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Petrochemicals and Climate Change

Tracing Globally Growing Emissions and Key Blind Spots in a Fossil-Based Industry

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2022

Document Version:
Publisher's PDF, also known as Version of record

Link to publication

Citation for published version (APA):
Bauer, F., Kulionis, V., Oberschelp, C., Pfister, S., Tilsted, J. P., Finkill, G. D., & Fjäll, S. (2022). *Petrochemicals and Climate Change: Tracing Globally Growing Emissions and Key Blind Spots in a Fossil-Based Industry*. (IMES/EESS report; Vol. 126). Lund University.

Total number of authors:
7

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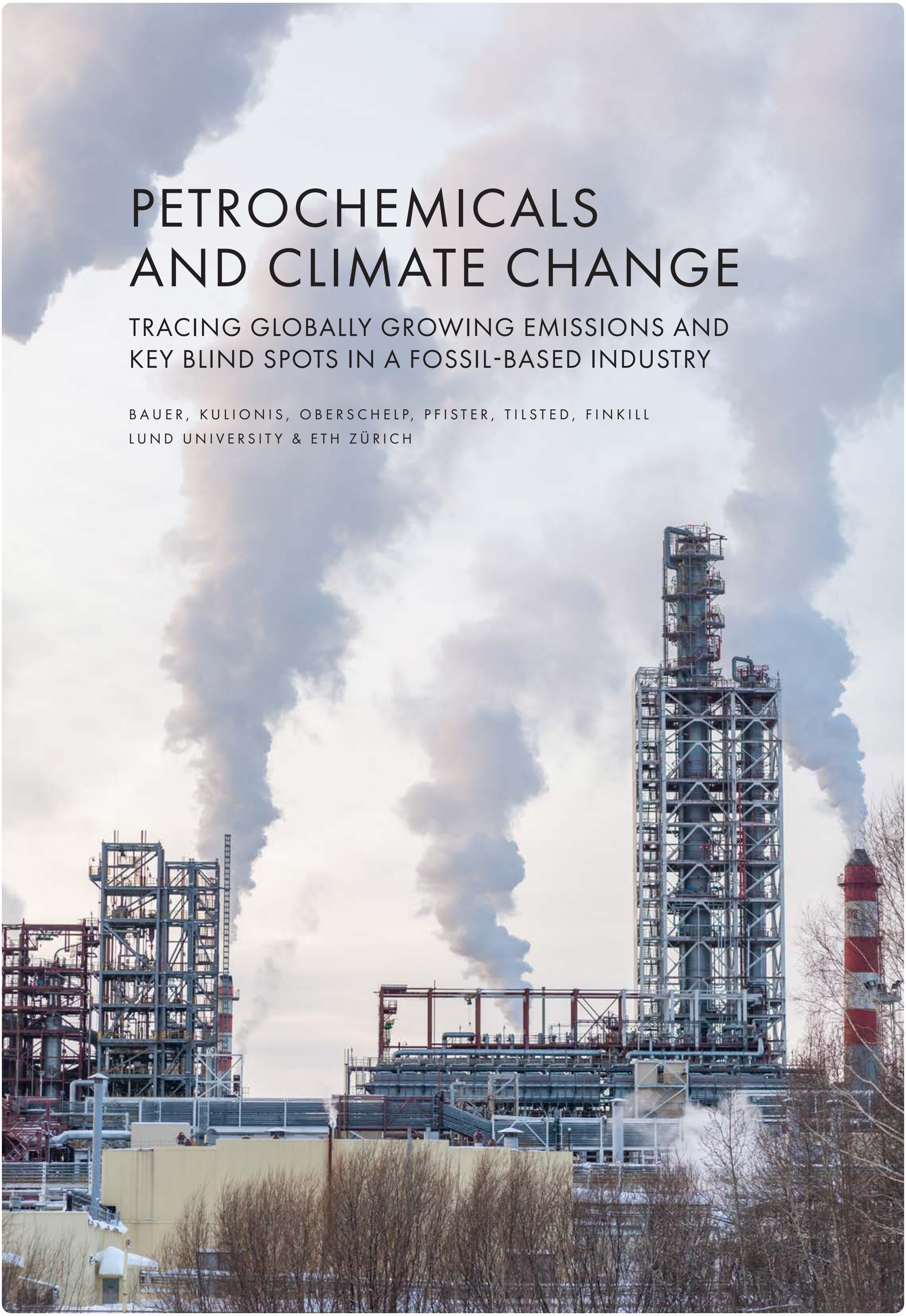

IMES/EESS REPORT NO 126
ISRN: LUTFD2/TFEM-- 22/3117--SE + (1-101)
ISSN: 1102-3651
ISBN: 978-91-86961-52-7

PUBLISHED 2022

COVER PHOTOS: ADOBE STOCK / ANATOLY SAVITSKY
LAYOUT & ILLUSTRATIONS: JOHAN CEDERVALL

ENVIRONMENTAL AND ENERGY SYSTEMS STUDIES
LUND UNIVERSITY, P.O. BOX 118, SE-221 00 LUND, SWEDEN

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TRACING GLOBALLY GROWING EMISSIONS AND KEY BLIND SPOTS IN A FOSSIL-BASED INDUSTRY

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The research presented in this report was funded by a grant from the V. Kann Rasmussen Foundation.

EXECUTIVE SUMMARY

With the risk of climate breakdown becoming ever more pressing as the world is on track for 2.7 degrees warming, pressure is increasing on all sectors of the economy to break with fossil fuel dependence and reduce greenhouse gas (GHG) emissions. In this context, the chemical industry and the production of important basic chemicals is a key sector to consider. Although historically a driver of economic development, the sector is highly dependent on fossil resources for use as both feedstock and fuel in the production of as well organic as inorganic chemicals.

The chemical industry demands both petroleum fractions and natural gas. Petroleum fractions such as naphtha and petroleum gases are used as feedstocks for building block chemicals and polymers (e.g., benzene and polyethylene), while natural gas is used for methanol and ammonia. Indeed, the sector is associated with both large process emissions as well as energy related emissions. Our results demonstrate that in 2020 direct GHG emissions from the petrochemical sector amounted to 1.8 Gt CO_2eq which is equivalent to 4% of global GHG emissions. Indirect GHG emissions resulting from the activities in other industries supplying inputs for the petrochemical industry accounted for another 3.8 Gt CO_2eq. The petrochemical industry is thus associated with a total of 5.6Gt CO_2eq of GHG emissions, equivalent to ~10% of global emissions.

Over the past 25 years, emissions associated with petrochemicals have doubled and the sector is the third most GHG emitting industry. This increase is fueled by large growth of petrochemicals production as well as growth in regions with high indirect emissions, i.e., in energy systems with high dependence on coal and other fossil fuels. Over the past decades, the industry has grown rapidly in the Asia-Pacific region especially in China which in 2020 was the source for about 47% of global GHG emissions associated with petrochemicals. USA accounts for 6% of the emissions from the industry and Europe for 5%. The BRIC group of countries, which except for China also includes Brazil, India, and Russia, currently accounts for 57% of GHG emissions from petrochemicals, showing that the emissions from this sector are more geographically clustered in these countries than emissions from other sectors.

Proper disaggregated and comparative analyses of key products is currently not possible. Data confidentiality and a high reliance on proxy data limit the reliability of LCA and stands in the way of mapping climate impacts. A strong demand of chemicals life cycle inventory (LCI) data for environmental footprinting has resulted in a general increase of chemicals data in many LCI databases, but the energy demands both for heat and electricity are typically not well-documented for production processes outside the main bulk chemicals. If incinerated at end-of-life plastics and other chemical products will emit embodied carbon as CO_2 and if landfilled there is a risk of slow degradation with associated methane emissions. Global estimates based on most LCA datasets will thus significantly underestimate emissions from the chemical industry.

The multitude of value chains dependent on the petrochemical industry makes it an important contribution to life cycle emissions in many sectors of the economy. Petrochemicals are used as an intermediate input in many industries and the emissions associated with them thus propagate through the economy, with final demand in manufacturing industries and services being associated with the largest shares of emissions from chemicals. The impacts and emissions downstream in value chains is however poorly understood and disclosure by petrochemical producers is lacking and insufficient.

While disclosure of emissions in the industry has increased over the past decades, it remains partial and shows inconsistencies over time. This is due to issues such as different reporting standards, large discrepancies in the extent of disclosure as well as various other gaps and inconsistencies in reporting. This holds for all scopes, although Scope 1 emissions are better covered. Only some firms disclose information about downstream Scope 3 emissions including end-of-life for final products. Emission targets set by firms in the industry do not correspond to the challenge of large and rapid emission reductions. Many targets include only parts of operations and transparent, standardized target-setting is lacking. Reported emission reduction initiatives to achieve targets are far from sufficient focusing mainly on efficiency improvements or insubstantial parts of the operation.

Shifting to renewable energy is a key for rapid emission reductions in the industry, yet few firms report strategic targets for this shift. As the industry has historically been closely linked to and integrated with the energy sector it holds a great potential for engaging with the deployment and adoption of renewable energy, although this implies a transformation of the knowledge base and resource allocation in the industry which is still focused on fossil fuels.

Roadmaps and scenario analyses show that apart from a shift to renewable energy, a transformation of the industry relies on the deployment of key technologies which are not yet fully developed. This includes new technologies for hydrogen production, e.g., electrolytic (green) hydrogen or hydrogen produced with carbon capture and storage (CCS). New chemical synthesis pathways based on captured carbon, so called carbon capture and utilization (CCU) is also highlighted, but the massive demand for renewable energy associated with this pathway is a significant barrier to its adoption in the near term.

The report shows how efficiency improvements continues to be the main focus for reducing the climate impact of petrochemicals, but that this is a completely inadequate approach for achieving the emissions reductions necessary in the coming decades. Breakthrough technologies are unlikely to be deployed at a rate consistent with international climate targets, and there is a great risk in relying on the promises of technologies which are yet to be proven at scale. The large knowledge gaps that remain are key barriers for effective governance of the transition.

CONTENTS

1 INTRODUCTION

With the risk of climate breakdown becoming more pressing as the world is on track for 2.7 degrees warming (UNEP, 2021) pressure is increasing on all sectors of the economy to break with fossil fuel dependence and reduce greenhouse gas (GHG) emissions. Significant research efforts have been devoted to study the possibilities of transitions within the energy and transportation sectors, which use the main share of fossil resources to produce heat, power and transportation fuels. Other heavy industry sectors face low-carbon transition challenges which are rather different as their dependence on fossil carbon is embedded in the processes and products themselves (Bataille et al., 2018; IEA, 2020; Rissman et al., 2020). In this context the chemical industry and the production of important basic chemicals is a key sector to consider as the sector is a driver of economic development (Arora et al., 1998) and highly dependent on fossil resources for use as both feedstock and fuel in the production of as well organic as well as inorganic chemicals. The industry has however not been the focus of much research on climate impact and mitigation as its climate impact has been hidden behind other industries closer to consumers in the global sustainability debate (Johnson, 2012).

The chemical industry demands petroleum fractions such as naphtha and petroleum gases as feedstocks for the production of organic building block chemicals and polymers, such as benzene and polyethylene, and natural gas, e.g. for the production of methanol and ammonia. Further, the use of coal for production of chemicals is large and increasing, mainly in China where it is used for primary chemicals and plastics. Yet, the climate impact of the chemical industry is not fully understood, neither on the global level, nor in specific regions or along specific value chains. The high level of complexity and the substantial share of emissions embodied in feedstock makes the petrochemical sector a challenging area to reduce emissions, compared to other industrial sectors with far simpler production processes such as the iron and steel or paper industry (IEA, 2020; IEA et al., 2013). Aside from the climate impact the chemical industry is also heavily implicated in other issues related to environmental sustainability, such as emissions of pollutants to surface and ground water, production and diffusion of endocrine disruptors, persistent organic pollutants, and other chemical compounds that negatively affect the human health, the ozone layer, and ecosystems (Persson et al., 2022). While this report focuses on climate change it is imperative that GHG emission reductions are addressed together with these other issues in the transformation of the industry towards more sustainable modes of production and use of chemical products.

The present report aims to provide an overview of the current knowledge of climate impact of the petrochemical sector through GHG emissions, as well as plausible future developments in the sector and key knowledge gaps. This will be achieved through an extensive literature and data review that will assess which petrochemical industry subsectors are accurately and comprehensively monitored. The review aims to capture the geography of the sector and its climate impact, include production is shifting geographically from the traditional strongholds of the industry in Europe and North America to rapidly growing economies in Asia-Pacific and the Middle-East and how this is reflected in the knowledge about the climate impact of the industry. The review will cover different literatures and data types to be able to provide comprehensive knowledge about both the current and future situation.

Well established research approaches used for environmental assessments include a top-down approach, based on Environmentally Extended Input-Output models (EEIO) and a bottom-up approach, based on Life Cycle Assessment (LCA) of a selection of products and processes. Both LCA and MRIO approaches have their strengths and limitations. They differ with respect to their level of detail, system boundaries and spatial and temporal resolution. The top-down approach quantifies the environmental impacts of different product categories at the national or global level and provides a macro-perspective on the issue of fossil resource use in different industries and the embodied climate impact in products such as plastics and petrochemicals. The bottom-up approach based on LCA describes the environmental and climate impact of different products throughout their whole life cycle and provides highly detailed information about the climate impact of the production, use, and disposal of petrochemicals and plastics from specific locations and in specific contexts. These two approaches complement each other and illuminate the environmental impact of petrochemicals from different viewpoints.

Another growing source of information about the environmental and climate impact is information published directly by the firms in the industry. The pressure on firms to disclose this type of information has increased in recent years as customers and investors request better insights into the environmental performance of firms they collaborate with or invest in. Legislation on so called sustainability reporting is also growing in terms of both scope and scale, improving the transparency of the climate impact of large firms, but accounting for GHG emissions is many times more complex than it may seem at first. In most parts of the world this type of disclosure is however still voluntary, which is why it can only give a partial image. Through this type of disclosure important insights are however gained regarding the ambitions firms have to reduce emissions and what types of initiatives they engage in to reach such targets.

The next chapter introduces the chemical industry, its structure and connections to fossil fuel resources, the complexity of tracing GHG emissions through the intertwined production processes and value chains of chemicals, and the problem of allocating GHG emissions to specific products. Chapter 3 presents the main findings from the review of EEIO literature and data. Chapter 4 presents the main findings from the review of LCA literature and datasets. Chapter 5 then reviews emissions and targets reported and disclosed by leading firms in the industry. Chapter 6 discusses future developments towards a petrochemicals sector with reduced emissions, based on published scenarios and information about the breakthrough technologies that many of emission reduction targets rely upon. Chapter 7 contextualizes the findings, while Chapter 8 presents the main conclusions and identifies key knowledge gaps that remain.

PHOTO: PIXABAY

2 THE PETROCHEMICAL INDUSTRY AT A GLANCE

2.1 A COMPLEX PRODUCTION SYSTEM

Petrochemicals are almost exclusively produced from fossil materials and with fossil energy – this resource base is the fundamental reason for the large carbon footprint of the industry. Petrochemicals include the common organic chemicals produced from petroleum fractions, coal, or natural gas as well as ammonia. The chemical industry is the largest industrial demand segment for petroleum – the sector accounts for 14 % of global petroleum demand and 8 % of natural gas demand (IEA, 2020). The petrochemical sector is growing rapidly and is projected to show the largest growth in petroleum demand until 2030 (IEA, 2018). The very high energy intensity of the industry and its production processes and the fact that this energy is mainly supplied in the form of the same fossil fuel resources that go into the processes as material, lead to the industry being associated with large GHG emissions.

The petrochemical industry uses coal, natural gas, natural gas liquids (NGLs), and refined liquid petroleum products to produce a group of key primary chemicals, also called high value chemicals, e.g., ammonia, methanol, ethylene, propylene, butadiene, and the aromatics benzene, toluene, and xylenes – commonly grouped as BTX. These primary chemicals are subsequently used in several downstream processes to produce more advanced chemical products. The two largest product groups are nitrogen fertilizers and plastics, fibres, and rubbers, with the remaining products being a diverse collection of additives, solvents, and explosives. Levi and Cullen (2018) estimated than almost 700 Mt of fossil fuels were used in the chemical industry in 2013, to produce more than 800 Mt of products, and direct emissions of almost 300 Mt of CO_2, as shown in Figure 1. Data shows that the global energy demand of the chemical industry was 15 EJ/y excluding feedstock and 42 EJ/y including feedstock (Boulamanti and Moya, 2017).

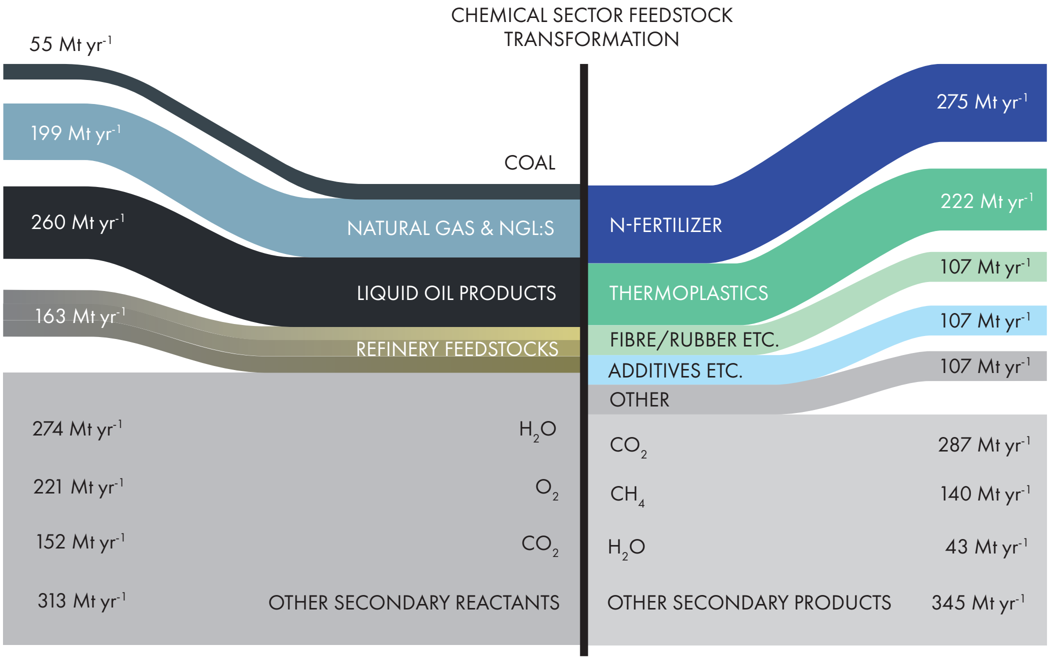

FIGURE 1 OVERVIEW OF GLOBAL MATERIAL FLOWS THROUGH THE PETROCHEMICAL INDUSTRY, FROM FOSSIL FEEDSTOCK TO CHEMICAL PRODUCTS IN 2013. SOURCE: LEVI AND CULLEN (2018). REPUBLISHED WITH PERMISSION FROM ACS, FURTHER PERMISSIONS RELATED TO THE FIGURE SHOULD BE DIRECTED TO THE ACS.

The complexity of production in the petrochemical sector also makes accounting of GHG emissions highly challenging due to the high number of chemical products (output complexities), the fact that many chemicals are not produced by a single production process, as well as diffuse and multi-staged emissions of different types of GHG, not least methane which is a gas with a very high climate impact – its global warming potential (GWP) is 83 times that of CO_2 over a 20 year period. Further difficulties include lack of publicly available detailed energy use data, complex production sites with high level of heat integration or high levels of combined heat and power (CHP) or integration with refineries (Boulamanti and Moya, 2017).

2.2 KEY VALUE CHAINS

The value chains from fossil feedstock to a consumer product are long and complex. From the fossil feedstocks a small number of fundamental primary chemicals are produced. These primary chemicals include the common olefins (ethylene, propylene, and butadiene), aromatics (benzene, toluene, and xylene), methanol, and ammonia. Figure 2 shows the estimated global production, energy use and associated CO_2 emissions for the key primary chemicals.

One of the most energy-intensive processes in the industry is the steam cracker, which is the core process for production of olefins and aromatics. In the steam cracker feedstocks such as ethane, propane, or naphtha are mixed with steam and rapidly heated to very high temperatures – up to 900°C – making the molecules crack into smaller ones. The primary chemicals from the steam cracker are subsequently primarily used to produce different plastic resins, but also solvents and other more advanced chemicals.

Methanol is produced in dedicated plants, in which natural gas, petroleum, or coal is converted into a synthesis gas through gasification or reforming. Both processes are highly energy intensive, with higher energy demand for processes using heavier feedstocks. The produced synthesis gas contains carbon monoxide and hydrogen which are then reacted in a catalytic process to produce methanol at medium-high temperatures of 200-300°C and high pressure of 5-10 MPa. Methanol is itself used as a solvent but it is also used extensively in downstream processes to produce adhesives, plastic resins, and fuel additives.

Ammonia is also produced from synthesis gas, just as methanol, but all carbon rich gases are removed from the gas to produce pure hydrogen which is then catalytically reacted with nitrogen to form ammonia. The reaction takes place at high temperatures of 400-500°C and very high pressure of more than 13 MPa which makes it very energy intensive. Fixated nitrogen in the form of ammonia is the foundation for nitrogen fertilizers, such as urea and ammonium nitrate, which make up the majority of the use of ammonia, but it is also used for the production of explosives and some plastics.

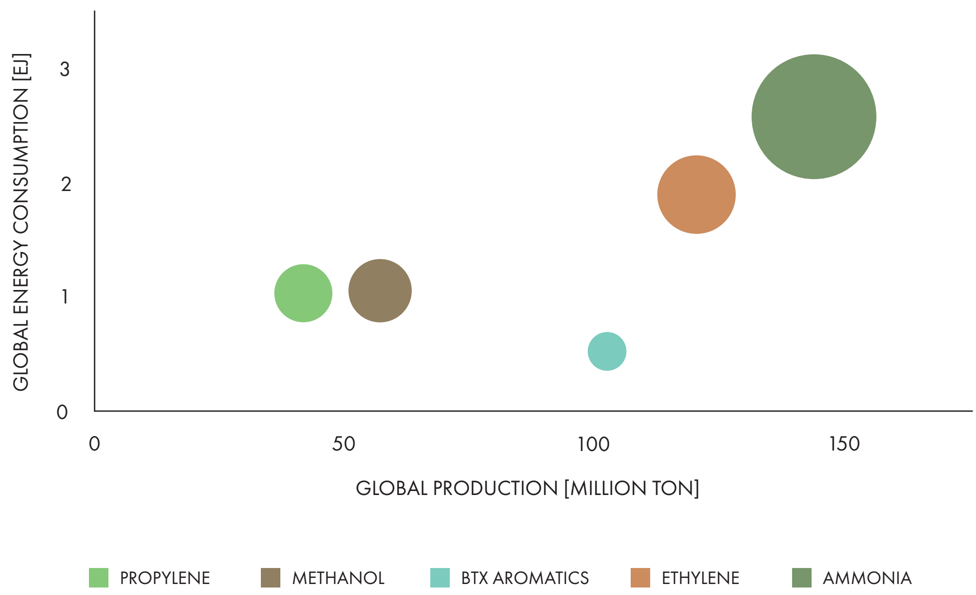

FIGURE 2 GLOBAL PRODUCTION AND ENERGY USE FOR KEY PRIMARY CHEMICALS IN 2011. THE SIZE OF THE BUBBLES CORRESPONDS TO THE GHG EMISSIONS ASSOCIATED WITH THEIR PRODUCTION. DATA FROM (IEA ET AL., 2013)

2.3 STRUCTURAL AND REGIONAL CHARACTERISTICS

As the chemical industry grew out of the industrial revolution in Europe and modern petrochemicals were largely developed in the US, these regions were for a long time dominating the global markets (Aftalion, 2001). However, following the era of globalization of many markets, value chains, and industries the landscape of the chemical industry and its geography of production has changed significantly. The new millennium has seen the most rapid growth in production in Asia-Pacific. At the same time production rates in the old strongholds Europe and North America have remained stable. Figure 3 shows the development of petrochemicals production in selected countries and global market shares since 1995.

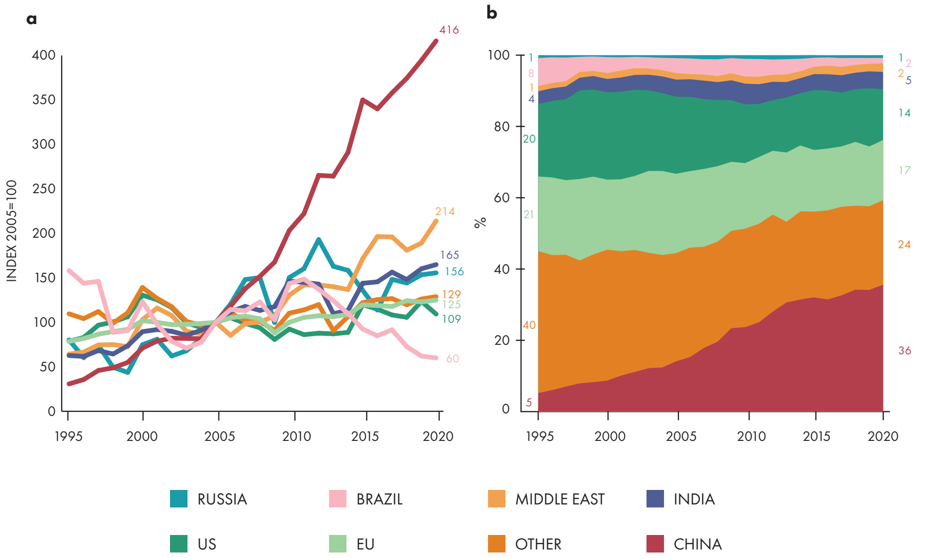

FIGURE 3 DEVELOPMENT OF PRODUCTION INDEX FROM 1995-2020 IN SELECTED COUNTRIES. BASED ON EXIOBASE 3.8.

The rapid growth of production in China has led to it now being the single most important country for petrochemicals. As GHG emissions are primarily associated with production of primary chemicals – although with variations depending on production technology – the macro-level image of emissions closely resembles that of production and sales, as will be shown in the next section.

2.4 FOSSIL RESOURCE USE AND GHG EMISSIONS IN THE CHEMICAL INDUSTRY

Although significant energy efficiency improvements have been achieved in the industry in ambitions to cut energy costs (Ren, 2009), it is still suffering from a troublesome 'carbon lock-in' (Unruh, 2000) largely due to factors such as integrated technologies and systems, sunk costs in existing production facilities, routines and standards for safety (Janipour et al., 2020). The fossil resource dependency of the industry for both feedstocks and energy is the main reason for its large GHG emissions.

While petroleum naphtha – a side-product from petroleum refining – for a long time dominated the feedstock use in the industry, the use of feedstocks is today more diverse, largely depending on regional availability and costs. Naphtha remains the most important feedstock in Asia-Pacific, Europe, and Latin America, whereas ethane has become the most important one in North America and the Middle East following a rapid development of gas extraction associated with large volumes of NGLs. Asia-Pacific and South Africa are the only regions in which coal – the feedstock widely used in the very early days of the chemical industry – remains in use in large scale. Coal is used due to it being a domestically available and cheap resource primarily in China.

Emissions depend on the use of feedstocks with production based on coal being associated with larger emissions, but to a large extent also on the product portfolio of the regions. Large production of the very energy intensive product ammonia – about half of it from coal – therefore leads to very high emissions from Asia-Pacific. The feedstock and product portfolios together with the associated emissions are presented in Figure 4 below.

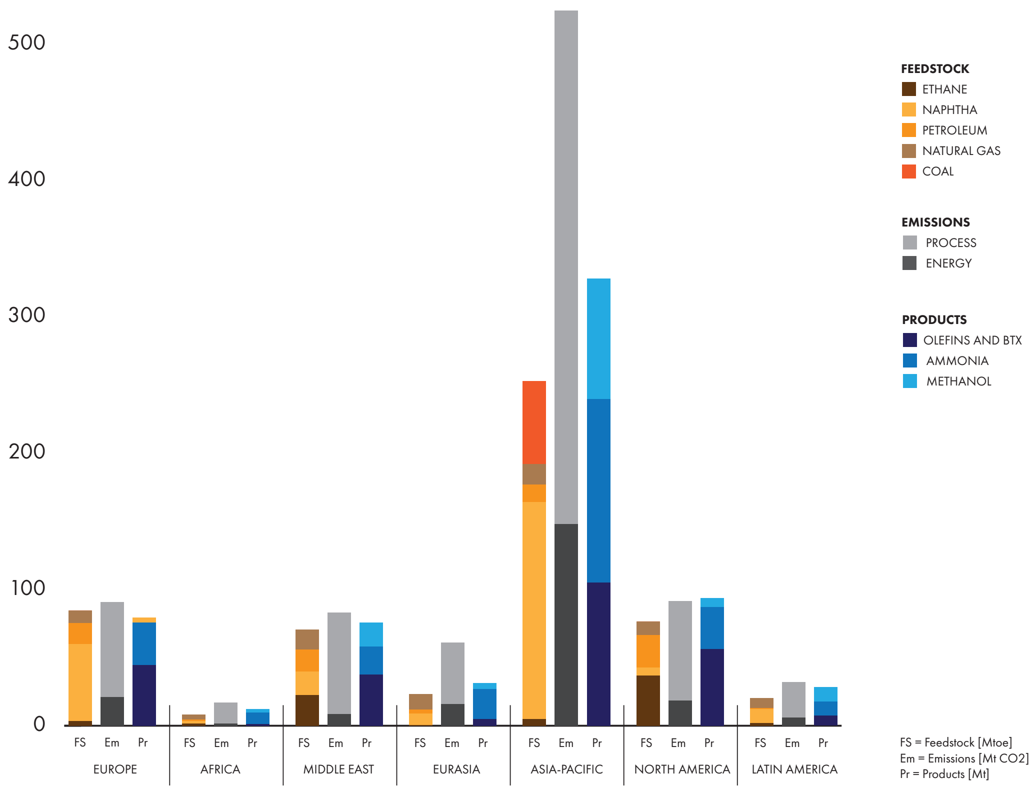

FIGURE 4 FEEDSTOCKS, PRODUCTS, AND GHG EMISSIONS ASSOCIATED WITH PETROCHEMICALS PRODUCTION BY REGION. DATA SOURCE: IEA.

