

Production of propane and propene via carbon capture utilisation: comparison of its environmental and economic performance against conventional production methods

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Supplementary Information

1 Conventional production of propane

Propane is a colourless and odourless gaseous aliphatic hydrocarbon with chemical formula C₃H₈. Propane is normally compressed and stored as a liquid due to its boiling point of -42.5 °C (Wypych and Wypych, 2019). Propane's uses include space and water heating, meeting grid CV (constant volume heat capacity) when injecting biomethane into the gas grid and as a fuel in vehicles. However, almost half of the propane consumed by industry is used to manufacture plastic (Bird Fuels, 2020).

Propane has two main origins: 60% is recovered from natural gas extraction and 40% is from refining crude oil (Figure 1). A small fraction is also made renewably from waste feedstocks (WLPGA, 2020). In 2021, global production of propane was estimated at 164.3 million tons (IMARC, 2022). The greatest producers of propane are the U.S., Saudi Arabia and Russia (Britannica, 2019).

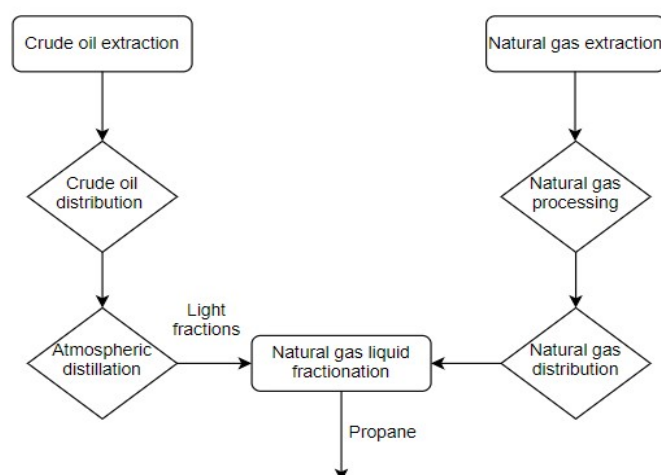


Figure 1. Overall flow diagram for propane production

Natural gas processing involves the removal of the impurities that are non-hydrocarbons and the natural gas liquids (NGLs), which are associated hydrocarbons. The “wetness” indicates the quantity of NGLs contained within it (WLPGA, 2020). Water vapour or “associated water” can be present and is removed by dehydration. The production of propane through NGL fractionation is achieved by separating out all the hydrocarbons present in natural gas. The

most common technologies used in recovery are refrigeration, cryogenic recovery, oil absorption and dry-bed adsorption (Speight, 2007).

Following the separation of the bulk NGLs, the different components are separated through fractionation. This consists of the following distillation columns (Maverick Engineering, 2020): de-ethaniser, de-propaniser, and de-butaniser, for ethane, propane and butane removal, respectively. This leaves pentane and heavier hydrocarbons.

The other common method of conventional propane production is via petroleum refining. Crude oil is a mixture of hydrocarbons that can be separated by distillation. The lighter, more volatile hydrocarbons such as propane are recovered at the top of the atmospheric distillation column (World Petroleum Council, 2020).

2 Conventional production of propene

Propene (also known as propylene) is a colourless gaseous aliphatic hydrocarbon that has a faint petroleum odour with formula C_3H_6 (PubChem, 2020). Propene is the second largest chemical produced globally by volume (IHS Markit, 2019) with a global production capacity of 133.18 million tons in 2020 (Statista, 2023). Propene is a key raw material to produce organic chemicals such as polypropylene, acrylonitrile, propylene oxide and oxo alcohols (IHS Markit, 2019). Acrylonitrile is used in the manufacture of acrylics such as Perspex and propylene oxide is used to produce propylene glycol. Polypropylene accounted for around two-thirds of the consumption of propene in 2017 (Wang, 2021), which is used for packaging and as plastic parts in various industries due to its high melting point, low density, stiffness, and strength (Moretti, 2020).

Propene production typically centres around steam cracking (SC) of naphtha. However, there has been a shift towards ethane and lighter feedstocks that yield less propene (PRNewswire, 2020) as naphtha use is discouraged due to the high price of crude oil and the emergence of shale-based ethane feedstocks (Dean, 2013). To meet this demand, “on-purpose” propene production technologies have increased in prevalence, such as propane dehydrogenation, methanol to propylene, high severity fluidised catalytic cracking and coal to propene (PRNewswire, 2020). For instance, the contribution of propane dehydrogenation to the global propene production will increase from 22% in 2018 to 32% in 2027 (Marsh and Wery, 2019).

SC to produce propene as a by-product of ethylene production accounts for 47% of global installed capacity in 2017, refinery operations contributed 32% and on-purpose technologies contributed the remaining 21% (Nexant, 2018). These are discussed below. The two main options to produce propene from crude oil are represented in Figure 2.

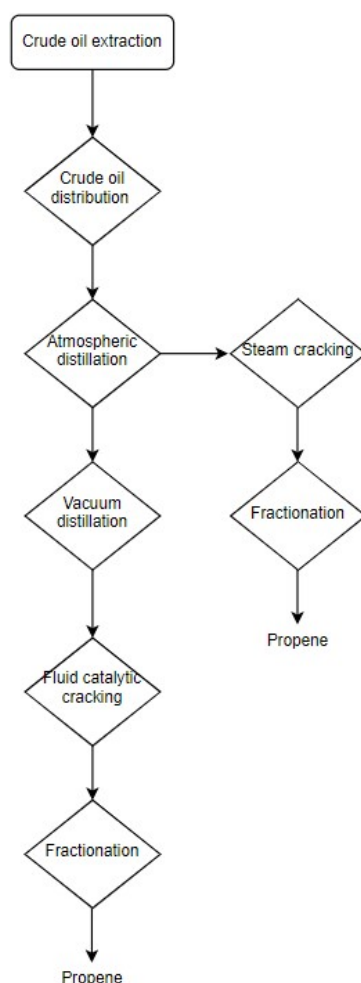


Figure 2. Overall flow diagram for propene production

2.1 Steam cracking (SC)

The prominent feedstocks for propene production from SC are liquid feedstocks such as naphtha. With the rise of NGLs from shale gas, propane, ethane and butane can also be used as reactant gases (Speight, 2011).

The feedstock used has a direct impact on the yield of products. SC of propane produces the highest yield of propene. However, naphtha, which is a more abundant feedstock in a refinery, produces a similar yield.

SC thermally decomposes saturated hydrocarbons with steam into shorter chain, unsaturated alkenes (i.e. olefins) in the absence of oxygen. The feedstocks are preheated, vaporised, mixed with steam and heated to 1050-1150 K in a tubular reactor to produce the olefins. Once the cracking temperature is reached, the product gas is immediately quenched with a colder fluid stream as product yield is dependent on furnace residence time, cracking temperature, hydrocarbon-to-steam ratio, and feed composition. Lower temperatures favour the production of propene (Kutz, 2017).

2.2 Fluid catalytic cracking (FCC)

The feedstock for FCC is usually vacuum gas oil and vacuum residue. When crude oil first enters atmospheric distillation, any of the heavy fractions that cannot be fractionated further are sent to vacuum distillation that produce the gas oil and residue. This is necessary because higher temperatures would cause thermal cracking (Corma et al., 2017).

FCC uses fine powdered catalysts such as zeolite, which are suspended in a flow of rising hydrocarbon feed. The feed of gas oil or residue is fed into the reactor, which vaporises due to heat transfer from the catalyst. The residence time within the reactor is between 2 and 5 seconds to promote selectivity of desirable products and prevent aromatisation and thermal cracking into by-products such as coke and fuel gas (Corma et al., 2017). Several reactions take place, such as isomerisation, cracking, alkylation and dehydrogenation.

2.3 Propane dehydrogenation

Propane dehydrogenation is highly endothermic and is carried out at high temperature and low pressure. There are only two commercially proven technologies for this process, known as CATOFIN, a fixed-bed reactor, and OLEFLEX, a moving bed reactor (Maddah, 2018).

The CATOFIN process passes propane over a fixed-bed of chromium-alumina catalyst. The process is highly endothermic, and the high purity propane is preheated in a charge heater to between 540 to 760 °C before entering the reactor for a residence time of 7 to 15 minutes. The reactor effluent is cooled to reject light ends before being compressed and separated in a flash drum into light products such as ethane and liquids such as propene (Maddah, 2018).

The OLEFLEX plant utilises a slowly moving bed of catalyst that circulates through the reactors before being regenerated after 5 to 10 days of operation. OLEFLEX uses a series of radial flow reactors with inter-stage heaters to supply continuous heat. The product gas is cooled, compressed, dried, and separated cryogenically. A by-product of the process is high purity hydrogen that can be sold to consumers to further improve the economics of the plant.

3 Carbon Capture and Utilisation

Carbon Capture and Utilisation (CCU) is a decarbonisation method that aims to reduce fossil resource depletion and greenhouse gas emissions by utilising captured carbon dioxide as a feedstock (Von der Assen et al., 2013). CO₂ can be transformed into chemicals, materials and transportation fuels (Al-Mamoori et al., 2017). This section analyses the different processes involved in this route.

3.1 Carbon capture

There are three main methods to capture CO₂ industrially:

- Post-combustion capture involves the use of a solvent that has a high affinity for CO₂ in a flue gas stream and is therefore contacted with the solvent in an absorber column. The rich solvent is regenerated by heating in a stripper column (Haszeldine, 2009). The industrial benchmark solvent is monoethanolamine (MEA) due to its relatively low cost and high capture rate (Khoo et al., 2020). However, piperazine (PZ) is an alternative solvent that is gaining momentum as it has a higher cyclic capacity which results in a lower circulation flowrate, a lower regeneration energy (Nwaoha, 2017) and lower corrosivity compared to MEA (Zheng, 2014).
- Oxyfuel combustion capture uses the process of cryogenic distillation in an air separation unit to burn fuel in power plants in the presence of pure oxygen combined with recycled flue gas to control combustion temperatures (Haszeldine, 2009).
- Pre-combustion capture involves reacting a fuel with steam and oxygen under high temperature and pressure to form syngas (NETL, 2020).

Sources for CO₂ are mostly large point-sources such as fossil fuel power plants, which emit 78% of all CO₂ from point sources globally (Von der Assen et al., 2013). The energy required for carbon capture is determined by the effectiveness of the solvent and the concentration of

CO₂ in the flue gas. Example concentrations and price of capture for such point-sources are detailed in Table 1.

Table 1 Table of different large point-sources of carbon dioxide, their concentrations (IPCC, 2005) and costs (Dieterich et al., 2020)

Source of CO ₂	Concentration of CO ₂ in gas stream by vol%	Cost (€/t CO ₂)
Direct air capture	412 ppm	222-268
Coal (power generation)	12 to 15	31-49
Natural gas (power generation)	7 to 10	47-90
Fuel oil (power generation)	8	N/A
Cement production	20	58-87
Integrated steel mills	15	70-73
Ammonia process	100	N/A
Ethylene oxide production	100	N/A

3.2 Carbon dioxide utilisation

The utilisation of CO₂ can be directly in applications such as enhanced oil recovery or conversion into products. Conversion can be split into carboxylation and reduction reactions, where the former produces carboxylic acids, whereas the latter involve the cleavage of carbonyl bonds to form products such as methane and methanol (Von der Assen et al., 2013). CO₂ has a high thermodynamic stability and kinetic inertness (Hong, 2018), so reduction reactions are inherently energy intensive, which is potentially disadvantageous (Von der Assen et al., 2013). Therefore, to have a net negative carbon saving relative to fossil fuels, the energy source must be renewable. To date, there have not been any analyses published comparing both environmentally and economically the conventional production of propane and propene versus methods that utilise captured CO₂ as a feedstock.

