

Life Cycle Greenhouse Gas Emissions of By-product Hydrogen from Chlor-Alkali Plants

Energy Systems Division

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Prepared by:

Dong-Yeon (D-Y) Lee, Amgad A. Elgowainy, and Qiang Dai

Systems Assessment Group, Energy Systems Division, Argonne National Laboratory

December 2017

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ACRONYMS

AC	Alternating current
ACC	American Chemistry Council
ASCC	Alaska Systems Coordinating Council
ATSDR	Agency for Toxic Substances and Disease Registry
BIT	Bituminous coal
CARB	California Air Resources Board
CC	Combined-cycle
CEH	Chemical Economics Handbook
CHP	Combined heat and power
CI	The Chlorine Institute
CT	Combustion turbine
DC	Direct current
DOE	U.S. Department of Energy
EC	European Commission
ECU	Electrochemical unit
EFC	Electrical fuel consumption
EIA	Energy Information Administration
EMF	Emission Factor
EPA	U.S. Environmental Protection Agency
ERCOT	Electric Reliability Council of Texas
FCEV	Fuel cell electric vehicle
FRCC	Florida Reliability Coordinating Council
FRED	Federal Reserve Economic Data
GDP	Gross domestic product
GHG	Greenhouse gas
GHGRP	Greenhouse Gas Reporting Program
REET	Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation
GT	Gas turbine
HHV	Higher heating value
HICC	Hawaiian Islands Coordinating Council
IPCC	Intergovernmental Panel on Climate Change
LCA	Life cycle assessment
LHV	Lower heating value
MRO	Midwest Reliability Organization

NAICS	North American Industry Classification System
NERC	North American Electric Reliability Corporation
NG	Natural gas
NPCC	Northeast Power Coordinating Council
PHR	Power-to-heat ratio
RFC	ReliabilityFirst Corporation
SERC	SERC Reliability Corporation
SMR	Steam methane reforming
SPP	Southwest Power Pool
ST	Steam turbine
TFC	Total fuel consumption
TRE	Texas Reliability Entity
UNEP	United Nations Environment Programme
WCC	World Chlorine Council
WECC	Western Electricity Coordinating Council
WHR	Waste heat recovery

1 INTRODUCTION

Current hydrogen production capacity in the U.S. is about 15.8 million tonne (or metric ton) per year (Brown 2016). Some of the hydrogen (2 million tonne) is combusted for its heating energy value, which makes total annual net production 13.8 million tonne (Table 1). If captive by-product hydrogen (3.3 million tonne) from catalytic reforming at oil refineries is excluded (Brown 2016; EIA 2008), approximately 11 million tonne is available from the conventional captive and merchant hydrogen market (DOE 2013). Captive hydrogen (owned by the refiner) is produced and consumed on site (e.g., process input at refineries), whereas merchant hydrogen is produced and sold as a commodity to external consumers. Whether it is merchant or captive, most hydrogen produced in the U.S. is on-purpose (not by-product) — around 10 million tonne/year.

Geographically, the Gulf Coast region and the State of California collectively produce 84% of total U.S. merchant hydrogen (Table 2), for which the market size has more than quadrupled over the last two decades (Brown 2015). The Gulf Coast area and California also account for 66% of captive on-purpose hydrogen production from refineries (EIA 2017a). For merchant hydrogen production, the steam methane reforming (SMR) process is the dominant technology (accounting for 80%). For overall (merchant and captive) on-purpose hydrogen production in the U.S., the contribution of SMR is approximately 90%.

TABLE 1 Captive and Merchant Hydrogen Production and Consumption in the U.S. (million tonne/year)

Industry	Consumption	Production	
		Captive	Merchant ^a
Oil refining	10.5	7.0 ^b	3.6
Ammonia	2.1	2.1	0.27
Methanol	0.60	0.45	0.15
Other chemicals	0.45	0.18	0.012
Metals	0.056	0.044	0.003
Food	0.036	0.035	0.001
Electronics	0.032	0.028	(< 0.0005)
Glass	0.002	0.002	(< 0.0005)
Total	13.8	9.8	4.0

^a Includes by-product hydrogen (0.3–0.4 million tonne/year).

^b Includes captive by-product hydrogen from oil refining (3.3 million tonne/year).

Source: Adapted from Brown (2016).

TABLE 2 Geography of Merchant Hydrogen Production in the U.S.

Geography	H ₂ State	SMR	By-product ^a	Others	Total
California	Liquid	0.2%			0.2%
	Gaseous	15.2%			15.2%
The Gulf Coast	Liquid	0.5%	0.2%		0.7%
	Gaseous	50%	7.9%	10.3%	68.2%
Other Areas	Liquid		0.6%	0.1%	0.7%
	Gaseous	14.6%	0.3%	0.2%	15%
Total		80.5%	9%	10.6%	100%

^a Not exhaustive. Does not include potential hydrogen production from chlor-alkali processes.

Source: Adapted from H2 Tools (2017).

At present, except captive by-product hydrogen for oil refining (3.3 million tonne/year) (Table 1), overall by-product hydrogen production capacity (not the amount delivered to the consumers) is about 2.3 million tonne per year (Brown 2016). The ethylene industry accounts for the largest portion (66%) of non-refinery by-product hydrogen capacity (1.56 million tonne), followed by the metals and chlor-alkali industry. However, most of the by-product hydrogen is combusted (e.g., 100% by-product hydrogen from the metals sector), and only a small fraction (0.3 million tonne) ends up in the merchant hydrogen market (EIA 2008; Brown 2016). Except for that from the oil refining industry, merchant by-product hydrogen accounts for less than 10% of merchant hydrogen and 4% of the overall hydrogen market (Brown 2016; H2Tools 2017; EIA 2008, 2017a).

Despite its small share, by-product hydrogen can play an important role by bridging the transition toward a wider adoption of hydrogen fuel cell electric vehicles (FCEVs) by utilizing the existing industrial resources to help meet the increasing demand of hydrogen fuel. In California, for example, the population of hydrogen FCEVs on the road, currently in the range of a few thousands, is expected to be around 40,000 in the next several years (CARB 2017). To fuel this new fleet of FCEVs, an additional 8,000 tonne of hydrogen fuel is needed annually, assuming a fuel economy of 65 miles/kg H₂ and a travel distance of 13,000 miles/vehicle/year. To meet the increasing demand in California as well as in the rest of the country, the remaining production capacity of conventional SMR plants could be tapped, achieving maximum possible capacity factor. As shown in Figure 1, however, existing daily production capacity of gaseous merchant hydrogen for non-oil applications in California is just around 29 tonne (or 10,600 tonne/year). The additional hydrogen fuel demand of 8,000 tonne/year for FCEVs is equivalent to 75% of the current merchant hydrogen market in California (or 40% when including liquid merchant hydrogen, 26 tonne/day). That said, sourcing hydrogen from existing markets and diverting it from current end uses to a transportation fuel will very likely face

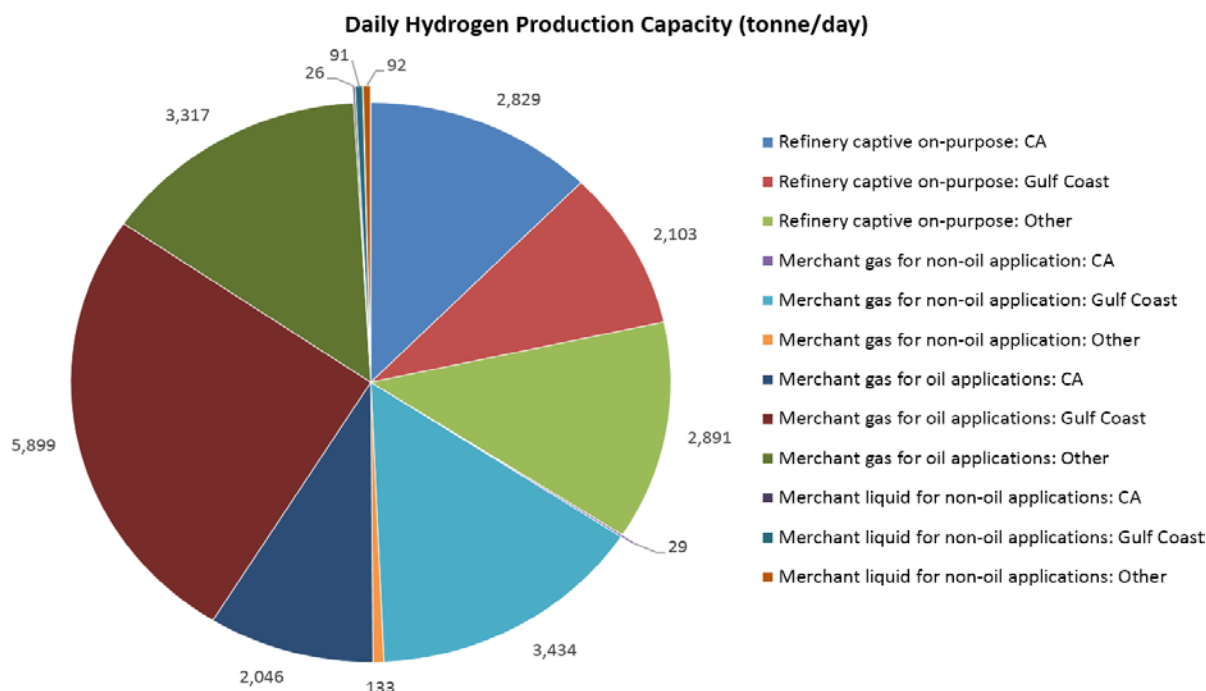


FIGURE 1 Daily Hydrogen Production Capacity in the U.S., by Region and Product Type, Excluding By-product Hydrogen from Chlor-Alkali Plants or Captive On-purpose Hydrogen at Ammonia Plants (around 6,000 tonne/day) (Source: Based on H2Tools 2017 and EIA 2017a)

market resistance. In fact, hydrogen demand from other end uses (other than transportation) has also been increasing (EIA 2016). To avoid the disruption in existing markets, new plants could be built for overall production capacity expansion, but market risk and uncertainty will be a challenge. Also, new capital investment can require a long lead time. In contrast, utilizing by-product hydrogen, readily available from existing industrial processes, does not need a long lead time and will be less sensitive to market risk, all of which can help lower the hydrogen production cost and fuel price in the near term.

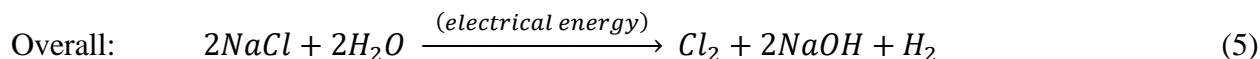
Chlor-alkali processes make up one of the potential by-product hydrogen sources, from which 0.4 million tonne of hydrogen fuel could be produced per year nationally (EIA 2008). The chlor-alkali hydrogen production pathway can help meet the near-term hydrogen fuel demand growth for FCEVs. However, information is lacking as to whether it brings overall environmental benefits. To fill this knowledge gap, we evaluated life cycle greenhouse gas (GHG) emissions of by-product hydrogen from the chlor-alkali processes in comparison with those of hydrogen from conventional SMR plants. In doing so, we considered different chlor-alkali process technologies and corresponding energy requirements, geographical variations in production capacity, and co-products market condition. We present the life cycle GHG emissions results for a baseline case in which by-product hydrogen is combusted on site to produce heat for internal use. As the hydrogen is taken out of the combustion fuel stream and sold to external customers, natural gas is burned as a substitute to generate the equivalent heat energy. Because of the substitution (natural gas replacing hydrogen as a combustion fuel), we assessed overall net GHG emissions in comparing the chlor-alkali and SMR pathways.

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2 BY-PRODUCT HYDROGEN FROM CHLORINE PLANTS

2.1 THE CHLOR-ALKALI PROCESSES

Typical industrial chlor-alkali production is based on the following electrochemical reactions in electrolytic cells (O'Brien et al. 2005; Karlsson and Cornell 2016):



The chlor-alkali process separates chlorine (Cl_2) from the brine (aqueous sodium chloride — H_2O and NaCl) and simultaneously produces sodium hydroxide (NaOH , often referred to as caustic soda, caustic, alkali, or lye) and hydrogen (H_2). Graphical illustration of the chlor-alkali process, characterized by Equations (1)–(5), is shown in Figures 2 and 3, for diaphragm and membrane cells, respectively. Stoichiometry tells us, for every kg of chlorine produced, 1.13 kg of caustic soda and 0.0285 kg of hydrogen are produced (EC 2000; WCC 2002a). The co-product mass composition of chlorine (1 tonne) and caustic soda (1.13 tonne) is called an electrochemical unit (ECU), which is sometimes used as a collective reference unit for energy intensity and cost calculation. From the manufacturer's standpoint, depending on the end-uses, either chlorine or caustic soda becomes the primary product, and the other the by-product (EC 2000). In general, chlorine, caustic soda, and hydrogen are all considered as co-products of chlor-alkali processes. Given the small mass ratio (around 3%) among the three co-products, however, hydrogen is typically called a by-product, making chlorine and caustic soda primary co-products, the basic properties of which are listed in Table 3.