PLASTICS IS THE MOST
IMPORTANT PRODUCT CATEGORY
FROM THE PETROCHEMICAL INDUSTRY

PHOTO: ADOBE STOCK

3 ENVIRONMENTALLY EXTENDED INPUT-OUTPUT ANALYSIS

This chapter presents a detailed overview of the top-down based EEIO approach by describing available IO models and databases and examining how the petrochemical industry is covered in these databases. Furthermore, we also quantify the environmental impacts of the petrochemical industry at the country and global levels.

3.1 ENVIRONMENTALLY EXTENDED INPUT-OUTPUT (EEIO) ANALYSIS

3.1.1 AN OVERVIEW

Input-output analysis is an analytical framework developed by Wassily Leontief (Leontief, 1936), in recognition of which he received a Memorial Nobel Prize in Economic Sciences in 1973. The key idea behind IO analysis is that a national or global economic system can be split into a number of sectors that are interlinked and whose relationship can be presented in a matrix form.

Performing IO analysis requires IO tables that record transactions between different industries (e.g., how much industry i buys/sells to/from industry j). National IO tables are usually compiled by statistical agencies and are an integral part of the System of National Account forming the central framework for the compilation of a single and coherent estimate of gross domestic product (GDP). The standards and guidelines for the data collection and compilation of IO tables are described by the United Nations System of National Accounts (see e.g. United Nations, 2018).

In their basic form, the IO tables show how goods and services are brought into an economy (either as a result of domestic production or imports from other countries), and how those same goods and services are used (intermediate consumption; final consumption by household, non-profit institutions serving households, and general government; gross capital formation; and exports). As such, they serve as a powerful analytical tool that can be applied to study various economic topics related to structural changes, productivity, employment, and value-added creation, to name a few.

One unique feature of the IO framework is that it can be linked with external data sources, often referred to as satellite accounts or extensions. Typical examples are satellite accounts for the environment, tourism, and employment. Satellite accounts are intended for particular purposes, for instance an environmentally extended input output (EEIO) model allows to evaluate environmental performance of a country or a specific industry including supply chains.

EEIO analyses have emerged in the late 1960s and 1970s at the time of the two oil crises. Given that energy was a critical factor of production for many industries, researchers and policymakers focused on understanding the role of energy in the economy. At the same time there was also growing concern over the environmental impacts associated with the use of fossil fuels and climate change (Miller and Blair, 2009). Today such environmental analyses are common and performed on a frequent basis by national statistical agencies (e.g. SCB Sweden, FOEN Switzerland, PBA Netherlands), supranational institutions (e.g. UN IRP, UNEP, OECD, Eurostat).

Early studies have investigated environmental impacts that occur within the borders of a single country. However, changes in international trade patterns and increasing international fragmentation of production processes led to a more global production system and distribution of environmental impacts across multiple countries. To understand these international interdependencies researchers have developed global multi-region input-output (GMRIO) databases and models (e.g. WIOD, EXIOBASE, Eora, GTAP). These databases allow to evaluate the environmental effects occurring in one country due to final demand (usually referred to as consumption) in another. For example, a car assembled in Germany and sold in the USA will contain parts made in multiple countries, in turn production of these parts will cause various environmental impacts. EEGMRIO models coupled with the environmental data allow to track and analyse where these impacts occur and where they are finally consumed.

3.1.2 IO MODELS AND DATABASES

Within the input-output framework, two methods are commonly used to assess environmental performance: the single region input-output (SRIO) model and the multi-region input-output (MRIO) model (Miller and Blair, 2009). Both methods are based on different underlying assumptions and have different data requirements. A detailed review of these methods and their application to environmental studies can be found in (Peters, 2008).

3.1.2.1 Single region IO (SRIO)

The SRIO models are typically applied to quantify the impacts on the producing sectors located in a particular region that are caused by new final demands for products made in the region (Miller and Blair, 2009, p71). These models rely on national input-output tables compiled by national statistical agencies, such as the Bureau of Economic Analysis (BEA) of the US, the UK's Office for National Statistics (ONS) and Statistics Denmark. Country specific SRIO tables may differ in the level of sectoral detail (ranging from roughly 35 sectors to more that 400 sectors), accounting conventions, classification systems, update frequency and other aspects. The USA and several other countries produce very detailed IO tables covering roughly 400 industrial sectors. More detailed sectoral classification enables to investigate a wider range of sectors. For example, in a very aggregate IO table there might be just one petrochemical sector, while in a more detailed table petrochemical sector is usually split into several sub sectors, such as Manufacture of chemicals and chemical products; Manufacture of basic pharmaceutical products; Manufacture of rubber and plastic products and in rare cases of very disaggregated IO tables these subsectors can split even further.

3.1.2.2 Multi-region input-output (MRIO)

The opening up of the world economy has led to unprecedented surges in international trade. As a result, it has become increasingly important to calculate environmental impacts embodied in trade. Early studies in this area relied on the SRIO models assuming that imported products are produced with the same technology as the domestic economy (Machado et al., 2001; Wyckoff and Roop, 1994). This assumption is often referred to as the domestic technology assumption (DTA) and it may lead to errors for countries with diverging technology and energy mixes (Andrew et al., 2009). This type of limitations associated with the SRIO models stimulated research in the use of multi-region input-output (MRIO) models.

The MRIO concept is not new and have been described already in the 1950s (Isard, 1951), though their application to environmental and other issues (e.g. trade in value added research) has gained traction only in the last two decades. This late start is often attributed to the data-hungry and computationally- intensive process of the construction of the MRIO table (Kanemoto and Murray, 2013). MRIO tables started to emerge in the late 2000s.

MRIO overcomes the issues associated with the SRIO method by eliminating the domestic technology assumption. The MRIO approach distinguishes between imports that are directed towards the final consumption and those that are directed towards the intermediate consumption (economic sectors). Imports that are directed towards the intermediate consumption can be allocated to either the production of goods for domestic use or the production of exports. This unique MRIO structure allows the tracing and analysis of the supply chain between regions and sectors.

Today a practitioner can choose from several MRIO databases such as WIOD (Dietzenbacher et al., 2013; Timmer et al., 2016, 2015), Eora (Lenzen et al., 2012, 2013), EXIOBASE (Stadler et al., 2018; Tukker et al., 2013; Wood et al., 2015), OECD ICIO (Yamano and Guilhoto, 2020), and GTAP (Aguiar et al., 2019). Below we describe the key features of these databases and how they cover petrochemical industry.

3.1.2.3 Spatially explicit input-output approaches

Spatially explicit input-output analysis is an emerging area of research which aims to connect top-down accounting techniques (such as MRIO) with localized impacts. Existing environmentally extended input-output models inform about the impacts at the national level (e.g., emissions in sector i in county r due to consumption of product j in country s) and in some cases at the subnational level (e.g., by splitting EU into 162 regions). As such they are suitable for broad national assessments of global environmental stressors such as CO_2 (1t CO_2 has the same GWP regardless of where it is emitted).

Spatially explicit input-output analysis aims to improve modelling of environmental impacts that have high local relevance e.g., water stress, biodiversity loss, or local air pollution (such as SO2, NOx, PM2.5, PM10). Sun et al. (2019) reviews key methods and limitations of various approaches that are used to integrate spatial data in input–output modelling. Typically, these approaches use maps and databases of environmental impacts or stressors generated from observations by monitoring stations and satellite remote sensing measurements. Moran et al. (2020) provides several examples where spatially explicit modelling has already yielded promising results that make environmentally extended supply-chain models more specific and actionable.

Some notable examples include studies linking supply chains to global biodiversity hotspots, fine-scale assessments of Europe's raw-material footprint and related global impacts or the impact of EU consumption on global water scarcity (Lutter et al., 2016). Spatially explicit assessment has also been used for dissolving Exiobase "Rest of the World" regions for land and water consumption (Cabernard and Pfister, 2021). The methods and databases developed in these research projects, many of which are openly available, provide evidence of the large potential to move supply-chain assessments to the next level by using spatially explicit information.

3.1.3 MRIO DATABASES

Below we describe the major EEMRIO that at least cover GHG emissions.

3.1.3.1 Eora

This database has one major advantage in comparison to other available MRIO databases. It covers 188 countries/regions (of which about 113 are estimated) and thus, allows performing nation-specific analysis for a larger number of countries/regions than any other MRIO database. Two Eora versions are available; the Full Eora and the Eora26. The difference between them resides in the sectoral classification. The former has a higher resolution, which varies depending on the country from 26 to ~500, whereas the latter includes 26 sectors for all countries. Even though Full Eora can be considered more accurate, using Eora26 avoids possible computational problems, since memory needs and server space would be significantly lower. However, this is not a major issue with current IT infrastructure. EORA 26 also provides more consistent results, since many countries have only 26 sectors also in full EORA.

3.1.3.2 EXIOBASE

EXIOBASE 3 covers 44 individual countries (28 EU members plus 16 major economies) and 5 Rest of the World regions (summarizing the remaining countries in Europe, Asia, Africa, America, and Middle East). The MRIO tables are provided in two forms: (i) a product-by-product table distinguishing 200 products, and (ii) an industry-by-industry table distinguishing 163 industries. EXIOBASE database also stands out in terms of the level of detail in the satellite accounts which are available for emissions, energy, land, water and employment.

The most recent EXIOBASE v3.8.2 covers the period 1995–2022. However, it should be noted that the original EXIOBASE 3 time series ends in 2011. The new time series are estimated based on trade and macro-economic data up to 2022. A lot of care must be taken when utilizing this data as it is only partially suitable for analyzing trends over time.

3.1.3.3 GTAP

The Global Trade Analysis Project (GTAP) database version 10 (released in 2019) covers 121 countries (plus aggregate 20 regions) and 65 industries for four benchmark years; 2004, 2007, 2011 and 2014 (no time series). GTAP consists of individual country input-output tables and in its original format is not suitable for an MRIO analysis. Peters et al. (2011) demonstrated how the GTAP database can be converted into an MRIO table. The GTAP database will be updated for the newest release including the energy and environmental extension and the land use and cover extension (no publication date available). However, neither water nor all greenhouse gas extensions are available. Furthermore, a license needs to be purchased.

3.1.3.4 WIOD

World input-output database (WIOD) contains two releases: (i) WIOD 2013 release, and (ii) WIOD 2016 release. The earlier WIOD 2013 release covers 35 industries and 41 countries/regions. This includes 27 EU countries, 13 other major economies alongside the rest of the world (ROW) region for the period 1995–2011. It comes with environmental accounts containing data for CO_2, other greenhouse gas emissions, energy, land, material and water use for the period 1995–2009. WIOD 2013 does not cover smaller countries (such as Switzerland) as a separate entity in the MRIO table. Instead, it is included in the ROW region. A more recent WIOD 2016 release provides monetary MRIO tables covering 56 industries and 44 countries (including e.g. Switzerland) for the period 2000–2014. The WIOD 2013 release tables adhere to the 1993 version of the SNA and the WIOD 2016 release tables adhere to the 2008 version of the SNA. Initially, the WIOD 2016 release did not contain any environmental extensions, but recently (July 2019), the Joined Research Center (JRC) launched the WIOD-based environmental extensions. However, the JRC environmental extensions contains data only for CO_2 emissions and energy use, data for other indicators (such as land and water) is not available. Both WIOD releases offer MRIO tables in current and previous years' prices, such tables are essential for the structural decomposition analysis.

3.1.3.5 OECD IO

The OECD database contains two releases: (i) ICIO SNA93, ISIC REV.3 released in 2016, and (ii) ICIO SNA08, ISIC REV.4 released in 2018. The OECD 2016 release covers 64 regions/countries (35 OECD, 28 non-OECD countries and ROW aggregate) and 34 industries (classified according to the International Standard Industrial

Classification revision 3) for the period from 1995 to 2011. The OECD 2018 release covers 65 countries/regions (36 OECD, 28 non-OECD countries and ROW aggregate) and 37 industries (classified according to the International Standard Industrial Classification revision 4) for the period 2005–2015. The OECD 2016 edition adheres to the 1993 version of the System of National Accounts (SNA) and the OECD 2018 edition adheres to the 2008 version of the SNA.

The OECD ICIO is built by internationally recognized organization and consequently can be seen as part of "official statistics". All other databases have been built by academic researchers and may face questions regarding credibility (Tukker et al., 2018). However, it is highly aggregated (34 sectors) and provides environmental extensions only for CO_2.

3.1.3.6 Coverage of petrochemicals in different MRIO databases

As shown in Table 1 Coverage of the petrochemical industry differs across different databases. OECD2016, OECD2018 and WIOD2013 editions cover only two sectors specialized in "Chemicals and chemical products" and "Rubber and Plastics products". This is a very aggregate classification where different manufacturing categories are presented in one group. For instance, "Chemicals and chemical products" aggregates sub-categories such as "Manufacture of pharmaceuticals, medicinal chemicals and botanical products", "Manufacture of fertilizers and nitrogen compounds", "Manufacture of basic chemicals" and other categories into one group. This level of aggregation allows only for a limited analysis of the petrochemical industry, for instance it is possible to assess the impact of rubber and plastic products, but not possible to evaluate the impact of nitrogen fertilizers or any other categories.

WIOD2016 and GTAP10 databases rely on a newer version of industrial classification (ISIC rev 4) which splits "Chemicals and chemical products" category into two parts: manufacture of chemical products and manufacture of pharmaceuticals. This classification enables to perform a somewhat more detailed analysis (compared with what OECD2016, OECD2018 and WIOD2013). Importantly it enables to separate the impact of pharmaceuticals from the rest of chemicals, which might be highly relevant for countries where the pharmaceutical industry plays a dominant role, since emission intensity per economic output is often lower for pharmaceuticals. It is important to note that often the importance of different industries is assessed in terms of employment and gross value added, assessment that take climate impacts into account are growing in importance.

EXIOBASE 3 provides the most detail representation of the petrochemical industry (see Table 1). It allows to assess the impacts associated with the manufacture of N-fertilizer; P- and other fertilizer; manufacture of basic plastic and; re-processing of secondary plastic into new plastic. However, it does not differentiate between manufacture of chemicals and pharmaceuticals. Another important aspect of EXIOBASE3 is that it covers a wide range of environmental accounts, which enables to assess not only climate but also other impacts such a biodiversity loss, water consumption and material use. Furthermore, a high sectoral resolution allows to perform a more detailed analysis in terms of where the inputs into the petrochemical industry come from (from which countries and sectors) and where the output is destined (to which countries and which sectors). We present the results of such analysis in Figure 11.

TABLE 1: OVERVIEW OF DATABASES

DATABASE	RESOLUTION OF PETROCHEMICAL SECTORS COVERED
EORA 26	• PETROLEUM, CHEMICAL AND NON-METALLIC MINERAL PRODUCTS
OECD2016	• CHEMICALS AND CHEMICAL PRODUCTS • RUBBER AND PLASTICS PRODUCTS
OECD2018	• CHEMICALS AND PHARMACEUTICAL PRODUCTS • RUBBER AND PLASTIC PRODUCTS
WIOD2013	• CHEMICALS AND CHEMICAL PRODUCTS • RUBBER AND PLASTICS
WIOD2016	• MANUFACTURE OF CHEMICALS AND CHEMICAL PRODUCTS • MANUFACTURE OF BASIC PHARMACEUTICAL PRODUCTS AND PHARMACEUTICAL PREPARATIONS • MANUFACTURE OF RUBBER AND PLASTIC PRODUCTS
GTAP10	• MANUFACTURE OF CHEMICALS AND CHEMICAL PRODUCTS • MANUFACTURE OF PHARMACEUTICALS, MEDICINAL CHEMICAL AND BOTANICAL PRODUCTS • MANUFACTURE OF RUBBER AND PLASTICS PRODUCTS
EXIOBASE 3	• PLASTICS, BASIC • RE-PROCESSING OF SECONDARY PLASTIC INTO NEW PLASTIC • N-FERTILIZER • P- AND OTHER FERTILIZER • CHEMICALS NOT ELSEWHERE CLASSIFIED • MANUFACTURE OF RUBBER AND PLASTIC PRODUCTS

3.1.4 GHG EMISSIONS OF THE PETROCHEMICAL INDUSTRY (BY SOURCE)

Global GHG emissions were 55.8 Gt CO_2eq in 2020, of which 1.8 Gt CO_2eq (or 4%) were direct emissions (often referred to as Scope 1) in the petrochemical industry. In addition to direct emissions, a significant share of emissions occurs indirectly (in other industries) as a consequence of the activities of the petrochemical industry. For the petrochemical industry, these indirect emissions were 3.8 Gt CO_2eq. In total the petrochemical industry accounted for 5.6 Gt CO_2eq or roughly 10% of global total. The largest share of indirect emissions came from the Utilities sector (31% of total petrochemical GHG emissions in 2020), followed by Mining (15%).

Furthermore, total GHG emissions of the petrochemical sector have more than doubled since 1995 (Figure 5b).

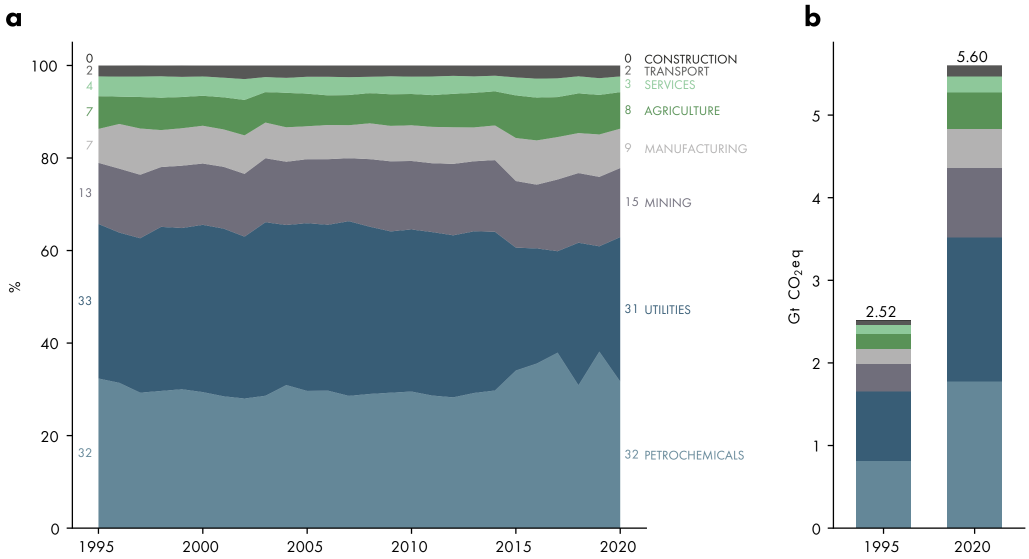

FIGURE 5 TOTAL GHG EMISSIONS FROM PETROCHEMICALS 1995-2020 BY SOURCE SECTOR.

Figure 6 display the total GHG of the petrochemical sector by the region where GHG are emitted. In 2020, China accounted for nearly half (47%) of the total GHG of emissions of the petrochemical industry. GHG emissions in other BRIC countries amounted to 10% (5% in Russia, 3% in India, 2% in Brazil). China had a substantial increase in the share of GHG emissions, as it accounted for only 24% of global GHG emissions in the petrochemical sector In 1995. A growing trend is also evident for the Middle East (from 4% in 1996 to 6% in 2020) region. In contrast, the USA and EU saw a strong decrease. In 1995, USA accounted for 17% of total GHG emissions from the petrochemical sector, while in 2020 it was responsible for 6%. European share dropped from 13% in 1995 to 5% in 2020.

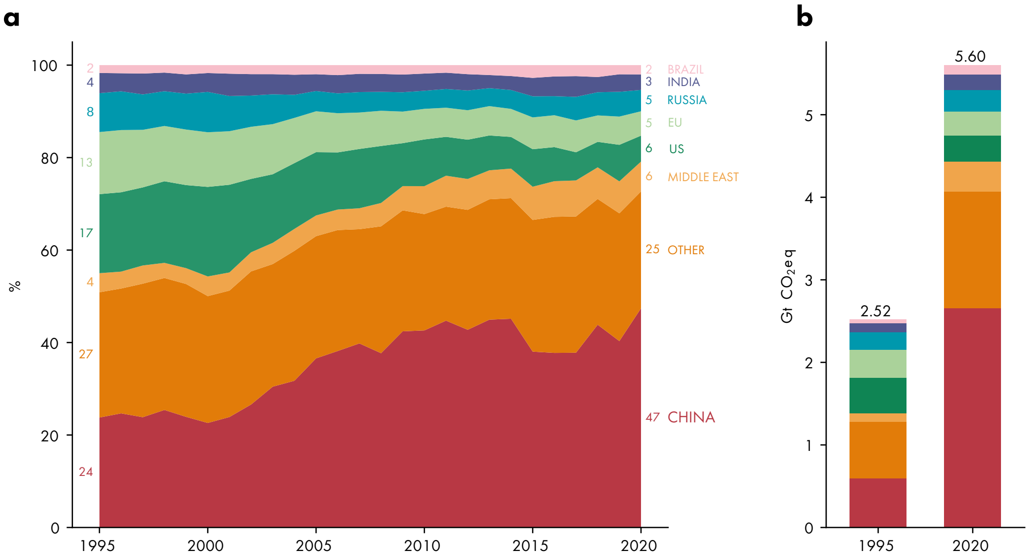

FIGURE 6 TOTAL GHG EMISSIONS FROM PETROCHEMICALS 1995-2020 BY SOURCE REGION

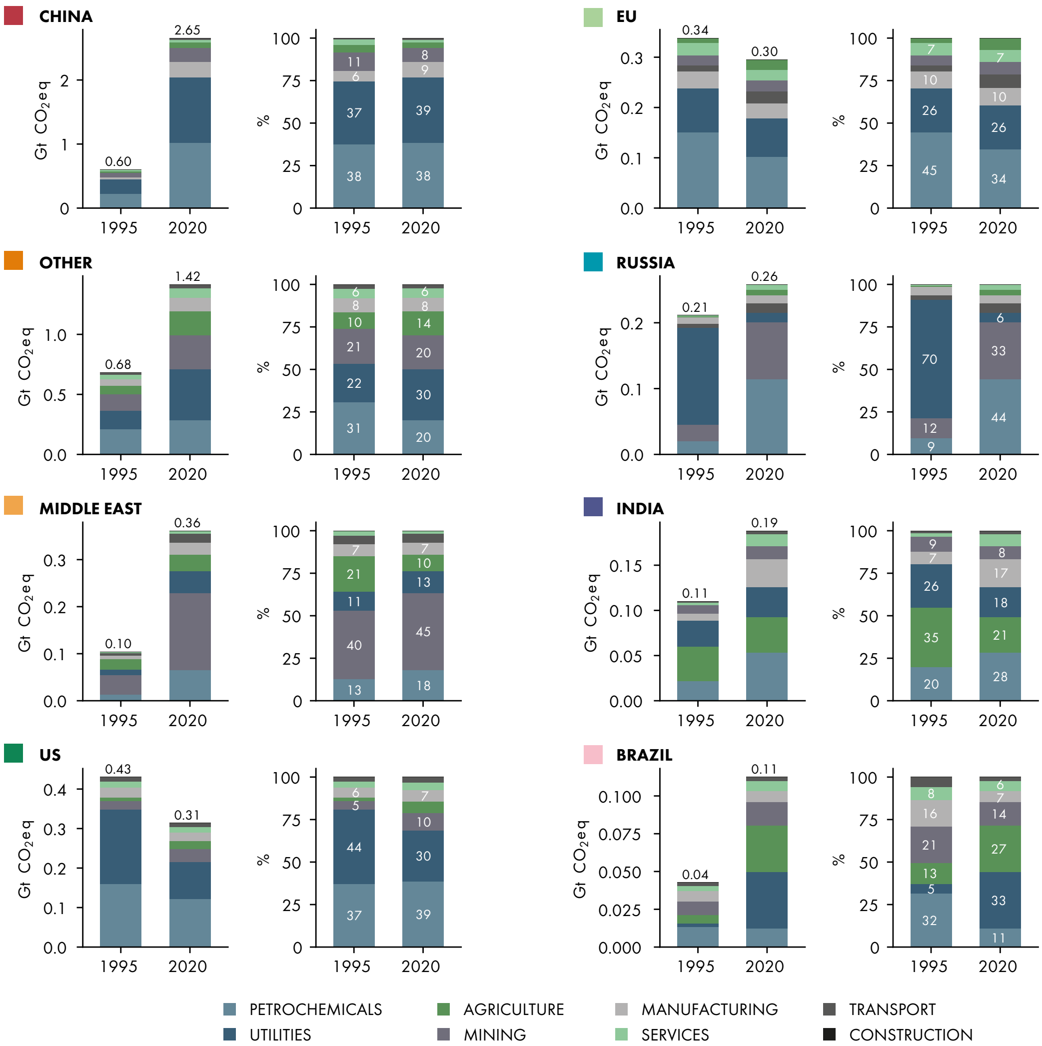

FIGURE 7 GHG EMISSIONS FROM PETROCHEMICALS IN KEY REGIONS AND COUNTRIES BY SOURCE

3.1.5 GHG EMISSIONS OF THE PETROCHEMICAL INDUSTRY (BY FINAL CONSUMPTION)

MRIO analysis is particularly useful to estimate flows of embodied GHG emissions through the global supply chain networks, which in turn can help identifying critical production stages and potential intervention points to reduce GHG emissions. Figure 7 presented above shows where impacts associated with the production of petrochemicals occur (by sector and country). Alternatively, we can look at where products finally end up, for instance plastics are used in many manufactured goods such as electronic devices which are sold for final consumers.

Figure 8a shows that in 2020, 23% of the total impact from petrochemicals was embodied in petrochemical goods sold for final use (e.g., soap, detergents, plastics bags, fertilizers, etc). This share has declined from 27% in 1995 to 23% in 2020.

Interestingly, we find that most impacts occurring in the petrochemical industry finally end up embodied in the provision of services (e.g., food sold in a restaurant will contain embodied GHG emission from the production and use of fertilisers needed to grow food; provisions of health services will contain embodied GHG emissions from the production and use of medical equipment that requires plastics as well use of drugs that require chemical inputs). The share of impacts that finally end up in the Services sector has grown from 25% in 1995 to 32% in 2020.

Manufacturing also plays an important role. In 2020, 27% of GHG emissions from the petrochemical sector were embodied in manufactured goods (e.g., plastic in TVs, etc.). In contrast, to the Services, the impacts embodied in the manufacturing sector have declined, from 30% in 1995 to 27% in 2020. It is also worth noting that GHG emissions embodied in the construction sector (e.g., impacts from petrochemicals in PVC windows) play an increasingly important role, as the share of impacts (from petrochemicals) embodied in the construction sector have grown from 10% in 1995 to 13% of the total impact in 2020.

Figure 9 displays GHG emissions from the petrochemical sector split by the destination country where the embodied impacts finally end up (e.g., impacts from manufacturing Chinese plastic components used in a Japanese car sold to Australian consumers, finally “end up” in Australia). This is typically known as the “consumption perspective”. When viewed from this perspective China, for example, displays a lower share of the total impact compared to results presented in Figure 6. On the other hand, the share of impacts that finally end in the EU and US is higher (compared to Figure 6). This implies that China is a net exporter while the EU and US are net importers of embodied petrochemical GHG emissions. It is worth noting that this should not be taken as evidence that China, for example, is a net exporter of petrochemical products. The results show that goods and services consumed in China embodied less GHG emissions from petrochemicals than total GHG emissions embodied in petrochemical goods produced in China.