3.3 Methanol to propene

Methanol is the simplest carbon-based fuel (Patterson et al., 2019) and considered one of the most important organic feedstocks as it can be used to form products such as formaldehyde, acetic acid and dimethyl ether (DME) (Guil-López et al., 2019). The synthesis of methanol industrially is predominantly from syngas produced from steam reforming of fossil fuels such as natural gas. However, the synthesis of methanol from carbon dioxide is far less exothermic and Karamé (2018) argued that the most straightforward method for methanol production is from the catalytic hydrogenation of CO₂ (Eq.1), with heterogenous catalysis being the preferred route industrially:



Due to the lower exothermicity of methanol synthesis from CO₂ a tube-cooled reactor can be used over a boiler water reactor type. The catalyst is commonly Cu-ZnO based (Guil-López et al., 2019).

Al-Mamoori et al. (2017) proposed the inclusion of the dry reforming of methane as an important pathway to produce methanol and other liquid fuels utilising the Fischer-Tropsch (FT) process.

An analytical review by Garcia-Garcia et al. (2021) found numerous CO₂ emission intensities for hydrogenation of CO₂ using Cu/ZnO/Al₂O₃ as summarised in Table 2.

Table 2. Different emission intensities of hydrogenation of carbon dioxide reported (Garcia-Garcia et al., 2021)

System boundary	Hydrogen and electricity source	CO ₂ emissions
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Gate-to-gate, excluding hydrogen generation and carbon capture	Hydrogen generation not included electricity use (for compression and pumping) from conventional pulverised coal power plant; 0.17 MWh t ⁻¹ for electricity requirements to produce methanol	0.13 t CO ₂ eq t ⁻¹ methanol
Emissions from flue gases, steam and electricity generation, hydrogen and oxygen production and the natural gas supply chain were considered	Electricity from natural gas, hydrogen from steam reforming	2.983 t CO ₂ eq t ⁻¹ methanol
	Electricity from natural gas, hydrogen from wind powered electrolysis	0.657 t CO ₂ eq t ⁻¹ methanol
	Electricity from natural gas, hydrogen from solar powered electrolysis	1.508 t CO ₂ eq t ⁻¹ methanol

Garcia-Garcia et al. (2021) emphasised the lack of studies that include not only emissions from hydrogen generation and carbon capture, but also the utilisation of CO₂ as a feedstock (as those shown in Table 2). Furthermore, the importance of the energy source, particularly for hydrogen generation, was highlighted as a key contributor to the overall environmental impact. Electricity requirements and how they are sourced (e.g. renewable vs fossil) are key factors in determining the environmental burden of the process.

The oil crisis in 1973 generated the first interest for methanol to olefins (MTO) and methanol to gasoline (Boltz et al., 2014). The MTO reaction involves the reversible dehydration of methanol to DME, before the conversion to light olefins (C₂ to C₄). The light olefins can be further converted into products such as methane, ethane, propane, heavier hydrocarbons and aromatics (Dimian et al., 2018).

The oligomerisation reaction occurs in a fluidised bed reactor at 350-500 °C, 2-3 bar and utilises a catalyst, usually SAPO-34, chosen for its activity and robustness (Dimian et al., 2018). To recover propene from the process, the components of the product gas, a mixture of olefinic and paraffinic components up to C₅, are separated out cryogenically in a front-end de-ethaniser set up (Keller et al., 2020). The yield of ethene and propene can be up to 40 wt.% each (Dimian et al., 2018). Vora et al. (1997) found that propene yield was 32 wt% when operating with SAPO-34 and at 450 °C, 1.5 bar.

Due to increasing demand for propene, a new process named methanol to propene (MTP) was developed. The process is characterised by the recycling of olefins to maximise propene selectivity (Boltz et al., 2014). Furthermore, while the MTO reaction utilises a fluidised bed reactor for efficient removal of reaction heat, the MTP uses a fixed-bed reactor. Although the MTO process can use crude methanol, it must be purified for MTP (Jasper and El-Halwagi, 2015).

Jasper and El-Halwagi (2015) simulated an MTO and MTP process and found that the direct CO₂ emissions were 20.9 and 16.1 t CO₂/t propene respectively. Xiang et al. (2015) carried out an LCA of olefins production comparing SC of naphtha to MTO where the methanol was produced from natural gas and coal. Coal to olefins resulted in significantly higher GHG emissions than from natural gas and crude oil, which were roughly equivalent. No studies were found that considered the techno-economics and environmental aspects of an MTP process that utilises captured CO₂.

Figure 3 shows the proposed production pathway for propene via CCU and subsequent MTP.

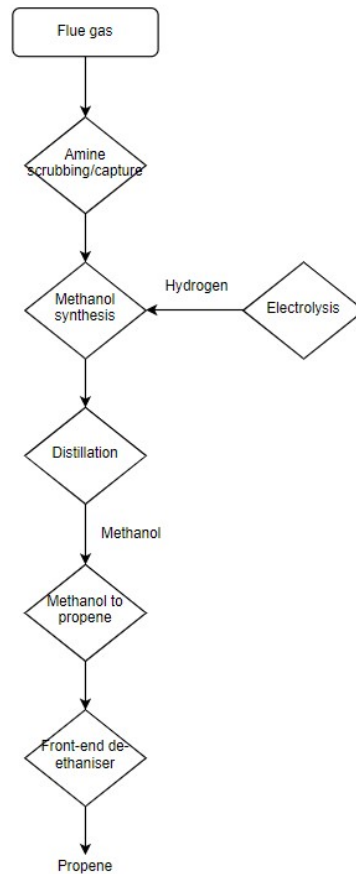


Figure 3. Simplified overview of CCU to produce propene

3.4 Propane

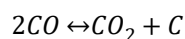
Al-Mamoori et al. (2017) stated there are two ways to convert CO₂ into liquid hydrocarbons. The conversion to methanol to produce propene (described in the previous section), has a low yield of paraffins. Therefore, the production of syngas from methane that is subsequently converted to long-chain hydrocarbons by the FT process is preferred for paraffins (Yao et al., 2020). The main products are paraffins, while olefins, oxygenates and aromatic compounds are produced with significantly lower yield (Dimitriou et al., 2015). The two main stages in this process are described in the following subsections.

3.4.1 Bi-reforming of methane

Syngas is produced from the oxidation of methane, where CO₂ can be used as the oxidising agent in the dry methane reforming process (DRM) (Eq. 2) (Lavoie, 2014). Therefore, the process can be considered a route for carbon dioxide utilisation.



Gangadharan et al. (2012) found that DRM results in significant coke deposition (Boudouard reaction, Eq. 3), which can be drastically reduced when combined with steam methane reforming (SMR), formerly known as bi-reforming of methane (BRM). SMR is the most common process for syngas production (Er-Rbib et al., 2012) as it provides a source of hydrogen for ammonia and methanol synthesis (Oyama et al., 2012). Additionally, Oyama et al. (2012) claimed that previous research on DRM had failed to recognise the issue of the reverse water gas shift reaction (RWGS) reaction, which consumes hydrogen to produce water, as studies mostly operated at atmospheric pressure where water production is small.



(Eq. 3)

Furthermore, Parsapur et al. (2020) and Er-Rbib et al. (2012) argued that the H₂:CO ratio is a critical operating condition in FT processes for selectivity of fuels and DRM obtains a syngas with ratio 1:1, which is limited to direct applications such as acetic acid synthesis. Therefore, DRM should be combined with SMR to achieve a more desirable ratio of 1.7 to 2.4. The use of water electrolysis for H₂ addition may overcome this issue, however, it ignores operational issues of coke deposition if DRM was used.

Youngsub et al. (2012) found that when SMR was combined with DRM, a net reduction of 67% in CO₂ emissions was achieved compared to SMR alone to form syngas.

3.4.2 Fischer-Tropsch (FT)

The FT process is highly exothermic and converts syngas to hydrocarbons at elevated pressures and temperatures within the range of 200 to 350 °C (Guettel et al., 2008). The production of gasoline and linear low molecular mass olefins is achieved with iron-based catalysts and temperatures between 300-350 °C, however, selectivity for high molecular mass linear waxes is achieved at 200-240 °C with iron or cobalt catalysts (Dry, 2002). Due to the exothermic nature of the reactions and to prevent catalyst deactivation, FT uses multi-tubular, slurry or fluidised bed reactors (Dry, 2002).

Figure 4 shows the proposed production pathway for propane via FT and CCU.

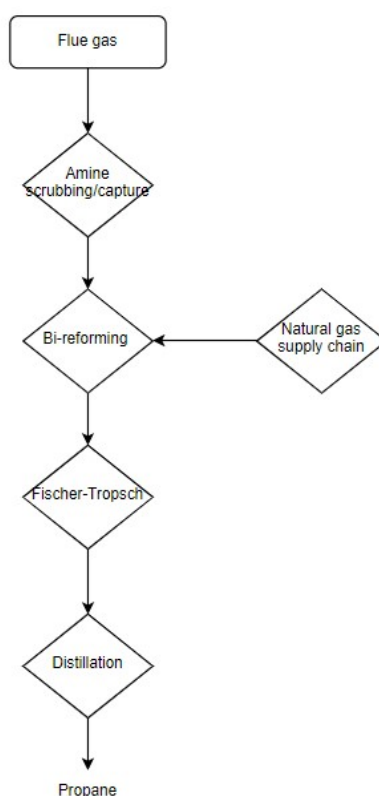


Figure 4. Simplified overview of CCU to produce propane

Reaction conditions such as pressure, temperature, H₂/CO, catalyst and reaction time governs the selectivity of the distribution of products (Krylova, 2014). These reaction conditions influence the chain growth probability, denoted α which varies between 0 and 1 (Kapteijn and Moulijn, 2020) and is a parameter used to evaluate selectivity where long paraffin yield

increases when α is close to 1 (Kapteijn and Moulijn, 2020). α relates to the catalyst surface where the adsorbed hydrocarbon species either desorbs, becomes hydrogenated or has another monomer added. Dry (2002) and Kapteijn and Moulijn (2020) have found that high H_2/CO ratio and high temperature decrease α and therefore increase selectivity of propane. Additionally, Corsaro et al. (2014) found that selectivity of propane varies from less than 5% to almost 15% between 523 and 623 K. Furthermore, Liu et al. (2020) found that C_2 - C_4 paraffin yield was highest (21-17.7 wt.%) when temperatures between 330 and 340 °C were used in combination with Fe_xO_y and $Fe/\alpha-Al_2O_3$ catalysts.

Currently, there is a lack of studies that evaluate the environmental impacts of propane production from FT with syngas derived from bi-reforming of methane. Some cradle-to-grave analyses exist for biologically-derived syngas (biogas or biomass) or from coal and natural gas to fuels such as gasoline.

