

Zero-Emission Pathway for the Global Chemical and Petrochemical Sector: Supplementary

Deger Saygin and Dolf Gielen*

International Renewable Energy Agency (IRENA), Innovation and Technology Centre (IITC), 53113 Bonn,

* Correspondence : info@irena.org

A. Recent developments in low-carbon chemical and petrochemical production

The following technology discussion covers five technology areas:

- Decarbonising process heat (energy efficiency and renewable energy)
- Biomass feedstocks (biomass feedstocks and bioplastics)
- Synthetic feedstocks (hydrogen and CO₂ based)
- Circular economy
- CCUS

Potentials and cost are summarised in Table A-1. The numbers are indicative as in all categories a rate of change is required that exceeds past experience. Except for synthetic feedstocks, the strategies have been pursued for the last few decades with limited uptake to date. This points to the importance of creating enabling frameworks to realise the transition that is needed in the coming three decades.

Table A1. Potentials and cost of key mitigation options.

	Current use	Potential 2030	Potential 2050	Cost 2030-2050 (USD/t CO ₂)
Decarbonising process heat, including renewable power (energy efficiency and renewable energy)	0.5%-1% improvement/yr <6% renewable energy share	1%/yr 40% renewable energy share	1%/yr 65% renewable energy share	0-125
Biomass feedstocks (biomass feedstocks and bioplastics)	<15 Mt	50 Mt	340 Mt	-100-400
Synthetic feedstocks (hydrogen and CO ₂ based)	<1 Mt	50 Mt	780 Mt	95 (-100-300)
Circular economy (of the total plastic waste generation)	10% mechanical recycling	20% mechanical recycling 10% chemical recycling	33% mechanical recycling 33% chemical recycling One third reduction in plastics demand	50-300
CCS for process emissions and energy recovery	<10 Mt/yr	100 Mt	940 Mt	0-150
BECCS for process energy generation	-	30 Mt	550 Mt	150-200

A.1 Decarbonising process heat: energy efficiency and renewable energy potentials

Studies and statistics have found an average annual rate of 0.5-1% improvement in the chemical and petrochemical sector's energy use. This improvement is based on energy efficiency technology retrofits, system-wide efficiency measures such as motor systems and process heat cascading as well as the implementation of new energy efficient process technologies (Saygin et al., 2013, 2012). Despite the efficiency gains the sector energy demand has grown by around 3% per year over the past decade due to the growing production volume. A 15% final energy savings potential remains if the sector were to implement best practice technologies widely (Saygin et al., 2011; Saygin et al., 2011b). Energy efficiency technologies are commercially available and they typically come with short pay-back periods (Neelis et al., 2008). The combination of continuous innovations and long-life process installations makes that a gap remains between the best available technologies and the global average efficiency. Also process integration and intensification techniques continue to contribute to energy efficiency gains (Klemeš and Varbanov, 2013). Because of the high share of feedstock energy, the efficiency potential is smaller than in other industry sectors. This is compensated by a high circular economy materials efficiency potential.

The share of direct renewable energy use in the sector's total final energy consumption and non-energy use is currently less than 1%. Biomass dominates renewable energy use. However biomass process energy and feedstock potential is much higher than its current share (Saygin et al., 2014).

A shift to renewable electricity can also increase the total renewable energy share. Electricity is traditionally used for chlor-alkali electrolysis process and for the operation of fans, pumps and compressors. However a large share of the fossil fuel use for steam and process heat generation could technically be replaced with electricity (Philibert, 2019). For low and medium temperature, highly efficient heat pumps can be deployed. The largest potential for heat pump integration is found in distillation, evaporation, drying and heating processes, which often take place at temperatures between 100°C and 500°C. Electrically driven heat pumps can be deployed at temperatures of up to 280°C, while higher temperatures might be reached depending on the availability of suitable heat sources (Zühlsdorf et al., 2019). Today's heat pumps do not achieve the required temperature level or the volume of heat required for basic chemical processes, further innovations will be needed.

Integrated sites use steam networks at different pressures to cascade the heat down in temperature, which increases overall efficiency (pinch technology).

Electricity-based alternatives to the traditional steam cracker process are also under development. Finally, efforts are currently aimed at greening gas supply using either green hydrogen (from renewable power) or biomethane. It is ultimately the economics that determine the type of energy use.

A.2 Biomass feedstocks

Various routes exist to deploy biomass feedstock, at the level of naphtha substitutes and syngas to primary building blocks such as methanol and ethylene, to direct production of plastics and fibers. Development efforts have been ongoing for decades, but technological feasibility is generally not matched by economic feasibility.

Plastics and olefins production

Today's bioplastics share is less than 2% of total production. Estimates shows that there could be an economic potential of 90-150 Mt for bio-based materials by 2030 (Saygin et al., 2014). Bioplastics can be split into drop-in bioplastics (same molecule as existing commodities) and dedicated new bioplastics (such as polyethylene furanoate, PEF, as replacement for PET) (Grau, 2019). Globally 2.1 Mt of alternative thermoplastics capacity existed in 2018. Biodegradable plastics altogether account for over 55.5% (over 1 Mt) of

the global bioplastics production capacities. The production of biodegradable plastics is expected to increase especially due to polyhydroxyalkanoates' (PHA) significant growth rates (Erickson et al., 2011). Global bioplastics production capacity is set to increase to approximately 2.4 Mt in 2024 (European Bioplastics, 2019). These values exclude biomass based PUR and epoxy resins use today (thermosets) that constitute another 6 Mt/yr in production capacity (Nova Institute, 2019).