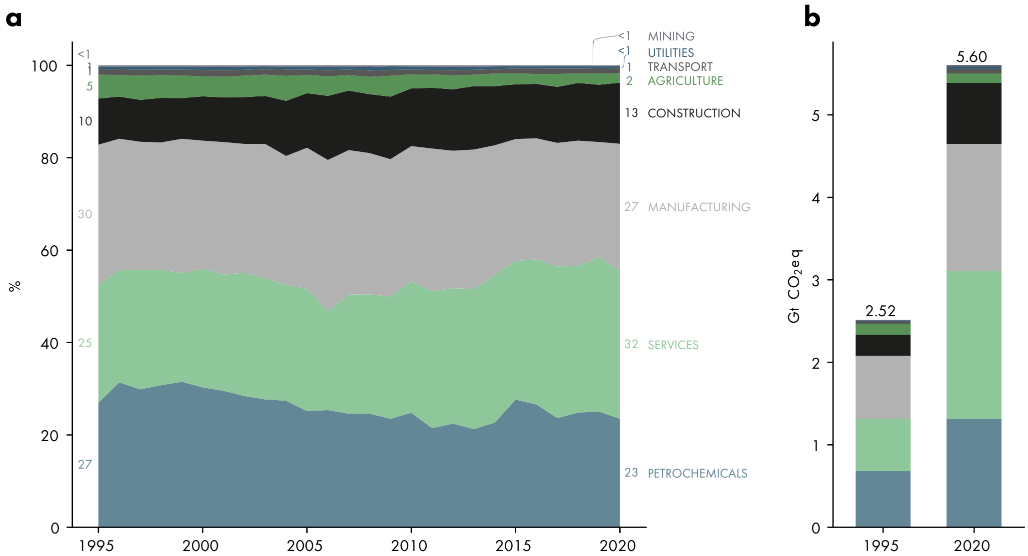

FIGURE 8 GHG EMISSIONS FROM PETROCHEMICALS CONSUMPTION, BY FINAL CONSUMPTION SECTOR.

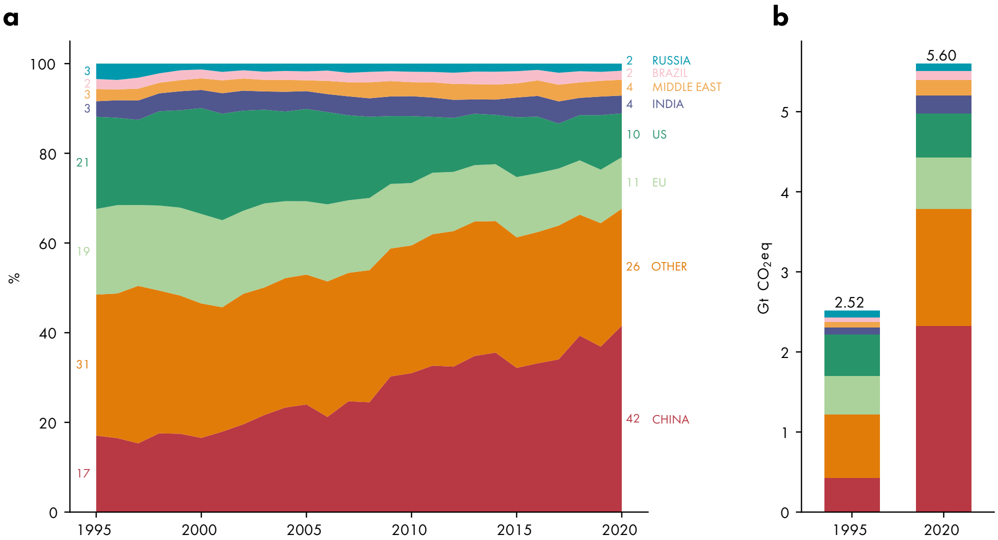

FIGURE 9 GHG EMISSIONS FROM PETROCHEMICALS CONSUMPTION, BY FINAL CONSUMPTION REGION.

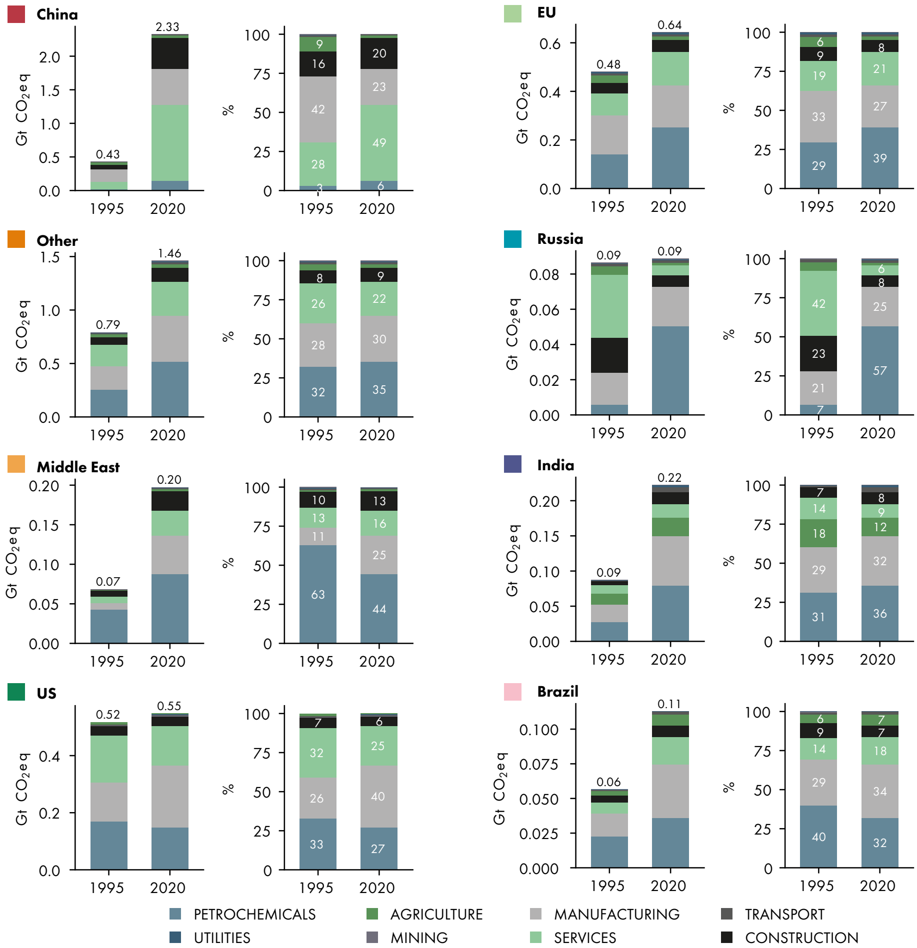

FIGURE 10
GHG EMISSIONS FROM PETROCHEMICALS IN KEY REGIONS AND COUNTRIES BY CONSUMPTION SECTOR

3.1.6 GLOBAL GHG EMISSIONS OF THE PETROCHEMICAL INDUSTRY (BY SOURCE AND FINAL CONSUMPTION)

Figure 11 maps embodied GHG emissions flows for the petrochemical sector in the global production system. The diagram can be split into two parts: upstream process shown on the left and downstream process shown on the right. The left part displays the source of GHG emissions associated with the production of petrochemicals. The source can be split into direct GHG emissions by the petrochemical sector (e.g., emissions due to fuel combustion in boilers, and furnaces) and indirect GHG emissions that occur in other sectors that supply inputs for the petrochemical sector (e.g., electricity, or transport services). The right part (reading from the midpoint to the right) displays destination of petrochemical products (and associated environmental impacts which are embodied in the petrochemical products). Petrochemical products can be sold as an input into further production process (e.g., plastic to produce car parts) or for final use (e.g., a plastic bag sold in a grocery store). GHG emissions embodied in petrochemical goods sold directly for final consumption (e.g., packaging material, fertilizers for private use) amount to 1.3 Gt CO_2eq.

The remaining 4.3 of Gt CO_2eq are embodied in the petrochemical products which are sold as intermediate inputs into further production process, mainly into the manufacturing (1.96 Gt CO_2eq e.g., plastic components into the automotive industry) and services (1.56 Gt CO_2eq) sectors. Use of intermediate products can continue through multiples stages. For instance, plastic can be used to manufacture car parts, which are then used in car manufacturing process, and this manufactured car is then sold to a logistics company that uses it to deliver goods either for business (this would be considered as a further intermediate step) or private customers (final demand). We do not show each of these transactions in the diagram, as such process can continue for many stages and would make a diagram very complex. Instead, we present the results for the first intermediate stage and the final stage in the supply chain (goods and services that are sold for final consumption and contain embodied emissions form the petrochemical industry). Notice that this is the reason why there is a gap in the flow diagram. Our results suggest that 1.8 Gt CO_2eq emissions from petrochemicals are embodied in services, and 1.54 Gt CO_2eq are embodied in the manufacturing sector.

It is worth noting that GHG emissions associated with petrochemicals might be larger if we account for emissions from waste incineration. This is because the carbon contained in fossil resources used as feedstock would be released if petrochemicals products were combusted. Recent estimates suggest that if all plastics produced in 2015 were incinerated, the global carbon footprint of plastics would increase by 19%(Cabernard et al., 2021).

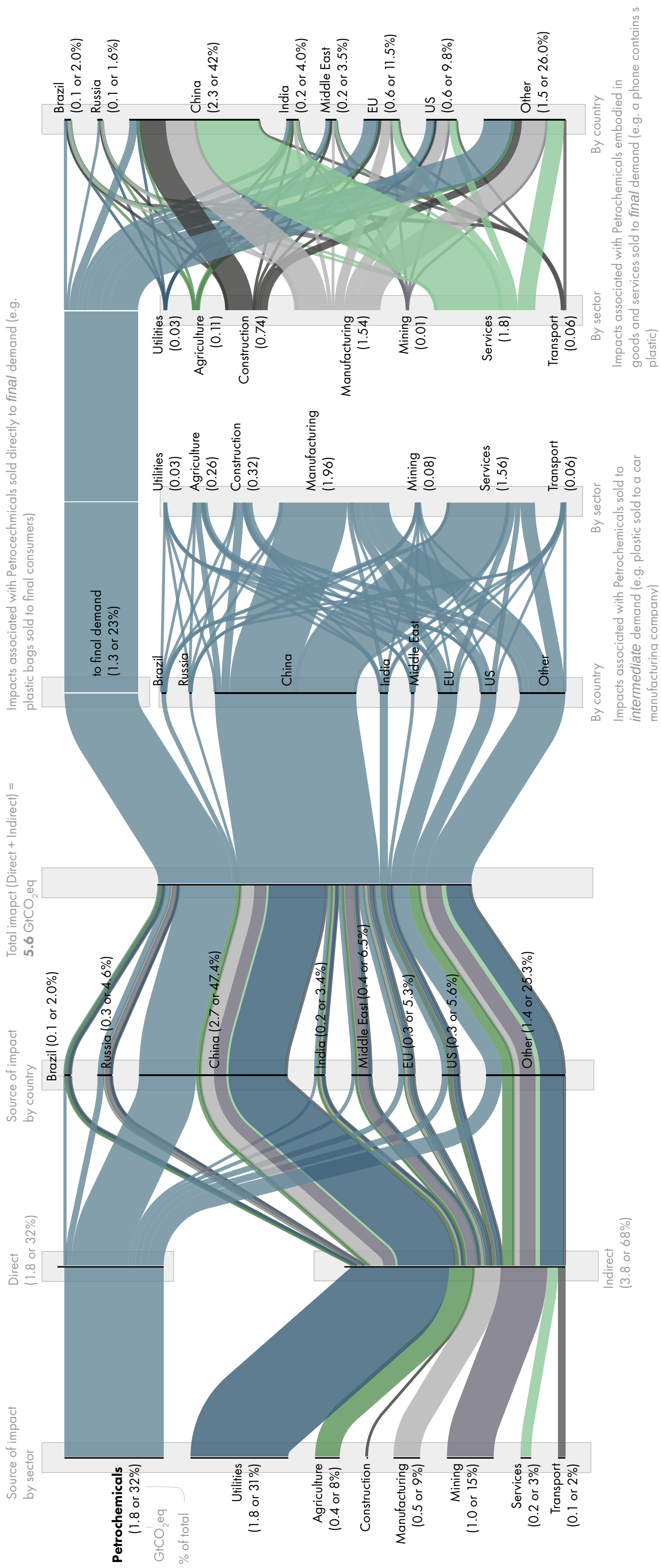

FIGURE 11 SANKEY DIAGRAM OF GHG EMISSIONS FROM PETROCHEMICALS BY SOURCE AND SECTOR OF CONSUMPTION. NOTE: THE GAP IN THE FLOW DIAGRAM REPRESENTS ALL INTERMEDIATE PRODUCTION BETWEEN THE FIRST INTERMEDIATE STAGE AND THE FINAL STAGE OF PRODUCTION. FEW ASPECTS WORTH HIGHLIGHTING FROM THIS SECTION:

PORT ARTHUR, TX (USA)
IS ONE OF THE PLACES WHERE THE
PETROCHEMICAL INDUSTRY IS CLUSTERED

PHOTO: PIXABAY

4 ASSESSING THE LIFE CYCLE OF PETROCHEMICALS

4.1 GENERAL OVERVIEW OF PETROCHEMICALS LCA

Life cycle assessment (LCA) is a standardized method for a comprehensive assessment of environmental impacts of products, services or consumption patterns (Hellweg and Milà i Canals, 2014; ISO, 2006a, 2006b). It assesses the emissions and resources uses of the system assessed in the life cycle inventory (LCI), including the supply chain, and the related impacts in the impact assessment step (LCIA). The LCA generally addresses the whole life cycle if a product or service, including production, use phase and end of life (disposal), which is called cradle-to-grave assessment. However, LCA can also focus on a production stage only and then usually referred to as cradle-to-gate assessment. The impacts are assessed concerning different impact categories, such as climate change, toxicity and particulate matter emissions, or also aggregated to an endpoint level to assess impacts on human health, ecosystem quality and resource depletion. In LCAs, this allows to evaluate trade-offs in environmental impacts (e.g. between GHG emissions and toxicity) but there are also methods to aggregate all impacts to a single score indicator that allows to quantify the environmental impact of the system in a single result.

LCA of petrochemicals is critical in the environmental evaluation of most product systems, be it for their use as energy carrier or material supply. A broad range of life cycle inventories (LCIs) for petrochemicals exists, both in the form of datasets in a number of major LCI databases, and as individual datasets for example published within scientific studies or environmental product declarations (EPDs). The scientific interest in the LCA of petrochemicals over the past decades has increasingly accelerated, even more so than for the LCA of chemicals in general (Figure 12). The demand for petrochemicals LCI data is driven by the increasing number of LCA studies that are being commissioned, and they serve to spot environmental hotspots within companies, product systems or supply chains at a higher resolution with more customization options compared to other assessments of environmental burdens such as the sector-level or country-level analyses using EEMRIO. With the option to tailor the LCIs to specific questions comes a large diversity in fundamental normative assumptions about the investigated system such as system boundaries, cut-off criteria, or temporal and geographic scope. That restricts the comparability of individualized studies in the field. Most of these studies, however, rely on background LCI databases as building blocks for providing more standardized LCI data with defined quality requirements and comparable methodological choices. The focus in the present review will be on these major background LCI databases, their fundamental principles, their coverage in terms of petrochemical data, their strengths and weaknesses, and their differences from each other.

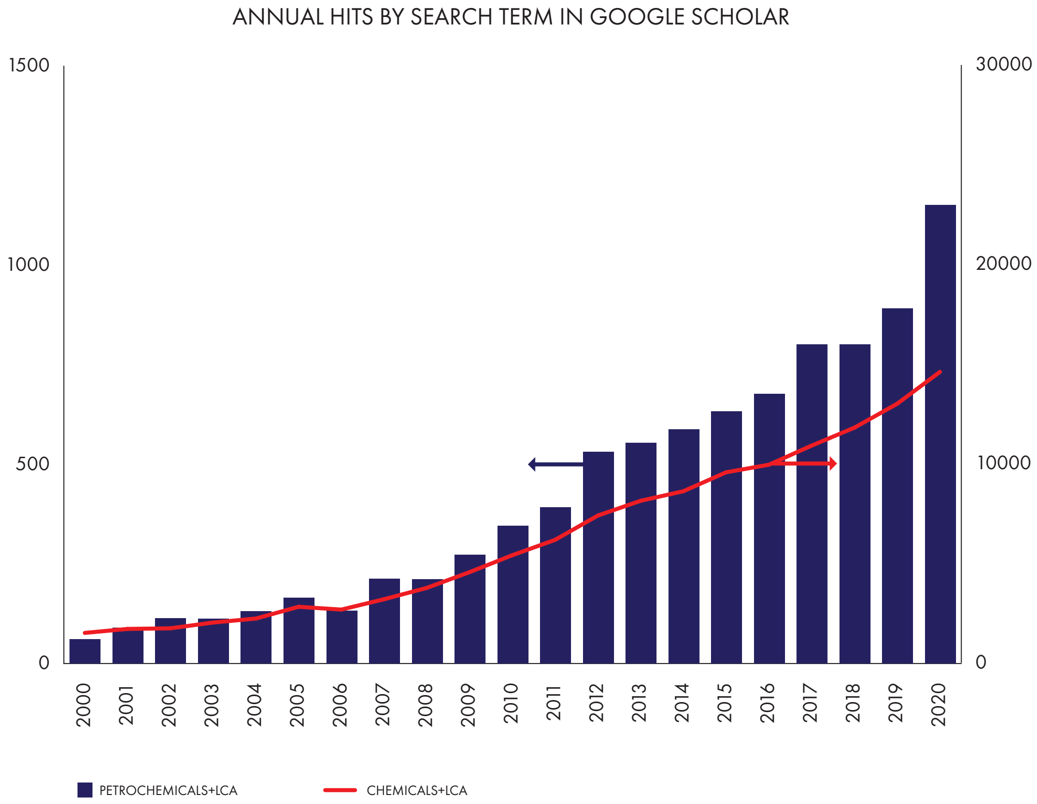

FIGURE 12: ANNUAL HITS OF SCIENTIFIC STUDIES IN GOOGLE SCHOLAR FOR CHEMICALS AND PETROCHEMICALS LCA

4.2 DATABASE OVERVIEW

4.2.1 ECOINVENT DATABASE

Ecoinvent in its most recent release (v3.8) is the most commonly used general-purpose LCI database and contains about 18000 datasets (Ecoinvent, 2021). Among these are producing activities as well as a large share of "market" datasets that represent regional supply mixes. About 3000 of the Ecoinvent datasets are related to chemicals with most of them being interconnected gate-to-gate processes, which combined represent complete supply chains. Four different "system models" of Ecoinvent are rulesets for allocation of emissions and impacts between products and life cycle stages in multi-output processes and waste treatment, and thus result in different database versions derived from the same raw data (see 4.3.3). Ecoinvent aims to be a global database, while it contains due to its Swiss origin many Swiss and European datasets, of which other regional datasets have partly been derived. The electricity supply and the respective fuel mixes are globally covered on a national level, with subnational resolution for large countries such as China, the US, Brazil, India or Canada. Ecoinvent has been used as background data source for several other, more specialized LCI databases or for disaggregation of sectors in EEMRIO, e.g. Exiobase, which was used for the analyses in chapter 3.

4.2.2 IDEA DATABASE

The Japanese IDEA database (AIST, 2019) contains about 4500 datasets as of version 2.3, which was released in 2019. In Japan, the release of version 3.0 has further expanded the database coverage, but this version is not yet available in English. Version 2.3 contains unit process data for about 750 chemicals based on different primary data and with a very different subset of chemicals compared to other LCI databases. The chemical sector is the sector with the largest and most detailed coverage within the database. A characteristic feature of the IDEA database is its use of Japanese input-output data, which allows to fill gaps in inventories systematically (e.g. for packaging requirements of chemicals that otherwise would be missing from bottom-up estimates) and furthermore provides representative sector averages for chemical products without covering all individual chemicals in details (as such data would also be unavailable). The regional scope of the database is mostly Japan with additional global datasets relevant for Japan imports or exports. The electricity supply and the respective fuel mixes are covered globally with a national resolution.

4.2.3 US FEDERAL LCA COMMONS (USLCI) DATABASE

The US Federal LCA Commons, also known as USLCI database, is the product of LCI data collection efforts of a broad range of US governmental agencies (NREL, 2021). The database in its most recent version largely contains gate-to-gate processes, of which about 120 are chemicals and petrochemicals. The dataset focus of the USLCI database is on the agricultural sector due to the involvement of the US Department of Agriculture and on the energy sector due to the involvement of the US Department of Energy while the coverage of chemicals is somewhat limited. In contrast to other LCI databases with disaggregated datasets, the US chemical datasets typically contain larger parts of the respective supply chains, so individual datasets for intermediate chemicals are frequently not available even though they are covered implicitly, which is a limitation for adjustments or comparisons. The regional focus of the database is mostly on the US and North America, while in some cases also for the US relevant countries in the most important supply chains are covered.

4.2.4 SPHERA GABI DATABASE

The GaBi database is a by-product of the consultancy work of the Sphera company, which has resulted in the creation of about 14500 datasets distributed over a basic LCI database, some topical satellite databases, e.g. for specific sectors like the chemical sector or specific regions, and a broad range of on-demand datasets (Sphera, 2021). Among these datasets, about 3000 are related to chemicals production with almost all of them being aggregated over the full supply chain (system processes), so no details on the inputs of intermediate inputs or energy requirements are available. However, a small number of partly disaggregated datasets (plans) related to chemicals are available. The full extent of connections within the database and its satellite products is however difficult to trace for users due to a lack of access to the disaggregated raw data. The general coverage of the database is global, with a lot of German and European datasets as the database has its origins in Germany.

4.2.5 PLASTICS EUROPE ECO-PROFILES

The eco-profiles provided by Plastics Europe are not a full LCI database but a collection of main chemical and petrochemical sector LCI datasets that are updated gradually over time (Plastics Europe, 2019). These datasets are fully aggregated (system processes) and have partly been derived from industry-reported data (emissions, inputs, outputs, etc.) and partly been modeled. The data covers the most relevant data for plastics supply chains like resource extraction, simplified energy supply, processing into basic polymer types at a European average level. This includes European average technology mixes, which are not further distinguished into different processing routes for the same products. Where more comprehensive data is unavailable, only the dominating technology is covered. For background data that is not covered by own data collection or models, the old Ecoinvent v2 database has been used as input, which is in the process of being replaced by GaBi. The Plastics Europe Eco-profiles are used in the current versions of GaBi and Ecoinvent for parts of their chemical and petrochemical sectors.

4.2.6 CARBON MINDS CM.CHEMICALS DATABASE

The cm.chemicals LCI database by Carbon Minds is a recent development specifically for the chemical sector, published for the first time in 2021 (Kätelhön et al., 2021). It contains at present (January 2022) in total about 100400 datasets for more than 1000 chemicals, which are individual production processes, individual chemical suppliers, supply mixes or consumption mixes for most countries of the world. Among the chemicals in the database, about 530 chemicals have been covered with low quality data, 390 chemicals with medium quality data, and 90 chemicals with high quality data, based on the self-classification of Carbon Minds (Kätelhön et al., 2021), which is generally more favorable than the standardized approaches for example used in GaBi or Ecoinvent (Weidema and Wesnæs, 1996). All datasets are fully aggregated system processes, and about 1160 chemical production processes have been included. The background data, for example for energy, steam, water, raw materials or missing chemicals is provided by the Ecoinvent database in the APOS ("allocation at the point of substitution") version, which is only marginally used by consultants and scientists, and therefore makes comparisons more difficult. Technology mixes are partly adapted to national conditions, and regional variation for specific processes seems to occur mostly through the use of national background data, but no documentation on the details is available and hence this pattern cannot be verified. Water flows in the database are not regionalized and in consequence, the inventories are not compatible with the AWARE LCIA method (Boulay et al., 2018), which is frequently used to assess the environmental impacts of water use as recommended by UNEP (UNEP/SETAC, 2017).

4.2.7 JLCA DATABASE

The JLCA database (JLCA, 2021) is a database of Japanese gate-to-gate life cycle inventories that were derived from measured industry data. It is not a fully connected database, so the inventories still need to be connected with individual background datasets from a more comprehensive database, but they nevertheless provide useful information on energy and material balances of the covered production processes. The sectoral coverage in the database is driven by available data rather than immediate user demands. While the total number of datasets is close to 700, the number of chemical sector datasets is about 120, most of which deal with the production of major bulk petrochemicals, important intermediates, as well as several types of polymers. More specialized chemicals like pharmaceutical or agrochemicals are not covered.

4.2.8 ENVIRONMENTAL FOOTPRINT (EF) DATABASE

The Environmental Footprint (EF) database of the European Union (Fazio et al., 2020) was formerly known as Product Environmental Footprint database and is a database of life cycle inventories that is under development for providing baseline European footprinting data and may in the future be used for regulatory activities such as European border adjustment taxes or product labels. The data in the database is added in several stages and is supplied by numerous established European data providers such as Ecoinvent, Sphera and a broad range of consultancies. Energy, transport and plastics datasets are adapted versions of GaBi datasets, while chemicals come from Ecoinvent. Due to the different methodological framework, the datasets in the EF database and their original LCI database differ from each other. Datasets are generally available in different forms, as aggregated system processes and partly disaggregated unit process datasets. The geographical scope of the database is Europe and the database contained 270 chemical datasets from Ecoinvent in phase 2, while about 190 more chemical datasets will be added or updated by Ecoinvent in the upcoming phase 3 version. The use of the EF database is restricted to a limited number of specific purposes outlined by European Union guidelines and therefore cannot be used for general LCA studies.

4.2.9 OTHER DATABASES

Beyond the databases mentioned above, there are several other LCI databases that contain data about chemicals. Among them is for example the UVEK database of the Swiss environmental agency FOEN, which is a derivative of the older Ecoinvent version 2.2 with partly updated data and a strong focus on Switzerland, but without the structural changes and the more global updates that have been introduced in Ecoinvent version 3. Similarly, the German environmental agency used to maintain an own LCI database by the name of ProBas, which has not been updated for several years, but still contains some LCI data on main chemical products for Germany. These and similar databases (e.g. the Chinese, Thai and Brazilian LCI database efforts) are not considered in this review any further due to their limited application range.

4.3 MODELLING PRINCIPLES

4.3.1 GENERAL APPROACH

The modelling principles of LCI datasets in the chemical and petrochemical sector generally resemble those for other sectors. In most cases (e.g. Althaus et al., 2007), the different production processes are modeled individually with their inputs and outputs from both technosphere and biosphere, and are then transformed into product-level datasets by combining them with the rest of the supply chains (e.g. from background LCI databases) and breaking the processes down per amount of product output (allocation, see section 4.3.3). The quality of the resulting datasets is typically limited by consistent and representative reporting of real-world petrochemical production data (Righi et al., 2020). As most chemical companies produce a wide range of products in different locations and with different processes, it is generally not possible to derive LCI datasets from site-level or company-level reporting as would be the case for less complex products. Instead, the scale-up of published lab data, the use of idealized process data sheets, process simulations, basic process models (based on energy and mass balances), reaction stoichiometry or black box data reported by industry associations are common data sources rather than available operational or measurement data. Such approaches can yield very good estimates of environmental releases for main pollutants, but turn very challenging in case of trace pollutants, side products of chemicals reactions, releases during non-steady-state operation, off-spec products, leakages and other emissions that are difficult to trace, predict or estimate.

Furthermore, the interconnectedness of petrochemical processes, e.g. in case of heat integration, multi-product processes, or waste utilization, make even the attribution of measured inputs and outputs to individual products and processes very difficult. With such a complexity in the processes and the supply chains, the number of possible modelling choices increases and hence has a potentially strong effect on the outcomes of LCA studies of petrochemicals production. While this has not yet been investigated broadly, yet, a rather simple case study with the same objective but six different modelers has provided some insights into how central this can be (Scrucca et al., 2020). Such issues, however, are not specific to petrochemical production alone but concern all types of products and processes in LCA. Of central importance in the evaluation of petrochemical products are the upstream supply streams with the utility use, and the allocation, which will be discussed in the following sections.

4.3.2 UPSTREAM SUPPLY CHAINS AND UTILITY USE OF PETROCHEMICAL LCI DATASETS

Across the available LCI databases and their petrochemicals datasets, the raw materials with their specific supply chains (oil, gas, coal, and in addition a limited number of other raw materials) and the energy requirements (both in the form of heat and electricity) play a central role for the overall life cycle impacts of the products and for climate change in particular. That is because the global energy supply for chemical sector is still mostly fossil-based, in the case of electricity supply from chemical sector power plants for example there is a share of 41% natural gas, 34% coal (mainly driven by Chinese production), 20% oil and about 2% renewables measured by capacity reported (S&P Global, 2021) (see Figure 13).

While the heat supply to chemical plants is distinguished by fuel types from generic regional heat supply averages in most LCI databases (e.g. in Ecoinvent, the Plastics Europe eco-profiles or IDEA), it is less common to distinguish the specific electricity mix. Here, the Japanese IDEA database represents a notable exception as a sector-specific electricity mix is used that is composed of the energy supply from power plants owned by chemical companies as well as surplus electricity supply from the public grid. Furthermore, Plastics Europe also provides a customized electricity mix for the chemical sector, but the documentation is not precise as to what exactly it covers as it only contains general descriptions of the electricity supply of chemical plants and aggregated LCI results (Boustead, 2005).