4 Overall environmental impacts to produce propane from crude oil refining

Table 3. Environmental impacts of processes involved to produce propane from crude oil refining

Crude extraction	Original value	Unit	Value in common unit	Unit	Characterised value	Unit
Crude oil required	16.30486	kg crude oil/kg propane				
Flaring	0.00379885	Nm ³ /kg OE	0.061939717	Nm ³ /kg propane	0.2623981	kgCO ₂ e/kg propane
Methane	0.000707	kg/Nm ³	4.37914E-05	kg/kg propane	0.0009196	kgCO ₂ e/kg propane
Carbon dioxide	3.71	kg/Nm ³	0.229796352	kg/kg propane	0.2297964	kgCO ₂ e/kg propane
Carbon monoxide	0.001	kg/Nm ³	6.19397E-05	kg/kg propane		
Non-methane volatile organic compounds	0.000196	kg/Nm ³	1.21402E-05	kg/kg propane		
Nitrogen oxides	0.00163	kg/Nm ³	0.000100962	kg/kg propane	0.0312981	kgCO ₂ e/kg propane
Dinitrogen monoxide	0.00002	kg/Nm ³	1.23879E-06	kg/kg propane	0.000384	kgCO ₂ e/kg propane
Particulates <2.5um	0.00054	kg/Nm ³	3.34474E-05	kg/kg propane		
Sulfur dioxide	0.17	kg/Nm ³	0.010529752	kg/kg propane		
Mercury	0.0000002	kg/Nm ³	1.23879E-08	kg/kg propane		
Radon-222	0.4	kg/Nm ³	0.024775887	kg/kg propane		
Venting	0.0007	Nm ³ /kg OE	0.011413402	Nm ³ /kg propane	0.1403734	kgCO ₂ e/kg propane
Methane	5.85E-01	kg/Nm ³	0.00667684	kg/kg propane	0.1402136	kgCO ₂ e/kg propane
Carbon dioxide	1.40E-02	kg/Nm ³	0.000159788	kg/kg propane	0.0001598	kgCO ₂ e/kg propane
Helium	1.00E-03	kg/Nm ³	1.14134E-05	kg/kg propane		
Non-methane volatile organic compounds	2.71E-01	kg/Nm ³	0.003093032	kg/kg propane		
Mercury	1.50E-08	kg/Nm ³	1.71201E-10	kg/kg propane		
Radon-222	1.00E-01	kBq/Nm ³	0.00114134	kg/kg propane		
Water Usage & disposal						
Fresh water usage	0.109	kg/kg OE			1.7772297	kg/kg propane
Water disposal intensity (onshore)	1.06	kg/kg OE			17.283152	kg/kg propane

Average oil concentration (produced water)	3.9	mg/l			67.404291	mg/kg propane
Emissions of energy usage for extraction					0.3513403	kgCO ₂ e/kg propane
Diesel burned in generator	0.026	MJ/kg				
NO _x	0.02123816	g/kg crude oil	0.346285222	g/kg propane	0.1073484	kgCO ₂ e/kg propane
PM	0.001117798	g/kg crude oil	0.018225538	g/kg propane		
CO ₂	1.844366509	g/kg crude oil	30.07213772	g/kg propane	0.0300721	kgCO ₂ e/kg propane
SO _x	1.69346E-05	g/kg crude oil	0.000276117	g/kg propane		
Electricity from grid	0.032	kWh/kg	0.41	kgCO ₂ /kWh	0.2139198	kgCO ₂ e/kg propane
Crude distribution						
Pipeline					0.3426169	kgCO ₂ e/kg propane
CO ₂	2.81	kg/bbl extracted	336.8871809	g/kg propane	0.3368872	kgCO ₂ e/kg propane
CH ₄	1.74E-03	kg/bbl extracted	2.08E-01	g/kg propane	0.0043732	kgCO ₂ e/kg propane
N ₂ O	3.65E-05	kg/bbl extracted	0.004375937	g/kg propane	0.0013565	kgCO ₂ e/kg propane
Atmospheric distillation						
Atmospheric distillation					0.2650081	kgCO ₂ e/kg propane
Fuel use (refinery gas)	1977.78	kJ/kg propane				
CO ₂	6.49E-05	kg/kJ	1.28E-01	kg/kg propane	1.28E-01	kgCO ₂ e/kg propane
CH ₄	1.27E-09	kg/kJ	2.51E-06	kg/kg propane	5.27E-05	kgCO ₂ e/kg propane
N ₂ O	6.16E-10	kg/kJ	1.22E-06	kg/kg propane	3.78E-04	kgCO ₂ e/kg propane
Electricity	184.2449	kJ/kg propane			0.0209834	kgCO ₂ e/kg propane
Steam (refinery gas)	1416.892	kJ/kg propane				
CO ₂	7.84E-05	kg/kJ	1.11E-01	kg/kg propane	1.11E-01	kgCO ₂ e/kg propane
CH ₄	1.25E-07	kg/kJ	1.77E-04	kg/kg propane	3.72E-03	kgCO ₂ e/kg propane
N ₂ O	9.85E-10	kg/kJ	1.40E-06	kg/kg propane	4.33E-04	kgCO ₂ e/kg propane
Water usage	0.513333333	m ³ /m ³ propane			0.9753333	kg/kg propane
Natural gas liquid fractionation						
Fractionation					0.0911077	kgCO ₂ e/kg propane
CO ₂	5.33	kg/bbl NGL	0.063691824	kg/kg NGL	0.0636918	kgCO ₂ e/kg propane
CH ₄	0.105	kg/bbl NGL	0.001254717	kg/kg NGL	0.0263491	kgCO ₂ e/kg propane
N ₂ O	0.000288	kg/bbl NGL	3.44151E-06	kg/kg NGL	0.0010669	kgCO ₂ e/kg propane
Propane transportation						
Transportation					0.0552893	kgCO ₂ e/kg propane
CO ₂	4.54	kg/bbl NGL	0.054252	kg/kg NGL	0.054252	kgCO ₂ e/kg propane
CH ₄	2.81E-03	kg/bbl NGL	3.36E-05	kg/kg NGL	7.06E-04	kgCO ₂ e/kg propane

N ₂ O	8.93E-05	kg/bbl NGL	1.07E-06	kg/kg NGL	3.32E-04	kgCO ₂ e/kg propane
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5 Environmental impacts of crude oil extraction

Table 4. Environmental impacts of crude oil extraction

Source	CO ₂	CH ₄	N ₂ O	Unit	Notes	Year
NETL, 2008	0.203219			kg CO ₂ e/kg crude oil	World average, extraction (includes venting and flaring)	2005
Zhou et al., 2019	4.108622	0.0024315	1.2625E-05	(g/ kg crude oil)	China, extraction and processing	

Table 5. Major crude oil producers and associated extraction GHG (NETL, 2008)

Country	Crude oil production (Mt/a) (ESU-Services, 2018)	GHG extraction (kg CO ₂ e/bbl crude oil) (NETL, 2008)
Nigeria	103	128.6
Iraq	193	19.6
Mexico	120	38.4
Saudi-Arabia	598	13.6
USA	556	24.5

Table 6. Conversion of extraction emissions for a bbl of crude oil to per kg (NETL, 2008)

Source	Weighted average (kg CO ₂ e/bbl crude oil)	Barrel of crude oil (kg) (Campbell, 2018)	Average (kg CO ₂ e/kg crude oil)
NETL, 2008	27.638	136	0.203219

Table 7. Direct and indirect emissions for crude oil extraction (Zhou et al., 2019)

Process	Indirect			Direct			Total		
	CO ₂ (g/MJ)	CH ₄ (g/MJ)	N ₂ O (mg/MJ)	CO ₂ (g/MJ)	CH ₄ (g/MJ)	N ₂ O (mg/MJ)	CO ₂ (g/MJ)	CH ₄ (g/MJ)	N ₂ O (mg/MJ)
Crude oil extraction and processing	16	0.05	0.27	71.867	0.002	0	87.867	0.052	0.27

Table 8. Total of emissions from Zhou et al. (2019) converted to per unit mass using (Norwegian Petroleum Directorate, 2020)

CO ₂ (g/kg crude oil)	CH ₄ (g/ kg crude oil)	N ₂ O (g/ kg crude oil)
4.108622	0.0024315	1.2625E-05

Table 9. Venting and flaring emissions

Crude extraction venting				Crude extraction flaring			
Process	Value	Unit	Source	Process	Value	Unit	Source

Crude extraction venting	1.46	Nm ³ /kg OE	ESU-Services, 2018	Crude extraction flaring	0.02	Nm ³ /kg OE	ESU-Services, 2018
Crude extraction venting	0.000092	kg/kg	NETL, 2008	Crude extraction flaring	0.00032	kg/kg	NETL, 2008
Crude extraction venting	1.028	m ³ /m ³	Rahman et al., 2014	Crude extraction flaring	5.796	m ³ /m ³	Rahman et al., 2014

Table 10. Venting and flaring emissions averaged and converted to per unit mass

Crude extraction venting conversion				Crude extraction flaring conversion			
Process	Value	Unit	Source	Process	Value	Unit	Source
Venting (World average)	1.46	Nm ³ /kg OE	ESU-Services, 2018	Crude extraction flaring	0.02	kg/kg OE	ESU-Services, 2018
Venting (U.S.)	0.000129	Nm ³ /kg	NETL, 2008	Crude extraction flaring	0.0004494	Nm ³ /kg	NETL, 2008
Venting (U.S.)	0.001268	Nm ³ /kg	Rahman et al., 2014	Crude extraction flaring	0.0071483	Nm ³ /kg	Rahman et al., 2014
Average	0.000699	Nm ³ /kg	ESU-Services, 2018 removed	Average	0.00379885	Nm ³ /kg	ESU-Services, 2018 removed

Table 11. Flaring of natural gas per kg of crude oil extracted. OE: oil equivalent (ESU-Services, 2018)

Origin	Flaring intensity (Nm ³ /kg OE)	Crude oil production (Mt/a)
Russia	0.02	547.00
Nigeria	0.05	103.00
Kazakhstan	0.02	79.00
Norway	0.00	90.00
Iraq	0.01	193.00
Mexico	0.03	120.00
Saudi-Arabia	0.00	598.00
USA	0.01	556.00
Algeria	0.09	65.00
Egypt	0.04	32.00
Great Britain	0.01	41.00
Weighted average	0.02	

The value of crude oil required was generated from Section 7.

Table 12. Composition of natural gas flared per Nm³. Bq; becquerel (ESU-Services, 2018)

Component	Unit	Sour natural gas
Methane	kg	0.000707
Carbon dioxide	kg	3.71
Carbon monoxide	kg	0.001
Non-methane volatile organic compounds	kg	0.000196
Nitrogen oxides	kg	0.00163

Dinitrogen monoxide	kg	0.00002
Particulates <2.5um	kg	0.00054
Sulfur dioxide	kg	0.17
Mercury	kg	0.0000002
Radon-222	kBq	0.40

Table 13. Flaring and venting for five conventional crude sites in North America (Rahman et al., 2014), conversion: Norwegian Petroleum Directorate, 2020

Crude site	Flaring	Unit	Venting	Unit
1	3.82	m ³ /m ³	0.68	m ³ /m ³
2	0.74	m ³ /m ³	0.74	m ³ /m ³
3	1.33	m ³ /m ³	0.78	m ³ /m ³
4	13.46	m ³ /m ³	0.95	m ³ /m ³
5	9.63	m ³ /m ³	1.99	m ³ /m ³
Average	5.796	m ³ /m ³	1.028	m ³ /m ³
Conversion	0.00677617	m ³ /kg	0.001201847	m ³ /kg
Conversion	0.00714827	Nm ³ /kg	0.001267844	Nm ³ /kg

The significance of natural gas venting in oil and gas production is on average 1.46 Nm³/kg oil equivalent (ESU-Services, 2018).