All major bulk plastics can be replaced with biopolymers (PE, PP, PET etc.). The production of bio-based PE is predicted to continue to grow, as new capacities are planned to come online in Europe in the coming years (European Bioplastics, 2019).

The production of bio-based ethylene is already commercial for several years in Brazil and India, though volumes are small (less than 0.5% of total global ethylene production). (Mello et al., 2019) conclude that a plant of 1.2 Mt/yr would result in production cost of USD 1,175 per ton, requiring a price premium in relation to petrochemical ethylene (around 1000 USD/t early April 2020 according to (Fibre2Fashion, 2020)).

In 2019, bio-based PP entered the market on a commercial scale with a strong growth potential due to the widespread application of PP in a wide range of sectors (Green Car Congress, 2020).

Intentions to increase production capacities for bio-based PET, however, have trailed predictions. Instead, the focus has shifted to the development of PEF, a new 100% bio-based polymer that is comparable to PET with feature superior barrier and thermal properties (Hwang et al., 2020).

Aromatics

Aromatics include benzene, toluene and xylenes (BTX), a group of chemicals that are characterised by an aromatic ring. Their total consumption is around 150 Mt per year, nearly a third of total petrochemical product volume. Efforts have focused on development of biomass alternatives. The chemical composition of the lignin component of biomass (a byproduct from chemical pulp making and other processes) is much closer to the functional aromatics. Therefore, if catalytic direct conversion routes can be developed this could work to the advantage of biochemicals. Currently bio-BTX aromatics production technology has reached readiness levels between 5 and 6 therefore the market entry on commercial scale is a few years away. A process for production of biobased p-xylene is currently being commercialised (IFP, 2019). While a first demonstration plant is planned, production on commercial scale will only be ready around 2025 ("BIO-HArT," n.d.). Because of the early stage of developments, reasonable estimates for price or cost development for lignin-based bio-BTX are missing. Preliminary price estimate for lignin-based bio-BTX indicates that the price may be as twice that of fossil oil based BTX (EC, 2018). Experts in this field indicate that commercial scale production could begin the earliest within 10-20 years (Fabbri et al., 2018).

Methanol

Methanol is a significant chemical component and fuel but it can also be used as a building block for other chemicals. Methanol to olefins (MTO) is a technology that is widely deployed in China to produce ethylene and propylene. Whereas methanol is produced from coal in China, it is also possible to produce methanol from biomass. Several bio-based methanol production plants are in operation or have operated in recent years in Canada, the Netherlands, Sweden and the United States. These produce methanol from various feedstocks such as biomethane, glycerine, black liquor or wood (IRENA and Methanol Institute, 2021). Biochemical company Enerkem is currently building a plant in Rotterdam that will turn 350 kilotons of waste, including unrecyclable plastic, into syngas and subsequently into 270 million liters of bio-methanol every year. Other feedstocks such as glycerine have been deployed in the past using steam reforming technology and

methanol synthesis. The bulk of methanol is produced from natural gas, which can be replaced with biomethane, which is produced through biogas upgrading. In the Netherlands 15% of BioMCN's is produced this way (67 kilotons per year). The parent company OCI operates a plant in Texas that applies the same technology. Biomethane price is 80 USD per MWh, roughly twice the long term European pipeline gas price (DENA, 2019).

A.3 Synthetic feedstocks

Electrochemical conversion of CO₂ in combination with hydrogen is another way to produce chemical feedstocks and building blocks with neutral or even net negative carbon balance. Water electrolysis is the most feasible power-to-chemicals conversion and several projects are underway:

- Yara and Engie partnered to test the renewable power-to-ammonia (P2A) technology in fertiliser production, investing USD 200 million, aiming to create a bankable prototype for creation of a larger project pipeline in the future. A feasibility study started in 2019 for the design of a 100 megawatt (MW) green hydrogen plant integrated with Yara's existing ammonia plant in Pilbara, Western Australia (Yara, 2019).
- Hydrogen Utility, a hydrogen infrastructure company partnered with ThyssenKrupp is developing a renewable P2A demonstration plant in South Australia. Australian dollars (AUD) 117.5 million are to be invested in a 30 MW electrolyser, for an ammonia production capacity of 18 kt/yr, together with two 16 MW open-cycle gas turbines fuelled by hydrogen (Brown, 2018; Port Lincoln Times, 2019).
- Haldor Topsoe is demonstrating efficiency improvements in the renewable P2A technology by incorporating waste heat to reduce power consumption (and costs). The company also works on reducing the initial capital costs by removing the air separation unit from the Haber-Bosch process. (Brown, 2019).
- The start-up Atmonia plans to build a USD 2 million prototype for an electrochemical catalyst process for generating aqueous ammonia directly from air and water, using renewable power (Brasington, 2019).
- Starfire Energy developed a new solution for renewable P2A production, including hydrogen production by proton exchange membrane electrolyser, nitrogen production by pressure swing adsorption, ammonia synthesis, and liquid ammonia storage. It built a 10 kg per day ammonia synthesis system in Colorado using its low pressure 'Rapid Ramp' ammonia process and plans to modulate the plant to 100 kg/day in 2020 (Beach et al., 2019).