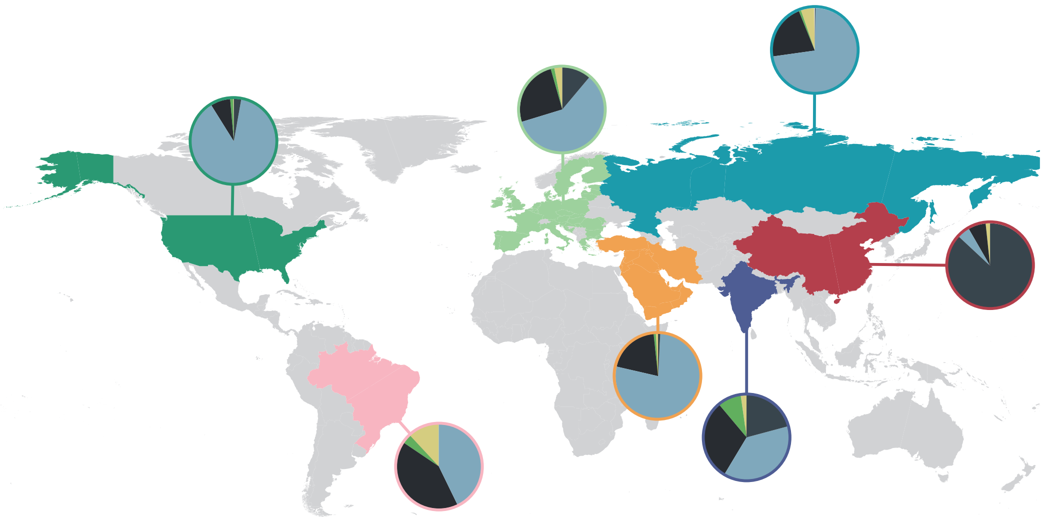

FIGURE 13: THE MAIN FUELS OF CHEMICAL SECTOR POWER PLANTS FOR DIFFERENT MAIN REGIONS OF THE WORLD IN 2021 (BY NET ELECTRICITY GENERATION CAPACITY) AS CALCULATED FROM S&P GLOBAL (2021).

On a regional level, the fuels used in chemical sector power plants differ distinctly from each other. For example, the widespread availability of inexpensive natural gas as well as stringent regulation of petrochemical sector emissions in North America have contributed to the widespread use of this fuel for chemical sector electricity production, whereas regions such as Europe need and parts of Asia (including China and India) lack the availability of high amounts of natural gas (IEA, 2021a). In such regions, natural gas is largely imported at higher prices and competes with relatively cheap domestically available or imported coal, which then reflects on the regional fuel mixes (S&P Global, 2021). In regions with large amounts of oil extraction such as the Middle East or Russia, the combustion of oil plays a substantial role in industrial energy supply, but still has a lower market share than natural gas. These patterns are not necessarily visible to the same degree in the public electricity mixes (IEA, 2021a) because petrochemical companies aiming to compete on the global market are much more sensitive to the economic implications of fuel choices. As a result, using the public electricity mix for chemical production LCA datasets can lead to high inaccuracies.

At the interplay of public and sector-specific electricity supply, the modelling principles of the Ecoinvent electricity sector cause some particular issues. The available electricity grid mixes in the database reflect the publicly traded electricity supply, from which the contributions of private auto-producer power plants (such as chemical sector power plants) have been excluded (Treyer and Bauer, 2016). There are, however, no complementary electricity mixes for these privately-operated power plants in the Ecoinvent database, neither in a sector-specific nor in a more general form. Auto-producers of electricity are thus implicitly dropped from the Ecoinvent database, which means that the petrochemical production datasets are using the generic national or regional electricity mixes unless a dataset author specified otherwise, which likely results in an overestimation of the contribution of renewable energy, especially for regions such as Europe. At the same time, electricity supply mixes in Ecoinvent are updated continuously every year while the heat markets and emissions intensities have not been updated in the past couple of years. Both electricity and heat supply are connected through the co-generation of heat and power from certain power plants, so this practice may cause a potential mismatch between electricity and heat with infeasible conditions in the overall energy supply compositions. Certified electricity mixes with Guarantees of Origin (GOs) have become an important issue in the reporting of GHG emission intensities of petrochemical companies (section 5.2), but are largely absent in LCI databases as of now.

High levels of energy integration between different processes represent a major competitive advantage of large chemicals sites besides sharing of other basic infrastructure such as waste treatment facilities, and educts or product transport infrastructure. The supply of thermal energy is covered in LCI background databases in different forms. Ecoinvent, for example, provides national datasets for different heat supply options and groups them into natural gas and non-natural-gas supply mixes. For each chemical sector dataset, it is then decided to which degree either of these two supply mixes, both of them with a specific ratio, or other types heat supply are most appropriate to a specific petrochemical production process (Althaus et al., 2007). GaBi, on the other hand, offers a more limited choice of heat supply mixes but instead has a larger number of modular energy supply datasets with additional conversion datasets for different qualities of heat and different boiler efficiencies available. Hence, the user of such datasets is required to make an active choice without the option to resort to more averaged default heat supply datasets. The GaBi modelling principle in this regard resembles the approach of earlier Ecoinvent versions, where combustion of fuels and its utilization for electricity or heat supply were covered by separate, but connected, datasets. In the IDEA database, there are several heat supply datasets for fuels that are specific to the chemical sector (e.g. combustion of dimethyl ether for energy supply) as well as a manufacturing industry heat mix that is mainly used as a default heat supply mix in their chemical datasets if the specific fuels are not known.

Upstream emissions of CO_2 and methane are important contributors to the overall climate change impacts of petrochemical products (Meili et al., 2021). Drivers for such emissions are mainly the extraction processes with their energy demands, the transportation of petrochemical raw materials (e.g. by pipeline or truck), fugitive releases (e.g. from leaking flanges or abandoned extraction sites), and flaring. In principle, these emission sources are all distinguished in the LCI datasets, but as extraction often takes place in remote regions with less strict environmental regulation and limited reporting requirements, and the emissions are distributed over a large number of sources, reliable data on such emissions is generally scarce. Hence, the amounts of LCI datasets is limited by data availability and generally has to rely more on assumptions and simplified models than for many other activities. Recently, an LCA study has been published on potentially higher amounts of flaring than in previous estimates (Meili et al., 2021), which may lead to overall higher contribution to climate change of petrochemicals production. The integration of that data into mainstream LCI databases has not been accomplished as of now, though. Nevertheless, high contributions of upstream emissions to the cumulative contribution to climate change of petrochemicals production are found across all the mainstream LCI databases, but the relevance of these contributions decreases for long petrochemical supply chains with high energy demands in the chemical processing.

4.3.3 ALLOCATION

The choice of allocation method is a central challenge of LCA studies and the petrochemical sector is no exception in this regard (Viganò et al., 2020). Allocation methods are used to sub-divide the environmental and technosphere exchanges as well as resulting environmental impacts for multi-output processes and attribute them to the individual products. This procedure is necessary in order to make products, that may be produced from different processes with different co-processes comparable. The allocation step always represents a normative choice with strong implications for the environmental performance of individual products and is thus often highly debated.

With the complex networks of processes and products in the petrochemical sector, this step is of higher influence on the result patterns than in the case of less complex sectors. Due to the unique conditions of the petrochemical sector, a large number of customized allocation procedures have been developed. In general, they can be classified by the properties they use for the allocation. Relying on physical properties such as mass, volume, calorific value or exergy content has the advantage of being independent of time and location, while in some cases also being able to reflect the purpose of some products (e.g. calorific values for fuel combustion). The disadvantage of this approach is that there are usually no objective criteria that make one of the physical properties a better indicator for allocation than others (e.g. mass or volumes). Furthermore, the petrochemicals are typically not used for one purpose alone, e.g. kerosene may be used as jet fuel but is also used as solvent, and so the calorific value is not a meaningful indicator for its utilization in the latter case.

Economic allocation on the other hand tries to allocate by prices in order to mirror the economic relevance each product has for the company that produces it as well as the relevance of the co-products on causing the activity, which in economic terms would be reflected in the price or value added. While this is in theory a strong concept, it proves challenging in practice due to regional differences in prices, high and unpredictable price fluctuations, products without observable prices (e.g. products that are traded between different parts of the same company), direct and long-term purchasing agreements without trade on the open market, and price differentiation by product quality. Furthermore, the price of a product is not quite as important as the profit a company is able to make with that product, which turns the prices into a surrogate allocation key.

Due to the challenges of selecting a clearly most suitable allocation method, there are substantially different approaches for different parts of the petrochemical supply chains in use, for example based on calorific values where products and co-products are used as energy source, but also a lot of economic allocation and even mass-based allocation. A special case within the petrochemical sector are the petroleum refineries, for which there are unique allocation procedures that then may have substantial downstream consequences (e.g. Fehrenbach et al. (2018): step-wise with bottom products considered as waste, Jungbluth et al. (2018): fixed energy-content factors by product). A comprehensive review demonstrated that differences in allocated results arise from whether refining processes are treated as dividable subprocesses or as aggregates, from the classification of outputs into by-products or wastes and from adopting a marginal or average perspective (Johnson and Vadenbo, 2020).

These factors were shown to have an especially high influence on the environmental impacts attributed to heavy fuel oil, bitumen, sulfur, and petcoke as these are assumed to either cause impacts or to avoid impacts based on the key assumptions (Johnson and Vadenbo, 2020). Furthermore, the choice of allocation method is also highly relevant for the petrochemicals sector in the case of raw material extraction where there is associated extraction of natural gas and oil, among which the related environmental impacts need to be distributed (Plastics Europe, 2012). The data for the extraction of these raw materials in Ecoinvent and GaBi is rather simple in this regard and does not cover the diversity of setups in the extraction of fossil raw materials while at least the USLCI database distinguishes different oil and gas fields in the US with their specific inputs and outputs in much more detail.

The complexity of allocation procedures and the consequences these have for the environmental impacts per product has led Plastics Europe to host a discussion roundtable about allocation for steam cracking as it wanted to ensure comparability of reported emissions and impacts between steam crackers in Europe. The result of this discussion was a recommendation for steam cracker allocation principles based on mass allocation with a specific list of substances declared as products (Plastics Europe, 2017).

Another example for the relevance of allocation choices is the case of energy supply. Due to the associated production of heat and power from co-generation power plants, it is necessary to apply allocation techniques in order to determine the environmental impacts for heat and electricity separately. It is customary for cases of energy products to allocate by exergy content in order to reflect the useful energy in each energy product. In Ecoinvent, an exergy allocation procedure has been established (Heck, 2007), but it has been derived from the properties of remote heating networks (with low heat temperatures), which may reflect global average conditions well, but do not match the conditions of chemicals production (higher temperature heat) and thus may lead to an underestimation of heat-related emissions and an overestimation of electricity-related emissions for petrochemicals production. GaBi in general follows a similar procedure but is not specific in the documentation so it is unclear whether GaBi is subject to a similar issue or not.

Economic allocation for petrochemical products is widespread in Ecoinvent (Althaus et al., 2007) but based on rather old prices (from around 2005). For refineries, the approach somewhat differs by country but mostly revolves around the energy content of each product (Fehrenbach et al., 2018; Jungbluth et al., 2018). Main outputs of petroleum refining are gasoline and diesel, which are mostly combusted to provide energy, but the material properties of several refining products are more relevant for the downstream petrochemical sector. For example, naphtha is often used as an intermediate product in the manufacturing of ethylene and propylene, which can then be used to make polyethylene and polypropylene, and is thus not primarily used as an energy source. Nevertheless, it is often still allocated like an energy product such as diesel or gasoline based on its calorific value.

System expansion or substitution are alternative approaches to ensure functional equivalence between two LCIs, which aim at avoiding allocation by adding or subtracting the exchanges and environmental impacts of single-output processes (ISO, 2006a, 2006b). For the example of a chemical process that has one chemical and some steam as output, this could mean that a single-output steam generation dataset is subtracted in order to only have a net production of the chemical. This approach is widely used in the cm.chemicals database of Carbon Minds, where for example steam generation from natural gas is used everywhere in order to balance the co-production of steam (Kätelhön et al., 2021). In practice, however, problems arise from the fact that the specific conditions for each site and each point in time may determine what a co-product substitutes, which may have a strong influence on the impact assessment outcomes (Hanssen and Huijbregts, 2019). For example, the heat supply by coal or oil are also widespread in the chemical sector and have their own unique site-specific environmental profiles. Thus, simply assuming natural gas heat supply is a pragmatic approach, but does not mirror the real setups at many chemical plants. In addition, more specific side-products such as other chemicals may not be produced via alternative production routes at a similar scale or are not produced from single-output processes. Such cases strongly limit the applicability of system expansion or substitution, and hence they are not used by most LCI databases.

4.4 SECTORAL COVERAGE

Data demand, production volume and data availability are the key drivers for the coverage of petrochemicals inventories in the investigated LCI databases. There are about 100 chemicals that are covered by all the databases due to their high importance for all the other supply chains in the database. These are mostly petrochemicals, focusing on the ethylene and propylene supply chains with their respective polymers, petroleum refinery outputs, ammonia, and a number of other base polymers with their supply chains (some of them have been described in more detail in section 2.2). Beyond that, the databases differ in their coverage. Due to differences in chemicals classification for these databases these are difficult to compare but the major part of datasets is made up by organic base chemicals.

For example, base chemicals in Ecoinvent make up a share of 50% of all chemical sector datasets, followed by fertilizers (14%), refined petroleum products (13%), plastics (10%), pesticides and other agrochemicals (5%), detergents (3%), and paints and coatings (2%). The total number of chemical sector datasets in Ecoinvent is about 3’000 datasets, of which a large number is market mixes. In the Ecoinvent database, there are mismatches along typical petrochemicals supply chains as downstream processes have been adapted with black box data from PlasticsEurope that does not use Ecoinvent refining data as inputs.

The sectoral coverage of the GaBi database is more difficult to assess as there is no straightforward classification of datasets provided and the chemical sector datasets are distributed over a broad range of sub-databases. Nevertheless, the focus also appears to be on base chemicals (52%), a higher share of plastics (24%) and refined petroleum products (19%), less fertilizers than in Ecoinvent (3%) and coatings (3%) at a total amount of about 2’900 chemical sector datasets. Where Ecoinvent provides market mixes of chemicals, there is a wider coverage of the same chemical from different regions. Subsets within the GaBi database are adapted from Plastics Europe, USLCI, and Fertilizers Europe data.

The chemicals datasets in the IDEA database are also roughly 50% organic base chemicals, but in contrast to the other LCI databases, they also have inventories for more than 150 inorganic chemicals (20%). Other large groups of chemicals are oil and fat products (9%), refinery products (4%) and chemical fertilizers (3%) at a total number of about 750 chemicals datasets. In Ecoinvent, GaBi and IDEA, the chemical sectors make up a major share of the total amount of datasets due to relevance and diversity of products.

The cm.chemicals database by Carbon Minds has a much larger number of chemicals life cycle inventories (about 100000) despite a smaller chemical coverage (about 90 mostly organic base chemicals with some different processing routes and different background data as well as 920 other mostly organic chemicals at lower data quality). The large number of individual datasets is based on combining a large number of national technology mixes, supplier mixes, and consumption mixes and the variation of national background data.

Other databases such as USLCI and JLCA basically cover the most common petrochemicals that are contained in all the databases.

End-of-life datasets (such as for waste incineration, landfilling or open burning) for some petrochemical products as well as recycling datasets (such as for PE or PET) are partly also available in the major LCA databases like Ecoinvent, GaBi and IDEA, but need manual linking with a product system under study to form an entire life cycle.

4.5 REGIONAL COVERAGE

The regional coverage in the chemicals sector of the different LCI database differs strongly. GaBi for example has a mostly European focus (63% of datasets) with more than 750 datasets for Germany alone, but North America and USA (21%), India (8%), China (3%), Brazil (2%) and Russia (1%) are also among the major regions in the chemicals sector of the database. There are hardly any global or generic datasets in the database and the degree of regionalization inside each of these datasets is currently unclear, while the documentation of some individual datasets indicates that often only a small number of parameters has been updated.

Ecoinvent has in contrast many global datasets (23%), which are only slightly fewer than the European (25%) datasets. In addition, 2% of datasets are available each for Switzerland, China, and South Africa, while 1% each cover Peru, Colombia, India, and Brazil. The extent of representativeness for global datasets is unknown as these datasets are typically derived from regional data, with adjusted inputs as far as possible – mostly in terms of electricity and heat supply, and key emissions.

The cm.chemicals database includes inventories for 2500 specific suppliers located in 190 regions. These datasets are developed by adapting basic process models with some regional background data, but the extent and implementation is unknown due to a lack of detailed documentation. Basic chemical product datasets are available in almost all countries without distinction of actually reported production capacities or facilities there. For example, the Vatican has datasets for domestic synthesis gas production, coke oven operation and in total about 65 chemical products, with one third of them being classified as medium or high-quality datasets (Carbon Minds, 2022). The practice of modelling chemicals production without any indication of actual production taking place may then also adversely affect the data quality along all petrochemical supply chains, for the different product consumption mixes that use such data as inputs and furthermore raises questions about how the regional differences in emission intensities captured when datasets are created without data inputs.

For the more regionally specialized USLCI database, the coverage is mostly the US and North America, while the two Japanese databases JLCA and IDEA contain mostly Japan-specific chemicals processes. In the upstream supply chains, all these databases aim at capturing the main regions of raw material extraction to the degree they are relevant for domestic supply.

4.6 CASE STUDIES

4.6.1 LCIS OF FERTILIZER PRODUCTION AND UREA

The production of fertilizers is crucial for the food and agricultural sectors, but has a limited number of applications in other sectors. In terms of environmental impact, the production of nitrogen fertilizers is central because of the fossil production routes that usually involve steam reforming of natural gas to produce syngas containing hydrogen gas (H2) and carbon monoxide (CO). The hydrogen is then used to produce ammonia (NH3), whereas the CO can be used for other chemical synthesis steps or a water-gas shift reaction in order to form additional H2 from water and CO with CO_2 as a by-product (Kulprathipanja et al., 2021). For the by-product CO_2, there are several use options that can then determine to a large extent the global warming impacts (section 2.2). For example, it can be used to further process ammonia into urea fertilizer (Brouwer, 2019), captured and used in other applications (like carbonation of beverages), or released to the air.

In the Ecoinvent database, prior to the release of v3.7 in 2020, the large-scale production of ammonia and urea had been disconnected and, due to a lack of data, the worst-case assumption of full CO_2 release to the atmosphere, and the input of industrial CO_2 to urea production from other sources had been modeled. This used to result in massive CO_2 releases from ammonia and urea production, which led to high contributions to climate change. For the release of v3.7, the decoupled model parts for ammonia and urea have been linked to connect the CO_2 supply from ammonia production with the CO_2 demand of urea production, which results in an impact reduction of around 35% in the European case based on ammonia production by steam reforming (Moreno Ruiz et al., 2020). Some types of water gas shift reactions are also covered implicitly by Ecoinvent, but these are difficult to make use of for specific needs due to high level of aggregation as they are contained in other datasets that cover a bigger part of the supply chains. There is no subdivision into smaller gate-to-gate processes, which is for example demonstrated by the syngas production that is part of the South African methanol and synfuel production datasets.

Beyond the syngas production from natural gas by steam reforming, there is also the gasification of coal to syngas, which can then be further produced into ammonia and urea (Kulprathipanja et al., 2021). Coal gasification has been employed in the South African chemical sector since the middle of the 20th century and has seen a recent surge in deployed sites in China in the past decade due to a local lack of oil and natural gas that is accompanied by an over-abundance of inexpensive coal resources. The CO_2 production from coal gasification is typically higher than from steam reforming and hence the global warming impacts of coal-based nitrogen fertilizer production may also be higher in case the CO_2 is released to the air. To date, only the cm.chemicals database covers this production route for China explicitly, while Ecoinvent instead covers the South African process variant.

The implementation of urea production from CO_2 and NH3, called the Bosch-Meiser process, is also a prime example of how the same process can be implemented in LCI databases in different ways, which can then have substantial consequences for the resulting environmental performance as quantified by LCA. Today, there are three major companies that have licenses for their large-scale urea production processes available (Brouwer, 2019): Toyo, Saipem, and Stamicarbon. Documentation and data sheets provide energy and mass balances for different process variations of the respective process technologies (Baboo et al., 2016; Saipem, 2019; Toyo Engineering, 2012). Connecting these balances with background energy supply datasets allows to quantify energy-related GHG emissions, which is shown for the case of natural gas-based heat and electricity supply based on Ecoinvent v3.8 cut-off in figure 4.3.

Toyo provides data for four versions of their ACES21 process, two of which are high in electricity demand and low in heat demand and two vice versa (Toyo Engineering, 2012). All of them supply the same product, granular urea. These process variants exist because there may be considerable differences in the inputs depending on local conditions, for example where a shift between heat and electricity may be favorable based on local costs and availability of fuels (Meyers, 1986). The US might for example be a case with abundant natural gas availability so the focus can there be more to burn this also for thermal energy supply, while countries like China have to import some raw materials and thus may try to recover more by-products while using other domestic fuels such as cheap coal as energy supply with more electricity-driven equipment instead of natural gas. Similar to the case of Toyo, Saipem offers four versions of their Snamprogetti urea process (Saipem, 2019) which also may prioritize low electricity or low heat consumption, but furthermore is available for two different product qualities that also impact the energy demands: granular urea or prilled urea (slightly lower impacts). In case of Stamicarbon, data is also available for a prilled urea case and allows for a direct comparison (Baboo et al., 2016).

In the development of life cycle inventories, the process-level material and energy balances would allow to set up inventories, connect them with background data (as we did with natural energy inputs) and implement them in a database. This approach is generally followed in the cm.chemicals database. Nevertheless, a critical information would remain how much each of the process variations is used in different regions and how the produced product quality differs in relation to this. Such data is difficult to obtain outside a few main bulk chemicals. In case this data cannot be collected, an average might be used instead, but then the granularity of the raw process-level data loses its value.

An even bigger problem becomes apparent, when the current Ecoinvent implementation (also adjusted to pure energy supply by natural gas) is compared to the best-case data reported by the licensing companies (see Figure 14). Ecoinvent makes use of measured and reported real-world data for Europe. Such data does not offer the full detail about the deployed technologies or detailed product property difference, but has the advantage of covering sub-optimal operating conditions, plant start-ups and shutdowns, equipment failures, operation outside design conditions, degradation of process equipment and other influences on process performance that are not included in the technology data sheets of the technology providers.

In environmental terms, these factors can cause a massive increase of environmental impacts that would otherwise be missed. For this illustrative case study of urea production, the real-world plants may cause on average about +60% higher greenhouse gas emissions, which represents a very substantial and environmentally relevant difference (Figure 14). Further differentiation of the specific energy supply (beyond the generic assumption of heat from natural gas everywhere as in the case of cm.chemicals) may then contribute to further substantial difference in emissions and impacts. The differences between real-world and idealized data exceed any differences between product qualities and processing variants by far. Thus, the example of urea production makes a strong case for favoring measured over modeled data for environmental accuracy of LCI data despite some losses of information in processing technology and product quality.

CO2 EMISSIONS OF ELECTRICITY AND HEAT FOR UREA PRODUCTION FROM CO_2 AND NH_3 (BOSCH-MEISER PROCESS) ASSUMING NATURAL GAS AS FUEL [kg CO_2/t UREA]

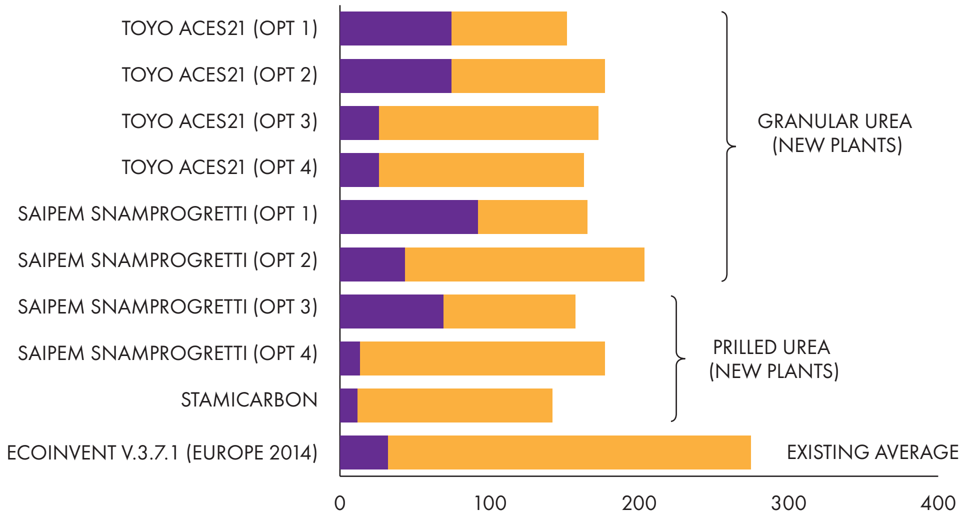

FIGURE 14: GATE-TO-GATE CO_2 EMISSIONS PER METRIC TONNE OF UREA FROM ELECTRICITY AND HEAT SUPPLY TO THE BOSCH-MEISER PROCESS ASSUMING NATURAL GAS AS FUEL FOR DIFFERENT REPORTED PROCESS OPTIONS (BASED ON COMPANY-REPORTED TECHNOLOGY SPECIFICATIONS) IN CONTRAST TO THE EUROPEAN OPERATIONAL AVERAGE CONDITIONS USED IN THE ECOINVENT DATABASE.

4.6.2 LCIS OF PLASTICS PRODUCTION AND IN PARTICULAR POLYPROPYLENE

As discussed in section 2.2, the production of polymers - especially from ethylene and propylene as monomers - represents one of the most widespread types of petrochemical production processes with the highest production volumes globally. The granularity and coverage for polymer production processes in LCI databases is generally high, but as in the case of fertilizer production, different types of data sources (manufacturer process specifications, operational averages, detailed models and others) are available, each offering different insights into the drivers for the related environmental impacts.

In ecoinvent v3, the major share of polymer production datasets for polyethylene (PE), polypropylene (PP), polyvinyl chloride (PVC) or polyethylene terephthalate (PET) are based on Plastics Europe Eco-profile datasets (Figure 15), which are generally created by merging European petrochemical plant operations data, acquired by Plastics Europe through surveys, with background LCI data from external data sources (Moreno Ruiz et al., 2019). Such background LCI data includes for example information on the fossil fuel supply chains and their environmental exchanges or electricity mixes as obtained from GaBi and ecoinvent v2 databases, which then have been derived with deviating data quality requirements, modeling principles or allocation procedures. Therefore, these datasets are partially inconsistent in background data and methodology compared to the rest of the ecoinvent v3 data. The Plastics Europe Eco-profiles are provided in an aggregated form, and in consequence, so are the ecoinvent datasets created from them, which restricts the depth of interpretation in that sector. A disaggregation of the polymerization step has recently been made available for ecoinvent, but in general their precursors remain aggregated black box datasets and do not use ecoinvent basic data (e.g. for ethylene or propylene). An exception of that are the polymer and monomer datasets outside Europe as they have been developed based on other data sources and are thus not subject to the same limitations (e.g. propylene production in South Africa). Polymer precursor supply chains related to petroleum refining activities would also be available to some degree in ecoinvent as they have been created even for Europe with separate refinery modeling and data collection, but these datasets are as of now not connected to polymer production as the input amounts for Eco-profiles are not known.

In the GaBi database, a major part of the European polymer supply chains is also derived from the Plastics Europe Eco-profiles, while additional data is available from internal refinery and steam cracker modeling. The self-modeled polypropylene polymer is then not created with the respective regional input mix from different processing routes but instead with propylene from steam cracking only (Figure 16). Additional datasets with mixes of other processing routes are available on demand or in extension databases. The Eco-profiles, in contrast, are considering both steam cracking (77%) and fluid catalytic cracking (23%) as most relevant processing routes for propylene and polypropylene production in Europe and hence depict a more representative split for European conditions.

The cm.chemicals data also represents aggregated datasets, but the different processing routes are more clearly distinguished from each other, while technology, production and consumption mixes are also available. The data sources and modeling techniques are not reported in detail, so the approach remains unclear, but upstream data and supply chains are obtained from ecoinvent v3, which is likely to then heavily influence the results. In contrast to ecoinvent, GaBi and Plastics Europe, the focus of cm.chemicals is more global and on the technical aspects (at least for bulk petrochemicals), so it covers more processing routes (e.g. by including propylene production by coal gasification via methanol or propane dehydrogenation) and prioritizes more by technological relevance (Figure 17). Nevertheless, the environmentally highly relevant coal gasification via Fischer-Tropsch liquids is only covered by ecoinvent among the analyzed LCI databases, which is somewhat in contrast to the statement by Carbon Minds that for propylene that “[a]ll relevant production technologies are considered for [propylene] and […] complete production and consumption mixes are used […].” (Kätelhön et al., 2021). This extends to the supply chains for several other petrochemicals in the cm.chemicals database.