Chlorine is a basic inorganic chemical and powerful oxidant that has a wide variety of end-uses. Chlorine demand is correlated with the gross domestic product (GDP) index (O'Brien et al. 2005), which means that a more affluent society consumes more chlorine. Vinyl (or polyvinyl chloride, PVC) accounts for the largest share (about 34%) of chlorine's end-uses, followed by organics and others (Bommaraju et al. 2002; WCC 2002b; O'Brien et al. 2005; Euro Chlor 2016). Caustic soda, an alkaline compound, is typically used for organics (about 20%), pulp and paper, aluminum, soap and detergents, textiles, and other applications (Bommaraju et al. 2002; WCC 2002a; O'Brien et al. 2005; Euro Chlor 2016). The by-product hydrogen is used on site to generate heat or sold externally as a fuel, if not vented to the atmosphere (EC 2000; Euro Chlor 2016).

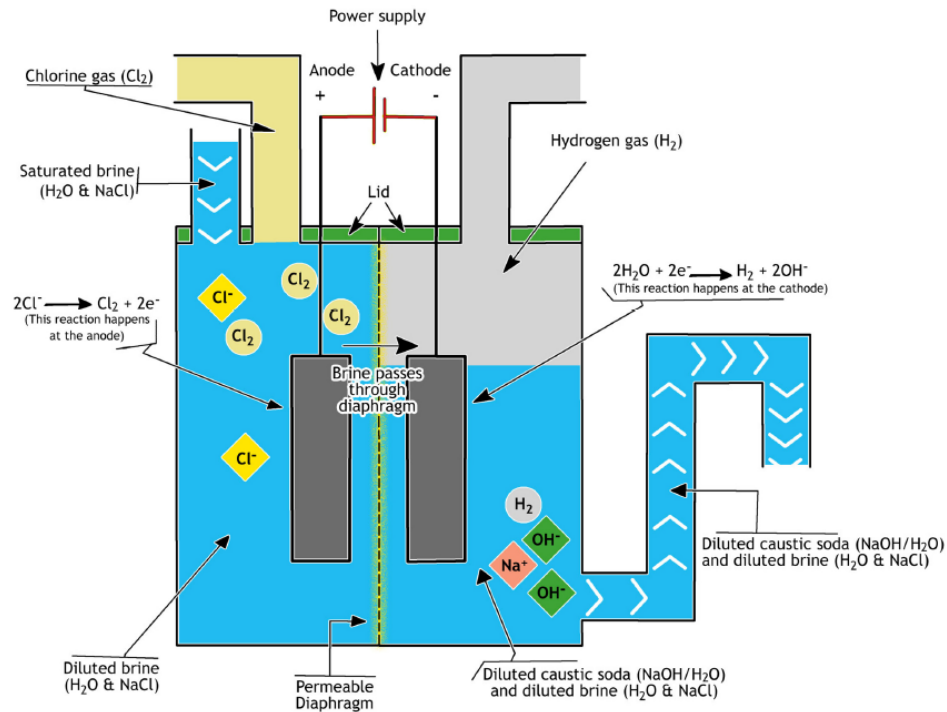


FIGURE 2 Chlor-Alkali Process in Diaphragm Cells (Image source: Euro Chlor 2017)

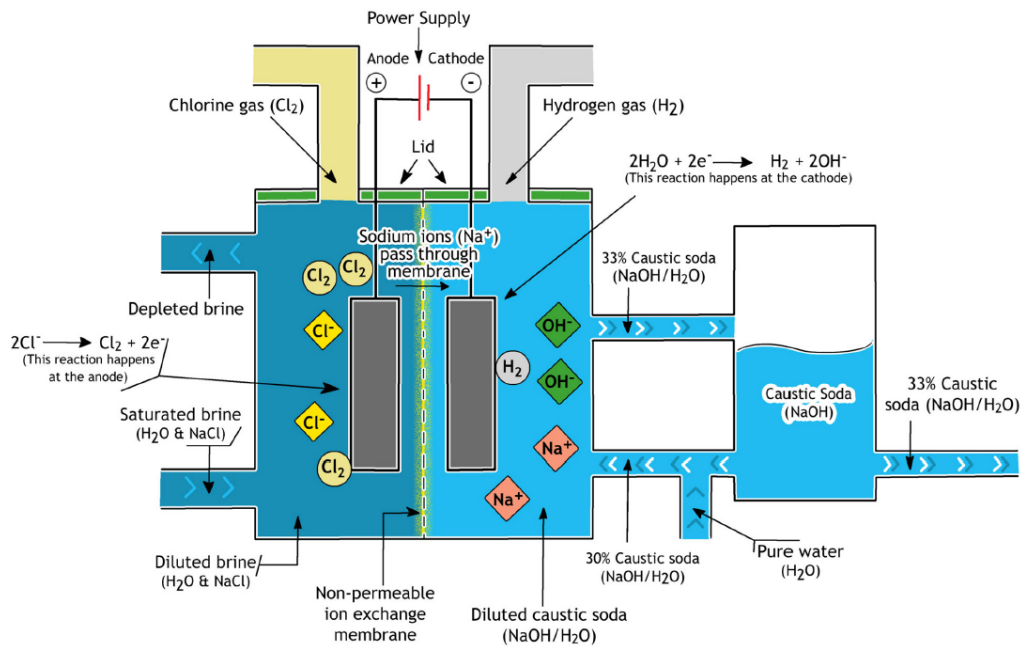


FIGURE 3 Chlor-Alkali Process in Membrane Cells (Image source: Euro Chlor 2017)

TABLE 3 Physical/Chemical Properties of Cl₂ and NaOH

	Cl ₂ (Chlorine)	NaOH (Caustic soda solution 50%)
Physical state	Gas	Liquid
Color	Green-yellow	Colorless
Odor	Characteristic “chlorine” odor	Odorless
Density	3.2 g/L	1.52 g/mL (20°C) (specific gravity)
Freezing temperature	−102°C,	14°C
Boiling temperature	−34°C	145°C
Molecular weight	70.9 g/mole	40.0 g/mole (anhydrous)

Sources: Euro Chlor (2017), Dow (2017).

2.2 CELL TECHNOLOGY

The electrolysis cell lies at the core of the chlor-alkali processes. Electrolytic cell technologies can be divided into three different types — diaphragm, membrane, and mercury cells (EC 2000; O'Brien et al. 2005; WCC 2007; Lakshmanan and Murugesan 2014; Euro Chlor 2016). Diaphragm and membrane electrolysis processes are illustrated in Figures 2 and 3, respectively. Figures 2 and 3 are used with a permission¹. In a diaphragm cell, the feed-in brine continuously migrates from the anode compartment to the catholyte through the permeable diaphragm. In a membrane cell, only sodium ions (Na⁺), not the brine, can pass through the membrane that separates anolyte and catholyte chambers. Whichever electrolysis cell type is used, direct current (DC) electricity is supplied to the electrolytic cell to convert brine to chlorine, caustic soda, and hydrogen.

Globally, the membrane cell is the most dominant technology, followed by the diaphragm cell (WCC 2007; Euro Chlor 2016). More than 70% of global chlor-alkali production capacity (about 80 million tonne of chlorine per year) is based on membrane cell technology (IHS Markit 2014). The mercury cell was once a popular chlorine production technology around the world but has been phased out, due to the increasing concerns of toxic mercury emissions (Winalski et al. 2005). In fact, the number of mercury cell-based chlor-alkali facilities has dramatically decreased over the last two decades (UNEP 2011, 2012), now representing only about 4% of global chlor-alkali production capacity (IHS Markit 2014). In the U.S., total chlor-alkali production capacity is 14 to 15 million tonne of chlorine per year, with a capacity factor around 80 to 90% (Bommaraju et al. 2002; CI 2016). As shown in Figure 4, diaphragm cells account for 55% of total capacity, and membrane cells represent most of the remaining 45%. The contribution of mercury cells in the U.S. has diminished from 17% in 1986 to less than 1% in 2015. For this reason, we did not consider the mercury cell.

¹ as stated in the Euro Chlor webpage: <http://www.eurochlor.org/the-chlorine-universe/how-is-chlorine-produced.aspx>

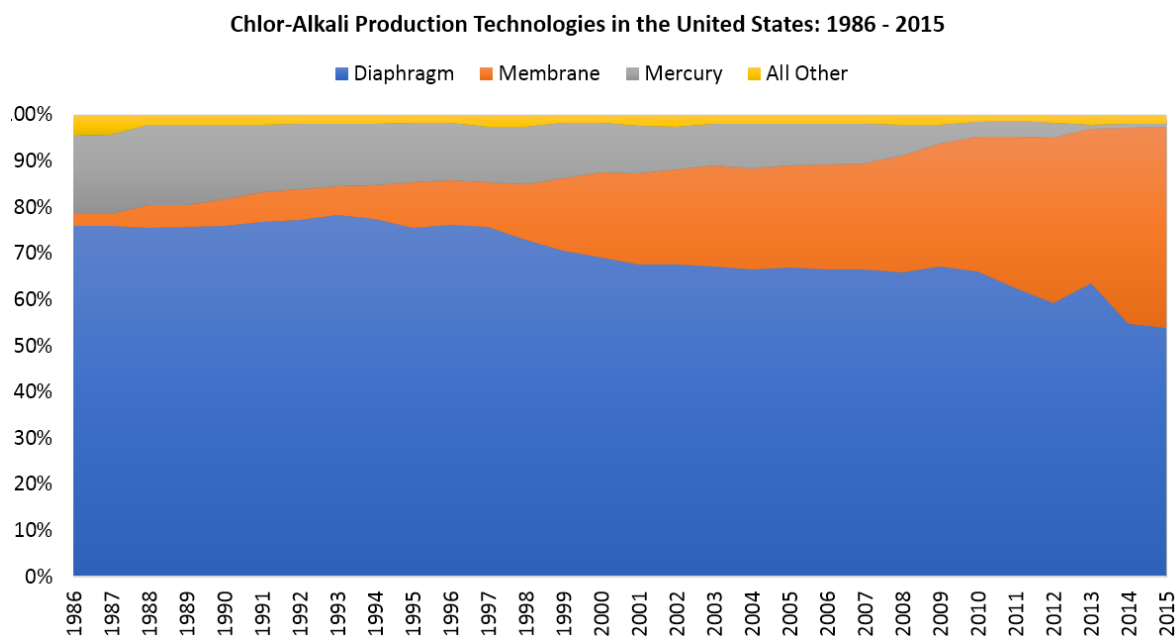


FIGURE 4 Historical Evolution of Electrolytic Cell Types and Their Share in Overall U.S. Chlor-Alkali Production Capacity (Source: Based on CI 2016)

Electrolytic cell technology can further be classified as bipolar or monopolar, depending on the way that the cells are constructed and assembled rather than the electrochemical reactions (Bommaraju et al. 2002; Schmittinger et al. 2011). In the bipolar system, cells are arranged in series, with the negative electrode of one cell connected to the positive electrode of the next. This system design entails higher cell voltage and lower amperage. In the monopolar configuration, all anode and cathode components are connected in parallel, operating at lower voltage and higher amperage in comparison with the bipolar design.

2.3 USE OF BY-PRODUCT HYDROGEN

Unlike on-purpose hydrogen manufacturing in which the process is primarily operated for (captive or merchant) hydrogen production, hydrogen from the chlor-alkali process is a by-product and thus may not always be 100% utilized. As mentioned earlier, for every unit of chlorine produced from the chlor-alkali process, 0.0285 unit of hydrogen is co-produced. Some of this by-product hydrogen is combusted to generate process heat energy required for chlorine and caustic soda manufacturing (Bommaraju et al. 2002; EIA 2008; Schmittinger et al. 2011; Euro Chlor 2016). Alternatively, the hydrogen can be sold as a commodity, shipped to customers by trucks or pipeline. If not combusted on site or sold to the hydrogen market, it is very likely that hydrogen gas is vented to the atmosphere or flared. Euro Chlor (2016) reports that about 10% of by-product hydrogen is vented or flared in European chlor-alkali plants. It has also been reported that as much as 50% of co-produced hydrogen from the chlor-alkali plants in the U.S. may be combusted (EIA 2008). According to Brown (2016), 30% of by-product hydrogen from the chlor-alkali plants is combusted; the rest is sold to the merchant hydrogen market. However,

there is limited information as to the exact end-use of by-product hydrogen. We assumed that the by-product hydrogen is to be burned on site to provide heat energy, as will be discussed in more detail in Section 8.

2.4 ENERGY REQUIREMENTS

Figure 5 shows processes involved in the production of chlorine, caustic soda, and hydrogen, in diaphragm and membrane cell-based systems, respectively. Overall process can be divided into three steps — pre-electrolysis brine preparation, electrolysis, and post-electrolysis product after-treatment. Brine preparation (e.g., saturation, purification, etc.) requires a heat input of 0.02 GJ/tonne of Cl_2 produced, which is assumed to be the same for diaphragm and membrane cells. Assuming 80% boiler efficiency (for steam generation), the natural gas fuel input is 0.025 GJ per tonne of Cl_2 (or 0.88 GJ per tonne of hydrogen).