This is a sample, 25-30 projects are being developed around the world (IRENA and Ammonia Energy Association, forthcoming). The cost of green hydrogen is critical for the process economics. Green hydrogen production cost can be split into electricity cost and capital cost for the electrolyser facility. At practical current densities, efficiencies (total of water electrolysis, hydrogen pressurisation, ammonia synthesis) range between 50% and 70% (Soloveichik, 2019). The energy conversion efficiency of the electrolyser is 65-67%, 50 kWh are needed per kg hydrogen. At USD 4 ct/kWh, the electricity cost amount to 2 USD/kg hydrogen. The electrolyser facility cost amount to 1000 USD/kW (input power). Given an annuity of 10% this translates into 0.6-1.8 USD/kg hydrogen, the range reflecting capacity factors. Today green hydrogen costs between 6 and 10 USD/kg. This may fall to 1.5 USD/kg in the coming years in the most favourable conditions. Still at such price a GJ of hydrogen (around 8 kg) would cost 12 USD, while a GJ or transmission pipeline natural gas costs currently between 2 and 6 USD/GJ in Europe and the United States. So hydrogen is more expensive. This does not account for any hydrogen transmission cost or electricity grid surcharges. At 20 GJ hydrogen per ton ammonia, the feedstock cost alone would be

240 USD/t and the ammonia production cost would be in the order of 400 USD/t. In comparison a ton of ammonia costs today 200-300 USD/t. Given 1.5 t CO₂ that is emitted per ton ammonia, mitigation cost are 65-130 USD/t CO₂.

Alternative to electrolysis, methane pyrolysis provides a new route for hydrogen production (BASF, n.d.). The by-product is carbon black or graphite, both chemicals with a comparatively small market of less than 10 Mt/yr. Therefore, the market size potential of this option will be limited. Moreover, such use would result in CO₂ emissions and it is therefore not a zero carbon solution.

Research and development into electrocatalytic materials for CO₂ reduction has intensified in recent years, with advances in selectivity, efficiency, and reaction rate progressing toward practical implementation. A variety of chemical products can be made from CO₂, such as alcohols, oxygenates, synthesis gas and olefins (Luna et al., 2019). Polycarbonates, polyurethanes, polyureas, polyesters can be produced from CO₂ by direct copolymerisation of CO₂ with co-monomers or by the synthesis of CO₂-based building blocks including (a)cyclic carbonates, carbamates, urea and lactones followed by their (co)polymerisation (Grignard et al., 2019). The success of the first approach depends highly on the catalyst design.

Crackers can be heated with renewables-based electricity in resistance heaters. Dry reforming of methane (instead of cracking naphtha) with CO₂ can produce a syngas that can subsequently be transformed into olefins (BASF, n.d.). Siemens is also working on a new pathway for electrochemical reduction of CO₂ to ethylene with the first customer-based power plant to be operational by 2021 (Siemens, 2018).

Synthetic methane can be used as a building block for methanol which can be converted into olefins using MTO technology (Palm et al., 2016). Carbon Recycling International (CRI) is already producing renewable methanol from carbon dioxide, hydrogen and electricity on a commercial scale at its production facility in Grindavík, Iceland. In total 4 kilotons of methanol are synthesised each year (IEA-ETSAP and IRENA, 2013a).

Also other players are looking into synthetic methanol production. BioMCN in the Netherlands is considering using CO₂ by-product from biomethane production and processes this with renewable hydrogen into methanol. This process is being developed at the scale of a 20 MW electrolyser.

The e-CO₂MET project consortium of Total and Sunfire investigates the conversion of renewable electricity to methanol. Hydrogen will be produced in a high temperature solid oxide electrolyser and CO₂ will be sourced from a refinery (Sunfire, 2020; Total, 2019).

A.4 Circular economy

A circular economy holds the promise of significant energy and climate benefits. But there is a need to enhance the understanding of its techno-economic potentials. The circular economy includes avoidance, recycling, reuse, materials substitution, more efficient materials design, and the use of sustainable feedstocks. The most common example of the circular economy relates to recycling. Another option is reusing the parts of a good after consumer use. Alternatively, the worn parts of a good can be repaired or remanufactured before turning them into new end products (re-use). Several examples today demonstrate how industry creates value from such a circular economy. A classic example is the beverage bottle. To avoid use, in many parts of the world, regulation is also tightening. Some 127 countries have placed limits on plastic bags, while the European Union will ban a range of items by 2021, including cutlery, plates and straws. Whereas some packaging is excessive, product quality may suffer without packaging. A typical example relates to fruits and vegetables where avoidance of packaging can result in rising amounts of food waste. Therefore the optimal strategy is often not evident and subject to debate.

Recycling of materials is often more energy efficient than production of primary materials from natural resources. A reduction of 50% and more of energy and resource use

can be achieved for many sectors and products (Gielen and Saygin, 2018). Yet the market for recycling remains small. One reason is the price dynamics and low profit margins. Recycled plastic prices depend on the cost of collection, sorting, and processing which can exceed those for primary material. Also the materials quality is often lower for recycled material.

Circular economy strategies require a good insight how materials are used and where waste materials arise. One aspect is that materials are stored in products. The life span of products varies. Whereas packaging materials may have a life span of a few days, use of materials in buildings and infrastructure may last decades or even hundreds of years. There is a clear trend for plastics towards shorter life spans. Notably the growth of the internet delivery economy in recent years has vastly increased the amount of packaging waste. In China (which accounted for 50% of global e-commerce in 2017), parcel packaging waste contributes 40% of municipal solid waste in 2017. Due to the rapid increase in express parcel garbage, the proportion of plastic and paper waste in domestic garbage has increased significantly. Over 90% of the parcel plastic packaging end up in municipal solid waste. Consequently, the proportion of plastic waste in China increased from 12% to 20%, and the proportion of paper waste increased from 9% to 14%. Total plastic waste recycling stood at 17–18 Mt in 2018 (the year plastic waste imports were banned) (1421 Consulting Group, 2018). Worldwide in 2010, more than 250 Mt plastic waste was generated per year (including processing waste) (Geyer et al., 2017). (Jambeck et al., 2015) estimate an even larger amount of 275 Mt of plastic waste.