Much like in the case of the different databases with a focus on Europe, the USLCI database covers the main polymer processing steps for the US, whereas IDEA and JLCA have a focus on the routes most relevant for Japan. The raw data pools for each of these three databases is separate from those of the different European databases and in addition, their level of disaggregation allows to further pinpoint the environmental hotspots in polymer supply chains. Hence, despite their regional coverage, these may offer deeper insights into the driving forces of environmental impacts within the supply chains than some of the other LCI databases do.

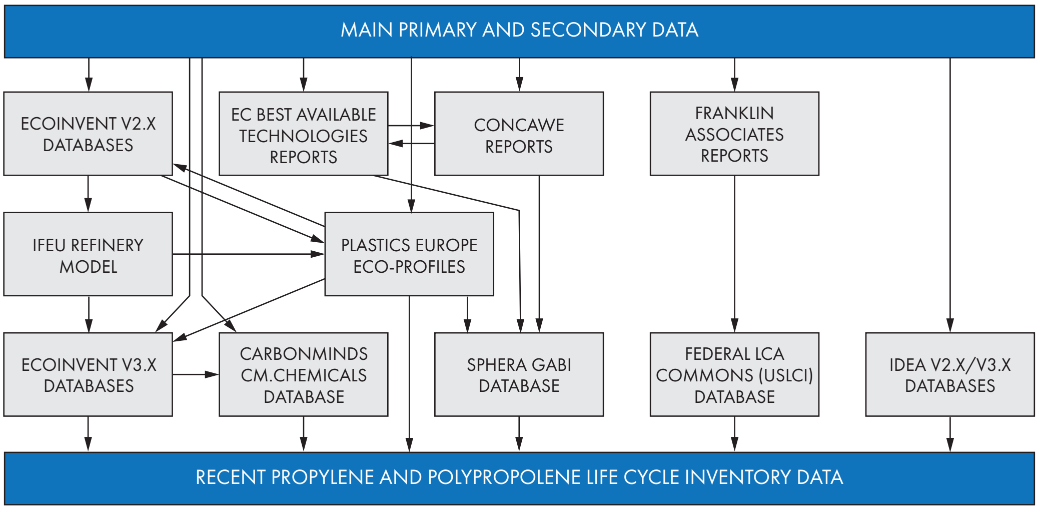

FIGURE 15: THE INTERCONNECTIONS OF DATA SOURCES FOR DERIVING PROPYLENE AND POLYPROPYLENE PRODUCTION LIFE CYCLE INVENTORIES.

By production volume, biogenic production of traditionally petrochemical-based polymers is rather limited, and so is at the moment the coverage in the existing LCI databases. For future projections or screening of promising biogenic alternatives to fossil supply chains, such data can be of high interest, and here at least the GaBi database has some coverage, for example for the production of biogenic polypropylene from four types of biomass (Figure 17). As there is a partial overlap of the raw material growing and processing with biofuels production, for which most LCI databases have some datasets based on different types of feedstock available, there are also some LCI databases with partial coverage of individual processing steps of biogenic polypropylene production (Figure 18), but only GaBi has complete and interconnected supply chains modeled. Outside of the GaBi coverage, there may be many other biogenic routes to produce polypropylene, but the coverage is limited to other scientific studies, which are difficult to compare due to a lack of standardized system boundaries and basic modeling assumptions (e.g. on carbon accounting or allocation) in the field.

Major processing routes of propylene and polypropylene have historically been via steam cracking, in Europe and Asia mostly of naphtha with crude oil as primary feedstock, and in the US supported by the availability of inexpensive natural gas and liquefied petroleum gas (LPG) (Kulprathipanja et al., 2021). A major contribution to global propylene production has come from fluid catalytic cracking (FCC) using mostly of vacuum gas oil (VGO) as input, which also makes crude oil the primary feedstock of that route. For more than half a century, coal chemistry in South Africa has been the notable exception, which led to the development of coal gasification to syngas, subsequent production of Fischer-Tropsch liquids and finally also propylene. In recent years (mostly in the past decade), a range of other coal-based processing routes of propylene has been firmly established in China, for example based on coal gasification, subsequent methanol synthesis, and finally methanol-to-olefins (MTO) processes to produce propylene. Some MTO plants may also import methanol obtained on the global market, which then usually originates from steam methane reforming with natural gas as original feedstock. In addition, build-up of propane dehydrogenation (PDH) capacity in the past decade with propane feedstock being supplied from refining operations (oil-based) or gas processing (natural gas-based) has been built up in China, the US and other parts of the world, which further increases the global propylene and polypropylene capacity. Biogenic routes for example via ethanol fermentation, ethylene and dimerization/metathesis are not common so far. Propylene is then polymerized to PP via gas-phase, bulk slurry or slurry polymerization with the first two dominating commercial processes today.

The coverage of these processes differs widely by database (Figure 17 and Figure 19), as especially recent developments in China are regularly not covered despite the possible relevance via global plastics product supply chains even in case of a regional LCI database focus. The partial aggregation of larger parts of the supply chains results in the fact that environmental impacts of intermediate chemicals regularly cannot be quantified and is further hindered where supply chains are not fully connected. Such cases exist for example where different processing routes exist towards the beginning of supply chains (e.g. in case of propylene production), but the subsequent polymerization processes then only use a subset of the available technologies as input (e.g. in GaBi where the German polypropylene dataset only uses propylene from steam cracking as input but not FCC propylene). A similar problem may arise from a mismatch of resolution between products, e.g. in case of the South African propylene production in ecoinvent, which misses a corresponding South African polypropylene dataset and hence ends up as minor input to the generic Rest of the World polypropylene production. The broadest and most consistent coverage of processing routes and resolution is present in cm.chemicals, which makes the polymer LCI data in that database a prime example for illustrating how much environmental impacts can differ based on feedstocks and local electricity mixes. Nevertheless, that approach is still lacking some major processing routes, real-world operational data and regional mixes of heat inputs as further main contributors to environmental impact differences.

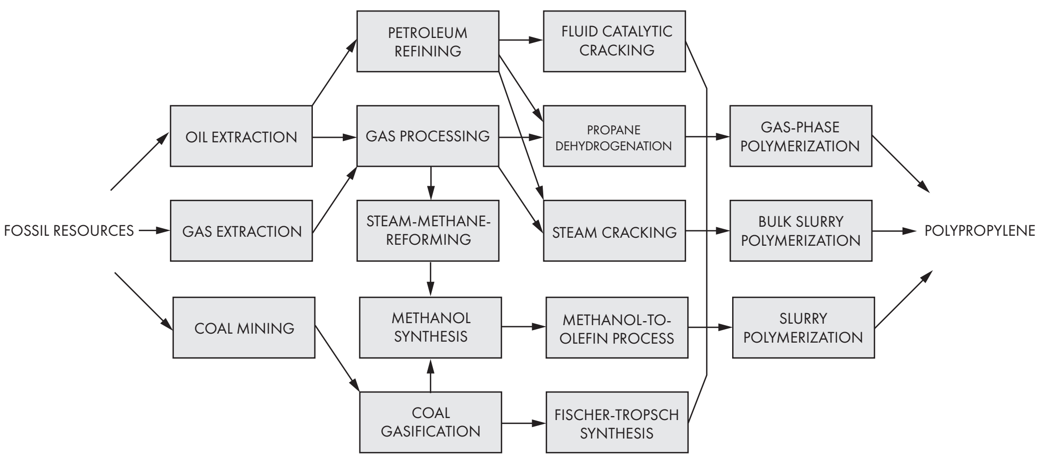

FIGURE 16: MAIN PROCESSING ROUTES FROM FOSSIL RESOURCES TO POLYPROPYLENE. BOXES SHOW PROCESSES WITH ARROWS SHOWING CONNECTIONS BETWEEN PROCESSES WITH MAIN SUBSTANCE FLOWS BETWEEN THEM. SOME MINOR PROCESSING ROUTES AS WELL AS SEVERAL INPUTS AND OUTPUTS ARE NOT SHOWN.

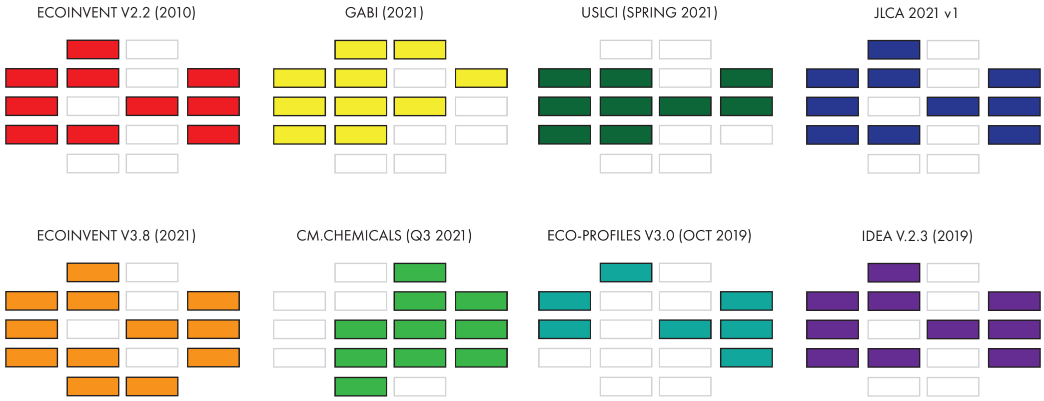

FIGURE 17: FOSSIL FEEDSTOCK-BASED POLYPROPYLENE-RELATED PROCESS COVERAGE OF DIFFERENT LCI DATABASES. EACH BOX REPRESENTS A PROCESS FROM THE FOSSIL PROCESS OVERVIEW (FIGURE 16) WITH A FILLED IN BOX MEANING THAT AT LEAST ONE CORRESPONDING DATASET FOR THE PROCESS STEP IS AVAILABLE IN THE RESPECTIVE LCI DATABASE.

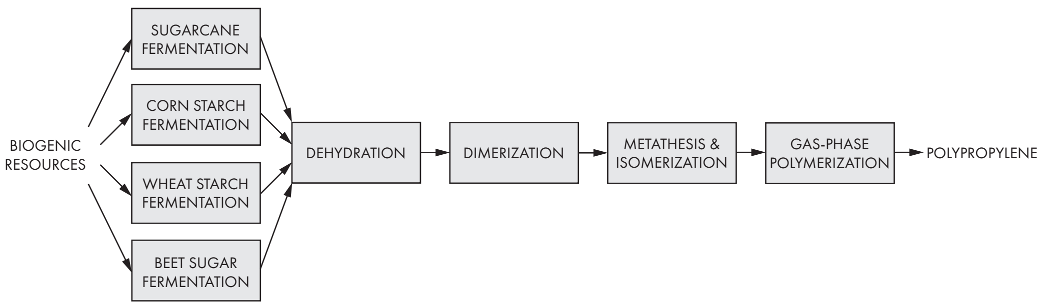

FIGURE 18 : MAIN PROCESSING ROUTES FROM DIFFERENT TYPES OF BIOGENIC RESOURCES TO POLYPROPYLENE AS MODELED IN THE GABI 2021 LCI DATABASE ("EXTENSION DATABASE XIX: BIOPLASTICS" FOR POLYPROPYLENE, "DATA ON DEMAND - SELLABLE CONTENT" FOR OTHER DATASETS). BOXES SHOW PROCESSES WITH ARROWS SHOWING CONNECTIONS BETWEEN PROCESSES WITH MAIN SUBSTANCE FLOWS BETWEEN THEM.

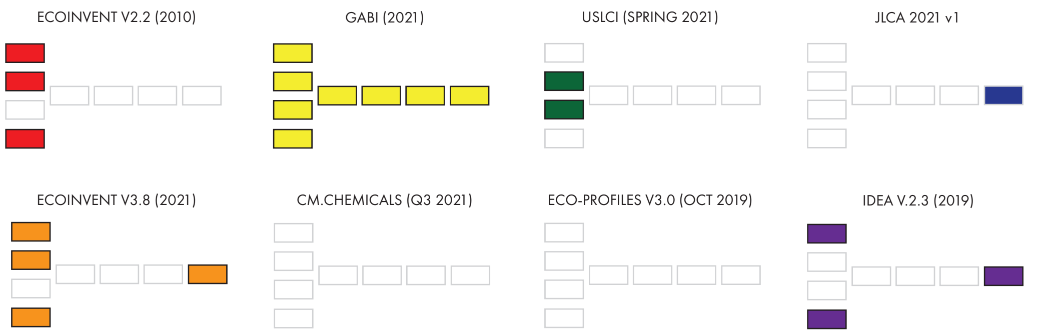

FIGURE 19: BIOGENIC POLYPROPYLENE-RELATED PROCESS COVERAGE OF DIFFERENT LCI DATABASES. EACH BOX REPRESENTS A PROCESS FROM THE FOSSIL PROCESS OVERVIEW (FIGURE 18) WITH A FILLED IN BOX MEANING THAT AT LEAST ONE CORRESPONDING DATASET FOR THE PROCESS STEP IS AVAILABLE IN THE RESPECTIVE LCI DATABASE.

In general, the LCI databases of Ecoinvent and cm.chemicals agree that coal-based processing routes show especially high global warming potentials due to the stoichiometric formation of CO_2 in the gasification-synthesis step (Figure 20). While part of the produced CO_2 may be captured and used as feedstock for other purposes, the emissions are still very high compared to other (fossil) production routes and are also contributing to pollution via very high heat and electricity demand of this process. At coal gasification sites, the heat and electricity are often supplied by dedicated coal co-generation power plants (e.g. in case of Secunda in South Africa (S&P Global, 2021)), which are not fully represented in the LCI databases as discussed in section 4.3.2 and may even lead to the underestimation of climate change impacts of coal-based petrochemicals production.

Oil and gas-based processing routes are more similar to each other concerning contribution to climate change per kg propylene across databases, but the specific levels depend a lot on individual allocation decisions especially due to refineries and steam cracking with many outputs and a very diverse set of allocation methods as discussed in section 4.3.3. Most LCI databases cover the main production route via steam cracking of naphtha in most detail, which allows to observe a range of values for different parts of the world (Figure 20). Steam cracking of LPG is covered less commonly, but the results nevertheless show that the performance in terms of contributions to climate change is in a similar range to steam cracking of naphtha. The steam cracking of ethane mostly plays a role for ethylene and polyethylene, while its outputs of propylene are comparably small. Hence, its data has not been collected with regards to propylene production and conclusion on its environmental performance cannot be drawn in this regard. The FCC route via VGO appears on average to have lower GHG emissions than steam cracking. The variability in supply and consumption mixes are high mostly due to the influence of coal-based propylene production in China.

The different polymerization technologies for propylene are often not specified in LCI databases or the polymerization step is covered as technology mix (Figure 21), which appears justified in the case of propylene polymerization as most processes are similar in utility demand despite some flexibility between electricity and heat (IHS Markit, 2021). Heat and electricity demand dominate the contribution to climate change of the polypropylene polymerization step. Since monomer trade data from producing site to consuming sites is generally not public, the LCI databases fill this gap to some degree with national and regional trade data, which evens out some of the very strong differences of environmental impacts in the specific monomer production routes. A higher resolution is available on demand from the supplier-specific datasets of Carbon Minds as they have site location data for some chemicals available and assume that production steps occurring in the same city are physically connected. Validation of that assumption, a critical discussion or an analysis of the consequences on model outcomes is so far not available. The global representativeness of most LCI databases has decreased in recent years in case Chinese and global processing developments in the petrochemicals sector with unique environmental profiles are missing. A similar picture for PE and other fossil-based polymers with feedstock variability compared to PP can be observed globally as coal-based syngas and methanol can be used for a broad range of petrochemicals.

Further manufacturing steps in the life cycle of PP products, the use phase, and the end-of-life treatment (e.g. by landfilling, incineration or recycling) further contribute to the overall contribution to climate change of PP use, but depend strongly on the specific products, and the waste treatment they undergo. These impacts lie outside the scope of the present study but are expected to be in a similar order of magnitude compared to the impacts up until polymer production (Cabernard et al., 2021).

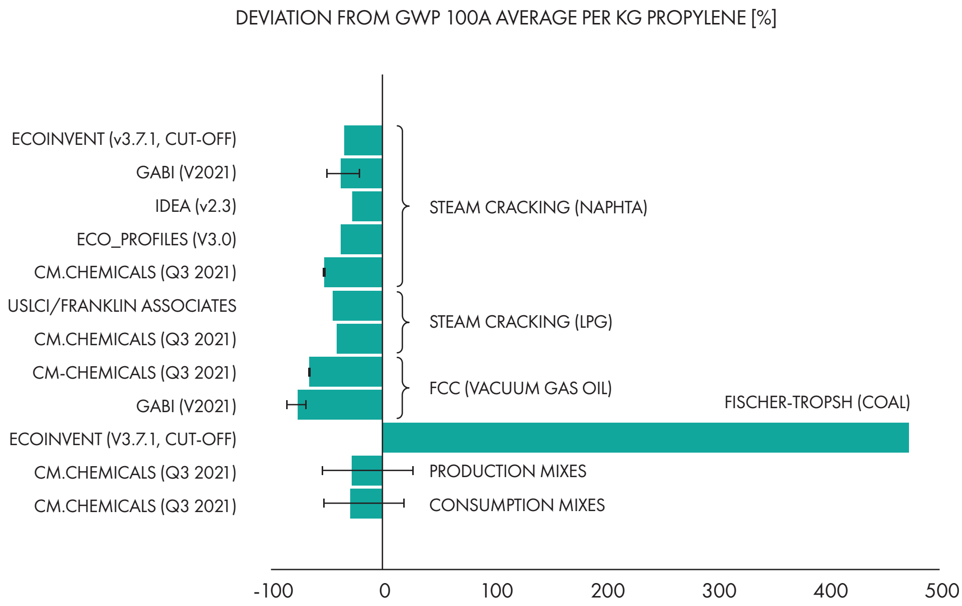

FIGURE 20: CLIMATE CHANGE IMPACTS PER KG OF PROPYLENE PRODUCTION FOR DIFFERENT PROCESSING ROUTES ACROSS LCI DATABASES IN COMPARISON TO THEIR AVERAGE IMPACT.

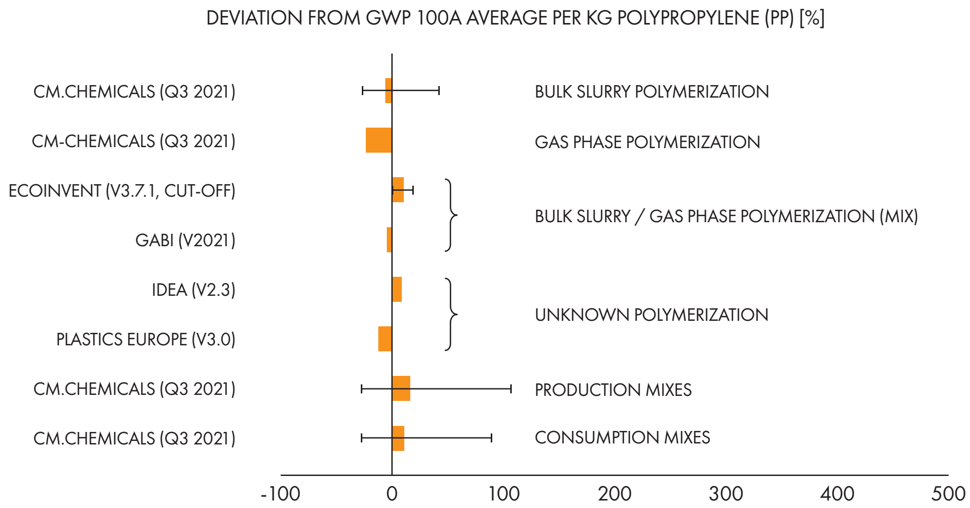

FIGURE 21: GLOBAL WARMING IMPACTS PER KG OF POLYPROPYLENE PRODUCTION FOR DIFFERENT PROCESSING ROUTES ACROSS LCI DATABASES IN COMPARISON TO THEIR AVERAGE IMPACT.

4.7 CRITICAL DISCUSSION OF PETROCHEMICAL LCI DATASET QUALITY

Across the available LCA databases, different aspects related to the environmental impacts of petrochemicals production are captured. In general, though, there is often a lack of recent large-scale operational data or measured data, which results in the major use of proxy approaches, assumptions or the use of rather old process data from more than twenty years ago. Such data may still represent the current situation sufficiently well, but from an LCA perspective at least requires basic documentation to be considered in the assessment. In that regard, several of the available databases show deficits, for example in case of cm.chemicals there is no documentation of where the process data comes from whatsoever, while other databases such as ecoinvent or GaBi refer to their data sources, but then sometimes these remain highly intransparent (e.g. in case of Plastics Europe data). Such practices not only limit the usefulness of the LCA data, but also prevent users occasionally from identifying gaps and limitations, and dealing with these appropriately.

Due to the high energy-intensiveness of the petrochemical sector, it is of particular importance that the energy supply for the sector is modeled in detail. Most databases make use of national electricity supply mixes of the public electricity grid, which then frequently dominates the regional patterns of environmental impacts per chemical as shown in Figure 22 for the example of adipic acid production. IEA data however shows that the public electricity mix is generally not representative of the electricity consumption of petrochemicals production with typically a much higher reliance on fossil fuels, which poses the risk of underestimating the underlying environmental impacts (IEA, 2021a). Furthermore, the IEA also provides data for the heat inputs of the sector, which has clearly been shown to be even more important for the environmental impacts of the petrochemical sector than electricity consumption (Kim and Overcash, 2003). Here, most databases also do not distinguish between regions, sectors and products, which is a key limitation for the environmental assessment of any petrochemical.

Finally, the available data on processing route alternatives for bulk petrochemicals is much better than for specialty petrochemicals or other types of chemicals, but even for the main one hundred products, so far, no LCA database has covered all the employed route alternatives. From the available data it is clear that the differences may in some cases be very significant, while they are almost negligible in other cases. As the different processing routes present options for reducing environmental impacts while still providing the same product output, it will be important for the LCA databases to close the remaining gaps, not only for providing a clearer picture, but also for highlighting improvement potentials in detail.

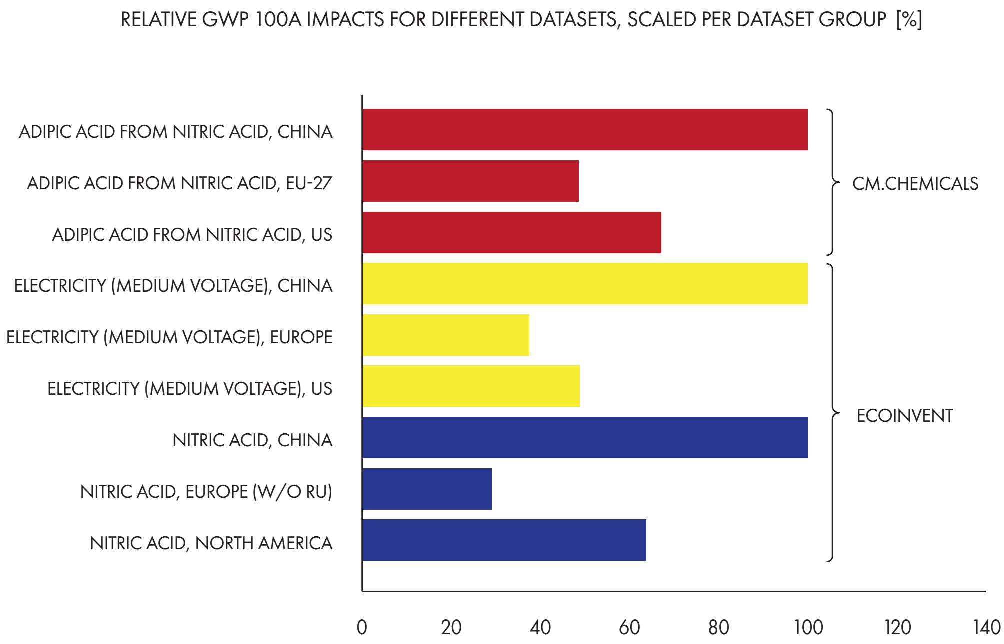

FIGURE 22: SIMILARITY OF RELATIVE CONTRIBUTION TO CLIMATE CHANGE PATTERNS FOR ADIPIC ACID, ELECTRICITY AND NITRIC ACID ACROSS DIFFERENT REGIONS DUE TO UNDERLYING MODEL SIMPLIFICATIONS. EACH GROUP OF DATASETS (ADIPIC ACID, ELECTRICITY AND NITRIC ACID) ARE SCALED TO 100%.

4.8 CROSS-CUTTING CONCLUSIONS

In general, it can be observed from the LCA data that the shale gas boom in the US and increasing development of coal-based chemical production routes in the past decade have led to a higher diversity in environmental impacts for the same petrochemicals in comparison to the mostly oil-based production of the past. The collection of primary data for production of bulk petrochemicals often dates back 10 to 25 years across LCI databases, even for the recently published cm.chemicals database. This can nevertheless provide a representative picture of environmental impacts where the age of plants and types of processing routes still match these conditions, but coverage of the newer processing routes in LCI databases is somewhat lagging behind. More specifically, the developments in China in the past five years have had great influence on the average environmental impacts per chemical due to the different production routes, the global outsourcing of energy-intensive processes to China and the coal-based energy supply there, but this development is not yet fully captured by most LCI databases. While there are generally many data products available for the creation of bulk organic chemical LCI data (Figure 23), there is still a gap in the availability of process data on bulk inorganic chemicals and even more so for fine chemicals such as agrochemicals, pharmaceuticals, additives, etc. Instead, proxy data is rather commonly used for petrochemical LCI datasets, but problematic where information on the use of the proxy data is lost from one process to another, the influence of the proxy data accumulates along multi-step supply chains, and process modeling is not updated once better data to replace proxies would be available. At least, unit-process LCI databases generally are more transparent on their modeling principles and offer the user substantially more depth in their analysis, while at the same time being somewhat restricted on the data they use for intellectual property reasons. System-process LCI databases, on the other hand, generally benefit from the fact that the raw data is not disclosed to the user, which allows them to use a broader range of data sources but would require more documentation on the modeling principles just so the users understand the implications for their results. In most cases, though, the documentation is less detailed for system-process data compared to unit-process data, which makes these databases less reliable for users as the data quality and suitability cannot be assessed.

In terms of data availability for LCA purposes, there has been major development in the data on upstream emissions, especially in terms of methane leakages, which are not yet fully incorporated into LCA datasets. Such data is particularly useful, where it includes operational practices or fugitive pollutant releases that cannot be calculated with engineering in a reliable way. Furthermore, there are substantial differences in process performance between idealized theoretical conditions (steady state, new plant, average design) and real-world conditions (start-ups and shut-downs, equipment degradation, machinery failures, operation outside optimal design conditions, site-specific design, specific energy supply, local regulation, outdated technology choices, influences of revamping and debottlenecking). Most LCI databases struggle with capturing such effects due to data availability, while some even neglect real-world conditions completely and may thus underestimate emissions and impacts considerably. Nevertheless, the available LCA data allows to quantify the contribution to climate change for major bulk petrochemicals on a product-level systematically (Figure 23), and as such allows to identify environmentally particularly harmful petrochemicals. For example, some of the LCA data could indicate that the breakdown of larger feedstock molecules into small primary petrochemicals such as ethylene and propylene, and the subsequent synthesis of other products out of these building blocks may result in higher contributions to climate change per product mass than the use of larger chemical structures as building blocks (such as aromatics). In addition, it becomes clear that the contributions of electrolytic processes for example in the manufacturing of vinyl chloride monomers (VCM) and polyvinyl chloride (PVC) can lead to high environmental impacts due to the large electricity demands. The available LCI data further allows to outline the major role of coal-based petrochemicals production as particularly problematic both in terms of their emission intensities as well as their major contribution to the global petrochemicals demand (Figure 24), for example for key petrochemicals such as methanol.

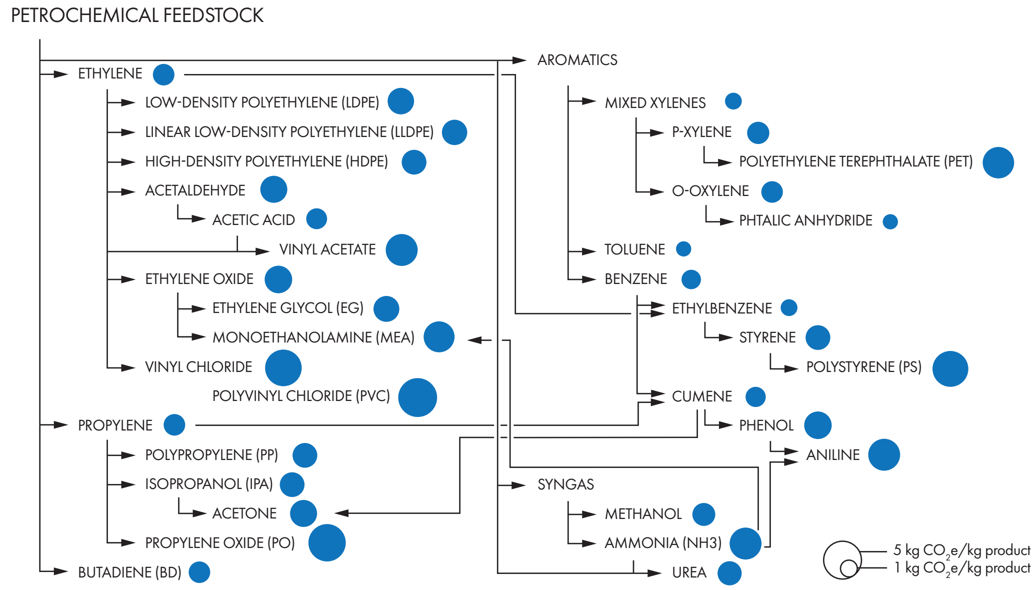

FIGURE 23: CRADLE-TO-GATE LIFE CYCLE CONTRIBUTION TO CLIMATE CHANGE PER KEY PETROCHEMICAL PRODUCT ACCORDING TO CM.CHEMICALS 2021 AND ECOINVENT V3.7.1, AND SIMPLIFIED REPRESENTATION OF CONNECTIONS BETWEEN CHEMICALS BY SYNTHESIS PATHWAYS.

