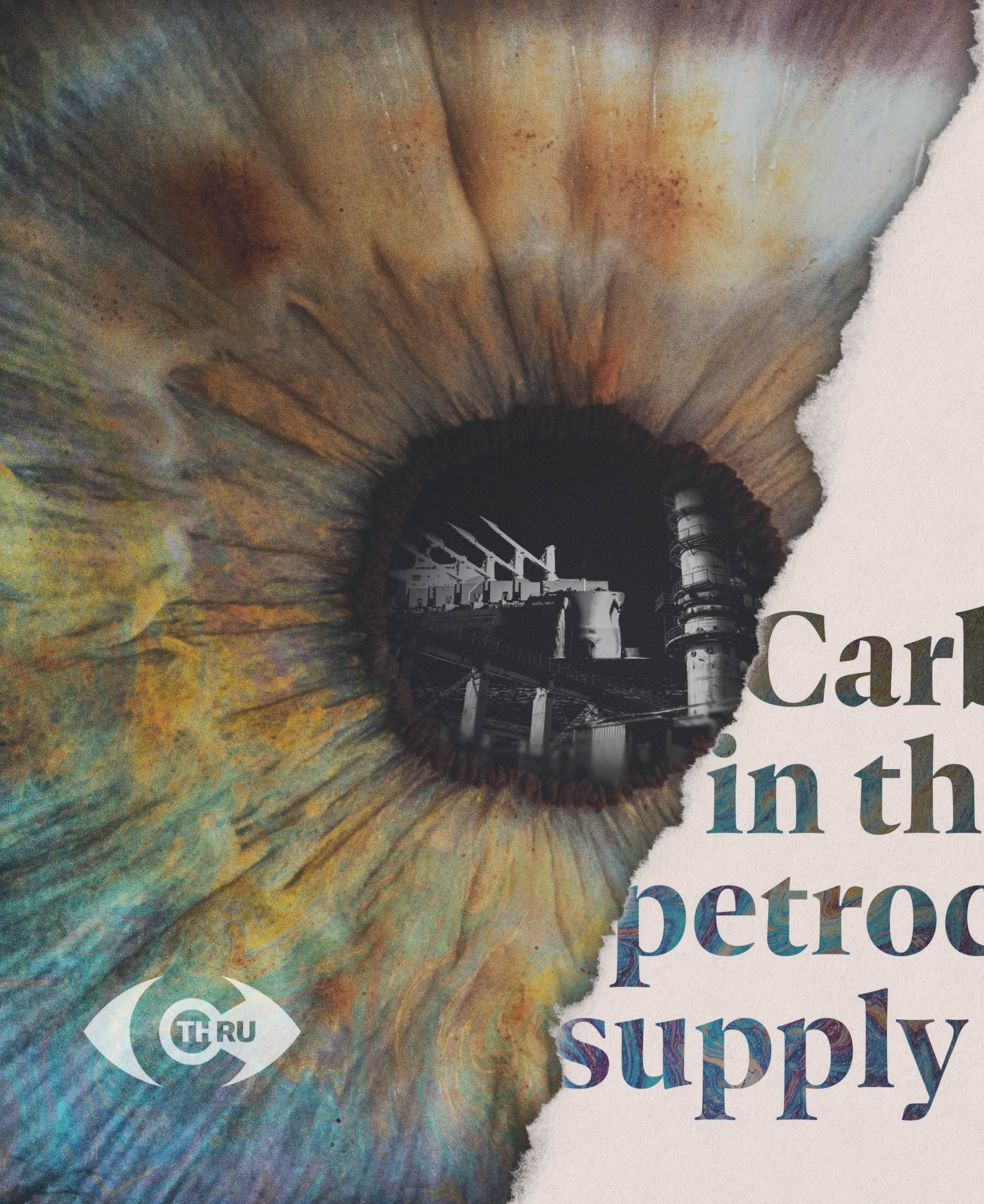

FIRST YEAR REPORT

Jonathan Cullen
Fanran Meng

Carbon clarity in the petrochemical supply chain

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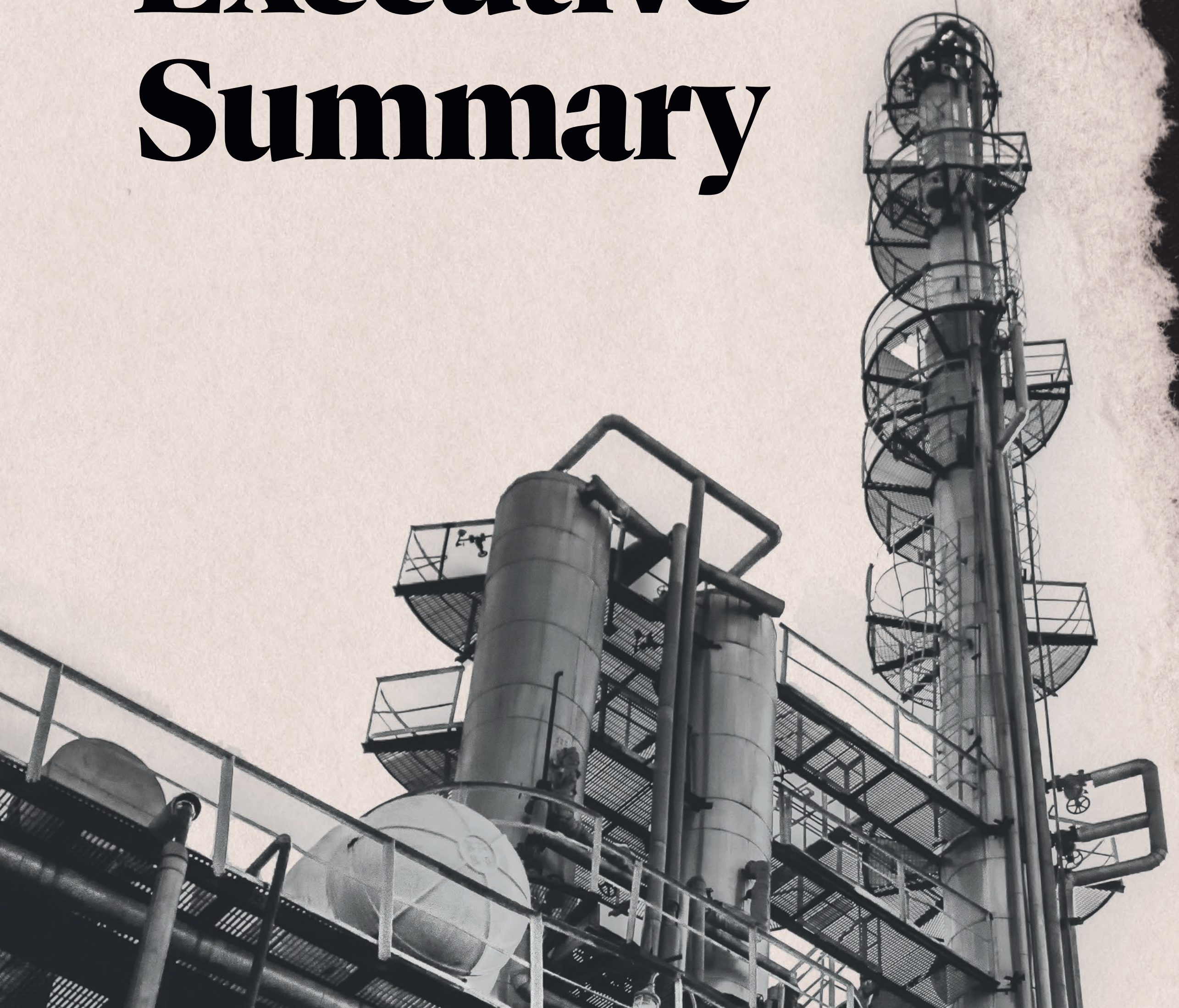
Executive Summary



Petrochemicals are integral to our modern way of life, but are also highly carbon-intensive, accounting for 17% of global industrial CO_2 emissions.