Unlike glass or metal, plastic packaging cannot be recycled infinitely because it degrades in quality. While scientists are working on so-called advanced recycling techniques to overcome this problem, they are not yet commercially viable. So, whereas mechanical recycling potentials are limited, chemical recycling does not face the same issue. Chemical recycling refers to a conversion where the plastic is converted into its building blocks, the so-called monomers. Feedstock recycling goes even a step further, the plastic is converted into an oil-like product. Although it is inherently restricted in its application to condensation-type polymers such as PET and polyamide, monomer recycling has the potential to generate some of the highest plastics recycling profitability levels. Monomer recycling can avoid the capital investments needed for steam crackers and aromatics plants, as well as the high-capital-cost plants required to make PET and polyamide intermediates (Hundertmark et al., 2018). Re-converting waste plastics into cracker feedstocks that could displace naphtha or natural-gas-liquids demand—most likely based on pyrolysis processes—may also be economically viable, and it is more resilient to lower oil prices, remaining profitable down to an oil price of USD 50 per barrel. Pyrolysis can be used to treat mixed polymer streams, which mechanical recycling technologies currently cannot handle. Pyrolysis also is an important back-up process to handle polymers that have exhausted their potential for further mechanical recycling. Several pyrolysis players offer a range of facilities from large-scale plants with capacities of 30 to 100 kilotons per year to much smaller-scale modular units with annual production capacity up to 3 kilotons per year (Hundertmark et al., 2018)

Approximately 100 international technology developers (United States, 52%; Europe, 35%; Asia, 13%) focused on providing chemical recycling solutions (Degnan et al., 2019). An Australian-based company, has developed Cat-HTR, a catalytic hydrothermal liquefaction process that uses supercritical water (250 bar, 450°C) to break down a range of polymers into light hydrocarbon gases and a liquid product that resembles a high-quality, sulfur-free synthetic crude (Degnan and Shinde, 2019). Feedstock recycling of polyolefins through thermal cracking has been trialled in the UK and in Germany. However, the latter plant was closed in 1999. Chemical recycling of PET has been more successful, as depolymerisation under milder conditions is possible. PET resin can be broken down by glycolysis, methanolysis or hydrolysis, for example to make unsaturated polyester resins (Hopewell et al., 2009).

However back-to-monomer and back-to-feedstock processes require energy to break down larger molecules to smaller building blocks, plus additional energy for separation and conversion of these building blocks back to plastics. This results in significant energy use and CO₂ emissions, higher than for back-to-polymer mechanical recycling.

There is already a market for waste plastic bales in each geographical region. As recycling activities pick up and markets expand, waste plastic bales will become an important new commodity with prices set by supply and demand. Sorting efficiency, collection costs, and quality will be reflected in the market price, similar to other commodities. In the last two decades Asia was the main importer and North America and Europe were the main exporters of plastic waste. National waste management decisions and waste material trade regulations will affect national waste infrastructure and trade patterns may change, as following the Chinese ban on import of plastic waste (Wang et al., 2020).

Further opportunities to increase plastic waste recycling include: developing better tagging or tracking of materials to significantly increase sorting and collection of higher-purity post-consumer plastics; providing blend stocks to compensate for somewhat inferior properties of recycled plastics; and developing new, large-volume markets that decrease use of recycled plastics for short life-cycle applications, such as packaging materials, with use for long life-cycle applications, such as textiles, pipes, or even housing construction materials. A second aspect is the collection and separation effort for the waste plastic feedstock. New AI based separation systems can facilitate the separation burden. While compatibilisation methods and the technique of dissolution–reprecipitation are already extensively studied, the delamination of packaging has not been investigated systematically. Technologies exist that can recycle multilayer packaging, but these have drawbacks such as a limited application scope or a high expenditure of energy (Kaiser et al., 2018). Given a European amount of 2 Mt multilayer plastics and composite packaging for liquids, global amount is estimated to be around 10 Mt. This is a category where recycling will remain challenging. However, it represents less than 3% of the total material volume.

Recycling and bioplastics efforts may interact. Bio-based plastic is to be considered as a potential source of contamination in current recycling practices (Alaerts et al., 2018). If biobased and biodegradable plastics are used on a more regular basis, then their disposal needs to be considered. Drop-in bio-based plastics can be recycled in the same stream. However, biodegradable plastics, which are chemically distinct from plastics currently on the market, represent a new stream of materials (Dilkes-Hoffman et al., 2019).