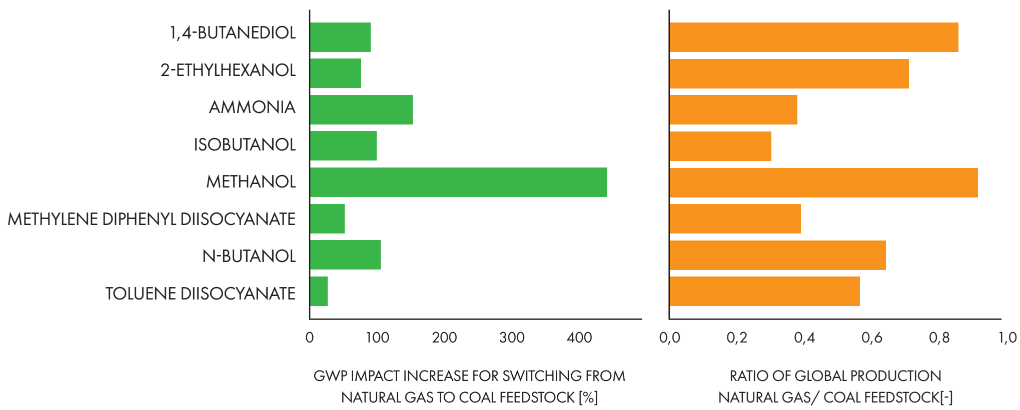

FIGURE 24: DIFFERENCE IN CRADLE-TO-GATE CONTRIBUTIONS TO CLIMATE CHANGE FOR THE PRODUCTION OF SEVERAL PETROCHEMICALS WITH NATURAL GAS AND OIL OR COAL FEEDSTOCK AND THE CURRENT RATIO OF GLOBAL PRODUCTION VIA THESE ROUTES BASED ON CM.CHEMICALS 2021 DATA.

4.9 OUTLOOK

In general, it can be said that the coverage of chemicals and petrochemicals in LCA databases is strongly increasing, driven by larger LCI data collection initiatives such as the data collection efforts of the European Union for environmental footprinting or by more specialized LCI data companies such as Carbon Minds, who for example added about 450 chemicals to their database in December 2021. The availability of process data that can be used in LCI databases as well as specific (measured) data for the key regions in Asia remains however a major problem as idealized best-case operational data for new plants may be to some degree available, but it typically differs strongly from the operational conditions across petrochemical plants of all ages. As unlinked process data and linking algorithms are not public for most LCI databases, database-wide consequences of fundamental normative modeling choices (such as allocation) remain unassessed and need to be better understood, especially due to the complexity of product and process interlinkages in the petrochemical sector. So far, however, the LCI data clearly confirms the central role of energy demand for contributions to climate change , as well as the role of raw material choice (coal, oil, gas, biogenic feedstock).

End-of-life data for chemical products may also make significant contributions, but the fate data and models on that particular aspect is patchy, much like for other sectors and so will require refinement. Especially the use of biogenic feedstocks as raw material for traditional petrochemical products is getting traction, but differs in fundamental aspects like the carbon balance, and hence the existing modeling principles need to be checked for whether they treat the specific features of such processes in an appropriate way, while there is also a clear need for more data on these processing routes to evaluate promising synthesis pathways.

In all of that, the environmental impacts beyond climate change remain challenging where pollutant releases cannot be derived directly from mass or energy balances (e.g. NOx emissions) or major inputs or outputs remain unknown (as operational data for plants at a product-specific resolution is largely unavailable). In order to prevent burden-shifting from climate change to other domains of environmental impacts such as the human health, more efforts will be necessary to include them as well in the raw data but also in all studies.

STEAM CRACKING IS A
CENTRAL PETROCHEMICAL PROCESS THAT IS
ASSOCIATED WITH LARGE GHG EMISSIONS

PHOTO: ADOBE STOCK

5 CORPORATE DISCLOSURES AND EMISSION REDUCTION TARGETS

In this report, the third type of data about emissions from the petrochemicals industry under review is information disclosed by leading firms in the industry themselves, as well as information about their targets for reducing these emissions. Over the past decades, the extent of various information disclosure programs has risen considerably (Matisoff, 2013). With growing pressure on firms to disclose their emissions, this is no different in the context of GHG emissions with significant increases in voluntary disclosure (Andrew and Cortese, 2011). Indeed, alongside pricing and target-setting, emissions disclosure is a key corporate carbon management strategy (Lister, 2018).

5.1 VOLUNTARY EMISSIONS DISCLOSURE

5.1.1 DISCLOSURE AND ENVIRONMENTAL GOVERNANCE

Information disclosure and transparency in sustainability governance often follows different rationales, ranging from market-oriented over technocratic to democratic visions (Gupta and Mason, 2016). Market-oriented arguments rests on different hypothesised mechanisms. Disclosure ensures the transparency which is needed for differentiated treatment across firms as poor environmental performance and/or non-disclosure arguably indicate poor risk management and represent a financial liability (see e.g. Khanna et al., 1998; Konar and Cohen, 1997; Patten, 2002). Such information is relevant for investors as well as for employees and other stakeholders. In other words, disclosure is meant to address information asymmetries (Weil et al., 2006). Moreover, the process of disclosure itself and the analysis it necessitates has been argued to enable more effective management practises, allowing companies to improve their environmental performance. However, evidence for any of these mechanisms appear mixed (Matisoff, 2013).

Notwithstanding the lack of consensus over the effectiveness of making information available, corporate disclosure can help track progress and scrutinize corporate practices. As the number of pledges to reduce emissions amongst corporate actors has proliferated following the Paris Agreement, the importance of disclosure has become increasingly clear (Lister, 2018). This chapter aims at examining corporate actors in the petrochemical industry through voluntary disclosures. Such arguments follow a democratization rationale, which among other things, highlights the need for accountability (Gupta and Mason, 2016).

Voluntary corporate reporting, however, is subject to a range of criticism. Many of these relate to the nature of voluntary self-reported disclosure. For one, the fact that corporate disclosures rests on self-declaration causes concerns over the reliability and quality of the available data (Depoers et al., 2016; Kolk et al., 2008; O'Dwyer et al., 2005; Sullivan and Gouldson, 2012). The international accounting firm KPMG (2015) found that differences in reporting within and across sectors and geographies made it 'all but impossible to accurately compare one company's carbon performance with another'. In this regard, Lister (2018) highlights the role of third-party assurance (LeBaron et al., 2017) and international standards in addressing such concerns. Other aspects of criticism include the limited potential for sanctions for non-disclosure as well as an overemphasis on process and procedure instead of mandating outcomes as in the end, disclosing emissions is not the same as acting to reduce emissions (Gupta, 2008; Mason, 2008).

Information disclosure can be governed in different ways (voluntary or mandatory) by different actors (private, public or hybrid). The globally leading platform for corporate GHG emission disclosure is the CDP (formerly Carbon Disclosure Project) which was established in 2000. Since then, it has grown rapidly, and the most recent dataset includes disclosures from more than 7000 companies. In this chapter, we therefore rely on the CDP database and the disclosures it contains to map the extent and form of corporate disclosure within the petrochemical industry.

In terms of governance, CDP submissions are voluntary with no penalty for non-compliance (Green, 2017). Moreover, it is formed from a hybrid arrangement with multiple stakeholders (Bäckstrand, 2008), funded mainly through corporate fees as well as public and private grants and collaborating with a range of private and public organisations. To convince companies of completing the CDP's reporting questionnaires, the organisation itself points to a 'high and growing market demand for environmental disclosure' and a number of claimed 'tangible business benefits' related to disclosure.

Importantly, the CDP database and the governance arrangement that underpins it has been subject to a range of the criticisms referenced above, perhaps most prominently that it enables powerful companies to dictate the conditions of climate governance and lacks effectiveness (see e.g. Andrew and Cortese, 2011; Gupta and Mason, 2016; Knox-Hayes and Levy, 2011; Lister, 2018; Matisoff, 2013). In terms of promoting reliability, understandability and comparability of data, the CDP grants a lower CDP score to companies that do not verify their data through a third party, although the CDP also publishes data that has received no third-party verification (Green, 2017).

Despite the criticisms, various environmental governance scholars argue that hybrid and private forms of governance arrangements have a role given decisive state-led actions. For example, Lister (2018) emphasises that disclosure should be regarded as a single element in a climate policy mix and argues for state co-regulation of corporate carbon management initiatives. Relatedly, Green (2017) posits that initiatives such as the CDP can be an 'initial building block toward meaningful climate action' while maintaining that their effectiveness is conditioned by government action.

5.1.2 CORPORATE DISCLOSURES OF GHG EMISSIONS IN THE PETROCHEMICAL INDUSTRY

Although far from all major petrochemical producers disclose emissions through CDP, the total number of companies in the chemical industry reporting has more than doubled in the period running from 2010-2020 (see Figure 25). The disclosing firms are clearly dominated by companies with headquarters in OECD member countries, Japan and USA being the countries with the highest concentration of disclosure, home to 71/145 of the reporting chemical companies in 2020. This has been the case for the entirety of the period under consideration with no noticeable exceptions illustrating a bias towards countries headquartered in the Global North in the reported data. As such, the findings are not necessarily indicative of the industry as a whole. This sort of regional bias, however, is not unique to the chemical industry but applies to the CDP more broadly, possibly due to differences in resource availability as well as social, economic and legal pressures (Luo et al., 2013).

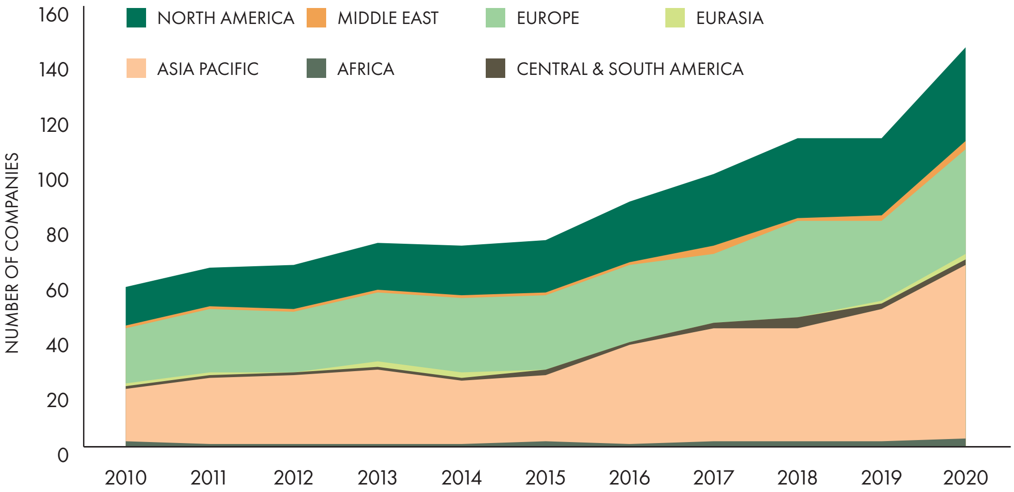

FIGURE 25: NUMBER OF CHEMICAL COMPANIES DISCLOSING EMISSIONS THROUGH CDP FROM 2010 TO 2020, BY REGION OF HQ. THE LIST ALSO INCLUDES 5 COMPANIES WHICH HAVE NOT LISTED THEIR PRIMARY SECTOR AS CHEMICALS IN ALL YEARS IN THE PERIOD BUT REMAIN AMONGST THE 50 LARGEST PRODUCERS IN THE WORLD.

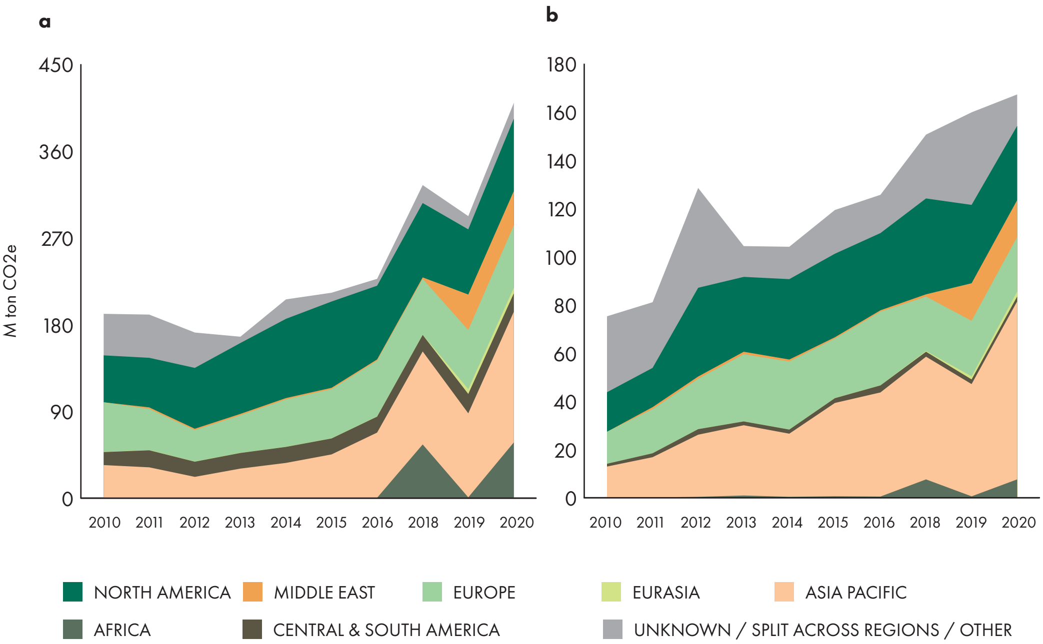

FIGURE 26: TOTAL REPORTED GHG EMISSIONS IN M. TON CO_2E ACROSS GEOGRAPHIES BY COMPANIES INCLUDED IN FIGURE 25. PANEL A DEPICTS GHG EMISSIONS REPORTED UNDER SCOPE 1 EMISSIONS. PANEL B SHOWS DISCLOSED LOCATION-BASED SCOPE 2 EMISSIONS. DISCLOSURES FROM 2017 ARE EXCLUDED DUE TO REPORTING INCONSISTENCIES. DATA SOURCE: CDP

As the number of disclosing companies has increased so have the total emissions figures reported by the industry (see Figure 26). In the period from 2010-2020, both scope 1 and location-based scope 2 emissions reported across regions have approximately doubled[1]. Despite the dominance of the regions where disclosing companies are headquartered, the regional dominance is not as one-sided in Figure 25 as in Figure 26.

For direct emissions (scope 1) especially but also generally, the disaggregation of data by region has improved with a decreasing share of emissions being reported without reference to a specific region. However, this hides the fact that there are substantial reporting gaps. That is, there are considerable disparities between total global emissions disclosed and totals aggregated across emissions reported across regions most noticeably in the 2013, 2018 and 2020 disclosures. For 2020, the gap for scope 1 is as high as around one third of the total disclosed scope 1 emissions.

Considering the total chemical sector emissions disclosed through CDP across scope (see Figure 27), the total amount of disclosed emissions has increased five-fold. This is largely due to an increasing amount of scope 3 emissions, which have increased by a factor ten in the 2020 disclosures compared to in 2010, despite the number of reporting companies increasing by no more than a factor 1.33.

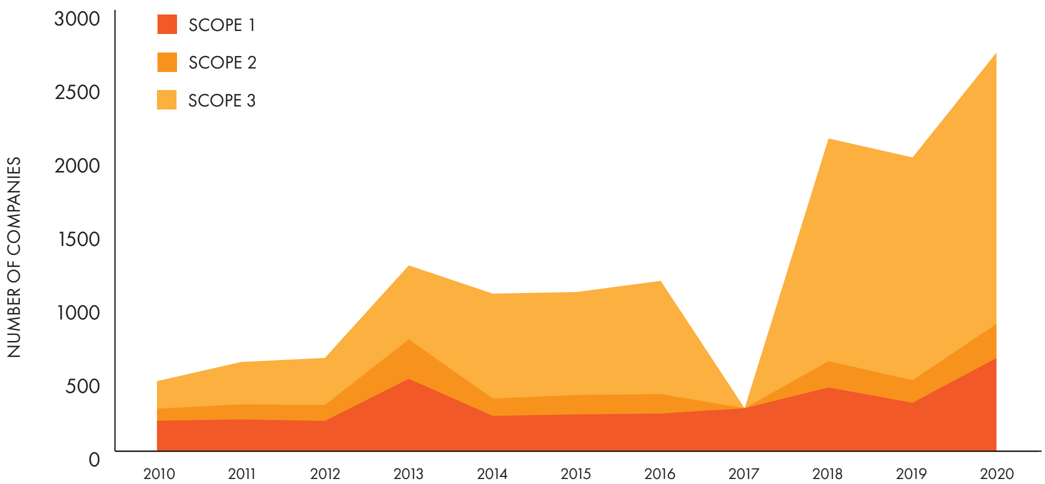

FIGURE 27: DISCLOSED EMISSIONS (IN M. TON CO_2E) BY CHEMICAL COMPANIES ACROSS SCOPES. FOR CONSISTENCY, THE DISCLOSURES OF TWO COMPANIES WITH EXTREME VARIABILITY IN THE REPORTED SCOPE 3 EMISSIONS IN 2018 ARE NOT INCLUDED IN THIS GRAPH. DISCLOSURES OF SCOPE 2 AND SCOPE 3 FROM 2017 ARE EXCLUDED DUE TO REPORTING INCONSISTENCIES. SOURCE: CDP

However, there are considerable year on year differences. Most noticeable is perhaps the lack of reported scope 2 and 3 emissions in 2017 but also the spikes in 2013 and 2018 (related to the aforementioned reporting gaps). For 2017 specifically, the relevant data reported by CDP could not be accurately mapped to such an extent that direct comparison with previous and later years was not possible.

1 SCOPE 1 GHG EMISSIONS REFER TO DIRECT EMISSIONS STEMMING FROM 'SOURCES THAT ARE OWNED OR CONTROLLED BY THE COMPANY' WHILE SCOPE 2 REFERS TO GHG EMISSIONS FROM PURCHASED ELECTRICITY. SCOPE 3 GHG EMISSIONS, IN TURN, REFER TO ALL INDIRECT EMISSIONS NOT COVERED UNDER SCOPE 2. EXAMPLES INCLUDE EXTRACTION AND PRODUCTION OF FEEDSTOCK; TRANSPORTATION OF PURCHASED FUELS; AND USE OF SOLD PRODUCTS (FOR PETROCHEMICAL PRODUCERS THIS MEANS THAT THE INCINERATION OF PLASTICS IS INCLUDED IN SCOPE 3) (WBCSD/WRI, 2004).

Such considerations arguably reflect the nature of self-disclosure and the lack of accountability referenced in section 6.1.1, which is further complicated by the differences in emissions accounting standards and protocols. Indeed, to collect activity data and report emissions the disclosing firms report a total of 71 variations and combinations of 21 different standards with no clear way of comparing the consistency between them.

Differences in accounting framework are also evident in the lack of standardization for how scope 3 emissions are reported, as disclosing companies have full discretion in choosing whether and how to report scope 3 (using different methodologies). Despite the fact that an increasing share of scope 3 emissions are disclosed relative to total scope 1 and 2 (total scope 3 emissions in 2020 doubled total scope 1 and 2), there are large varieties in which scope 3 emission categories that are reported. In the 2020 CDP disclosures, all reporting chemical companies disclosed scope 3 emissions associated with upstream transportation and distribution while around 1/3 did not report emissions from purchased goods and services (such as feedstock) despite its high climate impact (see Table 2). More critically, many companies did not report downstream scope 3 emissions despite their relevance in terms of climate impact as related to, for example, waste management and the incineration of plastics (Zheng and Suh, 2019). In fact, 94 firms did not report emissions related to the use of sold products while 82 out of the 145 companies reporting in 2020 did not disclose scope 3 emissions for end-of-life treatment of their products. For processing of sold products, a major source of emissions given the amount of intermediate product trade and use of chemicals across industrial processes, only 19 companies reported their scope 3 emissions.

The difficulties in reliably assessing and comparing emission estimates across the industry and its products and services (cf. chapter 4 and 5) further add to the challenges related to inconsistencies in accounting and reporting. Taken together, substantial issues with standardization, harmonization and transparency complicate and often render direct comparisons across companies very difficult.

TABLE 2: THE FIVE MOST REPORTED SCOPE 3 CATEGORIES BY CHEMICAL COMPANIES IN CDP IN 2020

SCOPE 3 ACTIVITY	REPORTING COMPANIES	TOTAL EMISSIONS (T CO_2EQ)	AVERAGE EMISSIONS (T CO_2EQ)
PURCHASED GOODS AND SERVICES	104/145	676,914,883	6,508,796
FUEL-AND-ENERGY-RELATED ACTIVITIES	97/145	59,679,546	621,661
UPSTREAM TRANSPORTATION AND DISTRIBUTION	145/145	25,678,651	270,301
WASTE GENERATED IN OPERATIONS	96/145	7,488,582	78,006
BUSINESS TRAVEL	105/145	2,196,020	20,914

In CDP, the chemical industry is grouped into 10 different sub-categories/activities. For the 2020 disclosures, most major petrochemical companies disclosing through CDP identified with the classifications of ‘other base chemicals’ and ‘specialty chemicals’ (see Table 3). Despite a majority of companies not reporting significant downstream scope 3 emissions (and the lack of commensurability due to differences in reporting and accounting standards), the total scope 3 are still two to three times that of combined scope 1 and 2 for these two main classifications.

Importantly, some of the largest petrochemicals producers are also fossil fuel companies with vertical integration across their value chains. Despite having some of the highest amount of chemicals production in the world, they identify their primary activity as belonging to the oil and gas sector and are therefore not included in the data we report in Table 3. The table therefore includes 142 of the 145 companies as above. This further complicates directly comparing disclosures across companies and illustrates the arbitrary character of sector boundaries between oil, gas, and chemicals. An illustrative example of this is the case of Sasol, which registered as a chemical company in 2018 and 2020 while identifying themselves as an oil and gas company in other years.

Considering the various CDP ratings which are decided based on CDP's own methodology and are meant to capture the quality of disclosure, most reporting companies obtained a score of either 'A' or 'B'. Some relevant exceptions apply most notably for companies listing their primary activity as 'basic plastics', where most companies obtained a 'D'. For the two classifications with most major petrochemical producers, 'other base chemicals' and 'specialty chemicals', around 1 out of 4 reporting firms obtained either a 'C' or a 'D'. As such, even though this list only includes companies which themselves choose to disclose in the first place and, as such, see an incentive in disclosing, there are still considerable shortcomings in disclosures. Indeed, many data points have not been verified by a third party to ensure the quality of their data. Across the 291 data entries covering emissions reported by the 145 chemical companies, 36 report no third-party verification at all while 70 companies or around half have no verification of scope 3 data. And for the companies which did use this third-party verification, the majority identified their primary activity as belonging to the 'personal care and household products' classification.

TABLE 3: FIRMS REPORTING TO CDP IN 2020 IDENTIFYING THEIR PRIMARY ACTIVITY AS PART OF THE CHEMICAL INDUSTRY

CDP CLASSIFICATION	# OF COMPANIES	TOTAL SCOPE 1 EMISSIONS (T CO_2E)	TOTAL SCOPE 2 EMISSIONS (T CO_2E)	TOTAL SCOPE 3 EMISSIONS (T CO_2E)	CDP RATINGS (# OF COMPANIES)					
					A	B	C	D	F	N/A
AGRICULTURAL CHEMICALS	2	697,989	430,834	1,598,526	1	1				
BASIC PLASTICS	6	4,433,393	3,757,756	10,484,624		2		4		
COMMERCIAL SERVICES	1	411,079	218,376	7,025,763	1					
INORGANIC BASE CHEMICALS	9	60,300,605	52,115,869	112,882,682	3	3	1	2		
NITROGENOUS FERTILIZERS	2	20,158,768	1,187,638	55,850,350		1	1			
NON-NITROGENOUS FERTILIZERS	5	21,874,197	6,761,816	31,479,594	2	2		1		
OTHER BASE CHEMICALS	40	267,539,618	84,662,538	681,292,212	12	18	7	3		
PERSONAL CARE AND HOUSEHOLD PRODUCTS	27	4,748,892	6,270,114	603,611,198	15	11	1	2		1
PHARMACEUTICALS	1	2,030,000	1,770,000	9,984,000	1					
SPECIALTY CHEMICALS	49	63,473,901	28,545,071	272,399,170	11	24	9	4		1
TOTAL	**142**	**445,668,442**	**185,720,012**	**1,786,608,119**	**46**	**62**	**19**	**16**		**2**

5.2 CORPORATE EMISSION REDUCTION TARGETS

5.2.1 INTRODUCING CORPORATE EMISSION TARGETS

A central corporate carbon management strategy other than emissions disclosure and reporting is the use of emission reduction targets (Lister, 2018). The use of environmental performance targets by corporations has long been commonplace (Mathews, 1997) although they have historically been rather arbitrary (Dahlmann et al., 2017; Rietbergen et al., 2015; Wang and Sueyoshi, 2018) and often low in ambition (CDP, 2009; Knox-Hayes and Levy, 2011).

In fact, multiple concerns have been raised in relation to corporate sustainability targets in general as well as emission reduction more specifically. These include inter alia that i) companies can choose base years with arbitrarily high emissions (Giesekam et al., 2018), ii) (misuse of emission offsets (Carton et al., 2020), iii) issues relating to renewable energy certificates (Brander et al., 2018), iv) concerns over targets based on emission intensity [2] (Krabbe et al., 2015) and v) measuring relative rather than absolute performance (Bjørn and Røpke, 2018). To combat such concerns, calls have been made to align corporate targets with environmental carrying capacities and/or external environmental goals (Bjørn et al., 2021, 2017).

Reflecting such an approach, the Science Based Targets initiative (SBTi) seeks to translate the temperature goals of the Paris Agreement to corporate level emission reduction targets. Through the SBTi, which was established in 2015 through a partnership between CDP, WWF, WRI, and the UN Global Compact, companies can access methods, tools, and guidelines for setting GHG emission targets with SBTi acting as a target certifier. This includes targets for both scope 1, scope 2, and scope 3 emissions set by a variety of different methods. Simplest of these is the absolute contraction approach, which dictates absolute emissions reductions by all companies at the same rate. Other methods differentiate across sectors and companies to take differences between them into account (SBTi, 2020a).

Despite the promise of aligning corporate targets with the Paris Agreement, the methods for setting so-called science-based targets (SBTs) have been subject to a range of criticisms. These include but are not limited to lack of regard for principles of equity, allowing purchases of renewable energy certificates, and misalignment between the different methods and overall temperature goals (for review of the literature and criticisms of SBTs see Bjørn et al. (2022)). For chemicals specifically, a further range of issues for setting SBTs are particularly relevant. These relate to the heterogeneity and unclear boundaries between chemicals and oil and gas including the extensive coproduction of various petrochemicals in integrated clusters and refineries.

The SBTi itself has recently addressed challenges and barriers for setting SBTs in the chemical sector (SBTi, 2020b). Three elements are identified as particularly relevant to address: 1) Developing sector-specific decarbonization pathways, which the SBTi suggests should include specific emission intensity pathways for the most important product categories; 2) Producing accounting and target-setting resources for key upstream and downstream activities including emission factors for purchased goods and services, processing of sold products, use of sold products, and end of-life treatment of sold products. 3) Creating consistency in accounting approaches and boundary-drawing across the scope 3 categories of purchased goods and services and end-of-life treatment of sold products.

2 WHICH, AMONGST OTHER CONCERNS, WILL NOT NECESSARILY LIMIT EMISSIONS WITHIN A STIPULATED CARBON BUDGET.

Additionally, industry actors have pointed to several issues to SBTi relating to setting SBTs (SBTi, 2020b). First, industry actors highlight low data availability and quality, relating to the purpose of this report. Moreover, chemical companies argue that there is a lack of 'technological readiness'. This, some companies claim, means that the time frame of SBTs (SBTi operates with a 5 to 15-year time frame) is too short. Finally, as mapped in chapter 3, the sector expects high demand growth and therefore opposes absolute reduction targets dictated by the absolute contraction approach.

