HGU					+
96	1	U		1 1	consumption, ie it helps to redu	1
97	On the other hand	d, the negative si	ign has a negativ	ve impact, indicating an increa	se in water consumption with	the application of the
98	measure.					
99		ADU – atmosphe	eric distillation u	ınit; VDU – vacuum distillatio	n unit; CRU – catalytic reformi	ing unit; HDT –
100	hydrotreatmen	t unit; RFCC – re	esid fluid catalyt	ic cracking; FCC – fluid cataly	ytic cracking; DCU – delayed c	oking unit; HGU –
101			hydro	ogen generation unit; CC: CO <sub>2</sub>	capture	
				<u>-</u>		
102	So	urce: WORRE	L and GALITS	SKY (2003); WORREL and	d GALITSKY (2005); CON	JCAWE (2008);
102						(,,
103			BERGI	H, 2012; MORROW III et a	al. (2013)	

105 Regarding water use, oil refining requires considerable amounts of water, which vary 106 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) 107 108 (SUN et al., 2018), and the products' requirements. Within this context, in Brazilian refineries, 109 water requirements deserve attention due to the processing of heavy-to-medium crude oils, as 110 well as to the increasingly stringent specifications of fuels that require the implementation of 111 hydrotreatment units, associated with the water-intensive steam reforming process (CASTELO 112 BRANCO et al., 2010; SZKLO, ULLER and BONFÁ, 2012; BARROS and SZKLO, 2015)<sup>1</sup>.

113 In addition, in Brazil, water availability is not evenly distributed. While the northern region 114 holds more than 80% of all water availability, the basins located in large urban centers, in the 115 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 116 117 stress, measured in relation to the level of water criticality of watersheds. This index measures 118 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 119 120 flow with permanence of 95%. In fact, REPLAN, REVAP, RLAM and REDUC, which account

<sup>&</sup>lt;sup>1</sup>In 2018, the Brazilian oil refining industry consisted of 17 refineries in operation, with a total installed nominal capacity of 2.2 Mbbl/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
- availability.
- 123



- 130 (OIL and GAS JOURNAL, 2018). Some CO<sub>2</sub> emission mitigation measures can positively or
- 131 negatively influence both withdrawal and water consumption at refineries. Within this context,
- this study aims to quantify the extent to which these measures can impact refineries' water use.
- 133 First, by developing an energy,  $CO_2$ ,  $H_2$ , water balance simulator for Brazilian oil refineries, and

applying it to different scenarios of  $CO_2$  mitigation, this study evaluates the  $CO_2$  mitigationenergy-water nexus at the country level. Then, this study analyzes the water supply of the hydrographic basin in which the largest Brazilian refinery, REPLAN, is located and how it behaves over time. This detailed analysis, at a local level, not only quantifies the water withdrawal impacts of  $CO_2$  mitigation options, but also identifies whether or not these impacts 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

## **2. Methods**

## 145

## 2.1. Methodological Procedure

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147 The methodological procedure applied by this study consisted of the following steps. The first step is the definition of GHG mitigation measures in oil refineries, according to the scientific 148 literature and the experience of the authors regarding Brazil's oil refineries<sup>2</sup>. Then, the study 149 150 simulates the baseline case for estimating the scenario without CO<sub>2</sub> mitigation, and simulates 151 the impacts of introducing CO<sub>2</sub> price scenarios into oil refineries, in terms of CO<sub>2</sub> 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 impacts of CO<sub>2</sub> mitigation options, but also identifies whether these impacts could be overcome 158 159 by the current water supply of REPLAN. In summary, the steps include:

160 161 1. To assess the  $CO_2$  mitigation options focusing on the saving potential for the consumption of fuels, steam, electricity and  $H_2$ .