A.5 CO₂ capture, utilisation and storage

CCS is close to be an economically viable option to capture CO₂ from high concentration flue gas streams. This includes ammonia, ethylene oxide and hydrogen production as well as and steam crackers. In fact, CO₂ capture is routinely applied in all ammonia and hydrogen production plant, in the order of 200-400 plant worldwide. However, the bulk of the CO₂ that is captured is vented or used for short term applications, for example to produce urea nitrogen fertiliser or in the beverage industry for fizzy drinks. Only a small fraction of the CO₂ that is captured is used for enhanced oil recovery (EOR, where part of the CO₂ stays underground) or it is stored underground in empty oil and gas reservoirs or in aquifers. Where capture occurs routinely the additional cost are limited to the pressurisation, transportation and injection, as well as monitoring systems to ensure the CO₂ remains underground. The cost of these steps varies on the distance to the storage and the electricity cost for pressurisation. Under favourable conditions these costs can be below USD 20/t CO₂. In less favourable conditions they can rise to more than USD 100/t CO₂. CCUS is at this moment mostly related to EOR. The oil revenues are sufficient to create a net benefit even in an environment without CO₂ price. However very few EOR operations monitor what happens to the CO₂ underground and long-term storage over thousands of years is not a given.

Also, industrial cogeneration units could be equipped with CCS, albeit at a higher cost. These depend on the specific operation and the local energy cost, but the capture part can add 25–50 USD/t CO₂, to which the transportation and storage cost must be added.

In terms of chemical and petrochemical industry or related industries 20 facilities are completed or operating worldwide (Global CCS Institute, 2020). Eight are ammonia fertiliser production units, five ethanol plant and three each hydrogen production units and various other chemicals. There is also one facility integrated with methanol production.

The combination of ethanol plant with CCUS results in net CO₂ removal from the atmosphere, as the carbon in biomass is produced from CO₂ that plants capture from the air (Biomass CCS, BECCS). There are 20 BECCS projects worldwide, which relate to various bio-energy technologies (waste-to-energy plants, ethanol plants, biomass combustion and co-firing, pulp and paper plants, biomass gasification) (Wienchol et al., 2020). CO₂ is also removed routinely at over 600 biomethane plants that upgrade biogas. There are currently three commercial BECCS plants operating in the USA, although these may not have been configured to achieve negative emissions on a life cycle basis; all capture CO₂ from fermentation-based biofuel production. The largest of these is the Illinois Industrial CCS Facility with a capacity of 1 Mtpa of CO₂ from bioethanol production from corn (Global CCS Institute, 2020).

Waste to Energy (WtE) with CCS is another form of BECCS. Municipal waste contains a mixture of biogenic (plant based) and fossil-based materials. There are currently almost 2.5 GW of WtE facilities operating around the world (1200 incineration plant according to (Wienchol et al., 2020). Currently about 60% of the carbon contained in MSW is biogenic. This means that capturing CO₂ from MSW incineration and sequestering the CO₂ permanently in geological reservoirs in a BECCS concept (Bio-Energy with CCS) will be carbon negative and represent an efficient measure to reduce CO₂ emissions over the long term (Midttun et al., 2019). If the biogenic component of the waste incinerated in a WtE facility is sufficiently large, and the CO₂ emissions are captured and stored, the plant will have net negative emissions. Grate boilers are used in 80% of WtE plants worldwide and, the CO₂ concentration was found to be about 6–12%. Oxyfuel combustion can reduce CO₂ capture cost but the feasibility is still unclear (Wienchol et al., 2020).

Four WtE plant with carbon capture are in operation: AVR in the Netherlands (0.06 Mtpa to be scaled up to 0.8 Mtpa) and Aker Solutions signed an agreement for the supply of a 0.1 Mtpa CO₂ capture plant in the Netherlands by 2021. Further, a 0.4 Mtpa CO₂ capture system with geological storage is in development at the Klemetsrud WtE facility in Oslo, Norway. This facility will have net negative emissions when operational (Kearns, 2019) A smaller pilot plant is operational in Saga City in Japan (0.004 Mtpa). Estimated capture cost for the Norwegian plant amount to 80 USD/t CO₂ (Midttun et al., 2019), resulting in total CCS cost of 100–125 USD/t CO₂.

The use of CO₂ from direct air capture or from bioenergy process flue gases for synthesis yields carbon neutral chemicals, provided the energy that is used in this conversion is carbon neutral (renewable hydrogen or electricity from renewable sources). A critical question relates to the CO₂ benefits of CCU (Kätelhön et al., 2019). From an emitter perspective, the elimination of emissions via CCU may suggest 100% emissions reduction. However, it depends on the application if this is true. An extreme example is the use of urea fertiliser: the CO₂ is stored but released soon after fertiliser application in the field.

If CO₂ is captured from fossil fuel combustion flue gases, the CO₂ impact is not a given. The emissions from fossil fuel combustion are eliminated but if the chemical products is used and incinerated, the carbon is ultimately released so overall there is a fossil CO₂ emission. (Fehrenbach et al., 2019) conclude a 35% reduction of CO₂ emissions in a scheme where coal power plant CO₂ emissions are captured and used for methanol production, with use of clean energy for the conversion. Such reduction is significant but it is not compatible with net zero strategies.

The cost of DAC or bioenergy flue gas capture tend to be higher than for fossil fuel combustion flue gases, typically USD 100-200/t by 2030 or today even USD 500-600/t for DAC, compared to 20-60 USD/t for fossil fuelled large scale processes.

(Hepburn et al., 2019) claim a 300-600 Mtpa CCU potential in chemicals by 2050, with associated cost of USD -80 to 320/t CO₂. They state that only a few of the technologies are economically viable and scalable. Some are commercialised, such as the production of urea and polycarbonate polyols. Some are technically possible but are not widely adopted, such as the production of CO₂-derived methanol in the absence of carbon monoxide (National Academies of Sciences, 2019). Breakeven costs per ton of CO₂, calculated from the scoping review, for urea (around -USD 100) and for polyols (around -USD 2,600) reflect that these markets are currently profitable.