Electrolysis is the largest component in terms of both cost and energy use. The electrolysis cell is the most expensive component of the chlor-alkali plant, representing 40% of total cost (Bommaraju et al. 2002). In addition, electricity for electrolysis represents around 30% of total production cost (UNEP 2012). In general, power consumption increases with cell voltage, which has a positively proportional relationship with current density (Schmittinger et al. 2011). Lowering cell voltage could help reduce the power consumption of a cell, but it could then require additional cells, which might lead to an increase in overall cost. Therefore, each plant may be designed differently and optimized to meet individual needs.

Equations (6) and (7) show the relationship between power consumption and cell voltage for diaphragm and membrane cells, respectively (Schmittinger et al. 2011):

$$E_{diaphragm} = \frac{U_{cell} \cdot 756}{\varepsilon_{cell}} \quad (6)$$

$$E_{membrane} = \frac{U_{cell}}{F \cdot CE} \quad (7)$$

where

$E_{diaphragm}$ = electrical energy consumption for the diaphragm cell (DC kWh/tonne of Cl_2),
 $E_{membrane}$ = electrical energy consumption for the membrane cell (DC kWh/tonne of NaOH),
 U_{cell} = cell voltage (V),
 ε_{cell} = current efficiency,
 F = Faraday constant for NaOH (1.492 kg/kAh), and
 CE = NaOH current efficiency.

Newer cells may achieve higher energy efficiency, as the performance improves with technological advancements, including voltage loss reduction and current efficiency optimization (Bommaraju et al. 2002). For the same manufacture year, aging could increase a cell's electricity consumption over time (Schmittinger et al. 2011). We used average energy intensity over a cell's lifetime.

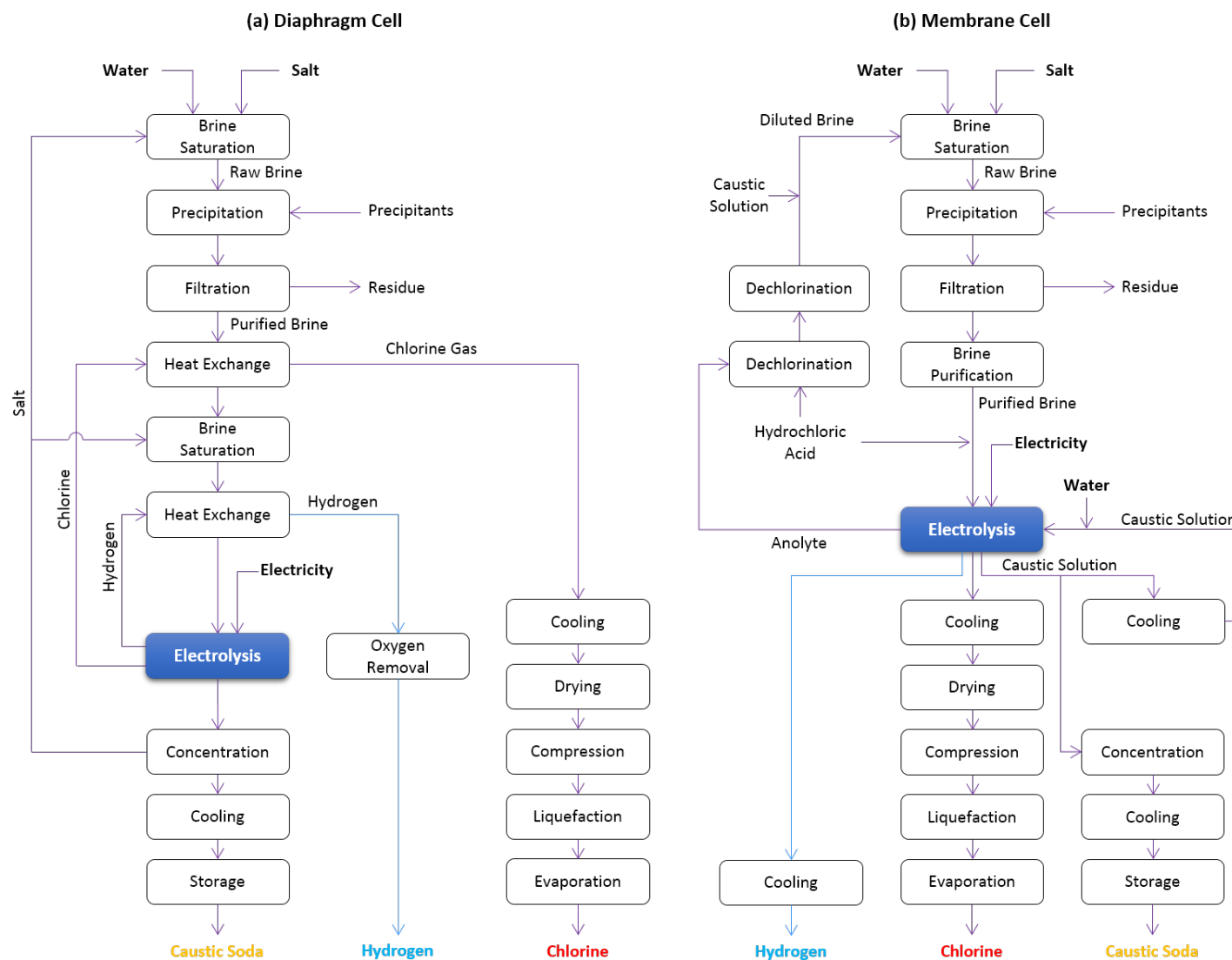


FIGURE 5 Overall Process of Chlorine, Caustic Soda, and Hydrogen Production from Chlor-Alkali Plants
 Sources: Adapted from EPA (1992), EC (2000), Bommaraju et al. (2002), WCC (2002c), Schmittinger et al. (2011), Brinkmann et al. (2014)

Table 4 shows the range of electricity consumption reported in the literature for mono- and bi-polar configurations and diaphragm and membrane cell types. Although the cell configuration (monopolar or bipolar) is an important factor, from the perspective of overall electricity use, the differences or variations are relatively small (within the range of uncertainty). All in all, average electricity intensity of electrolysis for the diaphragm cell is 9.42, and 9.78 GJ/tonne Cl₂ for the monopolar and bipolar configuration, respectively. For the membrane cell, it is 9.22 GJ/tonne Cl₂ for monopolar configuration, and 8.86 for bipolar. This is direct electricity consumption (DC electricity), and the electricity used in the rectifier (converting alternating current [AC] to DC) is 0.28 GJ/tonne Cl₂ (Worrell et al. 2000).

As Figure 5 indicates, each co-product requires a different set of after-treatment processes. Among the three co-products, hydrogen requires the simplest after-treatment, in part owing to the high-purity (>99.9%) hydrogen produced from the electrolysis. Only cooling/drying and compression are needed. For cooling/drying, we assumed that 8.59×10^{-3} kWh of electricity is consumed per kg of hydrogen, based on the reported enthalpy change (6.1 kWh/kg H₂) of hydrogen gas from the chlor-alkali process (O'Brien et al. 2005). Hydrogen gas compression (from 1.3 bar to 20 bar) at the plant gate, for external transmission and distribution, was estimated as 1.72 kWh/kg H₂, based on the following formula that has been adopted in the GREET® (Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) (Elgowainy et al. 2016) and H2A (DOE 2010) models:

$$E_{compression} = \left(\frac{1}{3,600} \right) \times \left(\frac{1}{\eta_{EM}} \right) \times n \times Z \times R \times T \times \left(\frac{1}{\eta_c} \right) \times \left(\frac{k}{k-1} \right) \times \left[\left(\frac{P_{outlet}}{P_{inlet}} \right)^{\left(\frac{k-1}{nk} \right)} - 1 \right] \quad (8)$$

where

- $E_{compression}$ = the energy requirement for hydrogen gas compression (kWh/kg H₂),
- η_{EM} = the electric motor efficiency (92%),
- n = the number of compression stages (4),
- Z = the mean compressibility factor (1.01),
- R = the gas constant for hydrogen (4.157 kJ/kg·K),
- T = the inlet gas temperature (293.15 K),
- η_c = the isentropic efficiency of compression (65%),
- k = the ratio of specific heat (or heat capacity ratio, 1.4 for hydrogen), and
- P_{inlet} and P_{outlet} = inlet (19 psi) and outlet pressure (290 psi), respectively.

TABLE 4 Electricity Consumption (DC kWh/tonne Cl₂) for Electrolysis in Diaphragm and Membrane Cells

Cell Technology	(Schmittinger et al. 2011)				(Brinkmann et al. 2014)	
	Monopolar		Bipolar			
	Min	Max	Min	Max	Min	Max
Diaphragm	2,200	2,900	2,400	2,800	2,540	3,040
Membrane	2,420	2,430	2,370	2,430	2,200	2,900

Chlorine and caustic soda each requires a more complex after-treatment process compared to hydrogen. Figure 6 shows the energy required for each of the chlorine product after-treatment processes. Most of the after-treatment energy is thermal (steam), generated by natural gas combustion. For after-treatment, required electrical energy is about half of the heat energy demand. The properties of chlorine product from diaphragm and membrane cells are similar, and thus the energy consumption in Figure 6 does not change between the two cell types. For caustic soda, however, diaphragm cells consume more energy than membrane cells because of very different product purity (Figure 7). The concentration of caustic soda from diaphragm cells is about 10 to 15%, which must be increased up to 50% to be sold as a commercial product. On the other hand, membrane cells produce much purer caustic soda (30–33%), and thus the energy requirement for after-treatment is relatively lower.

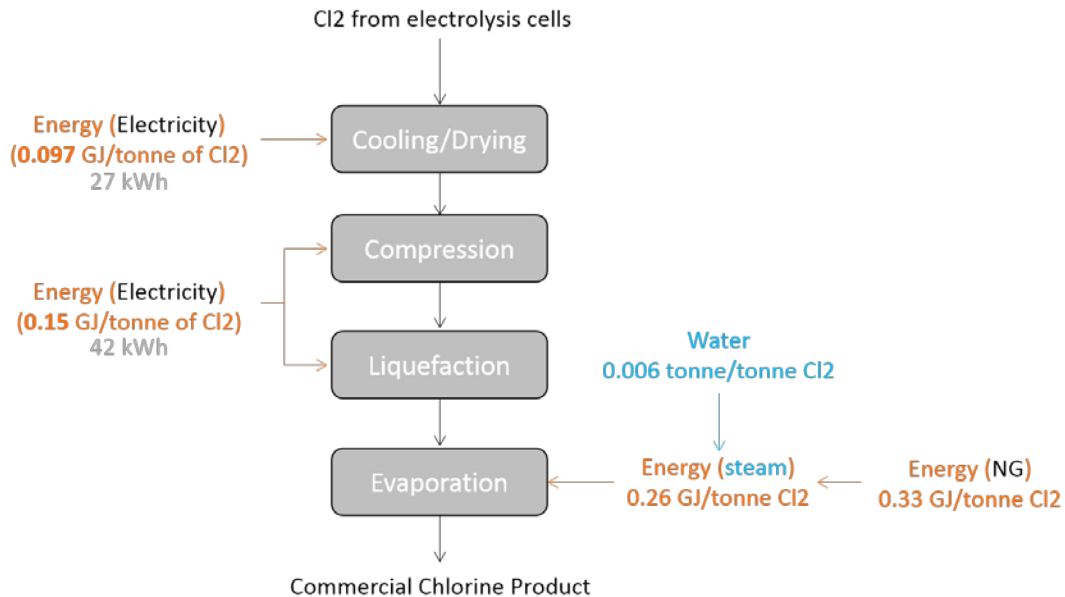
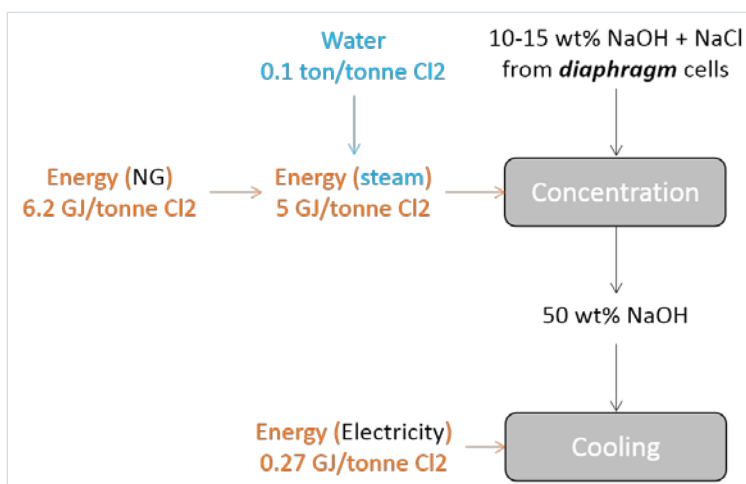
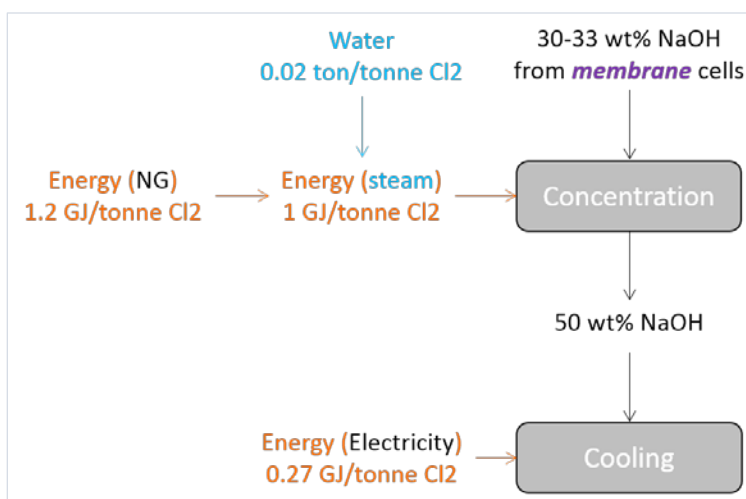