Table 14. Composition of natural gas vented (ESU-Services, 2018)

Component	Value	Unit
Carbon dioxide	1.40E-02	kg /Nm ³
Helium	1.00E-03	kg /Nm ³
Mercury	1.50E-08	kg /Nm ³
Methane	5.85E-01	kg /Nm ³
NM VOC	2.71E-01	kg /Nm ³
Radon-222	1.00E-01	kBq /Nm ³

Table 15. Venting and flaring parameters (NETL, 2008), conversion: (Unitrove, N.D.)

Parameter	Value	Unit	Value	Unit
Flaring	0.00032	lb/lb	0.00044944	Nm ³ /kg
Venting	0.000092	lb/lb	0.00012921	Nm ³ /kg

Table 16. Water usage and disposal sources for crude oil extraction

Category	Value	Unit	Source	Notes
Fresh water usage	0.109	kg/kg OE	ESU-Services, 2018	World average
Water disposal	1.06	kg/kg OE	ESU-Services, 2018	World average
Average oil concentration (produced water)	3.9	mg/l	IOGP, 2017	

Table 17. Fresh water usage intensity for major crude oil producers (ESU-Services, 2018)

Origin	Fresh water use intensity (m ³ /kg OE)
Russia	0.0000166
Nigeria	0.0000503
Kazakhstan	0.0000166
Norway	0.0000420
Iraq	0.00000314
Mexico	0.000360
Saudi-Arabia	0.00000314
USA	0.000360
Weighted average	0.000109

Table 18. Water disposal intensity for onshore production of crude oil (ESU-Services, 2018)

Origin	Water disposal intensity (onshore) (kg/kg crude oil)
Russia	1.37
Nigeria	0.42
Kazakhstan	1.37
Norway	-
Iraq	1
Mexico	1
Saudi-Arabia	1
USA	0.94
Great Britain	0.77
Average	1.06

Table 19. Energy intensity of crude oil extraction (ESU-Services, 2018)

Origin	Total fossil energy use	Diesel burned in generator	Electricity from grid
Unit	MJ/kg	MJ/kg	kWh/kg
Russia	2.78	0.014	0.060
Nigeria	4.13	0	0.012
Kazakhstan	2.96	0.03	0.017
Norway	2.04	0.057	0.025
Iraq	4.26	0	0.013
Mexico	5.22	0	0.051
Saudi-Arabia	1.01	0	0.013
USA	4.65	0.026	0.032
Average	3.98	0.15	0.02

Table 20. Diesel emissions for sulphur content <15 ppm (U.S. EPA, 1996) (DieselNet, 2019)

Category	Value	Unit
Fuel consumption (U.S.)	0.026	MJ diesel/kg crude oil
NOx	0.02123816	g/kg crude oil
PM	0.001117798	g/kg crude oil
CO ₂	1.844366509	g/kg crude oil
SOx	1.69346E-05	g/kg crude oil

Sulphur content of the diesel found to be 15 ppm which is the limit for non-road fuel that became effective post 2010 (DieselNet, 2009).

Table 21. Grid carbon intensity for U.S. in 2019 (U.S. EIA, 2020)

Country	Year	Source	Value	Unit
U.S.	2019	(U.S. EIA, 2020)	0.41	kgCO ₂ /kWh

6 Environmental impacts of crude oil distribution

Table 22. Environmental impacts of crude oil distribution

Source	CO ₂	CH ₄	N ₂ O	Unit
NETL, 2008	0.020662	2.40441E-05	2.68382E-07	kg/kg crude oil
ESU-Services, 2018		0.0000015		kg/kg crude oil
Average	0.020662	1.27721E-05	2.68382E-07	kg/kg crude oil

7 Process energy allocation and resources required for atmospheric distillation

Table 23. Process energy allocation and yield of petroleum products from 1 kg of crude oil feed (Wang, 2004)

Product	Mass (kg)	wt.%	Fuel (kJ)	Electricity (kJ)	Steam (kJ)	Total (kJ)
Residual oil	0.004	0.40	3.10	0.10	1.60	4.80
Fuel gas	0.044	4.36	92.90	6.20	42.10	141.20
Naphtha	0.001	0.10	0.50	0.10	0.90	1.50
Diesel	0.094	9.31	147.60	9.40	39.90	196.90
Kerosene	0.14	13.56	192.50	11.50	45.60	249.60
Gasoline	0.465	46.04	1334.70	53.60	184.40	1572.70
LPG	0.058	5.74	28.40	5.10	44.80	78.30
Gas oil	0.045	4.46	126.60	2.90	18.60	148.10
Heavy fuel oil	0.040	3.96	58.90	3.10	12.80	74.80
Lube stocks	0.07	6.93	111.40	5.30	202.10	318.80
Asphalt	0.02	1.98	46.80	1.50	23.50	71.80
Waxes	0.009	0.89	14.70	0.70	26.60	42.00

Coke	0.005	0.50	12.10	0.30	3.60	16.00
Hydrogen	0.005	0.50	21.20	0.80	1.40	23.40
Hydrogen sulphide	0.013	1.29	6.20	0.30	1.60	8.10
Total	1.01	100.00	2197.60	100.90	649.50	2948.00

Table 24. Resources/utilities required for generation of 1 kg propane (Wang, 2004)

Refinery product	Mass (kg)	Propane (wt.%)	Mass propane (kg)	Fuel (kJ)	Electricity (kJ)	Steam (kJ)	Total (kJ)	Mass crude oil (kg)
Fuel gas	0.717414	0.19	0.1363086	1514.722	101.0901	686.4347	2302.246	N/A
LPG	0.945682	0.9133	0.8636914	463.0581	83.1548	730.4578	1276.671	N/A
Propane	N/A	N/A	1	1977.78	184.2449	1416.892	3578.917	16.30486

Table 25. Total electricity environmental impact using U.S. grid carbon intensity

Utility	Value	Unit	Conversion	Unit	Notes
Electricity	184.2449	kJ/kg propane	0.02098345	kgCO ₂ /kg propane	Assumed grid intensity U.S. (U.S. EIA, 2020)

Table 26. Environmental impact associated with steam usage in refinery

Stream	CO ₂	CH ₄	N ₂ O	Unit	Source
Steam	0.000069			kg CO ₂ /kJ	Assumed steam boiler efficiency of 0.75 taken (Rahman, 2015) and assumed combustion of refinery gas (Ren et al., 2008)
Steam	8.77949E-05	1.25E-07	9.85E-10	kg/KJ	NETL, 2008
Average	7.83974E-05	1.25E-07	9.85E-10	kg/KJ	

Table 27. Environmental impact associated with refinery gas combustion

Stream	CO ₂	CH ₄	N ₂ O	Unit	Source
Refinery gas combustion (Fuel)	0.000069			kg CO ₂ /kJ	Assumed combustion of refinery gas (Ren et al., 2008)
Refinery gas combustion (Fuel)	6.08029E-05	1.269E-09	6.156E-10	kg/KJ	NETL, 2008
Average	6.49E-05	1.27E-09	6.16E-10	kg/KJ	

Table 28. U.S. Refinery water use for cracking, light cracking and heavy cracking (Sun et al., 2018)

Fuel	Cracking (L/L)	Light Cracking (L/L)	Heavy Cracking (L/L)	Average (L water/L product)
Propane	0.45	0.65	0.44	0.513333
Propene	0.24	0.25	0.24	0.243333

8 Natural gas liquid fractionation

Table 29. Values from NETL, 2008. Conversion made according to Norwegian Petroleum Directorate, 2020.

Process	CO ₂	CH ₄	N ₂ O	Unit
Natural gas liquids production and processing	5.33	0.105	0.000288	kg/bbl NGL
NGL production and processing	0.063691824	0.001255	3.44E-06	kg/kg NGL

9 Propane transportation

Table 30. Values from NETL, 2008. Conversion made according to Norwegian Petroleum Directorate, 2020.

Process	CO ₂	CH ₄	N ₂ O	Unit
Natural gas liquid transport	4.54	2.81E-03	8.93E-05	kg/bbl NGL
NGL transport	0.054252	3.36E-05	1.07E-06	kg/kg NGL

10 Overall environmental impacts to produce propene from natural gas extraction

Table 31. Environmental impacts of processes involved to produce propene environmental impacts from natural gas extraction

Natural gas extraction	Original value	Unit	Value in common unit	Unit	Characterised value	Unit
Natural gas required	901.2567	MJ/kg propane				
Extraction						
CO ₂	3.966628	g/MJ	3574.949611	g/kg propane	3.574949611	kgCO ₂ e/kg propane
CH ₄	0.105473	g/MJ	95.0585183	g/kg propane	1.996228884	kgCO ₂ e/kg propane
N ₂ O	0.000104	g/MJ	0.09412725	g/kg propane	0.029179447	kgCO ₂ e/kg propane
Sand	0.421252	g/MJ	379.6559653	g/kg propane		
Water	0.0134	kg/MJ	12.07683978	kg/kg propane		
Rock cutting	5.25E-04	kg/MJ	0.47278124	kg/kg propane		
Land use	2.38E-10	hectare/MJ	2.149E-07	hectare/kg propane		
Natural gas processing						
Processing						
CO ₂	2.097578	g/MJ	1890.456226	g/kg propane	1.890456226	kgCO ₂ e/kg propane
CH ₄	0.016203	g/MJ	14.60306231	g/kg propane	0.306664309	kgCO ₂ e/kg propane
N ₂ O	8.36E-05	g/MJ	0.07534506	g/kg propane	0.023356969	kgCO ₂ e/kg propane
Water	0.00266	kg/MJ	2.397157163	kg/kg propane		
Natural gas distribution						
Distribution						
CO ₂	2.005	g/MJ	1807.019684	g/kg propane	1.807019684	kgCO ₂ e/kg propane

CH_4	0.016775	g/MJ	15.11858114	g/kg propane	0.317490204	kgCO ₂ e/kg propane
Natural gas liquid fractionation						
Fractionation						
CO ₂	5.33	kg/bbl NGL	0.063691824	kg/kg NGL	0.063691824	kgCO ₂ e/kg propane
CH_4	0.105	kg/bbl NGL	0.001254717	kg/kg NGL	0.026349057	kgCO ₂ e/kg propane
N ₂ O	0.000288	kg/bbl NGL	3.44151E-06	kg/kg NGL	0.001066868	kgCO ₂ e/kg propane
Propane transportation						
Transportation						
CO ₂	4.54	kg/bbl NGL	0.054252	kg/kg NGL	0.054252	kgCO ₂ e/kg propane
CH_4	2.81E-03	kg/bbl NGL	3.36E-05	kg/kg NGL	0.0007056	kgCO ₂ e/kg propane
N ₂ O	8.93E-05	kg/bbl NGL	1.07E-06	kg/kg NGL	0.0003317	kgCO ₂ e/kg propane

The total amount of natural gas required to generate 1kg of propane is determined by converting first into total MJ:

- Propane has a gross heating value of 50.2 MJ/kg (The Engineering Toolbox, N.D.)
- The energy content of propane extracted from natural gas is 5.57% (U.S. EIA, 2020)
- Natural gas energy content 47.5 MJ/kg (IANGV, N.D.)