162 2. To estimate the energy and mass balances for a baseline case, including final energy
163 consumption, CO<sub>2</sub> emissions and water requirements. This case does not consider the
164 application of CO<sub>2</sub> 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

<sup>&</sup>lt;sup>2</sup> 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.
- 3. To run CAESAR with CO<sub>2</sub> emission prices<sup>3</sup> of 25, 50, 100 and 200 US\$/tCO<sub>2</sub>. In this case, the CO<sub>2</sub> emissions mitigation options are selected according to their marginal abatement cost that is, technological options with costs lower than or equal to the exogenously established CO<sub>2</sub> price are automatically selected by the simulation tool, allowing the construction of a CO<sub>2</sub> average abatement cost curve for all Brazilian oil refineries. The Supplementary Material provides the basic equation associated with the estimation of the abatement cost.
- 4. To develop a case study for REPLAN, the largest Brazilian refinery in terms of processing capacity, thus quantifying the water stress in detail, or locally. This allows investigating whether mitigation measures that were selected in step 3 can be adopted in cases where a greater water withdrawal is required. This case study is performed using the software tool Water Evaluation and Planning WEAP (see section 2.2. and Supplementary Material).
- 181
- 182 183

## 2.2. CAESAR tool – Carbon and Energy Strategy Analysis for Refineries

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The tool used for evaluating all Brazilian refineries, without detailing the water supply-demand
balance at a local level, is the simulator CAESAR – Carbon and Energy Strategy Analysis for
Refineries. It was originally developed by TOLMASQUIM and SZKLO (2000), later being
used by the Brazilian Government in its Long-Term Energy Plan 2030 (EPE, 2007). Finally, it
was updated by GUEDES (2015) and by VÁSQUEZ-ARROYO (2018) and MAGALAR (2018)
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 catalytic cracker, hydrotreaters (naphtha, diesel, kerosene and instable products), 195 196 hydrotreatment of finished gasoline, lube unit, and hydrogen generation unit. The processing units' capacities are determined, as well as the processed feedstocks, specific utilities 197 198 consumption (steam, fuel and hydrogen) and specific water consumption. The outputs of the 199 tool consist of the final energy consumption, CO<sub>2</sub> emissions, oil product output, and refineries' 200 water consumption and withdrawal.

<sup>&</sup>lt;sup>3</sup> They represent an established price to be paid for a given amount of  $CO_2$  emitted.

Therefore, CAESAR is a bottom-up model mostly based on the simulation of the mass (water, H<sub>2</sub>) and energy balances of Brazilian oil refineries. It has an additional feature for optimizing the energy consumption aimed at minimizing the cost of operation of oil refineries. The model also includes a list of  $CO_2$  mitigation options, which are detailed according to the processing units in which they can be implemented, their potential for saving fuel and/or electricity, their investment, operation and maintenance costs, and their penetration rates. In total, 204 options of technologies are available in CAESAR (see Supplementary Material for detailed data).

208 For the carbon price scenarios,  $CO_2$  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 scenarios for the current configuration of Brazilian oil refineries. As 204 CO<sub>2</sub> emission 211 212 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.

Therefore, depending on the  $CO_2$  emission price applied, the tool automatically selects different GHG mitigation options from the set list available, affecting the final energy use,  $CO_2$  emissions and water consumption. The Supplementary Material includes the basic data of the model and a 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 CO<sub>2</sub> 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 resources management (IWRM) developed by the Stockholm Environmental Institute (SEI). 227 228 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 and demand, demography, technology, operating rules and water management policies 231 (SIEBER and PURKEY, 2015). 232

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

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

The model simulates the use of water in hydrological basins by using a linear programming algorithm, which aims to maximize the water delivered to demand sites, according to a set of priorities defined by the user. When water is limited, the algorithm is formulated to progressively constrain water allocation to the lowest priority demand sites. More details of the model can be found in SIEBER and PURKEY, 2015. See the Supplementary Material for 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

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

253

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
· · · VDU	11 (11) (1 1 C

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

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

n	C	o
Z	σ	o
	-	_

Table 3 - Process Units' Utilities Specific Energy Consumption

Unit	HP Steam	MP Steam	LP Steam	Electricity	Fuel	Coke	H <sub>2</sub> Consumption	H <sub>2</sub> Production	BFW	CW
	kg/bbl	kg/bbl	kg/bbl	kWh/bbl	MJ/bbl	MJ/bbl	m³/bbl	m³/bbl	m³/bbl	m³/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 – hig	h pressure;	MP – medium p	oressure; LP	- low press	ure; BFW – boiler f	feed water; CW	- cooling	