FIGURE 6 Chlorine (Cl₂) After-Treatment Process and Energy Input



(a) Diaphragm cell



(b) Membrane cell

FIGURE 7 Caustic Soda (NaOH) After-Treatment Process and Energy Input

Our estimates of overall electricity and natural gas input for chlorine production are comparable to those in other studies. Franklin Associates (2011) reports 9.6 GJ/tonne Cl₂ of electricity and 6.2 GJ/tonne Cl₂ of natural gas input. This is similar to our estimates (10.3 GJ of electricity and 4.3 GJ of natural gas per tonne of Cl₂), although there are some differences. There can be numerous sources for the differences. The Franklin Associates report is based on 2003 data with 1.4 to 8.6% of mercury cell share, whereas our data are for 2015. As noted earlier, the chlorine production technology share has transformed significantly over the last two decades (Figure 4). More specifically, the share of the membrane cell has almost doubled between 2003 and 2015, while the share of the mercury cell has diminished drastically. Also, different assumptions of electricity-and-heat co-generation could lead to different results, especially for the heat energy requirement. Nevertheless, once we applied the electrolysis cell technology share

for 2003 (75% diaphragm and 25% membrane), our results became very similar, 10.45 GJ of electricity and 5.3 GJ of natural gas per tonne of Cl_2 produced, to those of Franklin Associates (2011). Overall energy requirement estimates are provided in Table 5.

Beal and Linak (2011) estimated energy input for diaphragm and membrane cells in the U.S., but the unit conversion (between chlorine and ECU) is not very clear. It is suspected that the energy intensity is not based on ECU, but on chlorine or caustic soda. Otherwise, the energy intensity reported by Beal and Linak (2011) is too high (e.g., 21–23.4 GJ/tonne Cl_2), compared to the values reported in other studies. Althaus et al. (2007) provide energy consumption estimates for diaphragm and membrane cells for European context. However, among the three sets of candidate values, Althaus et al. (2007) chose to use the lowest value from a somewhat outdated European Commission report (EC 2000), which, indeed, was updated in 2014 (Brinkmann et al. 2014). This led to an underestimation of the thermal energy requirement. Our thermal energy intensity estimate is comparable to the updated values in the most recent European Commission report (Brinkmann et al. 2014).

TABLE 5 Electrical and Natural Gas Energy Input (GJ/tonne Cl_2) for Typical Chlor-Alkali Plants

		Diaphragm	Membrane	Weighted (2003)	Weighted (2015)
Electricity	Rectifier	0.28	0.28		
	Electrolysis	9.6	9.04		
	Cl_2 After-treatment	0.248	0.248		
	NaOH After-treatment	0.27	0.27		
	H_2 After-treatment	0.88×10^{-3}	0.88×10^{-3}		
	H_2 compression	0.1765	0.1765		
	<i>Overall Electricity</i>	10.58	10.01	10.44	10.32
Natural gas	Brine preparation	0.025	0.025		
	Cl_2 After-treatment	0.328	0.328		
	NaOH After-treatment	6.21	1.24		
	<i>Overall Natural Gas</i>	6.56	1.59	5.32	4.32

3 GEOGRAPHY OF CHLOR-ALKALI MANUFACTURING IN THE U.S.

As of 2017, the U.S. chlor-alkali industry is dominated by three companies — Olin, Occidental Chemical (or OxyChem), and Westlake. Due to recent merger and acquisitions in the chlor-alkali industry, these three companies collectively account for 80% of total market share. Geographically, as Figure 8 illustrates, the Gulf Coast area (Louisiana, Texas, and Alabama) produces 11.4 million tonne/year, accounting for more than 80% of chlor-alkali production capacity in the nation.

For chlor-alkali plants in the U.S., we collected plant-by-plant data from numerous sources. The producer and location for chlor-alkali plants were identified based on a 2015 industry survey documented by The Chlorine Institute (CI 2016). Annual chlorine production capacity information is primarily from the ATSDR (Agency for Toxic Substances & Disease Registry) toxicological profile (ASTDR 2010), which is based on The Chlorine Institute report and IHS Markit (formerly SRI Consulting) Directory of Chemical Producers. Chlorine production data from the Kirk-Othmer Encyclopedia of Chemical Technology (Bommaraju et al. 2002) and the Chemical Economics Handbook (CEH) Marketing Research Report (Beal and Linak 2011) were also used as secondary sources for a few plants missing capacity information. Electrolysis cell type information is available in The Chlorine Institute report (CI 2016). Although somewhat old, similar information can also be found in the Kirk-Othmer Encyclopedia of Chemical Technology (Bommaraju et al. 2002). However, cell technology share evolves over time as mentioned previously (see Figure 4), and the exact production share of each

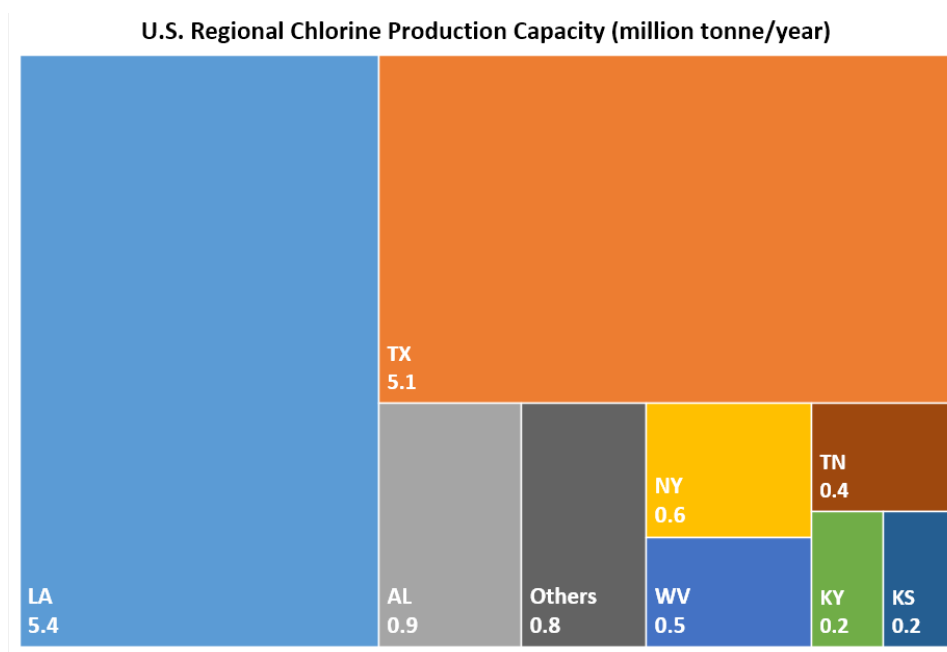


FIGURE 8 U.S. Chlorine Production Capacity (14 million tonne/year) by Region — Hydrogen Production Capacity from Chlor-Alkali Plants: 0.4 million tonne/year

electrolysis cell type for each plant is virtually unknown. In other words, there is a certain level of uncertainty not only for plant-by-plant production capacity, but also for electrolysis cell type and its production share in each plant.

With the reported chlorine production capacity, we estimated hydrogen production potential based on the stoichiometry (approximately 0.0285 kg of hydrogen for every kg of chlorine produced, see Section 2.1). Given the dominance of the Gulf Coast area in terms of chlorine production, for presentation, we divided the data into two groups — the Gulf Coast region (Table 6) and the rest of the country (Table 7). National annual by-product hydrogen production capacity from chlor-alkali plants is around 0.4 million tonne, with an 80 to 20 share between the Gulf Coast and the rest of the country.

TABLE 6 Chlor-Alkali Plants and Production Capacity in the Gulf Coast Area

Producer	State	County	City	Production Capacity (tonne/year)	
				Chlorine	Hydrogen
SABIC	AL	Lowndes	Burkville	82,000	2,340
Olin	AL	Washington	McIntosh	667,000	19,010
Occidental	AL	Colbert	Muscle Shoals	136,000	3,880
Other	FL	Hillsborough	Tampa	27,200	780
Occidental	LA	St. James Parish	Convent	353,000	10,060
Occidental	LA	Ascension	Geismar	243,000	6,930
Westlake	LA	Ascension Parish	Geismar	403,500	11,500
Westlake	LA	Calcasieu Parish	Lake Charles	1,247,000	35,540
Shintech	LA	Iberville Parish	Plaquemine	953,600	27,180
Georgia Gulf	LA	Calcasieu	Plaquemine	408,000	11,630
Olin	LA	Iberville Parish	Plaquemine	971,000	27,670
Olin	LA	Iberville Parish	St. Gabriel	163,000	4,650
Occidental	LA	St. Charles Parish	Taft	680,000	19,380
Occidental	TX	Harris	Battleground	500,000	14,250
Other	TX	Chambers	Baytown	363,000	10,350
Olin	TX	Brazoria	Freeport	2,939,000	88,760
Occidental	TX	San Patricio	Ingleside	548,000	15,620
Formosa	TX	Calhoun	Point Comfort	736,000	20,980
Sub-total				11,420,000	325,470

TABLE 7 Chlor-Alkali Plants and Production Capacity in the Rest of the U.S.

Producer	State	County	City	Production Capacity (tonne/year)	
				Chlorine	Hydrogen
K2	CA	Contra Costa	Pittsburg	73,000	2,080
Kuehne	DE	New Castle	Delaware City	15,000	430
Olin	GA	Richmond	Augusta	109,000	3,110
SABIC	IN	Posey	Mt. Vernon	87,000	2,480
Occidental	KS	Sedgwick	Wichita	239,000	6,810
Westlake	KY	Marshall	Calvert City	249,500	7,110
Olin	NV	Clark	Henderson	133,000	3,790
Other	NV	Clark	Henderson	5,000	140
Kuehne	NJ	Hudson	South Kearny	16,000	460
Occidental	NY	Niagara	Niagara Falls	304,000	8,660
Olin	NY	Niagara	Niagara Falls	259,000	7,380
Other	NC	Richmond	Hamlet	36,300	1,030
Other	OH	Ashtabula	Ashtabula	40,000	1,140
BleachTech	OH	Medina	Seville	18,100	520
Olin	TN	Bradley	Charleston	222,000	6,330
Occidental	TN	Humphreys	New Johnsonville	165,600	4,720
Other	UT	Tooele	Rowley	43,000	1,230
Westlake	WA	Cowlitz	Longview	79,000	2,250
Westlake	WV	Marshall	New Martinsville	463,000	13,200
Other	WI	Wood	Port Edwards	96,000	2,740
Sub-total				2,653,000	75,610

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4 COMBINED HEAT AND POWER FOR CHLOR-ALKALI PLANTS

Some chlor-alkali plants generate power on site, using a combined heat and power (CHP) system, as indicated in the CEH Marketing Research Report (Beal and Linak 2011). On-site electricity generation can be particularly advantageous for the chlor-alkali industry, because most of the energy required for chlor-alkali production is electricity for electrolysis (even more so for membrane cell type) — see Table 5. Typically, the operation of a CHP system is affected by bulk power as well as natural gas (fuel) market conditions, because on-site power generation may not always be cheaper than buying electricity from outside parties. Generating electricity on site can yield many benefits. From the energy efficiency and air emissions perspective, the benefit is mainly twofold, which varies with system efficiency as well as the type of electricity that on-site power displaces. First, overall on-site heating fuel use will be reduced, as waste heat is recovered and used to meet some or all on-site thermal energy demand. Second, electricity generated from the CHP system can provide a net reduction in air emissions over electricity from the grid, depending on what kind of fuel, combustion technology, operating condition (e.g., cold start, part-load), air pollutant emissions after-treatment system, carbon capture and storage, and waste heat recovery strategy are used for on-site power generation.

Figure 9 is a schematic showing the CHP system based on a combined-cycle power plant. For co-generation of heat and power, electricity can be the primary output and heat secondary, or vice versa. The former system configuration is usually called a topping cycle, and the latter a bottoming cycle. In the case of the combined-cycle power plant depicted in Figure 9, electricity is first generated at the topping cycle system (e.g., combustion/gas turbine). The heat generated from the combustion process is recovered and used as input energy at the bottoming cycle (e.g., steam turbine), which is then used to generate additional power. The overall waste heat stream from both the topping and bottoming cycles is directed to the heat recovery unit. Some of the recovered waste heat is used for power generation (in a steam turbine), and the rest is used to meet the process heat energy demand on site or could be exported externally.