The breakdown of dry natural gas (U.S. EIA, 2020) and associated natural gas liquids (U.S. EIA, 2020) was obtained:

Table 32. Total dry natural gas production and natural gas liquids in U.S. in 2019 (U.S. EIA, 2020)

Energy carrier	Volume		Energy content		Allocation (%)
	Value	Unit	Value	Unit	
Dry natural gas	962,773	Million m ³	36.62554	MJ/m ³	83.58
Ethane	667,609	Thousand barrels	3.249572	GJ/barrel	5.14
Propane	579,878	Thousand barrels	4.051414	GJ/barrel	5.57
Normal Butane	157,628	Thousand barrels	4.568392	GJ/barrel	1.71
Isobutane	152,579	Thousand barrels	4.568392	GJ/barrel	1.65
Pentanes plus	203,251	Thousand barrels	4.874358	GJ/barrel	2.35

Therefore, the energy allocation of propane against total natural gas production and associated liquids is 5.57%.

11 Environmental impacts of natural gas extraction

Table 33. Natural gas extraction emissions

Process	CO ₂	CH ₄	N ₂ O	Unit	Source
Extraction (U.S.)	42.7	2.34	0.004	tonnes/million m ³ NG	NETL, 2008
Extraction (China)	72.192	0.051	0.121	g/MJ	Zhou et al., 2019

Extraction (U.S. Shale)	2.13			g CO ₂ e/ MJ	Chen et al., 2019
Extraction (U.S. Shale)		539.46		g CH ₄ /MWh	California air resources board, 2018
Extraction (Canadian shale)	8.655			g CO ₂ e/ MJ	Sapkota et al., 2018

Table 34. Natural gas extraction emissions converted to per unit energy

Process	CO ₂	CH ₄	N ₂ O	Unit	Source
Extraction (U.S.)	1.11488251	0.06109661	0.00010444	g /MJ	NETL, 2008
Extraction (China)	72.192	0.051	0.121	g/MJ	Zhou et al., 2019
Extraction (U.S. Shale)	2.13			g CO ₂ e/ MJ	Chen et al., 2019
Extraction (U.S. Shale)		0.14985		g CH ₄ /MJ	California air resources board, 2018
Extraction (Canadian shale)	8.655			g CO ₂ e/ MJ	Sapkota et al., 2018
Average	3.9666275	0.1054733	0.00010444	g/MJ	China source removed from average

Table 35. Natural gas extraction resource and land use

Process	Sand	Unit	Water	Unit	Rock cutting	Unit	Land use	Unit	Source
Extraction (Canadian shale)	0.016134	kg/m ³ NG	0.005524	kg/MJ NG					Raj et al., 2016
Extraction (U.S. Shale)			0.021367	kg/MJ					Kuwayama, 2015
Extraction (Canadian shale)					5.25E-05	kg/MJ	2.38E-10	hectare/MJ	Raj et al., 2016

Table 36 .Average water consumption of U.S. shale gas and tight oil (Kuwayama, 2015)

Fuel	Average water consumption	Unit	Average water consumption	Unit
Shale gas	5	gallons/MMBtu	0.021528	kg/MJ
Tight oil	8.2	gallons/MMBtu	0.035305	kg/MJ

Table 37. Average water and sand use for Canadian shale gas (Raj et al., 2016)

Well	1	2	3	4	Weighted Average/Sum	Unit
Total water	9000	64000	23000	43000	34837.14	m ³ /well
Total sand	1300	3700	1500	4100	2511.87	t/well
Total shale gas	1.36E+08	1.81E+08	2.27E+08	1.13E+08	6.57E+08	m ³ /well
Share of total shale gas	2.07E-01	2.75E-01	3.46E-01	1.72E-01	1.00E+00	
Water use	6.62E-05	3.54E-04	1.01E-04	3.81E-04	5.52E-03	kg/MJ
Sand use	9.56E-06	2.04E-05	6.61E-06	3.63E-05	4.21E-04	kg/MJ

Rock cuttings and land use:

One gas well produces between 110 to 550 tons of rock cuttings and requires one to two hectares of land around the well for drilling rigs, waste storage, drill pipe storage and pump trucks (University of Michigan, 2020).

This source was combined with well data from Raj et al. (2016).

12 Upstream emissions for natural gas

Table 38. Upstream emissions for natural gas production from conventional and shale gas, all units gCO₂e/MJ natural gas extracted (Weber, 2012; California Air Resources Board, 2018; EPA, 2019)

Process/Activity	Conventi	Shale	Conventi	Shale	Shale	Conve	Shale	Conver	Shale	Conve	Shale	Conven	Shale	Convent	Shale
Well pad construction	N/A	0.1	0.2	0.1	N/A	N/A	N/A	1.6	1	N/A	1.5	0.0133	0.31313	0.6044	0.602626
Well drilling	N/A	0.2	N/A	N/A	N/A	0.3	0.3	N/A	N/A	N/A	N/A	N/A	N/A	0.3	0.25
Fracking water	N/A	0.3	N/A	N/A	N/A	N/A	0.3	N/A	N/A	N/A	N/A	N/A	N/A	0	0.3
Fracking chemicals	N/A	0.1	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	0	0.1
Well completion	N/A	1	0	1.3	4.7	0.4	1.6	0	0.8	0	8.6	N/A	N/A	0.1	3
Subtotal	N/A	1.7	0.2	1.4	4.7	0.7	2.2	1.6	1.8	0	10.1	0.0133	0.31313	0.5027	3.173304
Flaring	0.4	0.4	1.8	2	N/A	2.8	2.8	0.4	0.4			N/A	N/A	1.6667	1.4
Plant energy	3.7	3.7	N/A	N/A	N/A	N/A	N/A	4.3	4.1	4.1	4.1	N/A	N/A	4.2	3.966667
Vented CO ₂ at plant	1	1	0.2	0.2	N/A	N/A	N/A	0.8	0.8			N/A	N/A	0.5	0.666667
Fugitive at well	3.4	3.4	1.8	1.8	2.1	1.4	1.4	3.6	3.6	5	5	3.58	3.58	3.076	2.982857
Fugitive at plant	1.5	1.5	1.2	1.2	0.6	N/A	N/A	0.8	0.8	0.4	0.4	N/A	N/A	0.8	0.9
Workover	N/A	N/A	0	4.6	4.7	N/A	N/A	0	1.5			0	0.0637	0	2.715925
Liquid unloading	2.5	N/A	6.6	N/A	N/A	N/A	N/A	5.9	N/A	0.6		0.2389	0.2389	3.3347	0.2389
Subtotal	12.5	10	11.6	9.8	7.4	4.2	4.2	15.8	11.2	10.1	9.5	3.8189	3.8826	9.1038	7.997514
Compression fuel	0.4	0.4	0.4	0.4	N/A	0.2	0.2	0.3	0.3	0.6	0.6	N/A	N/A	0.375	0.38
Fugitive transmission	1.9	1.9	2.3	2.3	1.8	1.7	1.7	0.9	0.9	6.8	6.8	3.899	3.899	3.1198	2.757
Subtotal	2.3	2.3	2.7	2.7	1.8	1.9	1.9	1.2	1.2	7.4	7.4	3.899	3.899	3.2332	3.028429
Upstream subtotal	14.8	14	14.5	13.9	13.9	6.8	8.3	18.6	14.2	17.5	27	7.7312	8.09473	13.322	14.19925

13 Environmental impacts of natural gas processing

Table 39. Environmental impacts of natural gas processing

Process	CO ₂	CH ₄	N ₂ O	Water usage	Unit	Source
Processing (U.S.)	90.4	0.29	0.0032		tonnes/million m ³ NG	NETL, 2008
Processing (China)				129	kg/t	Zhou et al., 2019
Processing (U.S. Shale gas)	2.47				g CO ₂ e/ MJ	Chen et al., 2019
Processing (U.S.)		89.4			g CH ₄ /MWh	California air resources board, 2018
Processing (U.S.)	1.36				gCO ₂ e/MJ	EPA, 2019
Processing (U.S.)	2.2				gCO ₂ e/MJ	Tong, 2015
Processing (Amine gas treating)	0.013	0.000971		kg CO ₂ /kg NG		NETL, 2014
Processing (Dehydration)		3.40E-04		kg CH ₄ /kg		NETL, 2014

Table 40. Environmental impacts of natural gas processing converted to per unit energy

Process	Value CO ₂	Value CH ₄	Value N ₂ O	Water usage	Unit	Source
Processing (U.S.)	2.36031332	0.0075718	8.35509E-05		g /MJ	NETL, 2008
Processing (China)				0.002659794	kg/MJ	Zhou, 2019
Processing (U.S. Shale gas)	2.47				g CO ₂ e/ MJ	Chen et al., 2019
Processing (U.S.)		0.02483333			g CH ₄ /MJ	California air resources board, 2018

Processing (U.S.)	1.36				gCO ₂ e/MJ	EPA, 2019
Processing (U.S.)	2.2				gCO ₂ e/MJ	Tong, 2015
Average	2.09757833	0.01620257	8.35509E-05	0.002659794		
Sum (Amine gas & Dehydration)	0.273684	0.0276			g /MJ	NETL, 2014

To convert:

- Natural gas energy content 38.3 MJ/m³ (IANGV, N.D.)
- Natural gas energy content 47.5 MJ/kg (IANGV, N.D.)

14 Environmental impacts of natural gas distribution

Table 41. Environmental impacts of natural gas distribution

Process	CO ₂	CH ₄	N ₂ O	Unit	Source
Pipeline (Canadian shale)	1.82			gCO ₂ eq/MJ	Sapkota et al., 2018
Distribution (U.S.)		60.39		g/MWh	California air resources board, 2018
Distribution (U.S.)	2.19			gCO ₂ eq/MJ	EPA, 2019

Table 42. Environmental impacts of natural gas distribution converted to per unit energy

Process	Value CO ₂	Value CH ₄	Value N ₂ O	Unit	Source
Pipeline (Canadian shale)	1.82			gCO ₂ eq/MJ	Sapkota et al., 2018
Distribution (U.S.)		0.016775		g/MJ	California air resources board, 2018
Distribution (U.S.)	2.19			gCO ₂ eq/MJ	EPA, 2019
Average	2.005	0.016775	0	g/MJ	

15 Environmental impacts of natural gas liquid fractionation

Table 43. Environmental impacts of natural gas liquid fractionation

Process	Value CO ₂	Value CH ₄	Value N ₂ O	Unit	Source
Natural gas liquids production and processing	5.33	0.105	0.000288	kg/bbl NGL	NETL, 2008
NGL production and processing	0.063692	0.001254717	3.44151E-06	kg/kg NGL	

16 Environmental impacts of propane transportation

Table 44. Environmental impacts of propane transportation

Process	CO ₂	CH ₄	N ₂ O	Unit	Source
Natural gas liquid transport	4.54	2.81E-03	8.93E-05	kg/bbl NGL	NETL, 2008
NGL transport	0.054252	3.36E-05	1.07E-06	kg/kg NGL	

17 Overall environmental impacts to produce propene from steam cracking

Table 45. Environmental impacts of processes involved to produce propene from steam cracking