271

272

HANDWERK (2001); STANISLAUS et al. (2010)

water

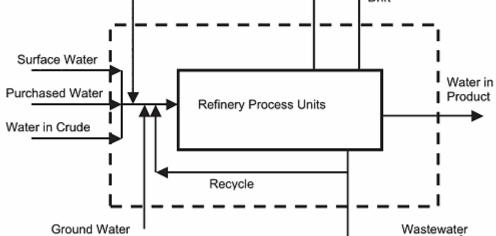
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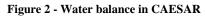
273

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

Table 4 - Water Use Coefficients per Process Unit

	CW (m³/bbl)	BFW (m³/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	-	-	-	-	-
0 by			water	re; BFW – boiler O et al. (2016)	
R	ain	Stea	am Losses	Cooling Evapor Drift	Tower ation &





- Source: Based on IPIECA (2010)

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 water used in the cooling towers, the make-up water for the boilers and the water used by the 292 processes (water incorporated into products, for instance, in the production of H<sub>2</sub>, because of 293 294 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  $Demand = (0.017 \times \sum_{i} CW_{i}) + \{0.497 \times \sum_{i} BFW_{i} + [0.33 \times \sum_{i} Steam_{i}]\}$  (1)

303

Where "CW<sub>i</sub>" represents the cooling system's circulating water of each process unit "i"; BFW<sub>i</sub>" is the amount of water used in boilers of each process unit "i"; "Steam<sub>i</sub>" is steam consumed in each process unit "i".

307

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

309

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

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

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

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

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

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

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

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

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

<sup>&</sup>lt;sup>4</sup> Lowest flow on seven consecutive days for 10-year return period.

<sup>&</sup>lt;sup>5</sup> Flow with 95% of permanence over a period.

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

- **358 3. Results**
- 359

361

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

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

- 365
- 366

**Table 5 - Utilities Consumption** 

-752,5	HP Steam (kt/year)
7,340.4	MP Steam (kt/year)
-375.9	LP Steam (kt/year)
<b>r</b> ) 12,162.7	Electricity (GWh/year)
284,018.2	Fuel (TJ/year)
58,952.6	Coke (TJ/year)
6,116.5	H <sub>2</sub> (M Nm <sup>3</sup> /year)

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)

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

As such, the water requirement of the existing Brazilian refineries is detailed in **Table 7**. The water intensity of 108.2 m<sup>3</sup>/bbl is compatible with the figures found in VANELLI (2004) for REVAP – Refinaria Henrique Lage; PETROBRAS (2005) and NOGUEIRA (2007) for REPLAN – Refinaria de Paulínia; SCHOR (2006) for REDUC – Refinaria Duque de Caixas; 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 3,720.4 Steam (t/h) 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<sup>3</sup>/bbl) 24.9 Withdrawal (m<sup>3</sup>/bbl) 108.2 Consumption (km<sup>3</sup>/year) 14107.9 Withdrawal (km<sup>3</sup>/year) 61351.7 BFW - Boiler feed water; CW - Cooling water

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391

It was also possible to estimate the CO<sub>2</sub> emissions of Brazilian refineries as of 2017, through the
multiplication of the emission factors reported by IPCC (2006) of the respective fuels used by
Brazilian refineries (**Table 8**). For electricity's CO<sub>2</sub> emissions, the average Brazilian grid
emission factor for 2017 was considered, equal to 92.7 tCO<sub>2</sub>/GWh (MCTIC, 2018).

396 397

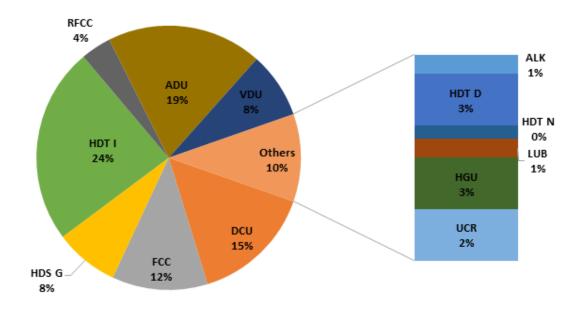
#### Table 8 - CO<sub>2</sub> Emissions (MtCO<sub>2</sub>/year) - Baseline