(Nyári et al., 2020) have considered CO₂ capture and use for methanol production. Through MTO this would open up a pathway to large scale replacement of petrochemicals. However they conclude that this is not economically feasible today, methanol production cost are at least twice those for current production. The green hydrogen supply cost are critical (set at 4.5 USD/kg). This assumed CO₂ would be available for free.

B. IRENA's REmap modelling framework and background data for countries and regions

Using its REmap modelling approach, IRENA has developed an extensive and data-rich energy scenario database and analytical framework, which is used to assess the projected impacts of policy and technology change:

- Planned Energy Scenario (PES) – IRENA's Reference Case, which includes current and planned policies and pledges announced by end of 2018. The energy-related CO₂ emissions are expected to increase each year until 2030 before dipping slightly by 2050 to below today's level.
- 1.5 °C case (1.5 C case) –An ambitious yet realistic climate compatible pathway to accelerate the energy transformation limiting climate change to 1.5 °C above pre-industrial levels. The total of CO₂ emissions from energy, process emissions and LULUCF are reduced to zero by 2050.

Details of IRENA's REmap modelling framework and its strength and limitations have been discussed previously (Gielen et al., 2019; Kempener et al., 2015; Saygin et al., 2015). The model has been applied previously at country and levels for the United Arab Emirates (Sgouridis et al., 2016) and the European Union (Collins et al., 2018) as well as to assess the economic impacts of climate policies at sector level (Saygin et al., 2019). IRENA's REmap framework has also been used to assess the renewable-hydrogen and decarbonisation potential of the global iron and steel sector (Gielen et al., 2020).

Table B-1 provides an overview of the production volumes, specific energy consumption and the fuel mix of the chemical and petrochemical sector's major products for the selected country/regions. Feedstock consumption values refer to net energy use for non-energy purposes which is the primary energy used as a feedstock without the required process energy (see Table B-2). The same feedstock value applies for all countries. No distinction is made between the feedstock values for different energy carriers.

Table B1. Estimated production volume, specific energy consumption and fuel mix of the major products in selected country/regions, 2017.

USA	EU-27	China	India	Japan	Rest of G20	Rest of the World	Global
Production volumes [Mt/yr]							

Ethylene steam cracking ¹	25.6	19.8	19.6	2.9	5.6	35.2	26.7	135.4
Propylene steam cracking	6.9	9.6	10.5	1.3	2.9	10.0	8.5	49.6
Propylene FCC	2.9	4.1	4.5	0.6	1.2	4.3	3.7	21.3
Benzene steam cracking	2.0	3.4	4.2	0.5	1.0	3.4	3.0	17.4
Benzene naphtha extraction	5.0	8.5	10.4	1.1	2.6	8.4	7.5	43.6
Toluene	5.0	1.8	6.6	0.1	2.1	4.9	4.9	25.5
Xylene	4.2	2.6	10.9	0.1	6.8	11.2	11.2	47.0
Butadiene steam cracking	2.4	2.9	3.3	0.4	0.9	3.4	2.8	16.1
Butadiene C4 separation	2.4	2.9	3.3	0.4	0.9	3.4	2.8	16.1
Butylene	5.7	4.4	4.3	0.6	1.3	7.8	5.9	30
Ammonia ²	14.1	16.2	52.9	13.1	0.9	37.4	37.8	172.4
Methanol ³	2.7	1.6	57.7	0.2	0.0	7.2	17.0	86.4
Specific energy consumption (excl. electricity and feedstock) [GJ/tonne]⁴								
Ethylene steam cracking	17.7	14.9	16.1	16.1	12.2	16.3	16.3	16.3
Propylene steam cracking	17.7	14.9	16.1	16.1	12.2	16.3	16.3	16.3
Propylene FCC	3.5	2.9	3.2	3.2	2.4	3.2	3.2	3.2
Benzene steam cracking	17.7	14.9	16.1	16.1	12.2	16.3	16.3	16.3
Benzene naphtha extraction	3.5	2.9	3.2	3.2	2.4	3.2	3.2	3.2
Toluene	3.5	2.9	3.2	3.2	2.4	3.2	3.2	3.2

Xylene	3.5	2.9	3.2	3.2	2.4	3.2	3.2	3.2
Butadiene steam crack- ing	17.7	14.9	16.1	16.1	12.2	16.3	16.3	16.3
Butadiene C4 separa- tion	7.9	6.7	7.2	7.2	5.4	7.3	7.3	7.3
Butylene	3.5	2.9	3.2	3.2	2.4	3.2	3.2	3.2
Ammonia	11.5	11.0	23.5	12.0	11.0	11.5	11.5	15.0
Methanol	10.0	10.0	12.0	10.0	10.0	10.0	10.0	10.0
Fuel mix [%]								
Steam cracking ¹								
Naphtha and gas oil	39	86	100	80	94	49	57	65
Ethane / propane / butane / oth- ers	61	14	0	20	6	51	43	35
Ammonia ²								
Natural gas	100	100	14	100	100	90	90	69
Oil	0	0	0	0	0	10	10	4
Coal	0	0	86	0	0	0	0	26
Methanol ³								
Natural gas	100	100	20	100	100	100	100	47
Coal	0	0	80	0	0	0	0	53