Crude extraction	Original value	Unit	Value in common unit	Unit	Characterised value	Unit
Crude oil required	87.4125874	kg crude oil/kg propene				
Flaring	0.00379885	Nm ³ /kg OE	0.332067308	Nm ³ /kg propene	1.4067523	kg CO ₂ e/kg propene
Methane	0.000707	kg/Nm ³	0.000234772	kg/kg propene	0.0049302	kg CO ₂ e/kg propene
Carbon dioxide	3.71	kg/Nm ³	1.231969711	kg/kg propene	1.2319697	kg CO ₂ e/kg propene
Carbon monoxide	0.001	kg/Nm ³	0.000332067	kg/kg propene		
Non-methane volatile organic compounds	0.000196	kg/Nm ³	6.50852E-05	kg/kg propene		
Nitrogen oxides	0.00163	kg/Nm ³	0.00054127	kg/kg propene	0.1677936	kg CO ₂ e/kg propene
Dinitrogen monoxide	0.00002	kg/Nm ³	6.64135E-06	kg/kg propene	0.0020588	kg CO ₂ e/kg propene
Particulates <2.5um	0.00054	kg/Nm ³	0.000179316	kg/kg propene		
Sulfur dioxide	0.17	kg/Nm ³	0.056451442	kg/kg propene		
Mercury	0.0000002	kg/Nm ³	6.64135E-08	kg/kg propene		
Radon-222	0.4	kg/Nm ³	0.132826923	kg/kg propene		
Venting	0.0007	Nm ³ /kg OE	0.061188811	Nm ³ /kg propane	0.7525612	kg CO ₂ e/kg propene
Methane	5.85E-01	kg/Nm ³	0.035795455	kg/kg propene	0.7517045	kg CO ₂ e/kg propene
Carbon dioxide	1.40E-02	kg/Nm ³	0.000856643	kg/kg propene	0.0008566	kg CO ₂ e/kg propene
Helium	1.00E-03	kg/Nm ³	6.11888E-05	kg/kg propene		
Non-methane volatile organic compounds	2.71E-01	kg/Nm ³	0.016582168	kg/kg propene		
Mercury	1.50E-08	kg/Nm ³	9.17832E-10	kg/kg propene		
Radon-222	1.00E-01	kBq/Nm ³	0.006118881	kg/kg propene		
Water Usage & disposal						
Fresh water usage	0.109	kg/kg OE			9.527972	kg/kg propene
Water disposal intensity (onshore)	1.06	kg/kg OE			92.657343	kg/kg propene
Average oil concentration (produced water)	3.9	mg/l			361.36364	mg/kg propene
Emissions of energy usage for extraction					1.8835836	kg CO ₂ e/kg propene
Diesel burned in generator	0.026	MJ/kg				
NOx	0.02123816	g/kg crude oil	1.8564825	g/kg propene	0.5755096	kg CO ₂ e/kg propene
PM	0.001117798	g/kg crude oil	0.097709605	g/kg propene		
CO ₂	1.844366509	g/kg crude oil	161.2208487	g/kg propene	0.1612208	kg CO ₂ e/kg propene
SOx	1.69346E-05	g/kg crude oil	0.001480301	g/kg propene		
Electricity from grid	0.032	kWh/kg	0.41	kgCO ₂ /kWh	1.1468531	kg CO ₂ e/kg propene
Crude distribution						

Pipeline					1.8368161	kg CO ₂ e/kg propene
CO ₂	2.81	kg/bbl extracted	1806.098313	g/kg propene	1.8060983	kg CO ₂ e/kg propene
CH ₄	1.74E-03	kg/bbl extracted	1.116438708	g/kg propene	0.0234452	kg CO ₂ e/kg propene
N ₂ O	3.65E-05	kg/bbl extracted	0.023459996	g/kg propene	0.0072726	kg CO ₂ e/kg propene
Atmospheric distillation						
Atmospheric distillation	6.99	kg naphtha/kg propene			1.8207261	kg CO ₂ e/kg propene
CO ₂	0.25960588	kg/kg naphtha	1.814645098	kg/kg propene	1.8146451	kg CO ₂ e/kg propene
CH ₄	5.07638E-06	kg/kg naphtha	3.54839E-05	kg/kg propene	0.0007452	kg CO ₂ e/kg propene
N ₂ O	2.46242E-06	kg/kg naphtha	1.72123E-05	kg/kg propene	0.0053358	kg CO ₂ e/kg propene
Water usage	0.243333333	m ³ /m ³ propene			0.4623333	kg/kg propene
Steam cracking						
Steam cracking					1.42E+00	kg CO ₂ e/kg propene
CO ₂	1.15E+00	kg/kg propene			1.15E+00	kg CO ₂ e/kg propene
CH ₄	2.62E-05	kg/kg propene			5.51E-04	kg CO ₂ e/kg propene
N ₂ O	3.40E-04	kg/kg propene			1.06E-01	kg CO ₂ e/kg propene
NO _x	5.18E-04	kg/kg propene			1.61E-01	kg CO ₂ e/kg propene
CO	5.58E-04	kg/kg propene				
SO ₂	1.27E-05	kg/kg propene				
VOC	7.97E-05	kg/kg propene				
PM2.5	1.27E-04	kg/kg propene				
PM10	1.27E-04	kg/kg propene				
Fractionation						
Fractionation					0.0911077	kgCO ₂ e/kg propene
CO ₂	5.33	kg/bbl NGL	0.063691824	kg/kg NGL	0.0636918	kgCO ₂ e/kg propene
CH ₄	0.105	kg/bbl NGL	0.001254717	kg/kg NGL	2.63E-02	kgCO ₂ e/kg propene
N ₂ O	0.000288	kg/bbl NGL	3.44151E-06	kg/kg NGL	1.07E-03	kgCO ₂ e/kg propene

18 Environmental impacts of steam cracking

Table 46. Environmental impacts of steam cracking

Process	CO ₂	CH ₄	N ₂ O	NO _x	CO	SO ₂	VOC	PM2.5	PM10	Unit	Source
Naphtha steam cracker	6.83E-01	1.52E-05	7.39E-06							kg/kg propene	Ren et al., 2008
Naphtha steam cracker	0.881973	1.97E-05	9.54E-06							kg/kg propene	Ren et al., 2006 (Converting energy use into fuel)

											grade by product emissions)
Naphtha steam cracker	1.7									kg/kg propene	Ren et al., 2006
Naphtha steam cracker	1.3		1.33E-03								Keller et al., 2020
Naphtha steam cracker	1.195166	4.38E-05	1.59E-05	0.000518	0.000558	1.27E-05	8E-05	0.000127	0.000127	kg/kg propene	Lee and Elgowainy, 2018 (Natural gas is combustion fuel)
Average	1.15E+00	2.62E-05	3.40E-04	5.18E-04	5.58E-04	1.27E-05	7.97E-05	1.27E-04	1.27E-04	kg/kg propene	

Table 47. Average steam cracker yield of propene when naphtha used as feedstock

Feedstock	Value	Unit	Source
Naphtha	13	% wt.	Akah, 2015
Naphtha	14.5	% wt.	Ren et al., 2006
Naphtha	15.4	% wt.	Lee and Elgowainy, 2018
Average	14.3	% wt.	

Yield of naphtha is 8 wt.% crude oil (Ren, 2008)

Table 48. Environmental impact of producing naphtha from atmospheric distillation of crude oil (Ren, 2008)

Process	CO ₂	CH ₄	N ₂ O	Unit	Source
Naphtha production (world average)	2.60E-01	5.08E-06	2.46E-06	kg/kg naphtha	Ren et al., 2008

19 Overall environmental impacts to produce propene from fluid catalytic cracking

Table 49. Environmental impacts of processes involved to produce from fluid catalytic cracking

Crude extraction	Original value	Unit	Value in common unit	Unit	Characterised value	Unit
Crude oil required	33.38214248	kg crude oil/kg propene				
Flaring	0.00379885	Nm ³ /kg OE	0.126813752	Nm ³ /kg propene	0.5372271	kg CO ₂ e/kg propene
Methane	0.000707	kg/Nm ³	8.96573E-05	kg/kg propene	0.0018828	kg CO ₂ e/kg propene
Carbon dioxide	3.71	kg/Nm ³	0.47047902	kg/kg propene	0.470479	kg CO ₂ e/kg propene
Carbon monoxide	0.001	kg/Nm ³	0.000126814	kg/kg propene		
Non-methane volatile organic compounds	0.000196	kg/Nm ³	2.48555E-05	kg/kg propene		
Nitrogen oxides	0.00163	kg/Nm ³	0.000206706	kg/kg propene	0.064079	kg CO ₂ e/kg propene
Dinitrogen monoxide	0.00002	kg/Nm ³	2.53628E-06	kg/kg propene	0.0007862	kg CO ₂ e/kg propene

Particulates <2.5um	0.00054	kg/Nm ³	6.84794E-05	kg/kg propene		
Sulfur dioxide	0.17	kg/Nm ³	0.021558338	kg/kg propene		
Mercury	0.0000002	kg/Nm ³	2.53628E-08	kg/kg propene		
Radon-222	0.4	kg/Nm ³	0.050725501	kg/kg propene		
Venting	0.0007	Nm ³ /kg OE	0.0233675	Nm ³ /kg propane	0.2873969	kg CO ₂ e/kg propene
Methane	5.85E-01	kg/Nm ³	0.013669987	kg/kg propene	0.2870697	kg CO ₂ e/kg propene
Carbon dioxide	1.40E-02	kg/Nm ³	0.000327145	kg/kg propene	0.0003271	kg CO ₂ e/kg propene
Helium	1.00E-03	kg/Nm ³	2.33675E-05	kg/kg propene		
Non-methane volatile organic compounds	2.71E-01	kg/Nm ³	0.006332592	kg/kg propene		
Mercury	1.50E-08	kg/Nm ³	3.50512E-10	kg/kg propene		
Radon-222	1.00E-01	kBq/Nm ³	0.00233675	kg/kg propene		
Water Usage & disposal						
Fresh water usage	0.109	kg/kg OE			3.6386535	kg/kg propene
Water disposal intensity (onshore)	1.06	kg/kg OE			35.385071	kg/kg propene
Average oil concentration (produced water)	3.9	mg/l			138.00178	mg/kg propene
Emissions of energy usage for extraction					0.719325	kg CO ₂ e/kg propene
Diesel burned in generator	0.026	MJ/kg				
NOx	0.02123816	g/kg crude oil	0.708975277	g/kg propene	0.2197823	kg CO ₂ e/kg propene
PM	0.001117798	g/kg crude oil	0.037314488	g/kg propene		
CO ₂	1.844366509	g/kg crude oil	61.56890559	g/kg propene	0.0615689	kg CO ₂ e/kg propene
SOx	1.69346E-05	g/kg crude oil	0.000565314	g/kg propene		
Electricity from grid	0.032	kWh/kg	0.41	kgCO ₂ /kWh	0.4379737	kg CO ₂ e/kg propene
Crude distribution						
Pipeline					0.7014649	kg CO ₂ e/kg propene
CO ₂	2.81	kg/bbl extracted	689.7339732	g/kg propene	0.689734	kg CO ₂ e/kg propene
CH ₄	1.74E-03	kg/bbl extracted	0.426358687	g/kg propene	0.0089535	kg CO ₂ e/kg propene
N ₂ O	3.65E-05	kg/bbl extracted	0.008959178	g/kg propene	0.0027773	kg CO ₂ e/kg propene
Atmospheric & Vacuum distillation						
Atmospheric & Vacuum distillation	18.69399979	kg unfinished oil (gas oil/residue)/kg propene			1.87E+00	kg CO ₂ e/kg propene
CO ₂	9.73E-02	kg/kg unfinished oil	1.82E+00	kg/kg propene	1.82E+00	kg CO ₂ e/kg propene
CH ₄	1.17E-04	kg/kg unfinished oil	2.19E-03	kg/kg propene	4.60E-02	kg CO ₂ e/kg propene
N ₂ O	1.71E-06	kg/kg unfinished oil	3.19E-05	kg/kg propene	9.90E-03	kg CO ₂ e/kg propene
Water usage	0.243333333	m ³ /m ³ propene			0.4623333	kg/kg propene