The decarbonisation of the sector is challenging given the complexity of supply chains and thermodynamic constraints of the chemical reactions. Emissions are released throughout chemical products' life cycles, with varying stages dominating for different products. Mitigation options are therefore less straightforward than in other industries, requiring a system-wide approach. The nature of the sector also makes data collection and analysis challenging, meaning there is currently no reliable, comprehensive picture of GHG emissions or energy, mass, and trade flows in the petrochemical sector.

Our critical review of 33 emissions databases and 20 key studies revealed that the current method of gathering petrochemicals emissions data i.e., top-down methods, lack integration, transparency, and robustness.

There are inconsistencies and gaps in the data across six dimensions:

- Product – there is a scarcity of data on material flows through the highly interconnected supply chain.
- Life cycle stage – the emissions at extraction and end-of-life stages are not disaggregated at the product level.
- Region – some countries only report as the sector in total or do not have consistent monitoring standards.
- GHG emissions – there are inconsistencies in the methodologies used for aggregating emissions.
- Time series – data is not consistently collected over time.
- Uncertainty – only a minority of data sources explicitly consider uncertainty.

The current accounts do not allow us to answer the questions that we need answer to work towards net zero carbon emissions. The lack of clarity and transparency in published emissions data, both from companies and governments, heightens these difficulties. An alternative approach to top-down methods is to use derived measurement – bottom-up –where material flows are reconciled with the underlying chemical reactions, thermodynamic principles and carbon intensities to model GHG emissions.

C-THRU will address the complexity of supply chains and processes in the petrochemical sector by developing an integrated model that combines life cycle analysis with material flow analysis.

We will provide an accessible and reliable repository of global resource flows, emissions data, and mitigation options for the petrochemical sector, accounting explicitly for uncertainty. Based on these accounts, we will catalogue and model mitigation options and their potential impacts on emissions reductions. Our accounting will be mutually exclusive and collectively exhaustive, respecting mass and energy balancing across products, life cycle stages and regions. This project will create an open-source database on decarbonisation technologies that will be instrumental in documenting the technical viability, environmental impact, and economic performance of different decarbonisation scenarios.

This report has four chapters. Chapter 1 outlines the motivation for understanding the GHG emissions impact of the petrochemical sector. Chapter 2 describes the distinctive characteristics of the petrochemical sector and details the sources of emissions throughout the life cycle stages and across the different groups of petrochemicals. Chapter 3 examines how GHG emissions are reported, how supply chains are analysed, and how uncertainties in these data are managed. To conclude, Chapter 4 details the overall approaches of the C-THRU project.

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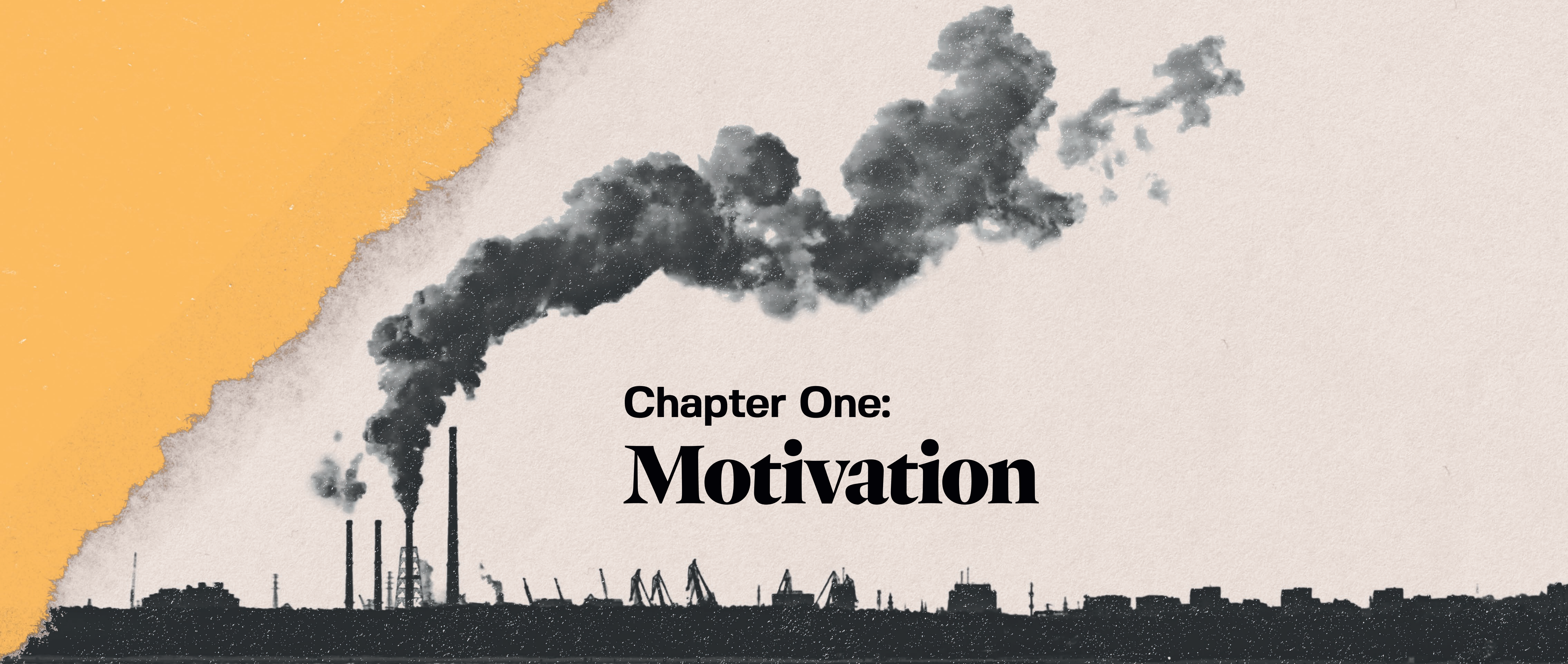


Chapter One:

Motivation

Chapter Summary

The products of the petrochemical sector are ubiquitous in the modern world: plastics and synthetic textiles are everywhere we look; agriculture and food systems use fertilisers; pharmaceutical products save lives every day. Chemicals and their derivatives currently contribute more than 1% of global GDP. The petrochemical sector has a significant carbon footprint, accounting for 17% of global industrial CO_2 emissions. Demand for petrochemicals is rising and, without intervention, the sector will continue to release greenhouse gases (GHGs) at an increasing rate.

The C-THRU project seeks to answer ever more urgent questions from the public, industrial stakeholders, and governments. Consumers want to know which products are most sustainable, companies are concerned about financing, and governments want to know how we can achieve emission reduction targets.