¹ Production of steam cracking products are based on the “International survey of ethylene from steam crackers – 2015” of the Oil and Gas Journal (Koottungal, 2015). The survey provides the ethylene production capacities and fuel mix of 261 steam crackers from across the world with a breakdown by country and plant name for the year 2015. Country data has been estimated based on the weighted average of individual power plants. If the fuel mix of a plant is missing in the survey, it has been assumed equivalent to the average of all other plants. Each fuel type that enters the steam cracking process has a different yield of products for ethylene, propylene, butadiene, and benzene. We estimated the production of these products based on the ratio of their output to ethylene (Neelis et al., 2005). In a subsequent step, we scaled the 2015 production volumes to 2017 for each country/region based on the production growth in the 2015-2017 period. The production of propylene from fluid catalytic cracking (FCC) process in petroleum refineries is based on other sources (Deloitte, 2019). Production of toluene and mixed xylenes is based on various industry sources (China (L’Élémentarium, n.d.; ICIS, 2020), EU-27 (Aromatics Online, 2015), India (“APIC Conference 2017,” 2017), Japan (“APIC Conference 2019,” 2019), US (Garside, 2020a, 2020b)). Production in the rest of the world and the rest of the G20 has been assumed same and volumes have been estimated by subtracting the total of 5 countries/regions from the world (Garside, 2019) as a whole. Country-level production of butylene is derived from the global total (GlobalData Energy, 2019) based on the share of HVC production. To estimate production from capacity data, a utilisation factor of 85% is assumed. ² Production data for ammonia was collected from the US Geological Survey for nitrogen (USGS, 2021). ³ Global methanol production is available from the Methanol Institute (Methanol Institute, 2021). Country level data has been collected from various industry sources (China (Liang, 2019; Xu et al., 2017a, 2017b), EU-27 (Ellis, 2018), India (Jaganmohan, 2020), US (EIA, 2019) and other countries (HDIN Research, 2019)). ⁴ Specific energy consumption of the chemicals are based on the IEA (IEA, 2009a) and the UNIDO (UNIDO, 2010).

Table B2. Feedstock consumption per unit of product (IEA, 2009a).

	[GJ/t]
Ethylene steam cracking	45.0
Propylene steam cracking	45.0
Propylene FCC	45.0
Benzene steam cracking	0.0
Benzene naphtha extraction	40.1
Toluene	20.3
Xylene	41.0
Butadiene steam cracking	0.0
Butadiene C4 separation	44.6
Butylene	45.0
Ammonia	20.7
Methanol	20.0

In 1.5 C case there are profound changes in the technology mix at country/region level (see Table B-3 for the technology penetration rates by country/region) and the growth and relocation of production (see Figure B-1) that follows the dynamics in supply-demand of chemicals and plastics and that favours renewable energy resource availability in different regions. In addition, the end-of-life waste treatment options of plastics change significantly in 1.5 C case compared to the PES where landfill is no longer an option, and the waste treatment is equally split between chemical recycling, mechanical recycling, and incineration (see Table B-4). By comparison in 2017, globally only 17% of all plastic waste collected was being recycled and 23% was incinerated with energy recovered. 60% ended up in landfills. There are differences in recycling shares between the countries: India and the EU-27 countries have the highest recycling shares of around 60% (including the informal sector) (MOHUA India, 2019) and 32.5% (Plastics Europe, 2020), respectively. In China and Japan (PWMI, 2019) recycling rates are around 25% of all plastic waste generated. Chemical recycling has a share of around 3% in Japan. The share of recycling in the United States is 9% (Geyer et al., 2017). The share of energy recovery ranges from as low as 16% in the United States to as high as 65% in Japan. On the contrary, Japan has the least share in landfilling at 8%. 75% of all waste is landfilled in the United States.



Figure B1. Estimated change in production of chemicals in the PES and 1.5 C case by 2050 compared to the 2017 level.

Table B3. Technology penetration assumptions in the 1.5 C case in 2050.

[%]	USA	EU-27	China	India	Japan	Rest of G20	Rest of the World
Energy efficiency (savings compared to 2017 level)							
BPT (PES only) ¹	15%	15%	15%	15%	15%	15%	15%
Breakthroughs	35%	35%	35%	35%	35%	35%	35%
Breakthroughs (other)	40%	40%	40%	40%	40%	40%	40%
Renewables (substitution potential of fossil fuels)							

CCU/S, BECCS (process emissions)	100%	100%	100%	100%	100%	100%	100%
CCU/S, BECCS (plastic waste incineration)	75%	75%	75%	75%	75%	75%	75%
Renewables for electricity	85%	85%	85%	85%	85%	85%	85%

¹ We assume 0.5% autonomous improvements in energy efficiency that will lead to 15% less demand in fuel use by 2050 compared to 2017. This is equivalent to the savings that would be achieved by implementation of best practice technologies today (Zuberi and Patel, 2019).

Table B4. Estimated plastics production, demand and waste generation in the PES and 1.5 C case, 2017-2050.