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

TOTAL	38.2
-------	------

399 By dividing the total emissions by the processed feed, this study estimated an emission intensity 400 of 0.4 tCO<sub>2</sub>/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)<sup>6</sup>. Just for comparison, worldwide several works in the literature present CO<sub>2</sub> emission intensities of oil refineries 402 403 hovering between 0.1 and 0.4  $tCO_2/t$  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  $CO_2$  emissions and water withdrawals, the 408 estimative for the baseline scenario is 0.62 t $CO_2/m^3$ . Figure 3 and Figure 4 present, for this 409 scenario, the most representative units in terms of water consumption and  $CO_2$  emissions, 410 respectively.

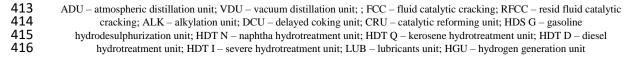


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<sup>6</sup> Equal to 0.45 tCO<sub>2</sub>/ t of oil processed in 2012. Of course, this intensity may vary slightly among years given the focus of the ADU campaign (in our study we focused on diesel), the possible maintenance of downstream units, which 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.

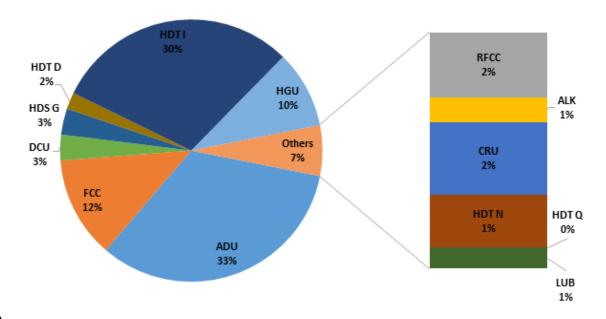


#### Figure 3 - Water consumption per processing unit in the baseline scenario





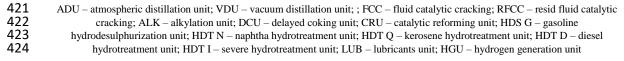








#### Figure 4 - CO<sub>2</sub> emissions per processing unit in the baseline scenario



425

426 According to SZKLO and SCHAEFFER (2007), most CO<sub>2</sub> emissions from Brazilian refineries 427 come from burning fuels. Interestingly, the fuel consumption of refineries in absolute terms 428 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 429 vacuum distillation units account for 35-40% of a refinery's final energy use (API, 2000) 430 because any barrel of oil entering a refinery passes through the topping separation units. This 431 432 explains their share of CO<sub>2</sub> emissions. Also, for global refining, between 16% and 20% of the total are non-energy emissions associated with the chemical reactions of hydrogen production 433 434 and cracking of the FCC (SZKLO AND SCHAEFFER, 2007). This average figure agrees with 435 our findings for Brazil. Finally, severe hydrotreatment (for unstable and unfinished distillates) results in both higher water consumption and CO<sub>2</sub> emissions due to the severity (temperature 436

higher than 450°C, H<sub>2</sub> partial pressure up to 21 MPa, and low liquid hourly space velocity<sup>7</sup> and hydrogen pressure) under which reactions must happen (GARY et al, 2007; STANISLAU et al, 2010).

440

441 442

## **3.2.** CO<sub>2</sub> Price Scenarios for all Brazilian Refineries

443 As described above, four  $CO_2$  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  $CO_2$  prices (and the emission factors of each possible fuel to be used). **Table 9** 447 summarizes the results for different  $CO_2$  prices, and **Figure 5** shows  $CO_2$  emissions and water 448 requirements for different  $CO_2$  emission prices scenarios.

449

#### **Table 9 – Summary of Results**

Final Energy Use (PJ/year)

CO<sub>2</sub> Emission Price (US\$/tCO<sub>2</sub>)

	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 Eletricity (GWh/year)	7252.71	7393.02	7199.61	7772.97	7643.62
Water requirements					
Consumption (km <sup>3</sup> /year)	14107.86	14143.04	14143.04	14154.36	14154.36
Withdrawal (km <sup>3</sup> /year)	61351.69	62191.48	62191.48	62228.12	62228.12
CO <sub>2</sub> emissions (MtCO <sub>2</sub> /year)	38.20	34.43	34.38	28.18	27.46

<sup>&</sup>lt;sup>7</sup> This is expressed in m<sup>3</sup> of fresh feed per m<sup>3</sup> of catalyst per hour. The inverse of LHSV is generally called residence time (STANISLAU et al, 2010).