The complexity of supply chains and processes within the petrochemical sector makes data collection and analysis challenging. The lack of clarity and transparency in published emissions data, both from companies and governments, heightens this difficulty. C-THRU aims to promote carbon clarity in the global petrochemical supply chain by delivering a comprehensive, data-driven model of the petrochemical sector; its life cycle contributions to current and future GHG emissions at global and regional levels; and methods to reduce emissions to net zero.

It is hard to imagine a world without the modern ***petrochemical*** sector: chemicals and their derivatives are widespread and directly contribute more than 1% of global GDP[1]. Plastic, rubber, and synthetic textiles adorn our buildings and vehicles and fill our cupboards and wardrobes; modern agricultural and food systems could not function without synthetic fertilisers; synthetic pharmaceuticals save millions of lives annually, with few known substitutes.

Although petrochemical products such as plastics and fertilisers are useful in many applications, we must confront their dark side: the release of plastic waste into the environment and the ***greenhouse gases*** (GHG) emissions generated by the industry.

The accumulation of mismanaged plastic waste in the environment has become a global concern[2]. Developed countries, such as the US and in the EU, regularly export plastic waste to developing countries. However, many developing countries have poor waste management systems, resulting in developed countries' mismanaged waste polluting inland waterways and oceans[3]. The material flows and in-use stock of plastic products must be understood to improve regional and global management of waste and to implement plastic pollution mitigating policies.

The petrochemical sector contributes a significant proportion of GHG emissions including 17% of global industrial CO_2 emissions. Achieving net zero GHG emissions by 2050 is consistent with efforts to limit the long-term increase in average global temperatures to 1.5°C. The number of countries and corporations announcing pledges to achieve net zero emissions over the coming decades has grown rapidly. Therefore, it is vital to develop emission mitigation strategies in the petrochemical industry to deliver a future net zero society[4].

Decarbonising the petrochemical sector is challenging for many reasons, including: chemical plants have capital-intensive, long-lived assets; the methods of production and the applications of chemical products are difficult to replace, economically and technically; demand for products, especially energy-intensive petrochemicals, are expected to at least double by 2050.

Furthermore, there is concern that declines in fossil-based transport fuels might drive a shift in production towards higher-value chemicals and polymers, increasing sector emissions even further. In light of emerging targets, achieving absolute emissions reductions, against a doubling in demand, requires twice the reduction effort in emissions per unit of production. The accurate measurement and forecasting of GHG emissions is critical to guide the petrochemical sector through this transition to a more sustainable future.

This report is the first deliverable of the C-THRU project and provides a critical review of GHG emissions data reporting from the petrochemical sector. The report is divided into four sections:

- Chapter One outlines the motivation for understanding the GHG emissions impact of the petrochemical sector.
- Chapter Two, Petrochemicals: a unique sector, includes the background information on life cycle stages, product groupings, and the uniqueness of the sector.
- Chapter Three presents a comprehensive review of literature and data sources. It covers how chemical sector emissions are reported, a review of supply chain databases and literature, and emerging data quality issues and gaps.
- Chapter Four details the overall approaches of the C-THRU project. The research will address the data gaps found and build a more complete and transparent evidence base for: answering the questions put to the petrochemical sector; exploring current and emerging emission mitigation options from every stage in the chemical products' life cycles; examining pathways to net zero carbon emissions, considering economic and business inputs and viewpoints.

Petrochemical

petrə(ʊ)ˈkɛmɪk(ə)l

We use the words petrochemical and chemical interchangeably, to mean all chemicals which are today derived from fossil fuel feedstocks.

Greenhouse gases (GHGs)

GHGs are gases that trap heat in the atmosphere, contributing to climate change. The petrochemical industry releases three main GHGs: carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O).

A. Rising demand for chemical products

Key points:

- Plastic products account for 40% of the mass of chemical products leaving the chemical sector, and nitrogen fertilisers make up 33%. The remainder output comprises solvents, additives and explosives, among others.
- The production of plastics and nitrogen fertilisers relies on seven primary chemicals - ammonia, ethylene, propylene, methanol, benzene, toluene and mixed xylenes.

The attractiveness and popularity of chemical products stems from their range of properties, their cost-effectiveness and the utility they deliver in society.

Increasing demand for petrochemical products, such as plastics and synthetic fertilisers, is a relatively recent phenomenon. Plastic production grew rapidly from the 1950s, driven by an ever-increasing range of new plastic materials, their exceptional properties, (being strong, lightweight, durable, and low-cost) and the numerous new products on offer. Similarly, the wide-spread availability of nitrogen-based fertilisers from the 1950s underpinned the Green Revolution which vastly increased global agricultural production. Today, the global petrochemical sector makes nearly 1 billion tonnes of chemical products, including 420 Mt of plastic products, 290 Mt of nitrogen fertilisers, fibre and rubber, and 250 Mt of other products including solvents, additives and explosives.[5] Demand for the seven primary chemicals—ammonia, ethylene, propylene, methanol, benzene, toluene, and mixed xylenes—is anticipated to increase in the future, with many products expected to double in demand by 2050. Rising demand for future chemical products makes action to achieve net zero emission targets more challenging and pressing.