Based on the list of chlor-alkali plants identified (see Section 3), we collected on-site CHP system information from the EIA-923 survey data (EIA 2015), which covers an array of industry types. To create a customized data set specifically for the chlor-alkali industry, we first filtered the CHP plants in the EIA-923 data, using NAICS (North American Industry Classification System) codes — 325 (Chemical Manufacturing), 32518/325188 (Other Basic Inorganic Chemical Manufacturing), and 325211 (Plastics Material and Resin Manufacturing). We then compared the filtered CHP plants with the reported chlor-alkali plants and selected only those that match in terms of producer name and location (physical address). For topping cycle CHP units, to avoid extremes or biases, we excluded the CHP plants that have too low (< 10%) or too high (> 50%) electrical efficiency. For the bottoming cycle, we did not apply the minimum electrical efficiency threshold, because heat production (not power generation) is the main purpose of the system.

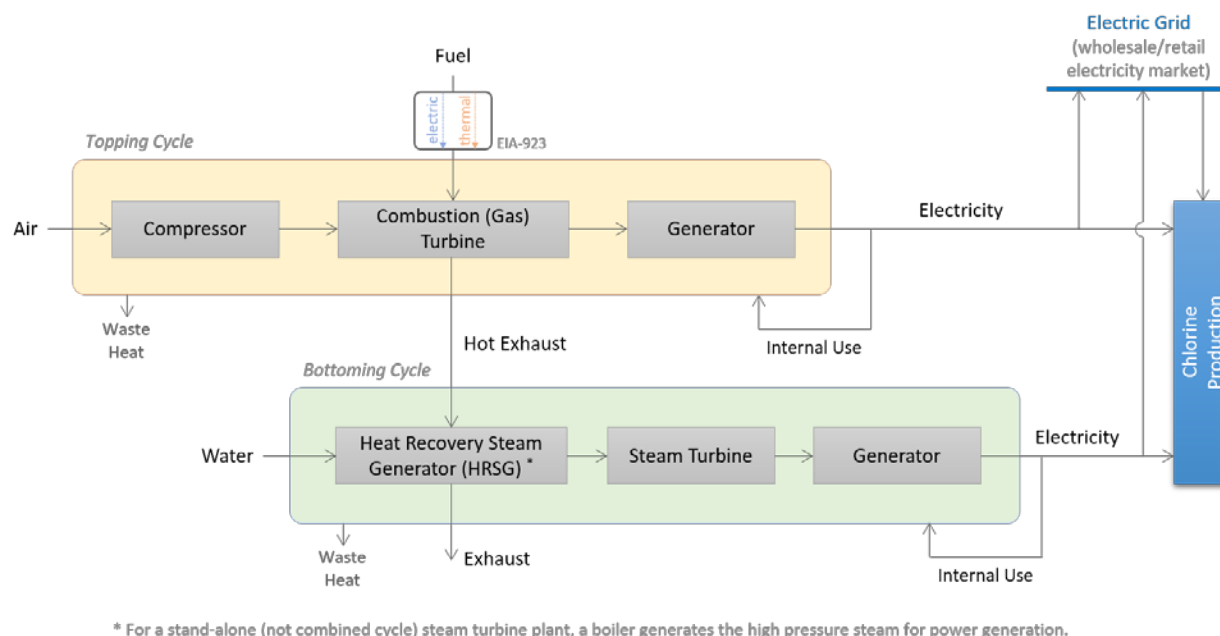


FIGURE 9 Schematic of a Combined Heat and Power (CHP) System

We found a total of eight chlor-alkali plants that have a CHP system with matching records in the EIA-923 survey data. Table 8 summarizes the identified CHP units for those eight chlor-alkali plants. Most of the CHP units are in the Gulf Coast region, which all are topping cycle systems. As can be seen in Table 8, individual CHP units are heterogeneous in terms of electricity generation capacity and the balance between import and export. However, some general patterns can be observed. The largest CHP units are natural gas-powered combined-cycle (NG-CC) systems, representing 83% of total net generation and 70% of total on-site electricity use of the entire CHP units at chlor-alkali plants across the country. Also, total electricity import and export are not always exactly balanced but similar. Overall industry-wide characterization of entire CHP units at chlor-alkali plants is shown in Figure 10. Out of 18.5 TWh of gross generation, 0.5 TWh is consumed for internal station use. Combined with 3.8 TWh of imported electricity, 21.8 TWh of electricity is available for chlor-alkali plants, of which 12.97 TWh is used specifically for chlorine production. The remainder is either exported or consumed for other on-site purposes, which may not be directly related to chlorine production. To estimate electricity generated and consumed on site for chlorine production, we used the electrical energy intensity (Table 5) and plant-by-plant annual chlorine production capacity. For simplicity, we did not consider credits for electricity export from CHP units. All in all, the U.S. chlor-alkali industry requires 25.8 TWh of electricity from the grid, of which 1.6 TWh is hydro-electric power in the Niagara Falls area. On-site CHP units supply around 32% of total electricity (40 TWh) consumed by the chlor-alkali industry.

TABLE 8 On-site Combined Heat and Power (CHP) Units at Chlor-Alkali Plants

State	Company	Annual Chlorine Production Capacity (million tonne)	Fuel Type ^a and Prime Mover ^b	Cycle ^c	Annual Electricity (TWh)			
					Net Generation	Import	On-site Use ^d	Sales or Export
TX	OxyChem	0.55	NG-CC	T	1.91	0.09	1.52	0.47
	Olin	2.94	NG-CC	T	4.05	1.93	5.6	0.38
			NG-GT	T	0.31	0.24	0.55	0
LA	Westlake (Plaquemine)	0.41	NG-GT	T	1.56	0.02	1.44	0.14
			OG-GT	T	0.08	0	0.07	0.01
	OxyChem	0.68	NG-CC	T	4.81	0.04	1.36	3.48
	Olin	0.97	NG-CC	T	4.15	0	2.2	1.94
	Westlake (Geismar)	0.4	NG-GT	T	0.62	0.25	0.87	0
WV	Westlake	0.46	BIT-ST	T	0.48	0.39	0.87	0
			OG-ST	T	0.03	0.02	0.05	0
IN	SABIC	0.09	BIT-ST	B	0.00041	0.26	0.26	0
			NG-ST	B	0.00083	0.53	0.53	0
Total ^e					18	3.8	15.4	6.4

^a Fuel type: NG = natural gas, OG = other gas, BIT = bituminous coal.

^b Prime mover: CC = combined-cycle, GT = gas turbine, ST = steam turbine.

^c Cycle: T = topping, B = bottoming.

^d On-site use includes electricity used for chlorine production (12.97 TWh) and other purposes.

^e Total may not exactly match the sum because of rounding.

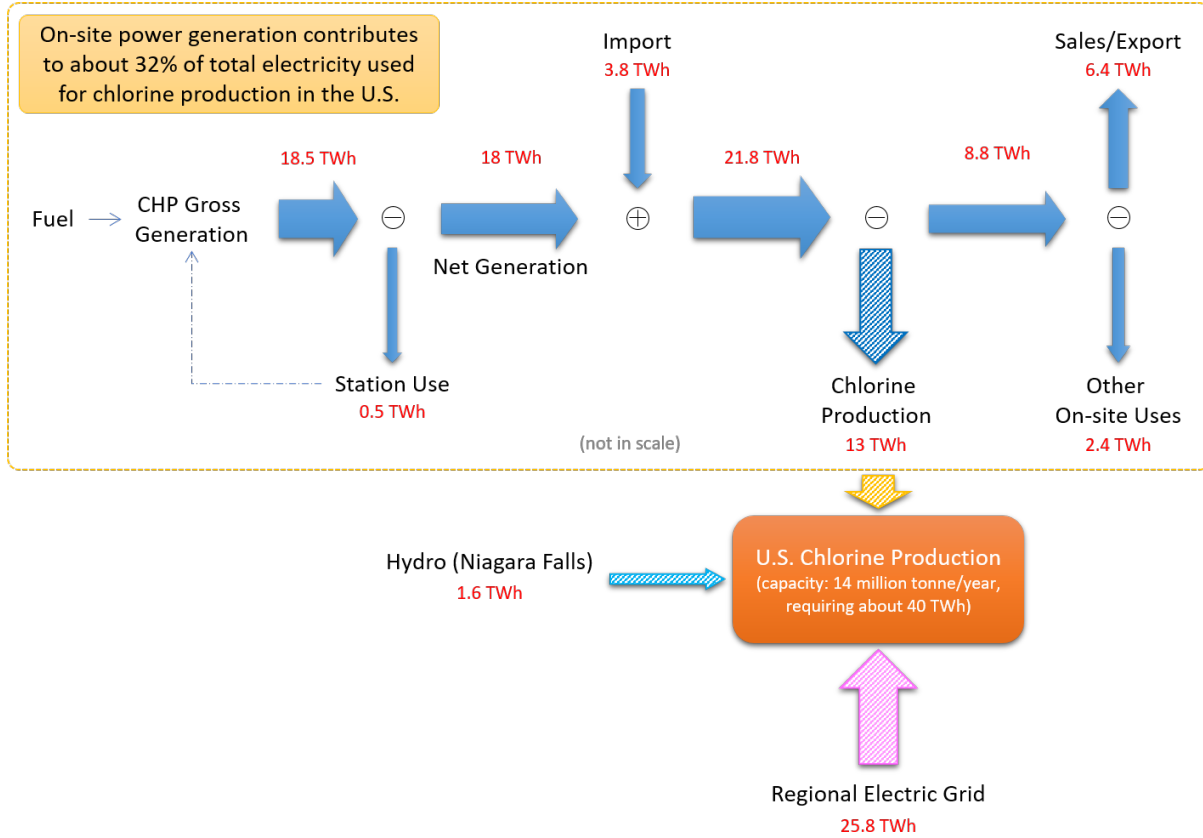


FIGURE 10 Overall Characterization of Electricity Flow for On-site CHP Systems at Chlor-Alkali Plants

In addition to the high-level characterization of electricity flow in CHP plants in the chlor-alkali industry (Figure 10), we estimated key CHP performance metrics such as electrical energy efficiency, thermal energy efficiency, overall system efficiency, and power-to-heat ratio (PHR). Overall effective electrical efficiency is 53%, which is based on electrical fuel consumption (EFC) reported in the EIA-923 form. If we use total fuel consumption (TFC) instead of the pre-allocated EFC values, electrical energy efficiency becomes 38.5%. Assuming 80% efficiency of the waste heat recovery system, overall maximum thermal energy efficiency is 49.2%. Overall CHP system efficiency then becomes 87.7% (theoretical maximum) and PHR is 0.78. Fuel consumption data from the EIA-923 form are based on a higher heating value (HHV), which we converted to a lower heating value (LHV) for consistency in our overall system analysis. The following equations show our methods and plant-by-plant aggregation:

$$\eta_{EffectiveElectric} = \frac{\sum \left[\left(\frac{NetGen_i \times 3.412}{EFC_i \times \frac{LHV_i}{HHV_i}} \right) \times NetGen_i \right]}{\sum NetGen_i} \quad (9)$$

$$\eta_{Thermal} = \frac{\sum \left\{ \left[\frac{(TFC_i \times \frac{LHV_i}{HHV_i} - NetGen_i \times 3.412) \times \eta_{WHR}}{TFC_i \times \frac{LHV_i}{HHV_i}} \right] \times NetGen_i \right\}}{\sum NetGen_i} \quad (10)$$

$$\eta_{CHP} = \frac{\sum \left\{ \left[\frac{NetGen_i \times 3.412 + (TFC_i \times \frac{LHV_i}{HHV_i} - NetGen_i \times 3.412) \times \eta_{WHR}}{TFC_i \times \frac{LHV_i}{HHV_i}} \right] \times NetGen_i \right\}}{\sum NetGen_i} \quad (11)$$

where

$\eta_{EffectiveElectric}$ = electricity generation efficiency;

$\eta_{Thermal}$ = thermal energy efficiency;

η_{CHP} = overall CHP system efficiency;

TFC_i = the total fuel consumption (mmBtu) of the i th plant;

η_{WHR} = the efficiency of waste heat recovery (WHR), assumed as 80%;

$NetGen_i$ = net electricity generation (MWh) of the i th plant;

$EF C_i$ = electric fuel consumption (mmBtu), fuel specifically used for electricity generation; and

LHV_i and HHV_i = the lower and higher heating values, respectively, for the fuel used in the i th plant.

Given that the PHR is lower than 1, it is worth noting that CHP units in the chlor-alkali industry generate more heat than power. As previously discussed, chlor-alkali manufacturing generally requires more electricity than process heat. For the heat generated on site that exceeds process heat demand for chlor-alkali production, we did not give credits. It is possible that the surplus heat generated on site is used for other purposes (not directly related to chlor-alkali production).