Fluid catalytic cracking						
<i>FCC</i>					1.7362352	kg CO ₂ e/kg propene
CO ₂	0.852311642	kg/kg propene			0.8523116	kg CO ₂ e/kg propene
CH ₄	9.44388E-05	kg/kg propene			1.98E-03	kg CO ₂ e/kg propene
N ₂ O	1.77073E-05	kg/kg propene			5.49E-03	kg CO ₂ e/kg propene
NO _x	0.002827262	kg/kg propene			8.76E-01	kg CO ₂ e/kg propene
SO ₂	0.000493836	kg/kg propene				
SO _x	0.027711887	kg/kg propene				
HCN	1.69203E-07	kg/kg propene				
<i>PM</i>	0.004581594	kg/kg propene				
NH ₃	0.00314796	kg/kg propene				
<i>Pb</i>	6.29592E-06	kg/kg propene				
<i>Hg</i>	1.37723E-06	kg/kg propene				
As	2.75447E-07	kg/kg propene				
VOC	8.46014E-05	kg/kg propene				
Fractionation						
<i>Fractionation</i>					0.0911077	kg CO ₂ e/kg propene
CO ₂	5.33	kg/bbl NGL	0.063691824	kg/kg NGL	0.0636918	kg CO ₂ e/kg propene
CH ₄	0.105	kg/bbl NGL	0.001254717	kg/kg NGL	2.63E-02	kg CO ₂ e/kg propene
N ₂ O	0.000288	kg/bbl NGL	3.44151E-06	kg/kg NGL	1.07E-03	kg CO ₂ e/kg propene

20 Environmental impacts of atmospheric & vacuum distillation

Table 50. Environmental impacts of atmospheric & vacuum distillation

Process	CO ₂	CH ₄	N ₂ O	Unit	Source
Vacuum distillation	14.7	0.0177	0.000258	kg/bbl unfinished oils	NETL, 2008
Vacuum distillation	0.0973032	0.0001172	1.71E-06	kg/kg unfinished oil	NETL, 2008

21 Environmental impacts of fluid catalytic cracking catalytic cracking

Table 51. Environmental impacts of fluid catalytic cracking catalytic cracking

FCC emissions	CO ₂	CH ₄	N ₂ O	NO _x	SO ₂	SO _x	HCN	PM	NH ₃	Pb	Hg	As	VOC	Unit	Source
FCC unit with ESP & CO boiler				0.00401		0.0278	2E-07	0.002518						kg/kg propene	U.S. EPA, 2015
FCC regenerator and reformer emissions				0.00393		0.0276		0.010821	0.0031	6.3E-06	1.4E-06	3E-07		kg/kg propene	EEA, 2016
FCC (China)	0.09													kg/kg propene	Jia et al., 2020
FCC	0.18261													kg/kg propene	Elgowainy, 2014
FCC (synthetic crude oil)	0.12374													kg/kg propene	Nimana et al., 2015
FCC	3.01289	9E-05	1.8E-05	0.00053	0.00049			0.000405					8E-05	kg/kg propene	Sun et al., 2019
Average	0.85231	9E-05	1.8E-05	0.00283	0.00049	0.0277	2E-07	0.004582	0.0031	6.3E-06	1.4E-06	3E-07	8E-05	kg/kg propene	

Table 52. Yield of propene from FCC when a gas oil feed is used

FCC yield	Value	Unit	Source
Vacuum gas oil feed	5.647922	wt.% propene overall	Stratiev et al., 2020
Gas oil feed	5.4	wt.% propene overall	Adewuyi et al., 1995
Vacuum gas oil feed	5	wt.% propene overall	Siddiqui et al., 2011
Average	5.349307	wt.% propene overall	

Table 53. Yield of gas oil and residue from atmospheric distillation (Babusiaux, 2007)

Yield of FCC feedstock	Value	Unit	Source
Gas oil	37	% wt.	Babusiaux, 2007
Residue	19	% wt.	Babusiaux, 2007

Table 54. Density of vacuum gas oil and residue

Feedstock	Density	Source	Density	Source	Unit
Vacuum gas oil	840 (288.15 K)	Mercuria, 2015	910	Mozyr Oil Refinery, N.D.)	kg/m ³
Residue	1200 (313.15 K)	Djimasbe et al., 2019	993 (343.15 K)	Ahmed, 2019	kg/m ³

Energy density of propene: 20.99 MJ/kg (The Engineering Toolbox, 2005)

22 Impact categories and global warming potentials

Table 55. Impact categories and global warming potentials (Sleeswijk et al., 2008; Hull, 2009)

Substance	Global warming potential	Acidification	Photochemical oxidant formation	Particulate matter formation	Human toxicity	Fossil resource energy depletion
Unit	kg CO ₂ e	kg SO ₂ e	kg NMVOCe	kg PM10eq	kg 1,4-DCBe	kg Sbe
SO ₂		35		26		
NO _x	310	22	33	26		
NM VOC			48			
PM10				29		
Mercury					3	
Crude oil						44
Natural gas						31
NH ₃		44				
Pb					9	
Hg					3	
As					12	
CH ₄	21					