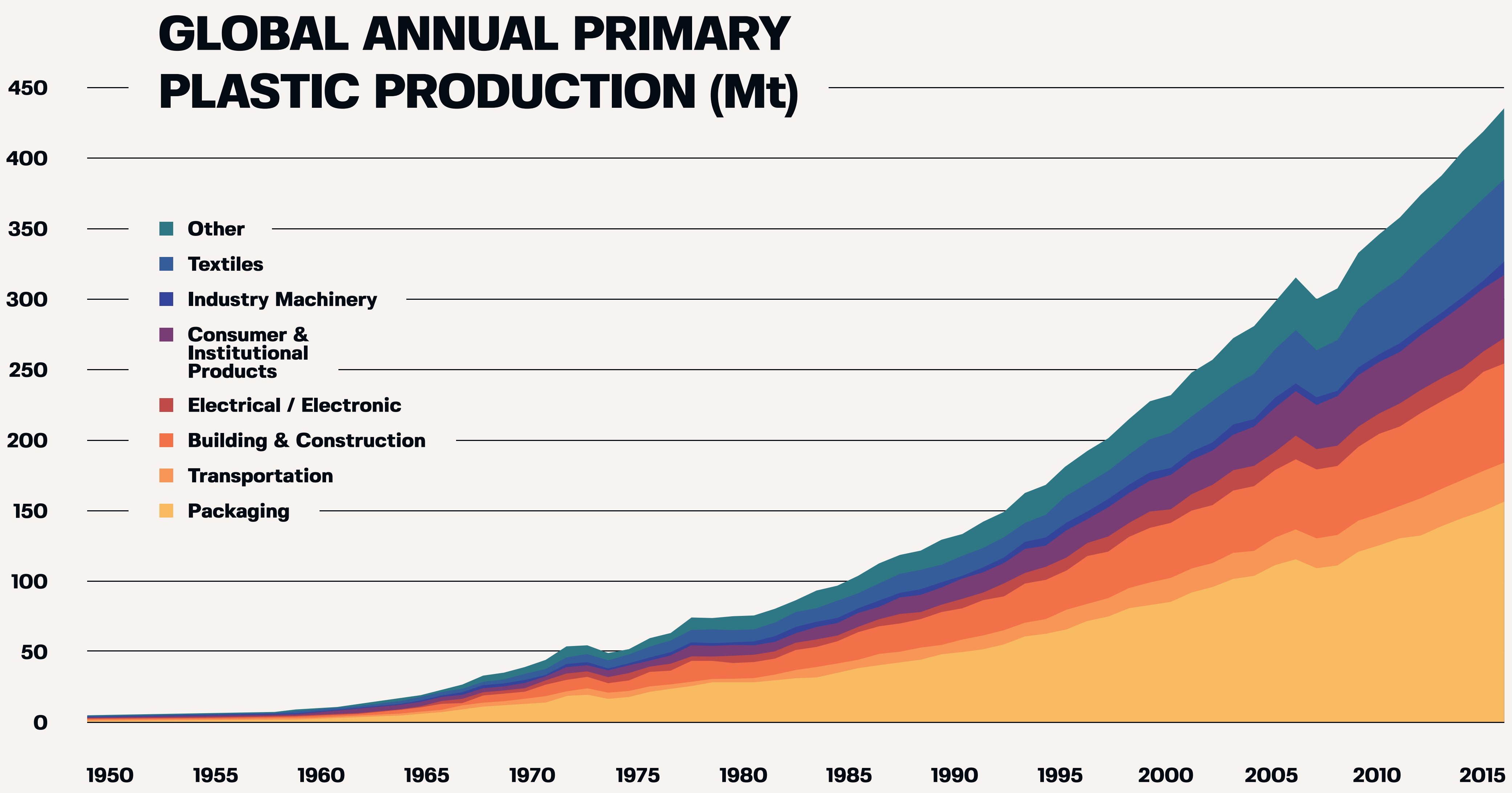


Figure 1-1: Global annual primary plastic production, a) by end-use; b) material types, in Mt (million tonnes) [6,7]

Anticipating the future demand for chemical products and their waste availability requires detailed knowledge of the end-use applications of these chemicals. For this reason, it is vital to track plastics, fertilisers and other petrochemicals from production through to end-use applications. This knowledge will enable the identification of additional climate change mitigation options in this sector.

As estimated by Levi et al., plastic products (consisting of thermoplastics and thermosets) accounted for 40% of the mass of chemical products leaving the chemical sector in 2013, and nitrogen fertilisers made up 33%.[8] For simplicity, in this section we only discuss the production and consumption of nitrogen fertilisers and plastics since these account for 73% of the production of the petrochemical industry. The remainder output comprises solvents, additives, and explosives, among others.

The production of plastics and nitrogen fertilisers relies on seven primary chemicals - ammonia, ethylene, propylene, methanol, benzene, toluene and mixed xylenes (collectively named as BTX), the building blocks of the petrochemical industry.[5] The production of these seven primary chemicals accounts for about two-thirds of the total energy demand and 60% of CO_2 emissions in the sector. Primary chemicals are mainly used as the raw materials of plastics and nitrogen fertilisers. For example, nitrogen fertilisers account for 80% of the ammonia consumed in the agricultural sector, and ethylene and propylene are used as the monomer to produce plastics, for instance, polyethylene and polypropylene. Approximately 60% of the methanol use of the sector is for the production of raw materials of plastics, for example, formaldehyde, acetic acid, ethylene and propylene, and around 30% is used as fuel, in the form of methanol, biodiesel, or methyl tert-butyl ether and dimethyl ether.[9] Regarding BTX, most of the toluene is converted to higher value benzene and xylenes; 45% of this benzene is adopted to produce polystyrene (PS) plastics via ethylbenzene; and 82% of these xylenes are used to produce polyethylene terephthalate (PET) plastics via terephthalic acid.[10]

Plastics are strong, lightweight, durable, and malleable. From the moment the first synthetic plastic, Bakelite, was produced in 1907, the world of materials was transformed. By 1941 more than 20 polymers had been invented and plastics had found their way into industrial applications and everyday household products. But plastic production really began to accelerate after the 1950s, growing from 1.5 Mt (million tonnes) in 1950 to 465 Mt in 2019[11], driven by an ever-increasing range of material properties and remarkably low production costs. Plastics are now ubiquitous in society, making up a large fraction of the products we use. They are used for wrapping foods, protecting hospital workers, and delivering water and electricity.

Figure 1-2 illustrates the plastic demand by sector and polymer type in Europe.[12] Around 40% of plastics are consumed as packaging, followed by 20% in building and construction. Plastics in each sector have different product lifetime distributions, ranging from less than one year as packaging to 35 years in building and construction. The worldwide in-use stock up to 2015 was estimated to be 2,500 Mt, while 6,300 Mt of plastic waste was generated in the same period. Among the plastic waste, approximately 800 Mt were incinerated; only 600 Mt were recycled; and 4,900 Mt of plastics were discarded to landfill or the natural environment.[6,7,13] Figure 1-3 shows that the stocks of plastics per capita in China, the UK and the USA increase with GDP per capita (purchasing power parity, PPP).[7,14,15] The increase rate slightly drops as GDP per capita increases, implying a saturation of stock per capita. Waste mismanagement leads to environmental issues including CO_2 emissions and plastic waste in waterways and oceans.

Chemical fertilisers and agrochemicals have risen to prominence with similar acceleration. The fertiliser industry produced 152 Mt of nitrogen nutrient in fertilisers in 2018. Historically the production of nitrogen fertilisers rose from 12.9 Mt in 1961 to 113.3 Mt in 2014, as shown in Figure 1-4. Ammonia was first produced at practical levels of