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5 OVERALL ELECTRICITY SOURCE AND CARBON INTENSITY

About two-thirds (68%) of total electricity consumed by the U.S. chlor-alkali industry is from the bulk electricity market (or the grid); the remainder (32%) is sourced from on-site power generation, as mentioned earlier. To account for the geographical heterogeneity of electricity generation sources, we examined production capacity and electrical energy consumption of chlor-alkali plants in each of the North American Electric Reliability Corporation (NERC) regions. We then took a bottom-up approach (production-weighted) for regional and national aggregation.

By and large, the U.S. electric grid is composed of three interconnections — Western, Eastern, and ERCOT (Electric Reliability Council of Texas). The Western interconnection is essentially Western Electricity Coordinating Council (WECC), and the ERCOT is Texas Reliability Entity (Texas RE, or TRE). The Eastern interconnection consists of six different regions — Florida Reliability Coordinating Council (FRCC), Midwest Reliability Organization (MRO), Northeast Power Coordinating Council (NPCC), ReliabilityFirst Corporation (RF, or RFC), SERC Reliability Corporation (SERC), and Southwest Power Pool, RE (SPP RE, or SPP). In addition to the three large interconnection systems in mainland U.S., Alaska and Hawaii each has an independent power grid — Alaska Systems Coordinating Council (ASCC, or Alaska interconnection) and Hawaiian Islands Coordinating Council (HICC), respectively. Sometimes, a state boundary (e.g., California or CA) is used to characterize a regional electric grid, but we based our analysis on the NERC regional entities because of data availability. Electricity is continuously exchanged across and within local and regional power markets, but we did not consider this exchange (import/export) aspect. We excluded ASCC and HICC in our analysis, as our focus is on the chlor-alkali industry in the contiguous U.S. Also, we are not aware of chlor-alkali plants in Alaska or Hawaii.

Figure 11 shows the electricity generation mix for the national average, NERC regions, ASCC, HICC, and California in 2016. Some regions rely heavily on coal (e.g., MRO) or natural gas (e.g., FRCC) for power generation. Nuclear and other renewables make up one-third of the total U.S. electricity generation source. The heterogeneity in the regional electricity generation fuel mix results in wide variations in GHG intensity (Figure 12). In general, GHG intensity for electricity generation increases with the total share of fossil fuels (e.g., coal, natural gas, and oil) in the generation mix. However, the composition of fossil fuels can also be an important factor, as can be seen in the cases of SERC and TRE. Fossil fuels account for around 66% of SERC's electricity supply source, whereas up to 78% of TRE electricity is based on fossil fuels. Despite the difference of fossil fuel contribution (66 vs. 78%), SERC and TRE have a very similar GHG intensity (0.58 kg CO₂e/kWh). TRE relies more on fossil fuels than SERC does, but natural gas accounts for 70% of total fossil fuel combustion in TRE (as opposed to 50% in SERC). As typical natural gas power plants emit roughly 50% fewer GHGs than coal (0.6 kg CO₂e/kWh for natural gas vs. 1.1 for coal, on a life cycle basis), overall GHG intensity becomes similar for SERC and TRE.

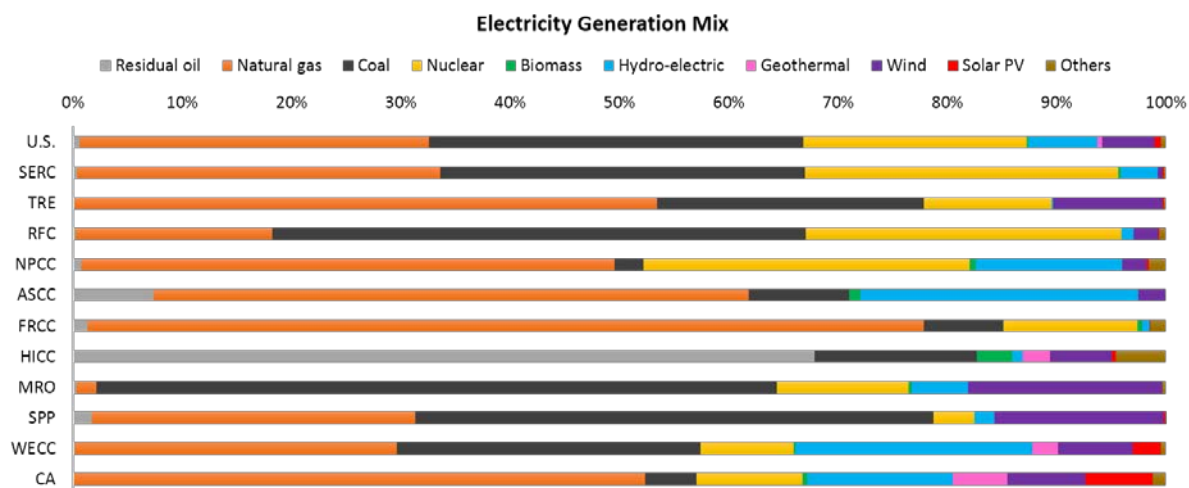


FIGURE 11 Electricity (stationary) Generation Mix Data source: GREET

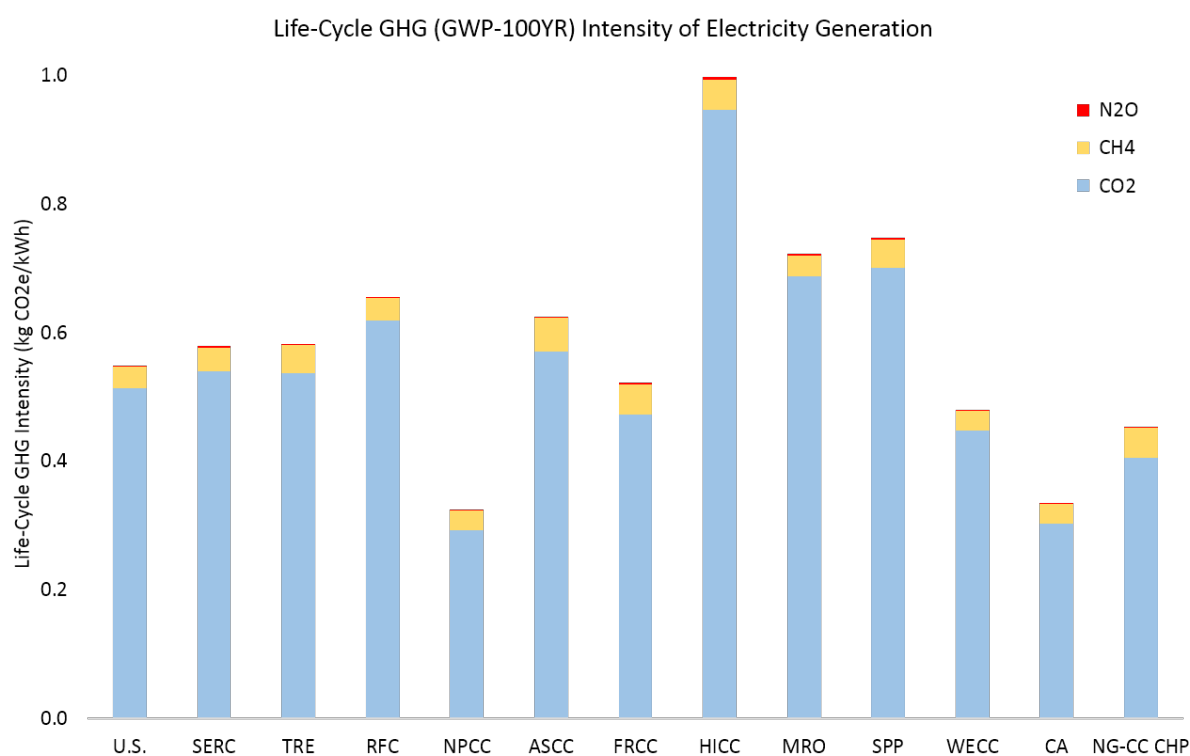


FIGURE 12 Life Cycle GHG Intensity for Electricity (stationary use) Generation, Based on the 100-year Time Horizon Global Warming Potentials (GWP = 100 year) Proposed in the IPCC Fourth Assessment Report (AR5) (IPCC 2015) Data source: for emissions and electricity generation mix: GREET. Greenhouse gases are weighted (multiplied by 1 for CO₂, 30 for CH₄, and 265 for N₂O) and shown in kg CO₂e

All in all, GHG intensity for bulk electricity in each NERC region (Figure 12) is used for 57.8% of total electricity consumption of the U.S. chlor-alkali industry. For chlor-alkali plants in Niagara Falls within the NPCC region, we assumed that 100% hydro-electric power is used, based on our communication with chlor-alkali industry experts in that region. Chlor-alkali plants in the Niagara Falls area account for 6.2% of total industry-wide electricity consumption. For on-site electricity (36%), we used NG-CC CHP as shown in Figure 12.

As for the net benefit of employing a natural gas-powered on-site CHP system, Figure 12 indicates that an NG-CC CHP system will provide net GHG emissions reduction in most of the regions except NPCC. However, as previously discussed, an overall GHG emissions reduction benefit for the chlor-alkali industry will also depend on the contribution of electricity in total energy consumption for chlor-alkali production, as well as how much of electricity consumed by the industry is generated from on-site CHP systems.

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6 EMISSIONS FACTORS FOR NATURAL GAS-POWERED INDUSTRIAL BOILERS

Except for those plants for which all thermal energy demand is met by an on-site CHP system, most chlor-alkali plants generate necessary process heat (including steam) by combusting natural gas in industrial boilers. We used the GREET model for air emissions factors of large natural gas-powered industrial boilers that have more than 100 mmBtu/hr of rated heat input. To see if GREET-based emissions factors are applicable to industrial boilers at chlor-alkali plants, we compared our carbon dioxide (CO₂) emissions estimates and those reported in the Greenhouse Gas Reporting Program (GHGRP) (EPA 2016). We identified four chlor-alkali plants that have matching records (e.g., NAICS code, location) in the GHGRP data. We assumed that all those plants adopt diaphragm cell type, based on the reported input heat rate and our thermal energy intensity discussed earlier. However, it is possible that some plants have both diaphragm and membrane cells in operation, producing chlorine from both cells, for which we are not aware of available data.

Table 9 shows four non-CHP chlor-alkali plants and their annual direct (on-site) CO₂ emissions from industrial boilers — our estimates vs. GHGRP. In calculating total CO₂ emissions, the challenge is to estimate total chlorine production, which is affected by production capacity (million tonne/year) as well as capacity factor. Our estimates of chlorine production capacity were based on the data sources previously discussed in Section 3. Using the production capacity information combined with thermal energy intensity mentioned before, we derived approximate heat input rate, which is a theoretical maximum. Once compared with the reported heat input rate in GHGRP, we obtained a capacity factor that ranges from 30 to 100%. As we use estimates of production capacity and thermal energy intensity (or natural gas fuel input), the actual capacity factor may change with those variables. Multiplying annual chlorine production (tonne/year), natural gas fuel input (mmBtu/tonne), and capacity factor results in annual total natural gas fuel consumed on site. With a CO₂ emissions factor (59.36 kg CO₂ per mmBtu of natural gas combusted in industrial boiler) from GREET, we estimated total annual CO₂ emissions from natural gas boilers. Because of the uncertainty related to actual chlorine production (tonne/year), we also considered cases in which capacity or production changes within $\pm 30\%$ range, in part based on historical capacity factor evolution in the U.S. chlor-alkali industry. For this, capacity can be higher than 100% of reported values, because plant capacity can change over time, as discussed earlier. As Table 9 indicates, the reported total CO₂ emissions in GHGRP fall within the range of our estimates. Our analysis was based on fuel input data for typical chlor-alkali plants; individual plants may vary, however, in terms of energy intensity. The uncertainty associated with annual chlorine production of each plant, as well as the national average capacity factor, may also differ from plant to plant. In addition, it is uncertain whether all reported thermal energy output from natural gas boilers is specifically used for chlorine production. It is possible that some of the thermal energy is used for other purposes that may not be directly related to chlorine production. For the CO₂ emissions intensity analysis in this section, we assumed that hydrogen produced on site (from chlor-alkali processes) is not combusted in boilers. If hydrogen is combusted in boilers, it can lower or eliminate CO₂ emissions from fuel combustion in boilers, depending on the fuel mix of hydrogen and natural gas. This adds another uncertainty in overall CO₂ intensity.

TABLE 9 Annual On-Site CO₂ Emissions from Natural Gas–Powered Industrial Boilers at Chlor-Alkali Plants

Company	Plant Name	Annual Chlorine Production Capacity (million tonne)	Capacity Factor ^a	Natural Gas Fuel Required (mmBtu)	CO ₂ (tonne/year)			GHGRP
					Estimated (GREET-based)			
					Δ Capacity			
					−30%	0%	+30%	
Occidental	Wichita, KS	0.239	100%	1,486,025	61,800	88,200	114,700	99,100
Occidental	Convent, LA	0.353	46%	1,015,675	42,200	60,300	78,400	76,500
Olin	St. Gabriel, LA	0.163	32%	319,460	13,300	19,000	24,700	26,400
Olin	Niagara, NY	0.259	42%	673,779	28,000	40,000	52,000	31,700

^a Based on GHGRP-rated heat input.