23 Process flow diagrams

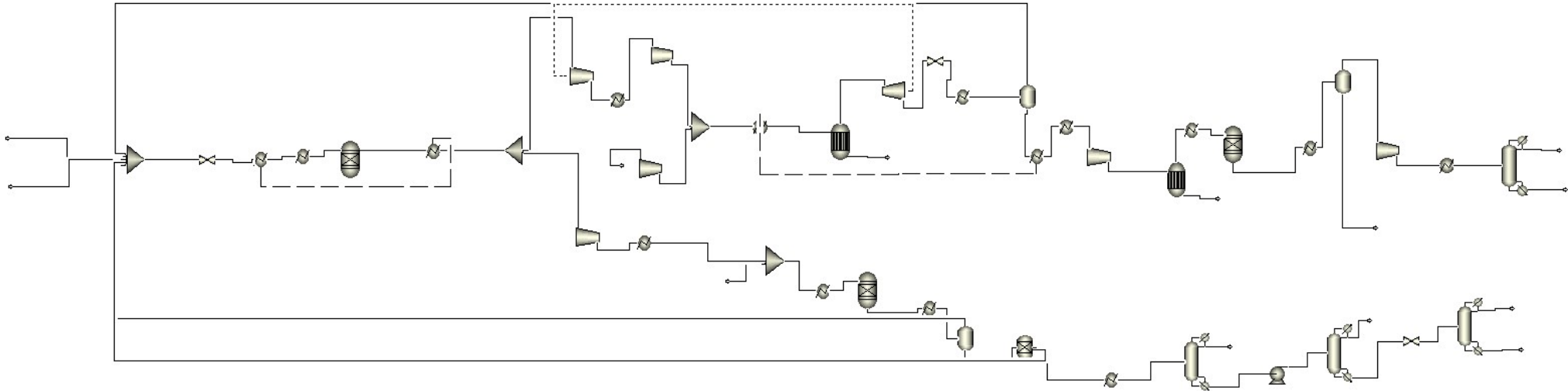


Figure 5. Overall chemical plant

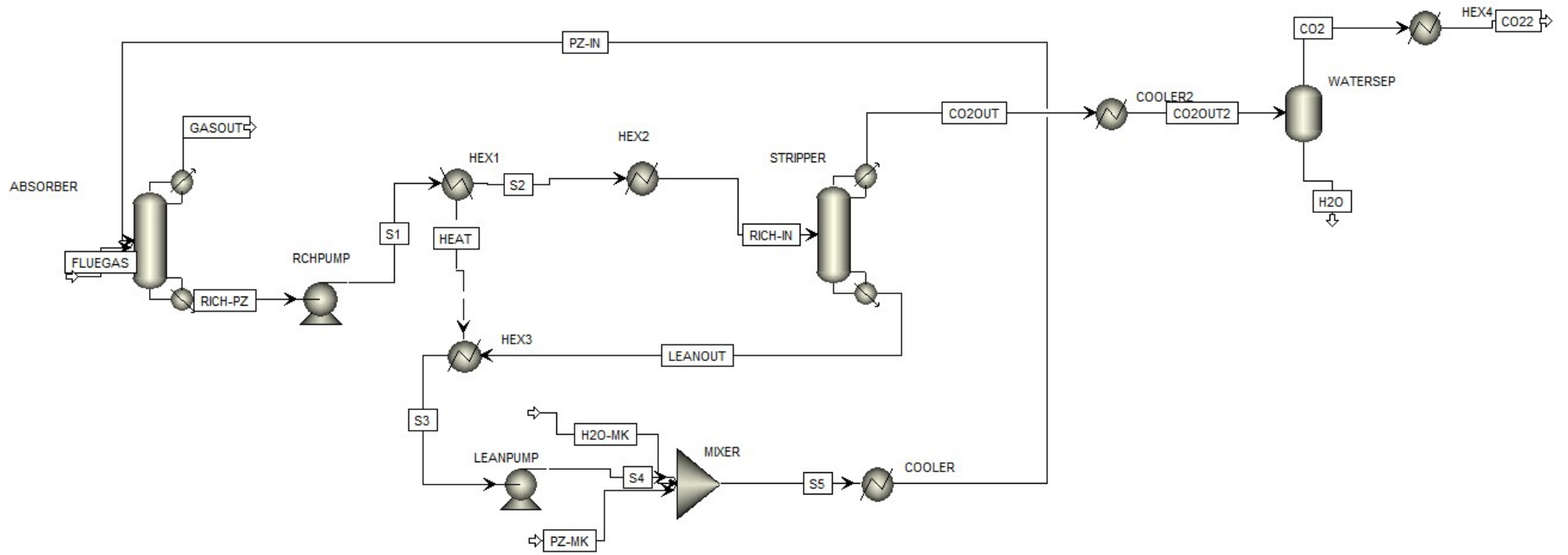


Figure 6. Carbon capture process

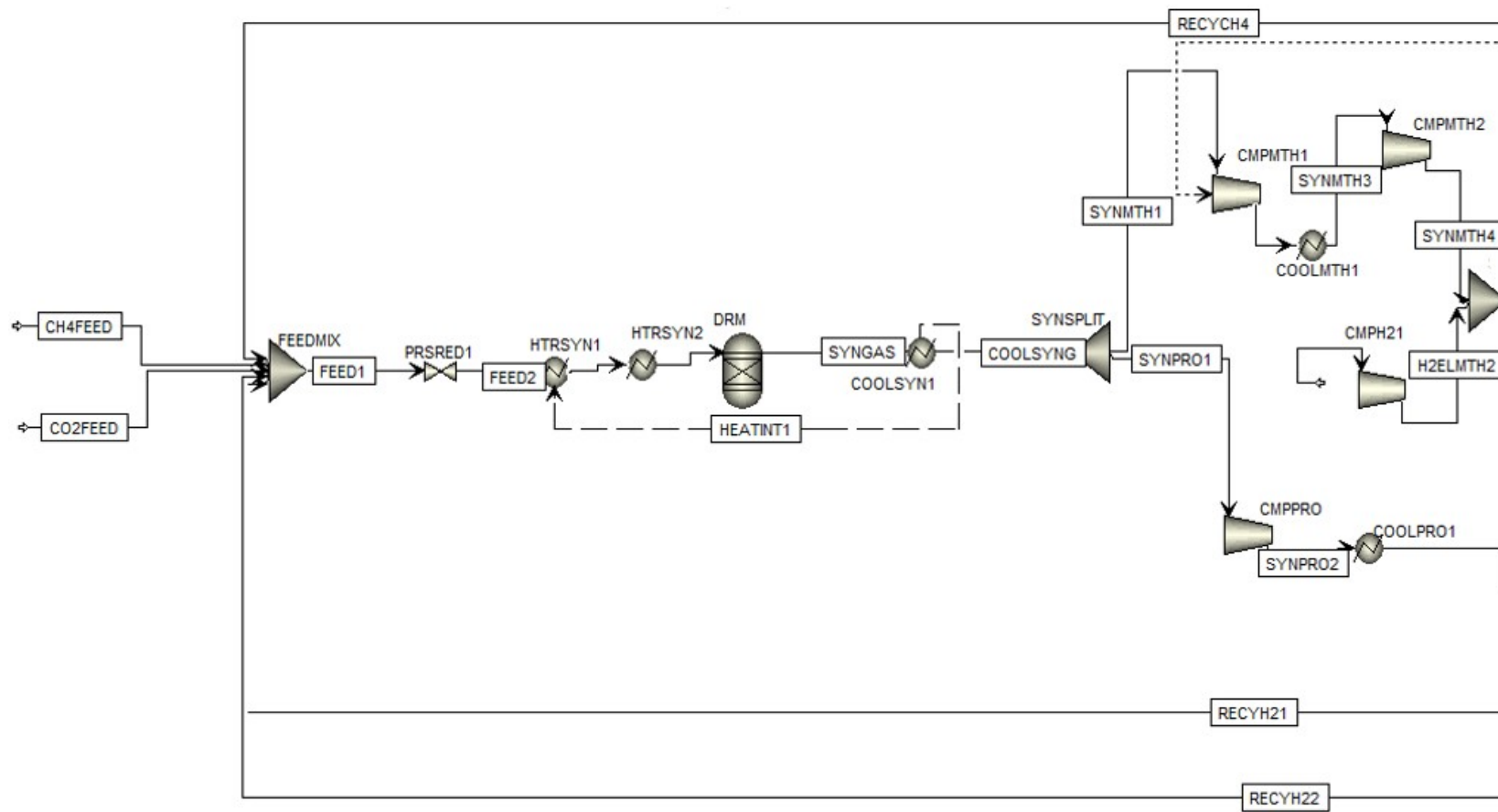


Figure 7. Process flow diagram for syngas production and common steps for propane and propene production

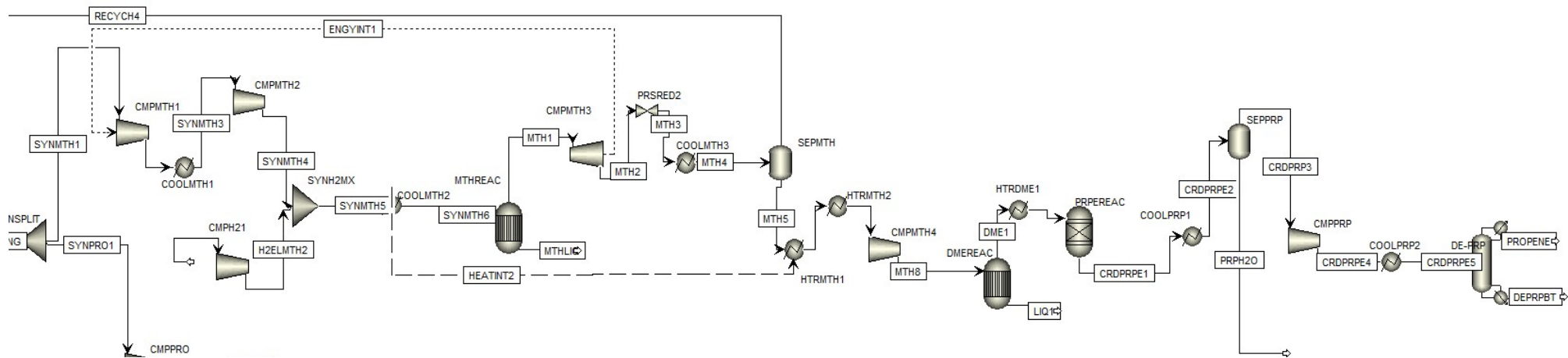


Figure 8. Process flow diagram for propene production

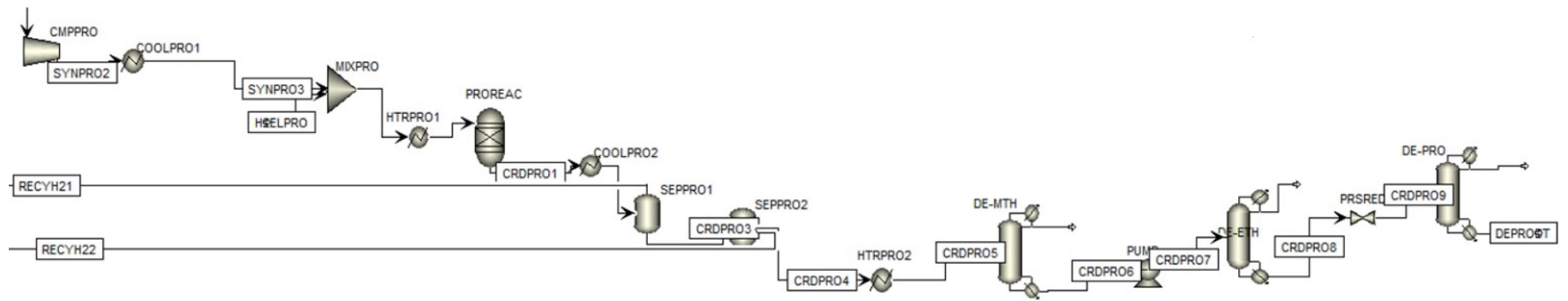


Figure 9. Process flow diagram for propane production

24 Carbon capture

Equilibrium reactions (Wang, 2021):



Rate-controlled (Wang, 2021):

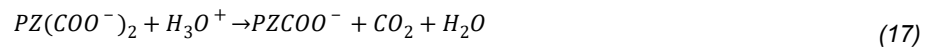
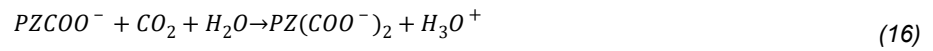


Table 56. Kinetic reaction parameters (Wang, 2021)

Reaction	Type	k_j^0 (m ³ /kmol.s)	E_j (kJ/kmol)
12	Kinetic	4.32e+13	5.55e+4
13	Kinetic	2.38e+17	1.23e+5
14	Kinetic	4.14e+10	3.36e+4
15	Kinetic	7.94e+21	6.59e+4
16	Kinetic	3.62e+10	3.36e+4
17	Kinetic	5.56e+25	7.69e+4

25 Utilities within the chemical plant

Table 57. Power of utilities

Name	Unit	Utility Type	Duty	Unit
RCHPUMP	Pump	Electrical	34,949	W
HEX1	Heat Exchanger	Heating	57,229,700	W
HEX2	Heat Exchanger	Heating	81,080,600	W
STRIPPER (Reboiler)	Distillation	Heating	49,510,000	W
STRIPPER (Condenser)	Distillation	Cooling Water	- 45,029,900	W
HEX3	Heat Exchanger	Cooling Water	- 57,229,700	W
LEANPUMP	Pump	Electrical	4,884	W
COOLER	Heat Exchanger	Cooling Water	- 51,170,000	W
COOLER2	Heat Exchanger	Cooling Water	- 18,318,500	W
HEX4	Heat Exchanger	Heating	1,213,750	W
HTRSYN2	Heat Exchanger	Heating	9,211,948	W
DRM	Reactor	Heating	95,423,026	W
COOLSYN1	Heat Exchanger	Cooling Water	- 50,936,504	W
CMPPRO	Compressor	Electrical	30,135,100	W
COOLPRO1	Heat Exchanger	Refrigeration	- 25,758,796	W
HTRPRO1	Heat Exchanger	Heating	5,709,128	W
PROREAC	Reactor	Cooling Water	- 210,146	W
COOLPRO2	Heat Exchanger	Refrigeration	- 21,548,600	W
HTRPRO2	Heat Exchanger	Refrigeration	- 561,795	W
DE-MTH (Reboiler)	Distillation	Heating	3,798,970	W
DE-MTH (Condenser)	Distillation	Refrigeration	- 259,279	W
PUMP	Pump	Electrical	22,603	W
DE-ETH (Reboiler)	Distillation	Heating	5,187,290	W
DE-ETH (Condenser)	Distillation	Refrigeration	- 3,875,810	W
DE-PRO (Reboiler)	Distillation	Heating	3,763,390	W
DE-PRO (Condenser)	Distillation	Cooling Water	- 4,434,360	W
COOLMTH1	Heat Exchanger	Refrigeration	- 8,671,419	W
CMPMTH2	Compressor	Electrical	22,981,303	W
CMPH21	Compressor	Electrical	781,924	W
COOLMTH2	Heat Exchanger	Cooling Water	- 15,045,922	W
MTHREAC	Reactor	Cooling Water	- 35,535,728	W
CMPMTH3	Compressor	Electrical	- 1,659,361	W
COOLMTH3	Heat Exchanger	Refrigeration	- 16,337,049	W
HTRMTH2	Heat Exchanger	Heating	1,709,815	W
CMPMTH4	Compressor	Electrical	955,207	W
DMEREAC	Reactor	Cooling Water	- 2,884,606	W

PRPREAC	Reactor	Cooling Water	- 10,903,690	W
HTRDME1	Heat Exchanger	Heating	2,860,464	W
COOLPRP1	Heat Exchanger	Refrigeration	- 22,984,909	W
CMPPRP	Compressor	Electrical	965,967	W
COOLPRP2	Heat Exchanger	Cooling Water	- 1,527,403	W
DE-PRP (Reboiler)	Distillation	Heating	837,587	W
DE-PRP (Condenser)	Distillation	Cooling Water	1,339,110	W

26 Cooling tower calculations

Makeup water (Perry et al., 1997):

$$Evaporation\ loss = 0.00085 * W_c * (T_1 - T_2) \quad (18)$$

Where W_c is water flowrate, temperature is for inlet and outlet water.

$$Drift\ loss = W_c * 0.002 \quad (19)$$

$$Blowdown = \frac{Evaporation\ loss}{(Cycles - 1)} \quad (20)$$

Typically, cooling towers are operated with between three and five cycles.

27 Operating costs

Table 58. Operating costs

Component	Fraction of total raw material and utility cost
Operating labour cost	0.05
Maintenance cost	0.01
Operating cost	0.01
Plant overhead cost	0.03
General and admin cost	0.09

28 Carbon tax sensitivity

Table 59. Carbon tax sensitivity

Price (\$/ton)	Carbon Revenue (\$/yr)	VP2	VP	NPV	Payback
0	0	2,123.55	13,366,017.64	- 695,557,394.13	-0.77488
25	11,326,392	3,553.65	24,692,409.64	- 521,442,987.80	-0.9141
50	22,652,784	4,983.75	36,018,801.64	- 347,328,581.47	-1.11431
75	33,979,176	6,413.85	47,345,193.64	- 173,214,175.14	-1.42682
100	45,305,568	7,843.95	58,671,585.64	900,231.19	-1.98293
99.87074143	45,247,007	7,836.55	58,613,024.31	0.00	-1.97894

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