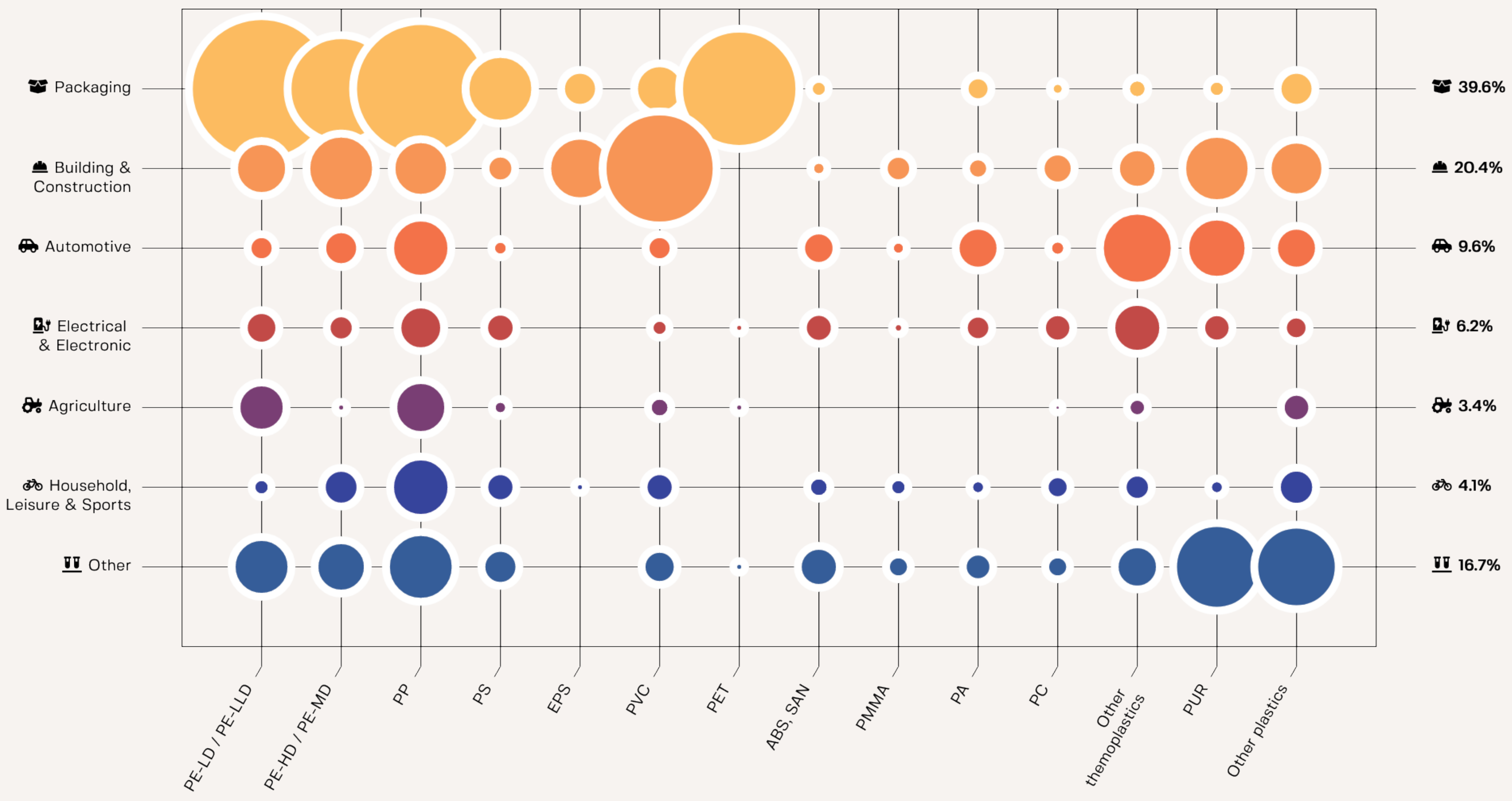


Figure 1-2: Plastics demand by sectors and polymer type in Europe in 2019 (total 50.7 Million tonnes) [12]

thermodynamic efficiency after the invention of the Haber-Bosch process in 1909, earning Fritz Haber and Karl Bosch Nobel prizes for chemistry in 1918 and 1931. For ease of transportation, gaseous ammonia is converted to various solid nitrogen fertilisers, for example, urea, ammonium phosphate and ammonium nitrate. This invention led to the rapid development of nitrogen-based fertilisers and went on to underpin the Green Revolution of the 1950/60s, which vastly increased agricultural production in developing countries. In fact, the Haber Bosch process is estimated to have provided the nitrogen for protein building in the bodies of two billion people alive today.[16] It is estimated that 48% of the current 7.38 billion global population is fed by synthetic nitrogen fertilisers.[17] Figure 1-5 shows a clear link between nitrogen fertiliser application and nitrogen contained in agricultural products. An important observed trend is that nitrogen use efficiency has increased in the US and China in recent years.

Other petrochemicals providing essential services in society include solvents (e.g. methyl alcohol), additives (e.g. carbon black) and explosives (e.g. ammonium nitrate). Overall, the petrochemical sector produces thousands of different materials and hundreds of thousands of different products. This diversity is unique in the world of materials, and the variety of possible chemical formulations leads to almost endless material properties which in turn creates utility in an increasing array of applications.

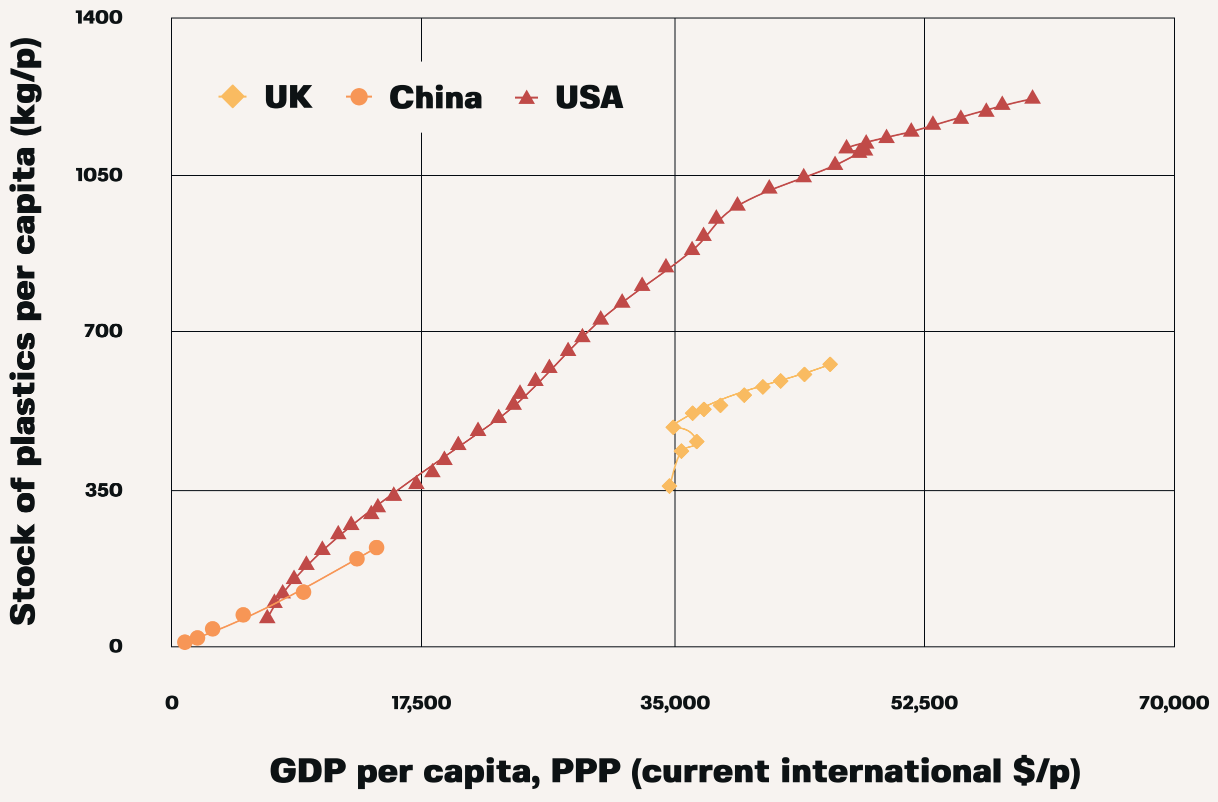


Figure 1-3: Relationship between the stocks of plastics per capita and GDP per capita, PPP (current international $/p) in China (1978-2017), the UK (2006-2017) and the USA (1973-2017). Data extracted [7,14,15]