Based upon the information of total annual CO₂ emissions and chlorine production, we also estimated CO₂ intensity, with capacity factor reflected (Figure 13). CO₂ intensity for each plant was estimated by dividing annual CO₂ emissions (Table 9) with estimated annual chlorine production (with capacity factor reflected). GREET NG Boiler EMF-based CO₂ intensity refers to the case in which the CO₂ emissions factor for NG boiler from GREET was used (Table 9). As can be seen in Figure 13, GREET EMF-based CO₂ intensity (0.37 kg CO₂/kg Cl₂) falls in the reported range based on GHGRP. Because GHGRP does not report actual chlorine production data, the inherent uncertainty here is the annual production. Overall, given the comparisons of annual total CO₂ emissions and intensity (Table 9 and Figure 13), it is deemed that GREET emissions factors for large natural gas–powered industrial boilers are applicable to the boilers at chlor-alkali plants.

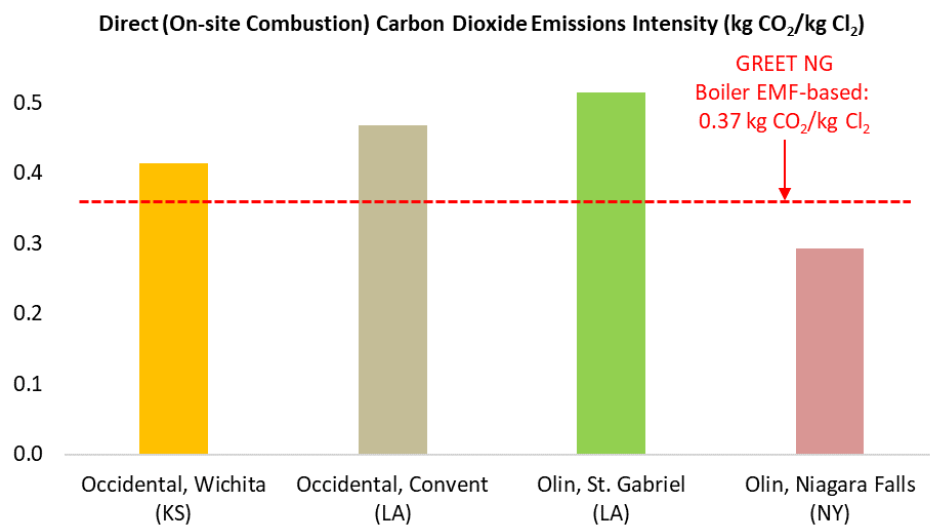


FIGURE 13 CO₂ Intensity of Natural Gas Boilers for Chlorine Production, Based on Reported Annual CO₂ Emissions in GHGRP, Natural Gas-Powered Industrial Boiler Emissions Factors (EMFs) in GREET, and Annual Chlorine Production Capacity

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7 MARKET VALUES OF CHLORINE, SODIUM HYDROXIDE, AND HYDROGEN

Market prices of chlor-alkali co-products (chlorine and sodium hydroxide) change over space (e.g., USA vs. Europe) and time, on which regional and national economic conditions (e.g., growth rate of GDP) have an overarching influence. We gathered longitudinal price data from the CEH Marketing Research Report (Beal and Linak 2011) and Tecnon OrbiChem (2013) materials. Figure 14 shows the historical evolution of chlorine and caustic soda prices in the U.S., which have been somewhere between \$57 and \$442 for chlorine and \$55 and \$1,058 for caustic soda (sodium hydroxide) in nominal U.S. dollars per metric ton. Although chlorine and caustic soda are co-produced from chlor-alkali processes, their prices are not correlated — see the correlation coefficient of 0.013 in Figure 14. The reason is that the two co-products are used for different applications (end products) (ACC 2017a, 2017b).

Figure 15 shows regional variations of caustic soda prices in the U.S. Although some regional differences can be observed, the overall price pattern in all regions follows the national trend shown in Figure 14. Caustic soda price is the lowest in the Gulf Coast area, home to most of the chlor-alkali plants, which has the largest regional share of U.S. chlor-alkali production. One of the contributing factors for the advantage of the Gulf Coast area for chlor-alkali producers may be the cheaper retail price of electricity. Although it differs from region to region, utility (mostly electricity) accounts for the largest cost of chlorine and caustic soda production (Prochemics 2007). In the U.S., 44% of total production

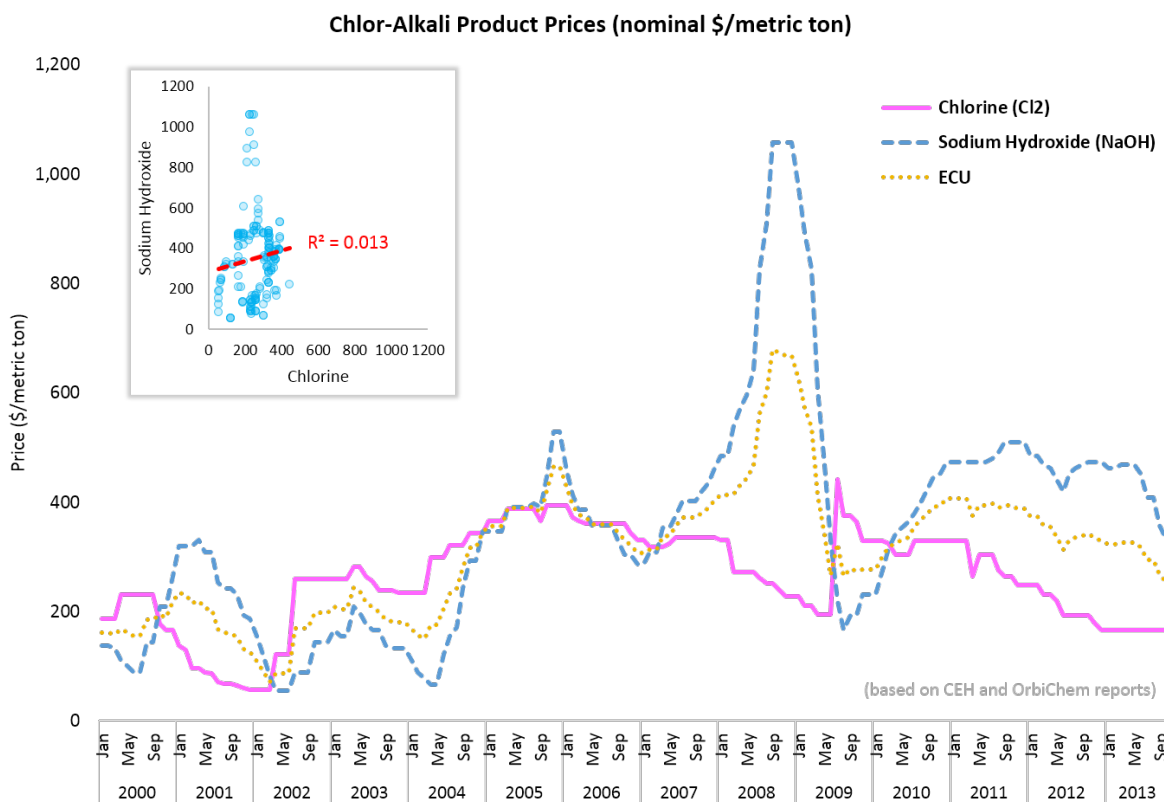


FIGURE 14 Historical Market Price for Chlorine and Caustic Soda in the U.S.

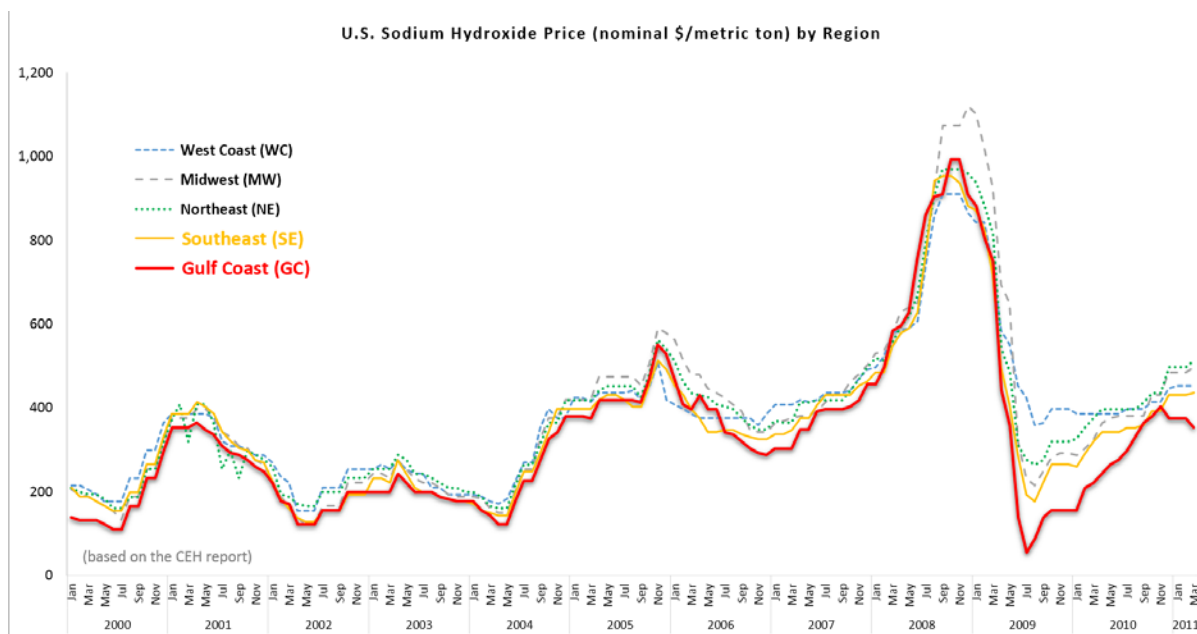


FIGURE 15 Historical Evolution of Regional Caustic Soda Prices in the U.S.

cost is attributable to utility (Figure 16), whereas the corresponding share of utility in overall cost is only 20% in the Middle East (Prochemics 2007). Because of the utility-dominant cost structure as such, chlor-alkali plants in the Gulf Coast area, including Texas and Louisiana (Figure 17), may benefit from the relatively cheap retail price of industrial electricity in the region (EIA 2017b). Other industrial facilities, for example, manufacturers converting chlorine or caustic soda to final products (e.g., polycarbonate for roof panels, polyurethane for insulation materials, soaps) available in the proximity could be another benefit of siting chlor-alkali plants in the Gulf Coast region.

The average 2010–2013 price, since the economic recession in 2008 and 2009, for chlorine and caustic soda has been \$255 and \$441 per metric ton in 2017 real U.S. dollars, respectively. Although more recent market prices are not readily available, the producer price index (PPI) for chlor-alkali chemicals between 2011 and 2017 (FRED 2017) indicates that current prices would not be very different from 2010–2013 averages. For the by-product hydrogen price, we assumed that the price range is \$1 to \$2/kg H_2 , based on personal communication with hydrogen market experts and the H2A model (DOE 2015). On a unit mass (tonne) basis, hydrogen is the most valuable product (\$1,000–\$2,000/tonne H_2) among the three products (chlorine, caustic soda, and hydrogen) coming out of chlor-alkali processes, in comparison to \$255/tonne of chlorine and \$441/tonne of caustic soda. On the other hand, the output mass of hydrogen is the smallest among the three products ($Cl_2:NaOH:H_2 = 1:1.13:0.0285$). What makes hydrogen a by-product is a combined effect of hydrogen price and mass ratio. If hydrogen was \$10,000/tonne H_2 (or \$10/kg H_2), for example, it would not be considered a by-product, but a co-product (like chlorine or caustic soda), providing a similar overall value proposition as the other products (chlorine and caustic soda).

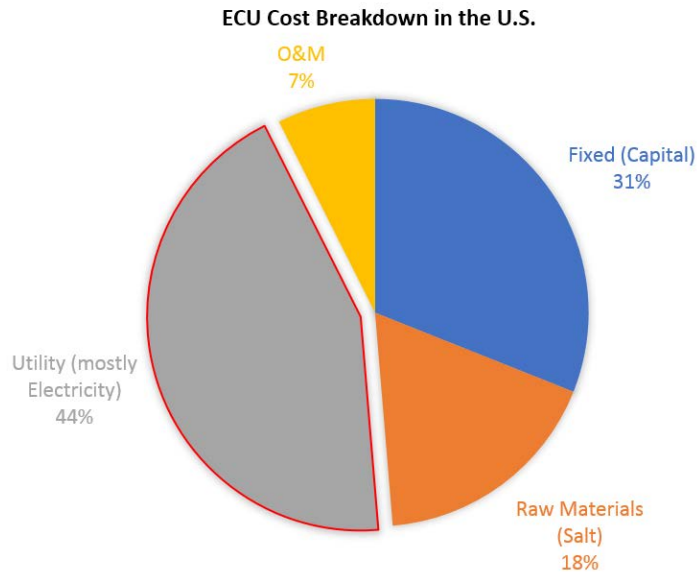


FIGURE 16 Breakdown of Chlor-Alkali Production Cost in the U.S.