The points raised here illustrate conflicts around the speed, form, and extensiveness of decarbonization in the petrochemicals industry. Therefore, it is worth mapping the adoption of emission targets (and their level of ambition) amongst the key emitters and scrutinize and critically examine these targets. At the very least, implementation of corporate emission targets reflects that petrochemical companies seek to signal that they intend to decarbonize, and, in this sense, target adoption reflects pressures on the sector to do so. This section aims to do exactly map and examine corporate emission reduction targets, again relying on the CDP database in which such targets are also disclosed.

5.2.2 CORPORATE EMISSION REDUCTION TARGETS IN THE PETROCHEMICAL INDUSTRY

Looking across the 2010-2020 period there has been an increased uptake of corporate emission reduction targets, related to the emergence of the debate about net zero and industrial decarbonization (see Figure 28 and Figure 29). Regarding the type of target, both absolute and intensity targets, either as GHGs as share of value added or as share of physical output, are frequently used each constituting roughly half of the reported targets. For the intensity targets specifically comes the worry referenced above, namely that they can be achieved despite lacking absolute reductions.

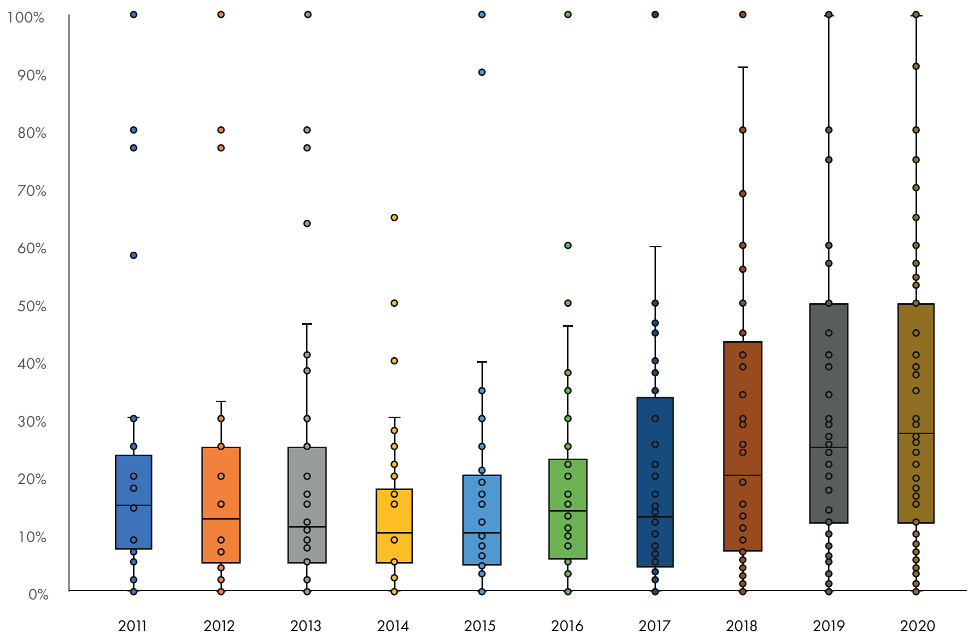

FIGURE 28: ABSOLUTE REDUCTION TARGETS REPORTED BY CHEMICAL FIRMS, BY YEAR. NOTE THAT BASE YEAR, TARGET YEAR, AND SCOPE OF TARGETS VARY. DATA SOURCE: CDP

Generally, the ambition level of targets has increased on average in recent years. Still, across the period under consideration, only a single of the major petrochemical producers (DuPont) reported a target of 100 % emission reduction across scope 1 and 2 (while including upstream scope 3 emissions). No major petrochemical producer reported a target of full decarbonization scope 1-3 across the entire value chain.

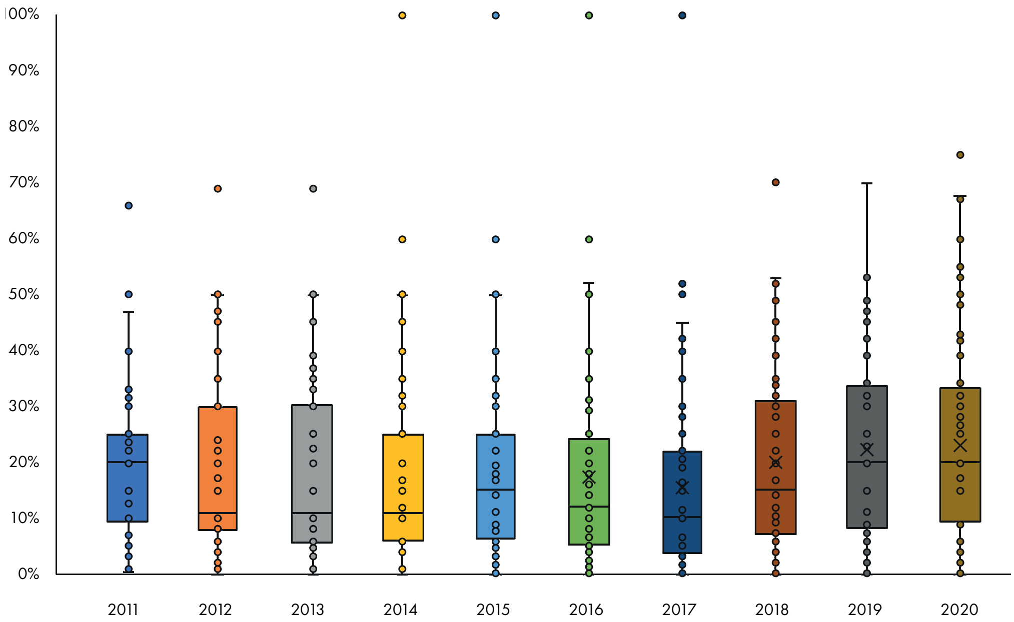

FIGURE 29: INTENSITY REDUCTION TARGETS REPORTED BY CHEMICAL FIRMS, BY YEAR. NOTE THAT BASE YEAR, TARGET YEAR, AND SCOPE OF TARGETS VARY. DATA SOURCE: CDP

For the 2020 disclosures, 132 amongst the 145 chemical companies which reported to the CDP in 2020 have set emission targets. For 19 of these companies, the adopted targets were reported as certified through the SBTi with a further 25 companies reporting targets that are not officially approved by SBTi but are considered "in-house" to be science-based. However, the fact that companies report that they have set SBTs via SBTi is no guarantee that this is actually the case due to lack of third party verification (Bjørn et al., 2022). Moreover, it is not clear what is meant when companies report certain targets to be 'science-based' nor is there consistency in target methodology. For example, BASF aimed for "carbon neutral growth" to 2030 meaning constant absolute emissions at the time of reporting (BASF has recently updated their target now aiming for reducing annual emissions by 2030). Despite this, BASF reported that their target was 'science-based'. For the companies that have set SBTs which have been verified by SBTi, only two of the 50 largest chemicals companies ranked according to sales are included, neither of which are in the top 10[3].

Relating to the issues flagged in previous sections in this chapter, only 14 companies include scope 3 targets. While most companies appear to have targets for scope 1 and 2, as many as 61 companies or almost half of the companies that report targets (61) do not specify the scope for their disclosed targets. By neglecting scope 3, companies can outsource the carbon-inten-

3 OF THE COMPANIES WITH AN SBT, SUMITOMO HAS THE HIGHEST CHEMICAL SALES, CHEMICAL & ENGINEERING NEWS RANKING THEM 16 IN THE WORLD IN 2020 IN THEIR GLOBAL TOP 50 (TULLO, 2021).

sive processes in their portfolios (that anyway usually have lower economic margins) and appear as if they are delivering on their promises, despite no overall reduction of the emissions. In fact, such outsourcing can lead to increases in total emissions, if increases in production are taking place in emission intensive facilities.

Considering differences in target years (Figure 30), companies should arguably both have short-term and long-term targets to ensure action in the near term while planning for full decarbonization by mid-century. When looking at the ambition of targets grouped according to end year, not many companies appear to have set targets beyond 2030. And for those who have there is great variety with both targets of 'carbon neutral growth' until 2050 (LG Chem) as well as 100 % reduction for scope 1 and 2 (DuPont). Such variance in reported targets is also evident for short and midterm targets where some companies (most of which classify their primary activity as 'personal care & household products') report targets of 100 % absolute emission reductions. These, however, include targets for 'avoided emissions' through product application and targets that are set for specific facilities (e.g., office buildings) as well as targets that are achieved using renewable energy certificates and offsets, both of which have been subject to strong criticism (see section 6.2.1). Therefore, the variance in targets reported here also reflect lack of standardization and issues of voluntary self-disclosure across reported targets.

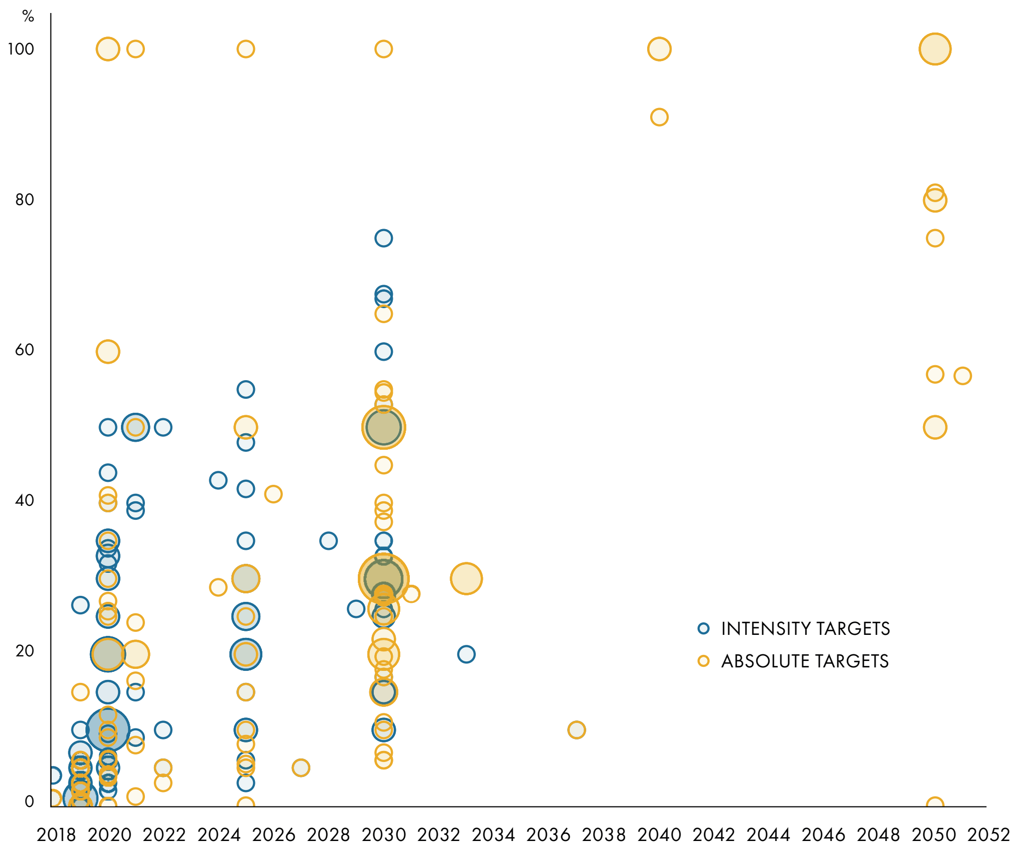

FIGURE 30: TARGETS REPORTED IN 2020 CDP DISCLOSURES FOR COMPANIES REPORTING THEIR MAIN ACTIVITY AS BELONGING TO THE CHEMICAL INDUSTRY (BASE YEAR VARIES). NOTE THAT BUBBLE SIZES REFLECT THE NUMBER OF TARGETS THAT MATCH THAT SPECIFIC TYPE, YEAR, AND REDUCTION. DATA SOURCE: CDP

Finally, it is worth noting that the targets reported here do not necessarily encompass the wider targets that companies may have set for themselves as these disclosures are geared around near-term targets to aid the decision-making of would-be investors.

5.2.3 CLAIMS OF EMISSION REDUCTION INITIATIVES IN CDP REPORTING

In addition to their stated emission reduction targets, companies can also report which initiatives they are pursuing in order to reach them in their CDP disclosures. These count various types of emissions reduction initiatives and are reported in Figure 31.

Across 575 reported initiatives that had been implemented by 2020, the reporting companies estimate annual emission reductions of 23.5 Mt CO_2eq. These estimated annual savings represent less than 3% of the annual scope 1 and scope 2 emissions across the 145 reporting companies in their 2020 CDP disclosures. The most commonly reported initiatives are energy efficiency measures, which despite being the clearly dominant strategy to reduce emissions has low overall impact considering the total disclosed scope 1 and 2 emissions. Another common form of initiative is energy efficiency in buildings, which despite a relatively high number of initiatives does nothing to change the production process and therefore unsurprisingly has low impact overall.

Considering the historical relationship between energy and chemicals (Bauer and Fuenfschilling, 2019; Bennett, 2007), one might expect that chemical companies would invest in renewables as is and has been the case for fossil-based energy. However, this is seemingly not a very common strategy and disclosing companies estimate almost no GHG savings from such initiatives, although reporting some initiatives in 'low-carbon energy generation'. Similarly, despite claims of a strong focus on circular economy, there are relatively few reported initiatives relating to waste reduction and material circularity and the strategy appears not to be a major driver of emission reductions in the sector.

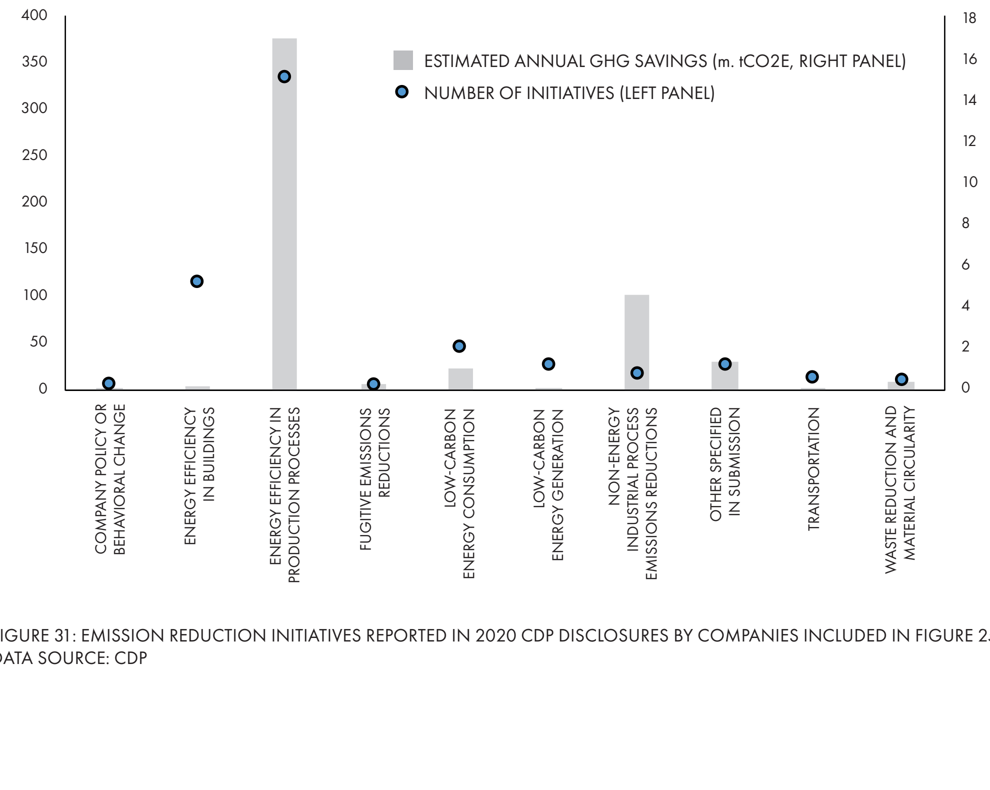

FIGURE 31: EMISSION REDUCTION INITIATIVES REPORTED IN 2020 CDP DISCLOSURES BY COMPANIES INCLUDED IN FIGURE 25.
DATA SOURCE: CDP

Across the reported initiative categories, it is not immediately clear what they entail. Looking into the non-energy industrial emissions reduction initiatives shows a clear focus on process optimization and energy efficiency. This mirrors the developments over time in the sector which have been characterized by a strong focus on incremental measures and process improvements (Bauer and Fuenfschilling, 2019). Even more critically, amongst the reported measures put in place was the use of captured emissions for enhanced oil recovery. As such, an effort put in place to increase and enhance fossil fuel extraction was reported as an emission reduction initiative. This adds to some of the arguments raised in this chapter concerning the nature of self-disclose and lack of transparency and comparability even in seemingly standardized reported initiatives such as CDP.

5.3 CONCLUSIONS

Taken together, corporate emission disclosures are nor suitable for large-N comparisons across regions or to understand trends over time. This is due to a strong regional bias, lack of standardization, and large discrepancies in the extent of disclosure as well as substantial gaps and inconsistencies in reporting. These criticisms relate to the nature of self-disclosure and voluntary action and illustrate the need for working towards standardized, transparent corporate disclosures for the petrochemical industry.

The disclosures, however, can still be used on a company level and to understand trends in company reporting over time. Here, notwithstanding the abovementioned issues, the review shows a trend towards increasing disclosure over time with higher disaggregation. This is largely due to more substantive scope 3 disclosures as well as a steadily increasing number of disclosing companies over time.

In terms of corporate emission reduction targets an increasing number of companies are setting targets. Also here, however, standardized, transparent disclosure is lacking. Moreover, most companies do not include scope 3 emissions in their targets despite its large share of overall emission and more ambitious targets are needed across the industry. The emission reduction initiatives disclosed as means of reaching those targets generally do not point towards industrial transformation and lack ambition.

PHOTO: ADOBE STOCK

6 DEVELOPMENTS AND FUTURES

6.1 SCENARIOS AND ROADMAPS

The chemical industry has not been the centerpiece of many research-based scenarios for decarbonization. However, the recent and growing interest in the challenge of decarbonizing heavy industries has led to more work on the topic and recent years have thus seen several publications focused on quantitative modelling of decarbonization scenarios in the industry. This section summarizes the key insights from key publications and compares their findings.

6.1.1 OVERVIEW OF SCENARIOS FOR CHEMICAL INDUSTRY DECARBONISATION

Broeren et al. (2014) showed how business-as-usual scenarios in the industry would lead to 50 % higher GHG emissions from the industry in 2030 than 2010, largely due to increased production and consumption in non-OECD countries. A scenario which implemented energy efficient best practice technologies was only partially successful at mitigating the emissions – ending up with a 10% increase in emissions in 2030 compared to 2010 – indicating the need to move far beyond best available practices to reach a properly low-carbon development. Removal of (fossil) energy subsidies to incentivise energy efficiency improvements and international carbon pricing could contribute to emissions reductions, but overall, this analysis showed no clear path to decarbonization.

DECHEMA published a well-cited report, commissioned by the European chemical industry trade association CEFIC, in 2017. In this report, they outline the maximum potential for transforming the European petrochemical industry to 2050, as well as two reasonably realistic scenarios. These scenarios assume a replacement of existing production to reach 35-50% production of key chemicals in proper low-carbon technologies by 2050, which together with efficiency improvements and low-carbon energy in conventional production facilities would mitigate 59-84% of GHG emissions compared to the BAU scenario. While the geographical scope of this report is Europe, its findings are in many ways relevant also for the global development of the industry. Interestingly, these scenarios completely exclude CCS – a breakthrough technology that is frequent in many later analyses – arguing instead that the industry will need all available CO_2 for use in CCU processes.

A paper by Kätelhön et al. (Kätelhön et al., 2019) investigated the environmental impacts of a chemical industry that completely transitioned to value chains based on captured carbon, i.e. a CCU-based chemicals industry. Two different CCU scenarios were developed, one based on processes with a high technology readiness level (TRL), mainly using methanol as a platform chemical for most downstream products, and one based on direct and selective conversion of

CO_2 to other chemical products. These scenarios show that a chemical industry decoupled from fossil resources and GHG emissions is theoretically possible if employing CCU technologies on a large scale. Relying on technologies and processes that are already or are close to being commercially available (a high-TRL scenario) is possible but leads to an electricity demand of about 32 PWh, which is more than current global electricity production and 97% of the estimated electricity supply in 2030.

The International Energy Agency has produced several versions of its scenarios for GHG emissions reductions from the chemical industry, both in its dedicated sector report on The future of petrochemicals (IEA, 2018) as well as in the more recent global analysis Energy Technology perspectives 2020 (IEA, 2020). The baseline scenarios, called Reference Technology Scenario (IEA, 2018) or Stated Policies Scenario (IEA, 2020), assumes development in line with current trajectories of technologies and policies, while the more ambitious mitigation scenarios, called Clean Technology Scenario (IEA, 2018) or Sustainable Development Scenario (IEA, 2020), aim to reach significant emissions reductions. None of the scenarios show a discontinued use of fossil feedstocks but rely on other measures to reach the emission reduction objectives.

The 2018 report reaches 60% reduction of GHG emissions compared to the reference scenario largely by improving the performance of existing technologies and processes, shifting from coal to natural gas, and adding carbon capture for utilization and storage. Implementation of breakthrough technologies for renewables is marginal, as is the contribution of increased plastic recycling. The result is a continued strong dependence on and integration with fossil energy – in fact chemical feedstock grows to more than 25% of global oil demand in this scenario as it the sector remains committed to fossil feedstocks.

A paper by Galán-Martín et al. (Galán-Martín et al., 2021) compares the environmental impacts across all planetary boundaries (Rockström et al., 2009) in a large set of scenarios to analyse the impact across categories for different types of mitigation measures. The analysis across climate boundary categories concludes that the contemporary petrochemical industry has not only a significant climate impact but it also "requires one-quarter of the entire carrying capacity of the planet to operate", indicating the need to consider impacts beyond climate change. The scenarios mainly rely on different types of CCU for the production of methanol as a key platform chemical, similar to the analysis by Kätelhön et al. The authors show that scenarios based on CCU powered by bioenergy with CCS (BECCS) perform best in terms of the carbon footprint but have very large and negative effects on biosphere integrity due to extreme demand for power from BECCS plants which also the authors conclude is unfeasible. Instead, different biomass-based pathways for the direct production of organic chemicals as well as pathways using other forms of low-carbon electricity for CCU show potential to reduce the negative environmental impacts of the industry across all planetary boundaries.

A recent analysis conducted by Saygin and Gielen (2021), with the International Renewable Energy Agency (IRENA), presents a scenario for net zero emissions from the industry, aligned with the 1.5 degree target of the Paris agreement. The single largest mitigation potential (26%) is identified to be in CCS for both combustion and processes, but the analysis finds approximately equal potential (~15%) in eletrolytic hydrogen, renewable power, energy efficiency improvements, and demand reduction.

TABLE 4: SUMMARY OF DETAILED GLOBAL CHEMICAL INDUSTRY SCENARIO ANALYSES

SOURCE	SCOPE	END YEAR	SUCCESSFUL GHG MITIGATION (INTERNAL REFERENCE EMISSIONS)	DEMAND GROWTH (REFERENCE/ MITIGATION SCENARIO)	KEY BREAKTHROUGH TECHNOLOGIES
BROEREN ET AL., 2014	PETROCHEMICALS AND CHLORINE	2030	9 – 25 %	74 %	
BAZZANELLA AND AUSFELDER, 2017	PETROCHEMICALS IN EUROPE	2050	59-179%	40%	CCU ELETROLYTIC HYDROGEN BIOMASS GASIFICATION
KÄTELHÖN ET AL., 2019	PETROCHEMICALS	2030	0-180% (2 GT)	NA	CCU
IEA, 2018	PETROCHEMICALS	2050	60 % (2 GT)	53 % / 40 %	CHEMICAL RECYCLING CCU CCS
IEA, 2020	ALL CHEMICALS	2070		60 % / 25 %	CCU CCS ELETROLYTIC HYDROGEN
SAYGIN AND GIELEN, 2021	PETROCHEMICALS	2050	100 % (4.79 GT)	164% / 145 %	BIOMASS RECYCLING CCS ELETROLYTIC HYDROGEN
GALÁN-MARTÍN ET AL., 2021	OLEFINS, AROMATICS, METHANOL	2020	-1110 – 3200%	-	CCU CCS BIOMASS ELETROLYTIC HYDROGEN
MEYS ET AL., 2021	PLASTICS	2050	0 – 104 % (4.73 GT)	255 %	BIOMASS CCU RECYCLING ELETROLYTIC HYDROGEN
IEA, 2021B	AMMONIA				

6.1.2 KEY INSIGHTS FROM SCENARIOS

The scenario analyses reviewed do not uniformly point towards a single specific pathway for mitigating the climate impact of the petrochemical industry. The diverse set of approaches to develop the scenarios, each with its own set of assumptions, do however underline some key issues that can contribute to mitigating a significant share of the GHG emissions from the industry.

Renewable energy is an absolute cornerstone for decarbonisation of the chemical industry. All scenarios show a large potential for reducing the climate impact by shifting to renewable energy, primarily electric power from renewables such as windpower and solar PV. This renewable power can directly substitute the large volumes electricity used in the industrial processes today – which in the key region Asia Pacific is mainly coal based – as well be used to electrify boilers and other applications which are currently supplied with heat through on-site combustion of fossil fuels. The energy demand in the chemicals industry has been assessed to be among the greatest opportunities to be electrified with available technologies (Madeddu et al., 2020), which points to the possibility for a significant and quick decrease of energy related emissions. Further, the implementation of processes based on CCU and eletrolytic hydrogen (see next subsection) will lead to a much larger demand for electricity in the sector. Several of the scenario analyses point to a situation where the demand for renewable electricity in the chemical industry will make up a very large share of total power generation, as forecasted in common energy models. Transmission grids will need to be upgraded to transfer this power to existing chemical clusters which are not located close to renewable generation capacity. Alternatively, it would mean large investments in new chemical production facilities in regions with significant renewable energy resources.

Energy efficiency measures remain important to reduce emissions from the industry as it is primarily the most energy intensive processes that are associated with large GHG emissions. Energy efficiency has steadily improved, but on a macro level seems to have levelled off according to the analysis by the IEA (2018) which shows that the share of fossil feedstocks that is used for energy has remained stable over the past decades. This macro level number hides important regional and technological differences, but the fact remains that improving the energy efficiency is a rapid way of reducing emissions. The scenarios are however also in complete agreement that improving energy efficiency will never be enough – more radical changes to the processes and value chains are needed in all scenarios to reach the emission reductions necessary.

Important energy efficiency measures include the integration and optimisation of heat use within and across chemical processes, the deployment of catalytic processes, and switching to more efficient energy sources and carriers. Optimisation and integration are specific to sites and facilities, often requiring both investments to modify heat exchanger networks as well as changes in operational routines. Catalytic processes can often achieve both higher selectivity and energy efficiency with a prime example being catalytic cracking of naphtha instead of thermal steam cracking. This does however often mean significant changes to the core processes and is thus neither quickly nor easily achieved. Switching from fuel heating to electric heating can lead to significant efficiency improvements, e.g., if it includes switching to heat pumps. There are however still limitations to the temperature range which heat pumps can deliver, restricting their deployment in the industry.

Demand reduction is a key measure that needs more analysis and attention – it is not explicitly considered in all scenario analyses reviewed above. Different types of demand side measures that can improve the material efficiency and reduce demand growth are important for reaching the necessary emission reductions. It is however also well known that the such interventions in chemicals as well as other material industries are poorly understood and implemented, and not promoted by industrial actors which prefer to focus on growth in material use (Allwood et al., 2010; Hernandez et al., 2018; Skelton and Allwood, 2017). As chemicals and plastics enter so many different value chains, as shown in Chapter 3, mitigating a growing demand implies interventions in a wide range of value chains. Restrictions on the use of plastic in different types of application, mainly single-use plastics and packaging, are being implemented in countries around the world, but these are commonly very narrowly defined and do not address the larger issue of reducing demand growth. This would mean addressing consumption patterns across market segments with use of chemicals, such as electronics, textiles, vehicles, and others. Exploring how to do this and what effects it could have, is thus an important field of inquiry.

Aside from the necessity of developing renewable energy capacity – central to the global energy transition – improving process and energy efficiency and reducing demand growth the scenarios all show the need for adopting breakthrough technologies, some of which are unique to the chemical industry.

6.2 BREAKTHROUGH TECHNOLOGIES FOR CLIMATE CHANGE MITIGATION

Several projects led by major institutions and organisations have in the past few years aimed to identify and review breakthrough technologies which would enable a shift towards low carbon emissions from the chemical industry (Bazzanella and Ausfelder, 2017; Boulamanti and Moya, 2017; IEA, 2020). As previously stated, the chemical industry is the third largest industrial sector in terms of GHG emissions globally and it is thus crucial to rapidly identify, scale up and adopt new technologies and other solutions which could immediately significantly reduce the emissions and be credible steps on the way towards zero emissions by mid-century. It is thus striking to note that the threshold for inclusion on the breakthrough technology list is commonly as low as a potential GHG emissions reduction of 5%.