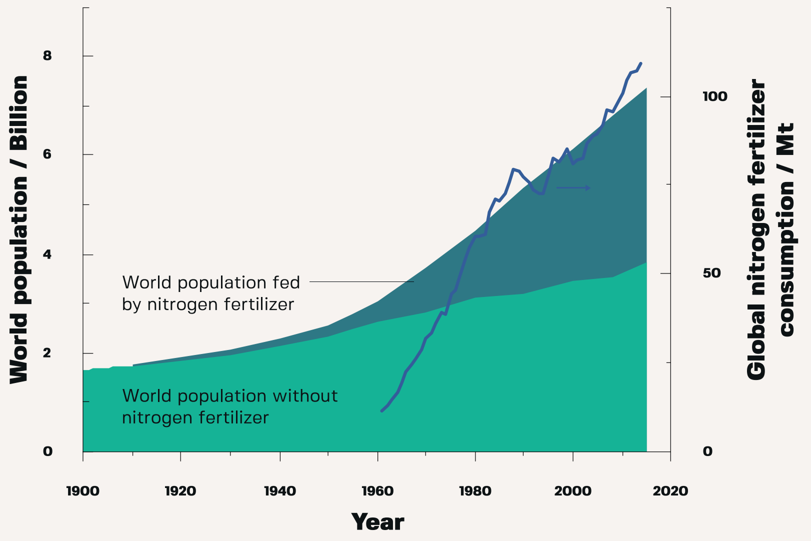


Figure 1-4: The world population with and without nitrogen fertilisers, as well as the global nitrogen fertiliser production, as a function of time [17,18]

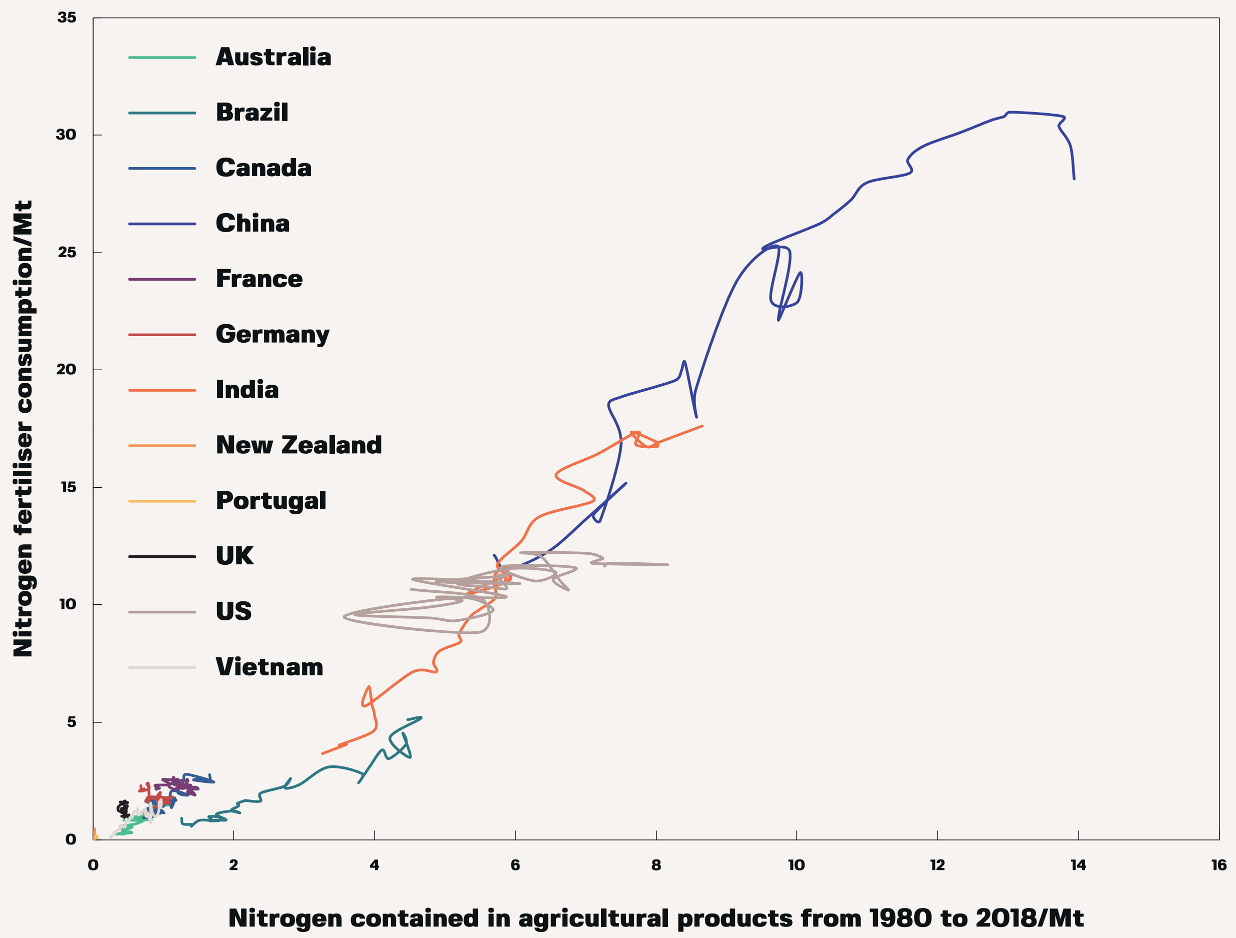


Figure 1-5: Relationship between nitrogen element contained in agricultural products and nitrogen fertiliser consumption in some countries. Soybean is not included in the calculation, since it only consumes 1.1% of the global nitrogen fertilisers and mainly relies on biological nitrogen fixation [19]

B. Hard to live with, hard to live without

The petrochemical sector is responsible for 30% of final industrial energy use, including 11% of global oil demand and 10% of global natural gas demand, and releases 17% of global industrial CO_2 emissions.[20] Emissions arise from chemical reactions and high temperature heat generation (direct process emissions); from energy conversion in the upstream energy sector (indirect emissions); and from end-of-life (EOL) treatment of products. Additional emissions are released from the use phase of some petrochemicals (e.g. fertilisers) and from fugitive emissions (e.g. methane) released from upstream oil and gas operations. Other non-GHG emissions have a significant environmental impact, such as fertiliser run-off contributing to eutrophication[21], bioaccumulation of toxic chemicals in organisms, and plastic waste in the world's oceans,[3] harming sea life [22]. Petrochemicals are hard to live with, but after years of dependency on them, they are almost impossible to live without.

The environmental strain magnifies as demand rises, with demand for the sector's most energy-intensive petrochemicals expected to at least double between 2010 and 2050.[5] Reducing emissions and environmental impacts against the backdrop of increasing production will be incredibly challenging. The petrochemical sector already operates efficiently relative to other sectors because of high shares of energy costs and advanced levels of process control and integration.

The highly positive social and economic impacts of the petrochemical sector are accompanied by a huge environmental burden.

A future sustainable petrochemical sector will need to innovate quickly to deliver products with dramatically lower GHG emissions and a reduced burden on the environment and natural resources.