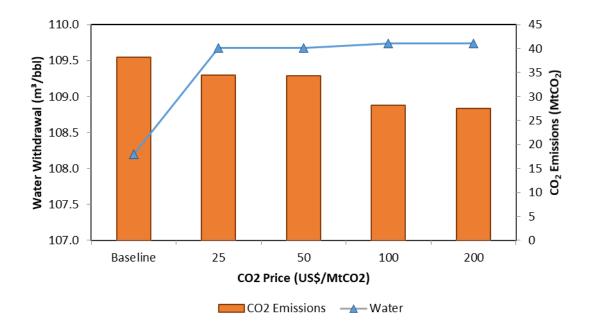
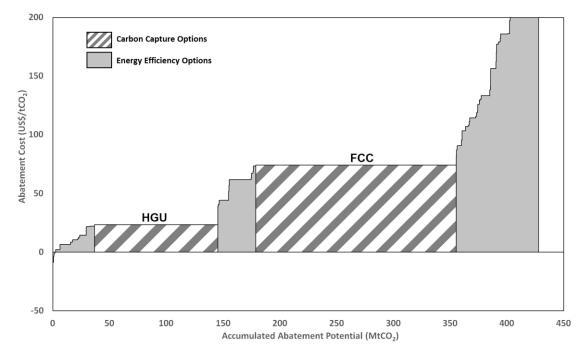




Figure 5 - Water withdrawal versus CO<sub>2</sub> emissions



The most significant CO<sub>2</sub> emission abatement occurs at 25 and 100 US\$/tCO<sub>2</sub>, 10% and 26%, 454 455 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 205.7 MtCO<sub>2</sub> (see Supplementary Material). In respect to water requirements, a slight change of 457 less than 1% occurs between the baseline scenario and 25 US\$/tCO2 scenario. In other 458 459 scenarios, the water withdrawals remain practically stable, with a small change, less than 0.5% in the 100US\$/tCO<sub>2</sub> scenario. To better illustrate the relationship between the abatement costs 460 and the accumulated abatement potential, the abatement cost curve (Figure 6) was produced, 461 462 including the 204 technologies considered in the study.





**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  $200/tCO_2$ , it would be possible to implement a series of measures that have a cumulative abatement potential of 423.78 MtCO<sub>2</sub>. 469 470 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 abatement potential of 145.5 MtCO<sub>2</sub>, refers to the HGU capture with SMR/MDEA, while the 472 473 second one, with 355.3 MtCO<sub>2</sub> 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.

In the end, the findings of this study show that the co-benefits of GHG abatement measures that
also reduce steam consumption (e.g., reduction of heat storage between ADU and VDU, steam
fouling reduction in ADU, installation of vacuum pumps to replace steam injectors in ADU,
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 chosen<sup>8</sup> by our

<sup>&</sup>lt;sup>8</sup> Steam fouling reduction in ADU and vacuum pumps to replace steam injectors in ADU are installed at 25 US\$/tCO<sub>2</sub>. Increase AGR solvent concentration in HDS G is chosen at 50 US\$/tCO<sub>2</sub>. Replace steam drive for electric in HDT N is chosen at 100 US\$/tCO<sub>2</sub>. CO-kiln in regenerative tower HRSG in FCC is installed at 200 US\$/tCO<sub>2</sub> 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, CO<sub>2</sub> mitigation impacts on water use by
- 484 oil refineries in Brazil are neutral. Figure 7 illustrates how steam consumption reduction from
- some mitigation measures is overcome by the increase required with CC implementation.