[Mt/yr]	USA	EU-27	China	India	Japan	Rest of G20	Rest of the World	Global
2017								
Production	38	54	104	13	14	97	29	348
Demand	48	61	84	8	16	137	31	385
Waste generated	35	34	61	9	9	76	17	241
Mechanical recycling	3	11	15	6	2	5	1	42
Chemical recycling					0.4			
Energy recovery	6	14	18	0	6	11	2	57
Landfill	26	8	27	4	1	60	15	141
2050 PES								
Production	91	65	334	40	22	232	138	922
Demand	114	73	270	25	25	330	148	986
Waste generated	83	41	195	30	14	183	82	628
Mechanical recycling	7	13	49	18	3	11	4	106
Chemical recycling	0	0	0	0	1	0	0	1
Energy recovery	13	17	59	0	9	27	8	134
Landfill	62	10	88	12	1	145	70	387
2050 1.5 C case								
Production	25	20	125	15	5	130	60	380
Demand	76	49	180	17	17	220	98	657
Waste generated	55	27	130	20	9	122	55	419

Mechanical recycling	18	9	43	7	3	41	18	140
Chemical recycling	18	9	43	7	3	41	18	140
Energy recovery	18	9	43	7	3	41	18	140
Landfill	0	0	0	0	0	0	0	0

C. Carbon flow analysis methodology

The chemical and petrochemical CO₂ emissions occur during the production and use of chemicals and plastics and during plastic waste treatment. Emission sources in each stage are:

- Production: emissions occur from the combustion of fossil fuels and as process emissions (oxidation processes, off-spec products etc)
 - Steam cracking process is responsible for the production of the bulk organic chemicals where intermediates and plastics are derived from. A share of the total carbon input is stored in olefins and other high value chemicals. The remainder is combusted in the steam cracking process and a small share flows back to refineries.
 - Ammonia production results in CO₂ emissions from both fuel combustion and feedstock use as process emissions since ammonia does not have any carbon. A share of the carbon emitted as process emission is captured to produce urea. The remainder is released to the atmosphere.
 - A share of the total carbon input is stored in methanol and carbon black. The remainder is combusted as process energy.
 - The total carbon stored in high value chemicals, methanol, urea and carbon black and the total combustion emissions and process emissions (only in ammonia) is equal to the total carbon input to the chemical and petrochemical sector.
- Use: High value chemicals, methanol (only 75% where the other 25% is used as transport fuel) and carbon black are processed into intermediate chemicals and they are subsequently converted to synthetic organic materials (e.g. solvents, surfactants) and plastics.
 - A share of the total carbon stored in products is released from the use of chemicals such as solvents and surfactants.
 - All carbon stored in urea is released during the application of urea fertiliser.
- Plastic waste treatment: Each year a share of all plastics in the material stock reaches the end of their life. There are three main options for the treatment of plastic waste, namely recycling, incineration and landfilling.
 - Incineration results in the release of the carbon stored in plastics as CO₂.
 - Landfilling buries the carbon stored in plastics underground.
 - During recycling carbon stored in chemicals is recycled back to the production of plastics.

The following emissions factors have been assumed to estimate CO₂ emissions from fossil fuel combustion (per GJ primary energy): 0.095 tons CO₂ for coal, 0.074 tons for oil products, 0.060 tons for ethane/propane/butane, 0.056 tons CO₂ for natural gas. Biomass stores around 0.1 tons CO₂ per GJ and it is used as fuel and feedstock in increasing amounts in the, however, it is regarded as carbon neutral energy carrier. On average 3 tons of CO₂ is stored in plastics and 2.8 tons CO₂ is stored in synthetic organic materials.

The carbon storage in olefins and other chemicals are as follows (in ton CO₂ per ton of product): 3.14 for ethylene and propylene, 3.26 for butadiene, 3.38 for benzene, 2.81 for toluene, 3.32 for xylene, 1.38 for methanol and 3.67 for carbon black. During use of surfactants and solvents on average 1.81 tons of CO₂ is emitted per ton of synthetic organic material.

Carbon flows are monitored from raw material to the end of life of plastics and chemicals following the steps described earlier in this section. Carbon accounting is crucial because carbon stored in chemicals is typically not accounted for. Use of biomass that is stored in chemicals and used as fuel in combination with CO₂ capture and storage yields net negative emissions, which complicates the accounting.

D. Investment cost assumptions of technology options

Table D1. Investment costs of technology options.

	Unit	Investment cost	Reference
Fossil fuel-based HVC production capacity	USD/t HVC	1,800	(Broeren et al., 2014)
Fossil fuel-based ammonia production capacity	USD/t ammonia	750	(Broeren et al., 2014)
Fossil fuel-based methanol production capacity	USD/t ammonia	350	(Broeren et al., 2014)
Energy efficiency	USD/GJ	50	(Broeren et al., 2014; IEA, 2019)
Solar process heat	USD/kW	200	(IEA-ETSAP and IRENA, 2015)
Biomass process heat	USD/kW	200	(Saygin et al., 2014)
Heat pumps	USD/kW	1,000	(IEA-ETSAP and IRENA, 2013a)
Mechanical recycling	USD/t/yr	500	(Cimpan et al., 2015)
Chemical recycling	USD/t/yr	1,200	(Solis, 2018)
Energy recovery	USD/t/yr	1,000	Own estimate
Bio-based chemicals and plastics (data for PLA)	USD/t/yr	3,300	(Chiarakorn et al., 2011)
Bio-based ammonia	USD/t/yr	4,000	(IEA, 2018; Sánchez et al., 2019)
Bio-based methanol	USD/t/yr	5,000	(IRENA and Methanol Institute, 2021)
Renewables-based hydrogen feedstocks	USD/kW	500	(Gielen et al., 2020)
Methanol to olefins	USD/t/yr	1,000	(IEA, 2018)
CCS for process heat	USD/t CO ₂ captured/yr	300	(Saygin et al., 2013)
CCS for CHP	USD/t CO ₂ captured/yr	250	(Saygin et al., 2013)

BECCS	USD/t CO ₂ captured/yr	350	(Restrepo-Valencia and Walter, 2019)
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