Indeed, energy efficiency as well as incremental process improvements, which are traditional modes of innovation for the chemical industry (Cesaroni et al., 2004; Ren, 2009) are important but far from sufficient for the transition currently necessary. Thus, we restrict this section to include those technologies that fulfil the dual criteria of independently delivering significant emission reductions of at least 20% and are aligned with pathways towards zero emissions. The section does not provide an extensive review of the development of all of these technologies, but briefly summarizes key developments and identifies key actors that are developing the technologies.

TABLE 5: OVERVIEW OF TECHNOLOGIES FOR CLIMATE CHANGE MITIGATION

TECHNOLOGIES	VALUE CHAINS	TRL
STEAM CRACKER ELECTRIFICATION	HIGH VALUE CHEMICALS, PLASTICS	3
ELECTROLYTIC HYDROGEN	HYDROGEN, AMMONIA, METHANOL AND DERIVATIVES	7-8
BIOMASS GASIFICATION	HYDROGEN, HIGH VALUE CHEMICALS, METHANOL AND DERIVATIVES	5-8
BIOMASS PYROLYSIS	HIGH VALUE CHEMICALS	6-7
CCS	HYDROGEN, AMMONIA	7-11
CCU	SYNTHETIC HYDROCARBONS, METHANOL AND DERIVATIVES	7-11
CHEMICAL PLASTIC RECYCLING	HIGH VALUE CHEMICALS, PLASTICS	7-9

6.2.1 ELECTRIFICATION OF STEAM CRACKERS

Steam cracking is currently central for the production of high value chemicals such as olefins and aromatics, and thus also for most plastic value chains. As previously mentioned the steam cracking process is one of the most energy and emissions intensive processes in the chemical industry. Steam crackers use combustion of fossil fuels, normally natural gas, to enable the furnace to reach a desired heating of up to 900 °C (Kulprathipanja et al., 2021). Substituting the energy supplied to heat the cracker for electricity is thus one opportunity to significantly reduce the direct emissions associated with the process, although if the cracker uses fossil feedstocks there will still be some process emissions as well as all of Scope 3 emissions.

The electric steam cracker is still under development with a TRL estimate of about 3, i.e. still at the stage of experimental proof-of-concept (IEA, 2020). Remaining challenges are to redesign and modify the steam cracker to utilize electricity as opposed to natural gas, such as selecting appropriate materials that can withstand immense currents necessary to provide the needed heat. A limitation today for the electric cracker is the surface temperature which the coils can withstand, where the maximum surface temperature of the available metals is 1150 °C (Amghizar et al., 2020) although new ceramic materials may be able to reslve this issue

There is currently a major investment of the electrified cracker made by several large chemical firms. BASF, Borealis, BP, LyondellBasell, SABIC and Total jointly formed The Cracker of the Future consortium in 2019. BASF and Linde are developing an electric furnace for the steam cracker based on electrical resistance heaters, aiming to eliminate all direct GHG emissions from the heat supply. Also Dow and Shell in 2020 formed a partnership for the development of an electrified cracker to reach their goals of carbon neutrality (Tullo, 2021a).

When looking at reducing the carbon footprint can both electrification and a feedstock substitute present possible ways of a lower net amount of GHG emission. According to LCAs done for producing thermoplastics was the mean emission reduction for implementing renewable electricity found to be 38 Mt CO2/year, decrease in GHG emission of 50-75 % compared of using fossil fuels. A substitution of the fossil-based feedstock to maize or switchgrass gives a higher uncertainty of reduction in GHG, from a decrease ranging from a 50 % decrease to a 10 %. To conclude, the more efficient route seems to be via renewable energy as supposed a renewable feedstock (Posen et al., 2017).

6.2.2 ELECTROLYTIC HYDROGEN PRODUCTION

Hydrogen as an energy carrier has gone through several hype cycles in past half century, but in recent years the driving interest for hydrogen has for the first time been from the industrial sector including the chemical industry (IEA, 2019a). Low-carbon hydrogen can be produced in different ways and the debate commonly describes hydrogen produced through electrolysis of water as green hydrogen, whereas blue hydrogen is produced from fossil fuels, e.g. natural gas, with carbon capture (see section on CCS below). Electrolytic hydrogen could thus be produced with no or very low GHG emissions, but the process demands large volumes of renewable energy.

The electrolysis process involves the split of the water molecule into hydrogen and oxygen by applying an electric current. Alkaline electrolysis is an established and mature process on the market to produce hydrogen and the most widely used, as it is the most efficient process today. The setup of the electrolysis consists of water mixed with a 20-40 % KOH solution, Ni coated electrodes and two half cells separated by a diaphragm ensuring no mixing of the gases. The process can be run at ambient pressure up to 30 bars. Proton-exchange-membrane (PEM) electrolysis is being rapidly developed and scaled up for industrial applications. It runs on pure water and can operate at higher pressure up to 100 bars unlike the latter technique. The advantage of PEM is that the stacks are more compact and dynamic, meaning that it combines well with non-constant electricity sources such as wind power (Bertuccioli et al., 2014).

Although electrolysis can be considered a mature technology, it is not yet so in the large scale relevant for commercially and economically viable operation in the chemical industry. The main challenge for the development of the establishment of water electrolysis is to be able to economically compete with the traditional route of producing hydrogen by steam reforming of natural gas (Grigoriev et al., 2020). Investment costs for electrolysers are large and have limited economies of scale. Projections show a significant potential for reducing investment costs over the next decade (Bertuccioli et al., 2014). It can be realized by reducing the amount of noble metal in the catalyst or operating with different materials (Mergel and Stolten, 2012). However, most focus on the development is focused on increasing the power density of the stacks, reducing the system size and improving the dynamics of the system (Mergel and Stolten, 2012). For large systems operating costs become very important with the cost of hydrogen closely following the price of electricity.

Hydrogen is central for the production of both ammonia and methanol, two of the most important platform chemicals. Several of the scenario analyses reviewed above rely to a very large degree on very large deployment of eletrolytic hydrogen for the production of methanol which is then used to produce most high value chemicals through methanol-to-olefins and methanol-to-aromatics processes.

Applications of hydrogen production via renewable electricity to manufacture methanol has been tested in small-scale operation by Carbon Recycling International on Iceland and is now being scaled up in China to a production capacity of 100’000 t/year (McCoy, 2021). This is however still small in comparison to regular commercial scale production. Several projects implementing electrolytic hydrogen for producing ammonia are being developed, e.g. by Yara and Fertiberia in Australia, the Netherlands, and Spain. These projects are all still limited in scale compared with conventional processes.

6.2.3 BIOMASS GASIFICATION

Through gasification of biomass the emission reductions in chemicals production can be achieved due to substituting the feedstock from fossil origin to renewable. Gasification is a high temperature process of thermal decomposition into volatiles, combustible gas and ashin the presence of an oxidizing agent, such as air, oxygen or water. The main product is a syngas with other light hydrocarbons but product formation is highly dependent on exact process conditions. A wide range of different types of gasifiers have been tested around the world over the past decades. Many organic chemicals can be manufactured from the syngas obtained from biomass gasification, such as methanol, ethylene, propylene, ammonia and BTX (Sansaniwal et al., 2017; Widjaya et al., 2018). Methanol is often identified as a key intermediate (Holmgren et al., 2012), which can then be used for the production of olefins or aromatics in subsequent processes. Finally, can ammonia be directly synthesised using the produced hydrogen in the Haber-Bosch process (Bazzanella and Ausfelder, 2017).

The gasification of biomass can be considered a mature process, as there are numerous of applications and commercials technologies, granting a TRL score of above 9. The main drawback for it to be a competing alternative is to source sustainable biomass and have an economic viable process with an acceptable efficiency. However, the main advantage and uniqueness of biomass gasification is that the technology can implement waste and residues from crops and wood as feedstock, providing the biomass gasification with a sustainable alternative with an economical advantage as well (Sansaniwal et al., 2017; Widjaya et al., 2018). To address the energy consumption is the major constraint the thermal efficiency of the gasification and the design of the gasifier (Ahmad et al., 2016). Biomass gasifiers can use different types of biomass – from wood chips to rice husks and waste or residue streams – allowing for adoption of the general technology to different regional conditions and resources.

Biomass gasification has been under development for a long time, primarily for energy purposes. Deployment of gasification technology at the scale relevant for production of ammonia or methanol has however not been very successful. Several actors are still working on different types of gasification processes using both biomass waste, e.g. BioMCN developing gasification for methanol production in the Netherlands (IEA, 2020).

6.2.4 BIOMASS PYROLYSIS

The general definition of pyrolysis is simply heating in the absence of oxygen, usually 450 - 600 °C, products formed are organic vapours, pyrolysis gases and charcoal. Pyrolysis can be categorized into slow, flash, and fast pyrolysis, the main difference between the process are the residence time as the names may indicate and the products formed. The high-value component formed in the pyrolysis process is the liquid bio-oil and has a weight percentage of 50-70 wt% of the input feedstock (Hu and Gholizadeh, 2019) . The pyrolysis oil can be used as a chemical intermediate for producing platform chemicals, such as aromatics, hydrocarbons, or biofuels (Kumar et al., 2020) after different upgrading processes (Jacobson et al., 2013).

The development of the pyrolysis technology has come quite far but for producing chemicals are most of the operations at the research or pilot stage, giving a TRL score of 5. There is great potential of manufacturing chemicals through the pyrolysis process, however there several obstacles that must be overcome such as a sustainable and reliable sourcing for the feedstock due to the fact that it accounts for the major cost of the operating (harvesting, collection and transportion). In addition, a reliable and vast characterisation data for the biomass and products should be derived to get the correct technical and economic parameters needed to make investment. Other challenges are to investigate the catalyst performance and increase the yields in the pyrolysis and for the upgrading steps. The available biomass types are similar as with the gasification method, such as wood and agriculture residues and different types of waste, but as it operates at lower temperatures it is less energy intensive.

Bio-BTX based on biomass pyrolysis is being developed and tested at pilot scale by several actors. The pyrolysis process takes place in one reactor, the vapor phase is transferred into a second reactor where BTX is formed through catalytic processing (Mruthyunjaya, 2022). Plans for scaling up have been announced by BioBTX, aiming to build a commercial scale production in 2023.

6.2.5 CARBON CAPTURE AND STORAGE – CCS

While some scenario analyses rely significantly on CCS being deployed to reach emission targets, other scenarios see CCS as a dead end, arguing that the chemical industry should focus on using carbon that is available rather than extracting more and then paying to bury it.

Overall CCS can be separated in two parts, the carbon capture (CC) and the storage (S). The capture part can be done by adsorbing or absorbing CO_2 from a flue gas or process stream. Compared with CCS in the energy sector applications in the chemical industry has some potential advantages as CO_2 could be captured from concentrated carbon dioxide streams such as in methanol and ammonia production (IEA, 2019b, 2018). The ammonia production accounts for the most promising carbon dioxide streams with 119.4 Mt of carbon dioxide available to capture each year (Zakkour Paul and Cook Greg, 2010). The main drawback of the CCS technology is the limited availability of concentrated carbon dioxide streams and the economic viability (IEA, 2019b). The cost of capturing carbon dioxide can be kept lower for concentrated streams compared to dilute streams such flue gases – some estimates show a difference in cost of a factor five (IEA, 2019b). Analyses show that the capacity for carbon capture of the chemical industry would to about 40 % consist of concentrated carbon dioxide streams and 60 % of dilute streams which originate from energy related carbon dioxide emissions (IEA, 2018).

Carbon capture storage can theoretically be implemented to eliminate emissions entirely from the chemical sector including use and disposal, thus decreasing its carbon footprint. A focal area for CCS deployment in the chemical industry is for the application of so called blue hydrogen, i.e. hydrogen produced from fossil sources but with CCS, which can then be used for ammonia production or other chemicals. Capture rates of 90% are possible, which would lead to very large emissions reductions, but the overall carbon footprint of such applications could still lead to significant climate impact due to the sensitivity of methane leakage. Analyses have shown that methane losses throughout the value chain are common and because of the high GWP of methane this can lead to a high climate impact of installations also with CCS (Bauer et al., 2022; Howarth and Jacobson, 2021). With decreasing costs for renewable energy the case for CCS may thus lose some of its attraction (Grant et al., 2021).

There currently 26 operational large-scale CCS projects scattered around the world, permanently storing 40 M tonne of CO_2 every year – although most of them are using the captured CO_2 for enhanced oil recovery (EOR) – and in addition are there several of pilot facilities. SABIC has deployed CCS (for to EOR) at an ammonia production facility and started delivering blue ammonia in 2020, showing the feasibility of the technology at commercial scale. An additional example of a CCS in commercial scale for ammonia is a plant in the US developed by Wabash Valley Resources and is expected to be finished 2022, which aims to build a near-zero CO_2 emission ammonia plant. The technology used will be integrated gasification combined cycle to capture the CO_2 formed in the chemical reaction of producing ammonia, with a capture of 1.5-1.75 Mt CO_2/year (Global CCS Institute, 2019).

6.2.6 CARBON CAPTURE AND USE – CCU

CCU technologies allow for capturing carbon dioxide either directly from the atmosphere, so called direct air capture (DAC) or from CO_2 rich gas streams and then using that carbon to produce different chemicals. Most commonly this includes mixing the CO_2 with hydrogen to form a syngas which can then be used to produce methanol and derivatives, or other syngas-based chemicals. The largest CCU process used in the chemical industry to date is the production of urea, which commonly captures CO_2 from an ammonia facility and uses that to process the ammonia into urea. As this carbon is emitted in the fields and of fossil origin the capture however yields no real benefit for the climate.

Several projects are looking at capturing carbon from other sources, such as blast furnaces in steel plants, and produce chemicals from these, mainly methanol as in the case of the Carbon2Chem project run by ThyssenKrupp in Germany. As the source of the carbon is still fossil, the reductions in climate impact from such production routes is however limited and strongly dependent on the life length of the products. Different sources of CO_2 can yield rather different carbon footprints for the CO_2 when used as feedstock (Müller et al., 2020) and is thus a key consideration for assessing the climate benefits of CCU pathways. Routes based on CO_2 captured from biogenic streams, e.g. flue gases from pulp mills, or even DAC could yield products with a better carbon footprint.

A major obstacle for CCU pathways and value chains is the resultant extremely high energy demand, as shown in the analysis by (Kätelhön et al., 2019), although there is a potential for innovative technologies to reduce the energy demand. This analysis does however clearly highlight that CCU is in no way a quick or easy way for the industry to break with its carbon lock-in.

THE USE OF COAL POWER IS A MAJOR SOURCE OF GHG EMISSIONS ASSOCIATED WITH THE GROWING PETROCHEMICAL INDUSTRY IN CHINA

PHOTO: ADOBE STOCK

7 DISCUSSION

This review of different research literatures and data sources has shown how the petrochemical industry is one the most important industrial sectors in terms of GHG emissions. Over the past 25 years emissions associated with petrochemicals have doubled and the sector is the third most GHG emitting industry. This increase in total emissions is due to a large growth of petrochemicals production as well as growth in regions with high indirect emissions, i.e., in energy systems with high dependence on coal and other fossil fuels.

7.1 GEOGRAPHICAL ASPECTS

Over the past 20 years the industry has grown rapidly in the Asia-Pacific region especially in China which is now the source for about 45% of global GHG emissions associated with petrochemicals. The BRICS group of countries, currently accounts for about 60% of GHG emissions from petrochemicals, showing that the emissions from this sector are more geographically clustered in these countries than emissions from other sectors. This is however not clear from voluntarily disclosed emissions data due to the fact that such disclosure is highly skewed towards firms headquartered and active in OECD countries. This mismatch also applies to LCA databases, which mainly focus on processes in Europe and partially US and Japan.

The shifting geography of the petrochemical industry has led to a divergence in terms of operations. While the industry in the late 20th century was rather homogenous in its use of petroleum naphtha as the primary feedstock for high value chemicals and their derivatives this has changed in the 21st century. The boom for shale gas and ethane-based production in the US, growth in coal-based production in China, and the development of crude oil-based production in the Middle East and Asia Pacific together led to a diversification of both scope and scale of the environmental impacts of petrochemicals – although these macro-trends are all still focused on fossil-based production. Especially the developments in China have had a great influence on the global average environmental impact of petrochemicals due to the different production routes and the coal-based energy supply there. However, both the geographical diversification and shift towards China is however only poorly captured in many environmental assessment tools and life-cycle inventory datasets as they often rely on data collected 20 years ago which reflect an industry that was more homogenous and dominated by Europe and North America.

Regional coverage differs across different GMRIO databases. Some databases, such as Eora, provide high regional resolution but relatively low sectoral coverage. Other databases with better sectoral resolution have relatively low regional coverage. Merged datasets, such as the ones by Cabernard and Pfister (2021) and Bjelle et al. (2020) are not consistent in terms of MRIO modeling but can help to improve spatial and sectoral detail for environmental extensions and impact assessments. In principle, a higher geographical resolution is better as it allows for more detailed and precise analysis. This is especially relevant for pollutants and resource use that vary over space and have highly local impacts (e.g. biodiversity loss, water stress and local pollutants sucsh as PM2.5). Regional detail is not an issue for global environmental stressors such as GHG emissions because the effect on climate change is the same regardless of where CO_2 is emitted and level of flue gas treatment has limited effect on GHGs. However, representation of technologies is also only possible with higher spatial resolution. Additionally, low regional resolution limits the depth of the analysis, for instance, in some cases, it may be unclear in which country the impact occurs if the database does not cover that country.

The SRIO models, by definition, contain only one country. In some cases, such models cover more sectors (e.g., US national input-output tables covers >400 sectors), but they suffer from the so-called domestic technology assumption. This assumption is that all imports are produced with the technology of the importing country which can introduce can introduce significant errors (Andrew et al., 2009).

Just like sectoral emissions, country-specific GHG emissions associated with petrochemicals can be viewed from different perspectives. It is common to consider where emissions are emitted (also known as a production perspective) and where they finally end up (a consumption perspective or a country's footprint). Our findings demonstrate that the importance of China as a key emitting region has grown considerably over time, in 1995, it accounted for 24% of global GHG emissions associated with petrochemicals and by 2020, their share increased to 47%. The share grew most rapidly between 2000–2010, and this coincides with the accession of China to WTO and its increasing participation in international trade. The share of impacts that finally end up in China followed a similar pattern, increasing from 17% in 1995 to 42% in 2020. EU and US collectively accounted for 10% of GHG emissions from petrochemical if we look at where GHG emissions occur and about 20% if we look at where emissions finally end up. From our results, we cannot determine the exact reason for these differences, but key factors that typically play a role are trade balance, production mix and technological differences between countries (e.g. use of coal vs natural gas). However, these results also indicate that action to decrease GHG impacts of petrochemicals might focus more on China and BRIC production than on EU or US domestic sectors.

7.2 VALUE CHAINS AND DOWNSTREAM SECTORS

The multitude of value chains dependent on the petrochemical industry makes it an important contribution to life cycle emissions in many sectors of the economy. Petrochemicals and their derivatives are used as intermediate inputs in many industries and the emissions associated with them thus propagate through the economy. Final demand in manufacturing industries and services are therefore associated with the largest shares of emissions from chemicals. The impacts and emissions downstream in value chains is however poorly understood and disclosed by petrochemical producers.

The LCA dataset review has clearly shown the importance of understanding the specificities of chemical value chains in order to appreciate the climate impacts of these chemicals. Chemicals produced from coal are associated with much higher emissions than those produced from petroleum or natural gas liquids such as ethane which has become an important part of the feedstock portfolio in North America. However, as methane has a very high GWP the climate impact of chemicals production based on natural gas and natural gas liquids is very sensitive to methane losses throughout the value chain and these losses are poorly mapped and accounted for. The contribution to climate change of gas based production could thus potentially be much higher than official estimates and this will also propagate throughout the value chains of these products.

While scope 3 emissions are increasingly reported and disclosed this primarily accounts for upstream scope 3 emissions. These disclosures are also inconsistent making it extremely difficult to paint a comprehensive picture of the impact. Only some disclose information about downstream scope 3 emissions – including end-of-life treatment for final products – or set targets for these emissions. All scope 3 emission reporting suffers from large uncertainties regarding the system boundaries of what is reported. The understanding of how the emissions diffuse through the economy thus to a large degree rely on the macro-level assessment provided by the MRIO data. Our results suggest that most impacts associated with petrochemicals finally end up in Services (32%), Manufacturing (27%) and Construction (13%).

Services play an increasingly important role. The share of impacts from petrochemicals that finally end up in Services increased from 25% in 1995 to 32% in 2020. The services sector covers a broad range of economic activities such as finance, education, health, public administration, etc. The health care sector heavily depends on petrochemical products, particularly on pharmaceuticals, plastics, and medical supplies, and few substitutes are available for petrochemical inputs (Hess et al., 2011). As the petrochemical producers have very few targets for downstream scope 3 emissions it is difficult to assess how the industry is aiming to support a reduction of the climate impact of the sectors that extensively rely on their products.

7.3 FUTURE DEVELOPMENTS

The literature covers a range of roadmaps and scenarios with different degrees of decarbonisation and great diversity in terms of developments across different geographies. Yet, relative to corporate emission reduction targets, the scenarios are seemingly far more ambitious. A direct comparison is however complicated by the lack of standardized and transparent corporate target setting making it difficult to even measure progress against stated targets (Bjørn et al., 2022). If the industry is to decarbonize in the pace that is needed while take impacts beyond climate change into account, actors have to increase their ambitions. Linking targets to scenarios (as is the case for SBTs) would be a step forward in that regard.

Relatedly, the roadmaps focus on deployment of breakthrough technologies on a scale large enough to decarbonize the entire industry. In sharp contrast, reported emission reduction initiatives primarily focus on process efficiency improvements or minor emission sources such as energy efficiency of buildings. In other words, disclosed sector initiatives do not point towards a decarbonization trajectory.

The so-called breakthrough technologies, however, also comes with a range of uncertainties. These also relate to their emission reduction potential. Thus, LCA of prospective technologies are always sensitive to assumptions and especially so when there is little or even no real data. For example, CCS plays a large role in many roadmaps and scenarios, but analyses show emissions intensity of production with CCS extremely sensitive to fugitive emissions, especially of methane.

More generally, data from the past has limited opportunities to tell us much about the deployment of breakthrough technologies or how they will integrate with the contextual energy system. Thus, the prospects of any mitigation pathway need to take factor in such considerations. From a precautionary perspective, relying extensively on prospective technologies with high sensitivity to assumptions warrants hesitation.

Notwithstanding differences across scenarios, renewable energy remains a cornerstone for emissions reduction in most analyses. Yet, this is not reflected in the emission reduction initiatives reported by firms. Given the central role of renewables and the uncertainties around prospective technologies, this is especially worrisome.

Going forward, future developments need to account for burden shifting across different ecological impacts from the industry. As highlighted in one of the reviewed scenarios, this requires extending the focus beyond climate change to assess mitigation pathways with reference to multiple planetary boundaries. This is important in terms of both EEMRIO and LCA analysis as well as corporate disclosures. The imperative to do so is especially clear given that the planetary boundary for so-called novel entities has been crossed due to massive chemical and plastic pollution (Persson et al., 2022).

8 CONCLUSIONS AND KNOWLEDGE GAPS

The climate impact of petrochemicals is difficult to map as they are produced in co-dependent processes in enormous integrated clusters and used across a multitude of complex, interconnected value chains. Using a combination of data sources and literature this report has attempted to bring together the knowledge about GHG emissions from different parts of the industry and identify key knowledge gaps.

Our results demonstrate that in 2020 direct GHG emissions from the petrochemical sector amounted to 1.8 $GtCO_2eq$ which is equivalent to 4% of global GHG emissions. Indirect GHG emissions resulting from the activities in other industries supplying inputs for the petrochemical industry accounted for another 3.8 $GtCO_2eq$. The petrochemical industry is thus associated with a total of 5.6$GtCO_2eq$ of GHG emissions, equivalent to ~10% of global emissions. Out of these GHG emissions, 1/3 were direct (scope 1), 1/3 were indirect from the utilities sector (scope 2), and 1/3 were indirect emissions in other sectors of the economy (scope 3 upstream). This amount of indirect emission shows the potential agency that the petrochemical industry sector has over supply chain emissions, which outweigh direct GHG emissions from the industry.

The analysis shows that emissions have increased rapidly over the past 25 years, and are likely to continue increasing if the growth envisioned by many actors materializes. There is overall a limited understanding of the implications of the geographical shift towards Asia-Pacific seen in the last two decades as LCA studies and datasets primarily reflect processes and production patterns used in Europe and North America. Key differences include the use of coal as feedstock, primarily in China, as well as the high dependence on coal-based energy. Another limitation is the limited connection to end-of-life treatments of products from the chemical industry. If incinerated at end-of-life plastics and other chemical products will emit embodied carbon as CO_2 and if landfilled there is a risk of slow degradation with associated methane emissions. Global estimates based on most LCA datasets will thus significantly underestimate emissions from the chemical industry.

Voluntary disclosure of emissions paints an incoherent picture with large gaps due to a strong bias towards OECD countries, different reporting standards, large discrepancies in the extent of disclosure, inconsistency in disclosures around regional emissions, and inconsistent sector boundaries. Scope 3 emissions are commonly not addressed at all in disclosures, and when they are it is only haphazardly. Emission targets set by firms in the industry do not yet fully correspond to the challenge of large and rapid emission reductions. Many targets include only parts of operations or focus on efficiency improvements.

It is absolutely imperative that emissions from the chemical industry do not continue growing in the same way that they have – requiring large-scale changes to operations in the industry both in the near and long term. The use of coal must be abandoned, both for feedstock and energy. A rapid shift towards using renewable energy in existing plants and processes could cut a significant share of emissions, but targets and strategic initiatives on this area disclosed by firms in the industry are inadequate in terms of both scope and scale. A focus on retrofitting fossil-based production with CCS is associated with large risks for continued diffuse emissions of methane throughout the value chain and also stranded assets if the costs for renewable energy continue to decrease. A strategic reorientation away from its connections with fossil fuels could however make the chemical industry a key partner for renewable energy. In the longer term more radical change is needed, towards truly circular and zero emission technologies for primary chemicals.

8.1 KNOWLEDGE GAPS AND FUTURE RESEARCH

With large emissions both upstream in oil and gas and downstream when products are used, discarded, and incinerated, the boundaries for assessing the sectors impacts on climate change are unclear. Perhaps not surprisingly, there are limitations to the current knowledge of the petrochemical industry's climate impact (as illustrated in the report at hand). Building on the findings above, this section maps current knowledge gaps and points to future research that is needed to fully understand how petrochemicals contribute to climate change.

Despite the clear advantages of EEGMRIO-modelling, the petrochemical sector often remains grouped in rather aggregated subsectors with considerable internal heterogeneity (as described in chapter 4). To address this, some national databases might provide more detail (as is the case for the national US IO data) but in general national databases also suffer from issues of aggregation (e.g., EU national IO tables cover roughly 60 sectors). This concern is of course not an issue that is only relevant for petrochemicals but is a relevant general limitation of MRIO-analysis. Therefore, the work which is continuously done to improve and update MRIO databases will also ensure a stronger foundation for analysing the climate impact of the petrochemical industry. In addition, future research to improve specifically chemical industry resolution is needed to further understand the impact of key processes and ensure the reliability and quality of data.

Notwithstanding such research, bottom-up LCA can in principle address the shortcomings arising from aggregation. However, as revealed in this report, proper disaggregated and comparative analysis of key products is currently not possible due to inconsistent modelling choices and data gaps. At present, data confidentiality, a high reliance on proxy data and regionally biased coverage limit the reliability of LCA and stand in the way of mapping climate impacts comprehensively. Adding the environmentally most relevant synthesis pathways, e.g. with a special focus on the technologies in use in China, is essential for providing a solid base for evaluation. In addition, there is also a strong relevance of energy supply on environmental impacts, which is currently to some degree captured by national electricity mixes and occasionally sector-specific electricity mixes, but in general, heat is for most petrochemicals more relevant. Here, there is a clear lack of regionalized and sector-specific data across all LCI databases even though raw data is readily available from the IEA. Adding the data by adapting existing heat mixes correspondingly will greatly increase the quality of LCA results. Finally, this improvement of energy supply data has to go hand in hand with improved data on the energy demand of individual petrochemical products and processes. Finally, replacing some of the generic proxy approaches in LCA with product or process-specific estimates, for example from process simulations or based on the nature of the involved synthesis steps, will be a main objective in order to reach a high reliability of the LCI data for petrochemicals.

Lastly, as referenced in the report, understanding the extent of fugitive emissions (methane in particular) are of high relevance, especially in relation to the desirability of CCS. Therefore, data on methane leakages must be incorporated into the different databases under review.

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ENVIRONMENTAL
AND ENERGY SYSTEMS STUDIES
LUND UNIVERSITY, P.O. BOX 118,
SE-221 00 LUND, SWEDEN

EESS REPORT NO 126
ISRN: LUTFD2/TFEM-- 22/3117--SE + (1-101)
ISSN: 1102-3651
ISBN: 978-91-86961-52-7

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