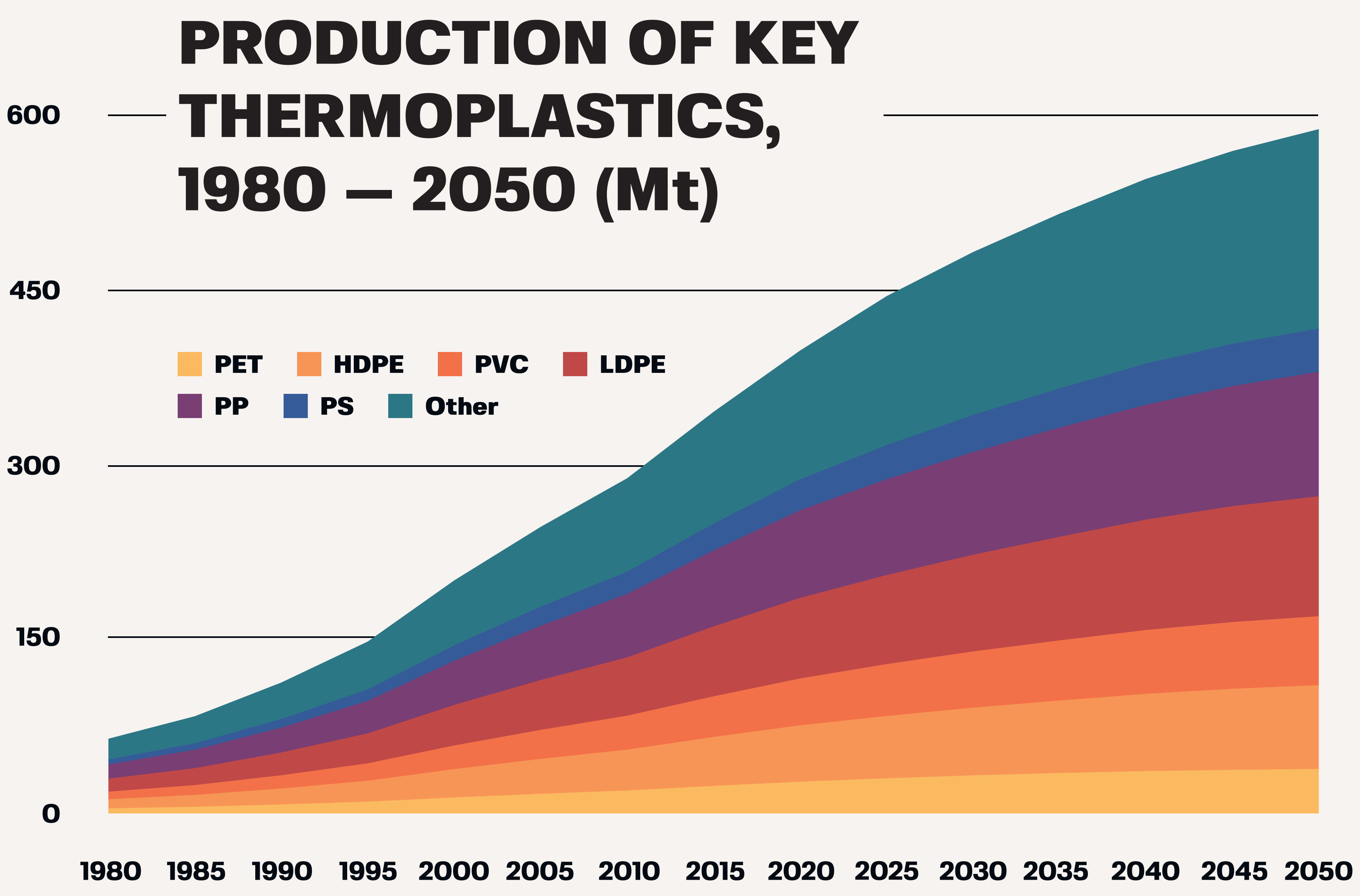


Figure 1-6: Historical and project future production of key thermoplastics based on the IEA Reference Technology Scenario 3. PET = polyethylene terephthalate; HDPE = high-density polyethylene; PVC = polyvinyl chloride; LDPE = low-density polyethylene; PP = polypropylene; PS = polystyrene.

C. Many questions, few answers

Consumers:

- Which petrochemical products are more sustainable?
- If single use plastics are so bad, why are they still used for food and medicine?
- Do plastic-free days or carrier bags charges make any difference?
- Do viable substitutes of our plastic straws exist?
- What is the emissions impact from fertilisers used to grow food?
- What are the environment and health risks of microplastics?

Governments:

- Can we trust the reported emissions from the industry?
- How we can achieve emission reduction targets?
- Can the petrochemical sector be made to operate more efficiently?
- What emerging technologies are available for mitigating emissions?
- What are the alternatives to using plastics and fertilisers?
- Why are we still exporting plastic waste overseas?

Advocacy Groups:

- Can we trust the reported emissions from industry and government?
- Can we achieve net zero emission plastics?
- How much methane emissions are released during fossil fuel extraction?
- How are refining emissions allocated onto downstream products?
- Why does so much nitrogen fertiliser end up in waterways?
- Why are the recycling rates for plastic so low?

Increased awareness of the prevalence of petrochemicals in society and their link to environmental impacts has raised many questions in the public domain directed at the chemical sector.

Consumers want to know which products are more sustainable, governments are asking how the chemical sector can deliver on ambitious emissions targets, and environmental advocacy groups are questioning the very need for many chemical products. At the same time, the petrochemical sector has often been reluctant to provide answers to these questions in an open and transparent way.

Amassing the evidence necessary to answer these questions is no trivial task. The myriad of different materials, products and actors involved in the petrochemical value chain makes data collection challenging.

GHG emissions data for petrochemical production are collected at a country level from individual plant operators, and then submitted to the United Nations Framework Convention on Climate Change (UNFCCC) for country level comparison. The comprehensiveness of the data submitted varies by country, with developed countries (Annex I Parties) expected to provide more detailed data than developing countries (Non-Annex I Parties). The result is a dataset which reports only country-level emissions for high level sectors, with the aim of tracking emissions against pledged targets over time. However, this data does not allow us to answer more detailed questions about the emissions associated with specific chemical products, across the full product life cycle and consumed in certain countries, because this data only reports isolated production emissions.

Data concerning the energy performance and material balances of chemical processes are often deemed commercially sensitive because they can contain clues about a company's operational strategy. Consequently, energy and material data are typically only available in aggregated form across spatial (by country or region) and temporal (annual) resolutions. Some good examples of aggregated data for the chemical sector include the datasets by Eurostat[23] and the IEA[20], with technical data being restricted at the regional level. Several proprietary databases exist behind paywalls, and are often only available to plant operators that submit data, such as the Solomon Associates Olefin Study[24], which plant operators use to gauge their own performance relative to competitors, usually anonymously. However, the restricted access to such databases limits their use for answering the questions posed.

D. C-THRU: carbon clarity in the global petrochemical supply chain

CARBON CLARITY IN THE GLOBAL PETROCHEMICAL SUPPLY CHAIN

c-thru.org

C-THRU is an international and multidisciplinary research project that aims to promote carbon clarity in the global petrochemical supply chain.

Accurate measurement of GHG emissions and modelling of future interventions to reduce emissions will be critical to guide the petrochemical sector to a more sustainable future. This will require new data frameworks and modelling tools to aggregate data from disparate sources, deal with the uncertainty in these data, and be designed flexibly to answer questions from different viewpoints.

C-THRU will achieve this by delivering a comprehensive data-driven model of the petrochemical sector and its life cycle contributions to current and future GHG emissions at global and regional levels. C-THRU is unique because it brings together several of the most rigorous modelling efforts that focus on analysing the environmental impacts of the petrochemical sector. Each modelling activity uses different tools to address different research questions across different parts of the life cycle in different geographical areas and time spans.

By the end of the C-THRU project we will have:

- Reviewed GHG emissions literature and data from the petrochemical sector and identified knowledge gaps.
- Provided an accessible and reliable repository of global resource flows, emissions data, and mitigation options for the petrochemical sector, accounting explicitly for uncertainty.
- Created accurate and verifiable accounts for current GHG emissions and environmental impacts (by chemical product, life cycle stage, sector, and region) and validated the accuracy of existing GHG emissions accounts.
- Catalogued and modelled supply-side mitigation options (i.e. new process routes, efficiencies, and technologies), demand-side mitigation options (i.e. materials efficiency, recycling, and recovery), and their potential impacts on future pathways and emissions reductions outcomes.
- Explored the petrochemical sector's influence on environmental policy, considering the implications of economic, legal, business, governance, regulation, and policy contexts.
- Supported an international response to climate change and co-created active stakeholder networks by delivering an unbiased, open, and rigorous approach to reducing GHG emissions from the petrochemical sector.