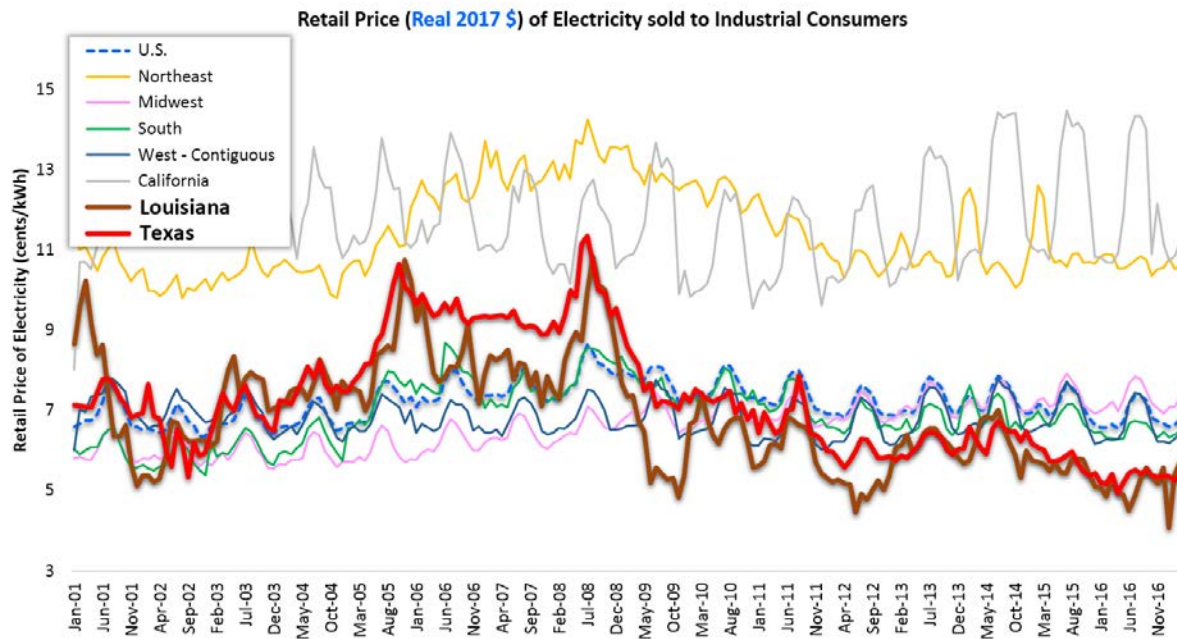


FIGURE 17 Historical Evolution of Retail Price of Industrial Electricity in the U.S. by Region between 2001 and 2016

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8 CASE STUDY: SUBSTITUTION OF HYDROGEN WITH NATURAL GAS FOR HEAT ENERGY

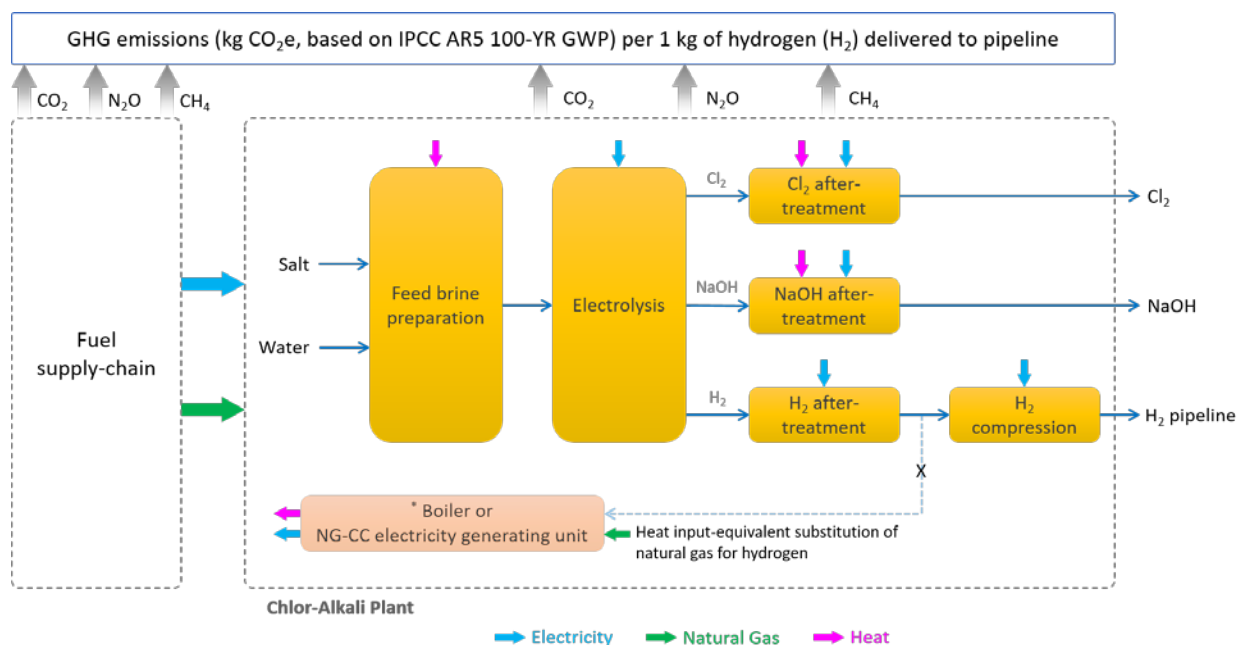
8.1 SUBSTITUTION SCENARIO

By-product hydrogen from chlor-alkali processes is sometimes combusted in industrial boilers to meet on-site heat energy demand. Alternatively, hydrogen can be taken out of the combustion fuel stream and sold to the external market as a commodity. In this case, the heat energy that could have been generated from hydrogen combustion is now provided by natural gas, which we define as a substitution scenario. As opposed to the baseline scenario in which hydrogen is combusted, natural gas substitutes hydrogen as a combustion fuel, generating equivalent heat energy. We assumed that the thermal efficiency (80%) of industrial boilers does not change, whether hydrogen, natural gas, or the mixture of the two is combusted. That said, supplying equivalent process heat energy for chlor-alkali processes by combusting natural gas instead of hydrogen is essentially identical to injecting a thermally equivalent amount of natural gas fuel into boilers. For the same heat input (0.1137 million Btu) of 1 kg of gaseous hydrogen to boilers, 2.545 kg of natural gas is to be combusted, on a LHV basis. In terms of energy use, the only difference between the baseline and substitution scenarios is compression (from 1.3 to 20 bar) for pipeline injection. Whether hydrogen is substituted by natural gas or not, hydrogen after-treatment is always required for safety.

8.2 LIFE CYCLE ASSESSMENT

We conducted a life cycle assessment (LCA) to assess overall GHG emissions benefits of substituting natural gas for hydrogen so that hydrogen can be sold to the merchant market rather than being combusted in industrial boilers or CHP units. The goal of our LCA was to compare the life cycle GHG emissions of two different hydrogen production pathways — chlor-alkali pathway (based on the substitution scenario mentioned above) vs. the conventional natural gas-based SMR pathway. The functional unit is 1 kg of hydrogen produced and delivered to the transmission pipeline.

Figure 18 shows the system boundary for the chlor-alkali pathway. The scope includes the upstream fuel supply chain (for natural gas and electricity) and on-site (e.g., boiler) components. Among individual processes at chlor-alkali plants, we considered only those directly and exclusively related to hydrogen production — hydrogen after-treatment (cooling) and compression. For example, although electrolysis is a main process in chlor-alkali plants, it is used to produce not just hydrogen but also chlorine and caustic soda, and thus we excluded it from our analysis of the substitution scenario. For more integrated analysis incorporating such mixed-use processes, other approaches (e.g., mass allocation) may be adopted, which are not addressed in this report.



(*Boiler generates only heat, whereas NG-CC electricity generating unit (e.g., CHP system) produces both electricity and heat.)

FIGURE 18 System Boundary of Chlor-Alkali Pathway for Hydrogen Production

We used GHG emissions factors in the GREET model for natural gas-based industrial boiler combustion as well as conventional centralized hydrogen production from SMR plants. To compare SMR and chlor-alkali pathways on an apples-to-apples basis, we did not include hydrogen pipeline transmission and distribution or the components (e.g., pre-cooling) related to hydrogen refueling station operation. In other words, as depicted in the system boundary (Figure 18), we accounted for energy use and GHG emissions only up to the point where hydrogen produced from SMR or chlor-alkali plants is compressed and injected into a transmission pipeline. Three types of electricity generation mixes were considered — non-CHP, CHP, and composite — as discussed earlier, all based on regional aggregation. For GHG emissions, we took a weighted sum of CO₂, nitrous oxide (N₂O), and methane (CH₄), based on the 100-year time horizon GWP in the IPCC Fifth Assessment Report (AR5) (IPCC 2015). More specifically, we used 30 for CH₄ and 265 for N₂O as 100-year GWP values relative to CO₂. We presented life cycle GHG emissions in CO₂-equivalent (CO₂e).

8.3 GHG EMISSIONS AND COMPARISON WITH HYDROGEN FROM SMR PLANTS

Compared to conventional hydrogen production from the natural gas-based centralized SMR pathway, hydrogen produced from chlor-alkali plants creates fewer GHG emissions on a life cycle basis (Figure 19). There are slight differences between CHP vs. non-CHP cases, but generally around 20% of life cycle GHG emissions reductions are achieved for hydrogen

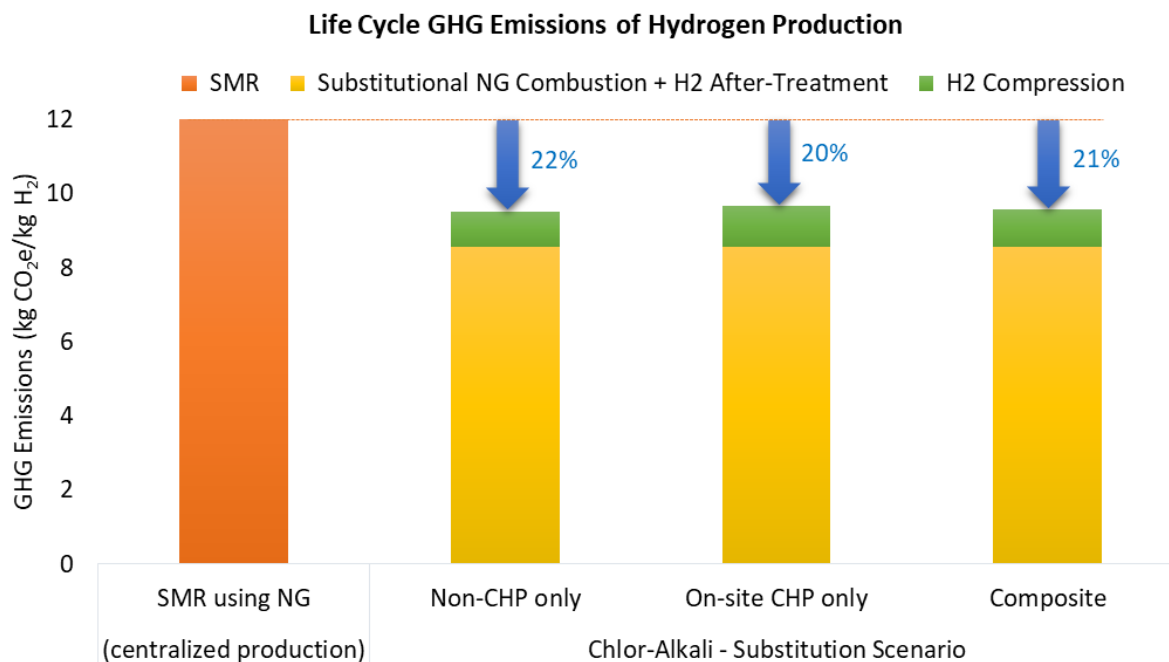


FIGURE 19 Life Cycle GHG Emissions of Hydrogen Production — Centralized SMR vs. Chlor-Alkali Pathways

produced from the chlor-alkali pathway compared to its conventional SMR counterpart. The reason that CHP does not make a big difference is due to the small contribution (5%) of electricity in overall energy use, particularly for the substitution scenario considered in this report. Natural gas, as a substitute for hydrogen, accounts for most of the energy consumed for the substitution scenario. About 3 to 10% of life cycle GHG emissions are attributable to hydrogen compression and hydrogen after-treatment (e.g., cooling), depending on CHP system configuration (3% for CHP-only and 10% for non-CHP-only). The remainder is associated with on-site natural gas combustion (for heat generation) as well as its fuel supply chain.

8.4 LIMITATIONS

In addition to the substitution scenario evaluated in this report, more integrated analysis accounting for the co-production characteristics of chlorine, caustic soda, and hydrogen would be necessary. For this, more detailed co-product treatment strategies (e.g., system boundary expansion, allocation) could be considered. Also, based on the data and method presented, a broader environmental impact analysis could be conducted; for example, looking at criteria air pollutant emissions impacts, water scarcity, and land use. Lastly, due to data availability, we did not consider energy and emissions involved in salt production and transport, which could be revisited in future work.

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Energy Systems Division

9700 South Cass Avenue, Bldg. 362

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