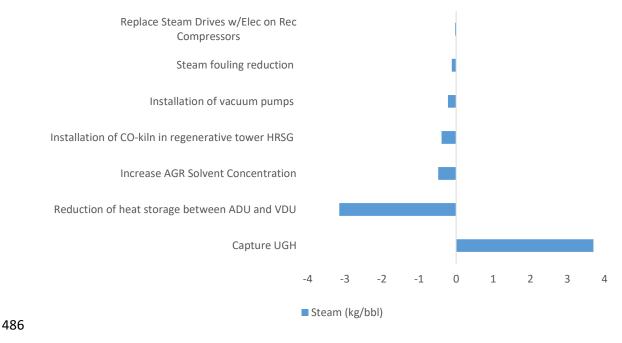


Figure 7 – Steam requirements impacts of CO<sub>2</sub> mitigation options

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#### 489 **3.3.** Case Study: REPLAN

At a local level, for the largest Brazilian oil refinery, the water balance undertaken showed that, 491 492 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.

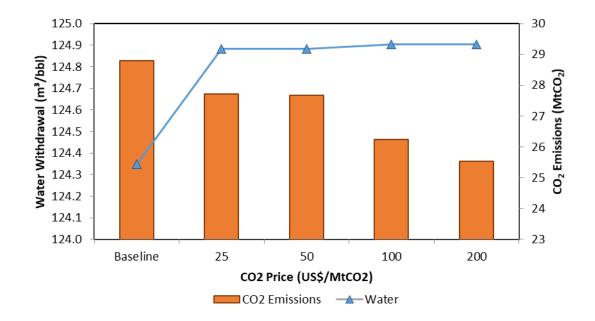






Figure 8 - Water withdrawal versus CO<sub>2</sub> abatement in REPLAN

**Figure 8** shows an increase in water withdrawal in all scenarios. Although some mitigation measures reduce steam consumption, in the refinery's overall water balance, this reduction is offset by the increase in the demand for boiler feed water and for cooling. Mitigation measures costing up to US\$  $25/MtCO_2$  were the ones that most demanded water due to the increase in boiler feed water need, which was 1.4% more than in the baseline scenario. In addition, the slight increase that occurred between scenarios US\$  $50/MtCO_2$  and 100 was due to the implementation of CC, which increased the demand for cooling water.

Nevertheless, as a final balance, a reduction of less than 1% was obtained when implementing all  $CO_2$  mitigation measures in REPLAN. This means that, contrary to what happens in other energy sectors (ZHAI and RUBIN, 2011; MERSCHMANN et al., 2012), the implementation of  $CO_2$  abatement in oil 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 measures not directly linked to  $CO_2$  abatement (no significant co-benefits). This is valid both at local and country levels.

516

## 517 **4. Final Remarks**

518

This study developed an energy,  $CO_2$ ,  $H_2$ , water balance simulator for Brazilian oil refineries, and applied it to different scenarios of  $CO_2$  mitigation (at 25, 50, 100 and 200 US\$/tCO<sub>2</sub>) aiming at investigating the climate-energy-water nexus. A Baseline scenario, i.e., a scenario without  $CO_2$  prices was also elaborated. Results for both scenarios included final energy consumption,  $CO_2$  emissions and water requirements. The most significant reductions in  $CO_2$ emissions were due to the implementation of the carbon capture. However, this option offsets the co-benefits of  $CO_2$  abatement measures that reduced the water requirements of Brazilian oil refineries, especially those already located in areas under water supply stress, such as the largest refinery in Brazil (REPLAN), whose water balance with carbon mitigation options was detailed in this study.

Nevertheless, as this study focused on the impacts of  $CO_2$  mitigation options on water requirements, it was not able to follow the reverse path of the nexus: from climate to water availability. This means that climate change can affect the water availability to oil refineries (water supply, instead of water demand side). Hence, future studies could focus on this issue, also including the analysis of alternatives to regularize river flows to deal with climate impacts on water supply. Another idea could be optimizing refineries for minimizing water consumption (or withdrawals).

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

Finally, although the 204  $CO_2$  mitigation options considered by this study represent an extensive list of measures, there are always new possibilities to be assessed. For example, some studies have evaluated the use of renewable energy sources to supply the energy demand (PINSKE et al., 2012) and the hydrogen consumption (SILVA, 2017) of oil refineries.

547

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549

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