The project is divided into seven workstreams (WS1 – 7) shown in Figure 1-7 and detailed on the following pages.

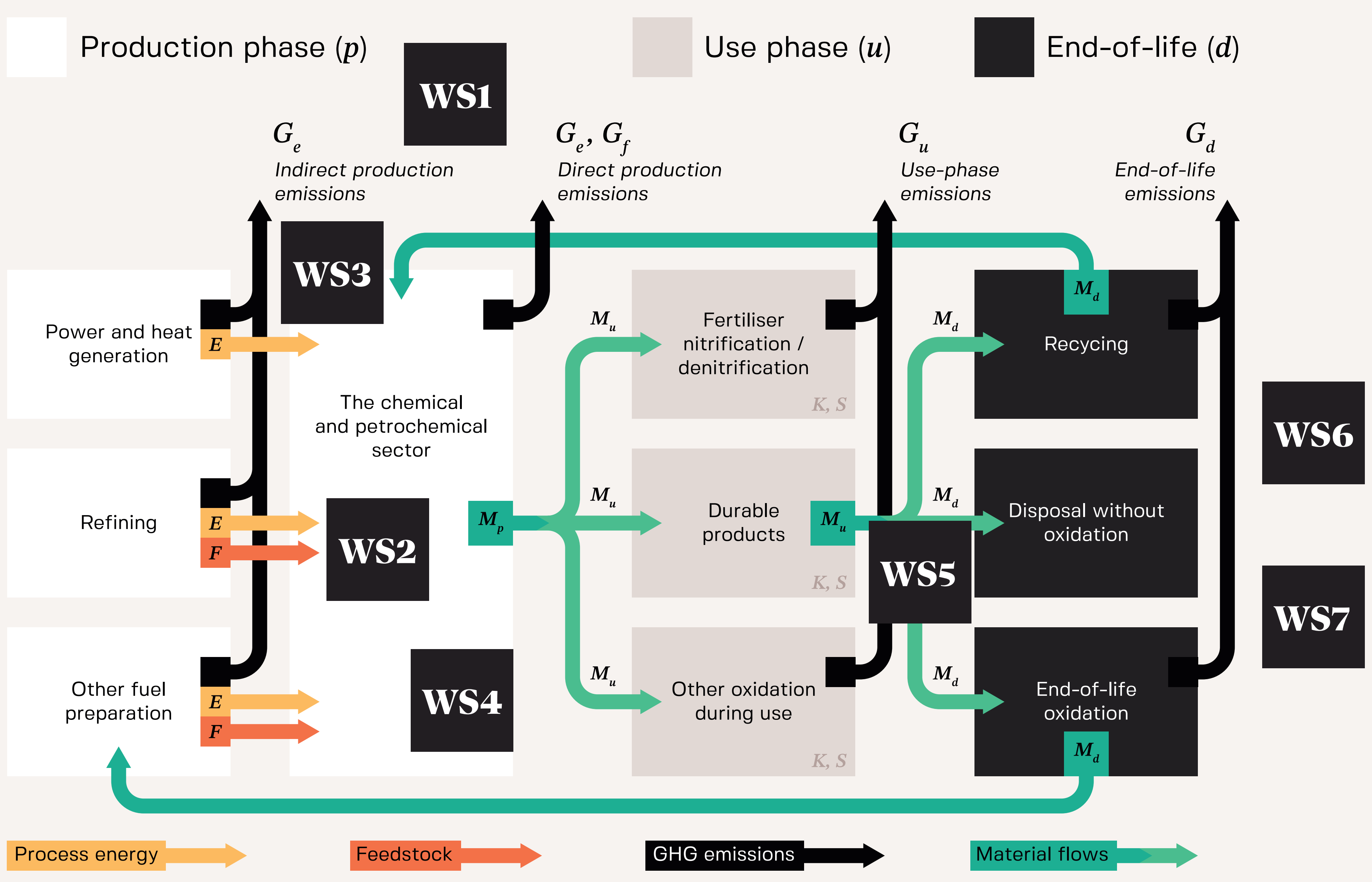


Figure 1-7: Overview of the Research Program structure and workstreams

CARBON CLARITY IN THE GLOBAL PETROCHEMICAL SUPPLY CHAIN

C-THRU project lead:

Prof Jonathan Cullen,
University of Cambridge

WS1

Literature Review

Provide an informed view of the accuracy and comprehensiveness of emissions data and monitoring regimes across petrochemical sectors.

Lead investigator:

Prof Jonathan Cullen,
University of Cambridge

WS2

Data Model & Uncertainty

Develop an open and comprehensive integrating model of global resource flows, emissions, and technologies in the petrochemicals sector. This will combine information, data, and learnings from the other workstreams (WS3–5) in an open repository, creating transparency and a process for accepting contributions to update or improve the dataset.

Lead investigator:

Dr Rick Lupton,
University of Bath

WS3

Energy & Emissions

Disaggregate WS1 energy use and emissions data into more detailed industry subsectors, products and processes for incorporation by WS2, 6 and 7, and use this technology richness to further explore different supply-side levers for dramatically decarbonising future chemicals production.

Lead investigator:

Prof Eric Masanet,
University of California, Santa Barbara

Lead investigator:

Prof Phillip Christopher,
University of California, Santa Barbara

WS4

Product Demand

Map the global flows of chemicals from production to end-use applications. This map will be used to build a dynamic model of product stocks, to test the impact of alternative interventions along the chemicals supply chain in future demand, waste generation and global life cycle emissions, and will provide mass flow information from production to use for the overall model in WS2.

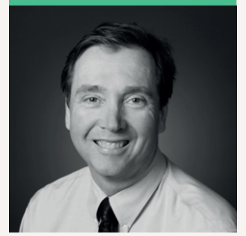
Lead investigator:

Dr André Cabrera Serrenho,
University of Cambridge

WS5

Recycling and EOL Options

Explore opportunities for enhanced circular polymer processing and the integration of waste plastic de-polymerisation using a model of US chemical manufacturing industry, as an interconnected network of approximately 1000 chemical processes.



Lead investigator:

Prof David Allen,
University of Texas at Austin

WS6

Economic Context

Create a high-level macroeconomic model of how the petrochemical supply chain, including recycling and capturing of GHG emissions (e.g. from industrial facilities) integrates within a large economy. The purpose is to model the dynamics and feedbacks of carbon mitigation efforts, exploring feedbacks from a circular economy. Information from WS3–5 will be applied in a macroeconomic model for the United States and serve as a template for other economic regions.

Lead investigator:

Dr Carey King,
University of Texas at Austin

WS7

Business Landscape

Analyse the business ramifications of future changes to petrochemical supply chains, which are identified in WS3, 4 and 5, and fully modelled in the scenario analysis in WS2.

Lead investigators:

Chris Hamlin & Penny Hamlin,
HancockHamlin Ltd

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2

Chapter Two:

Petrochemicals: A unique sector

Chapter Summary

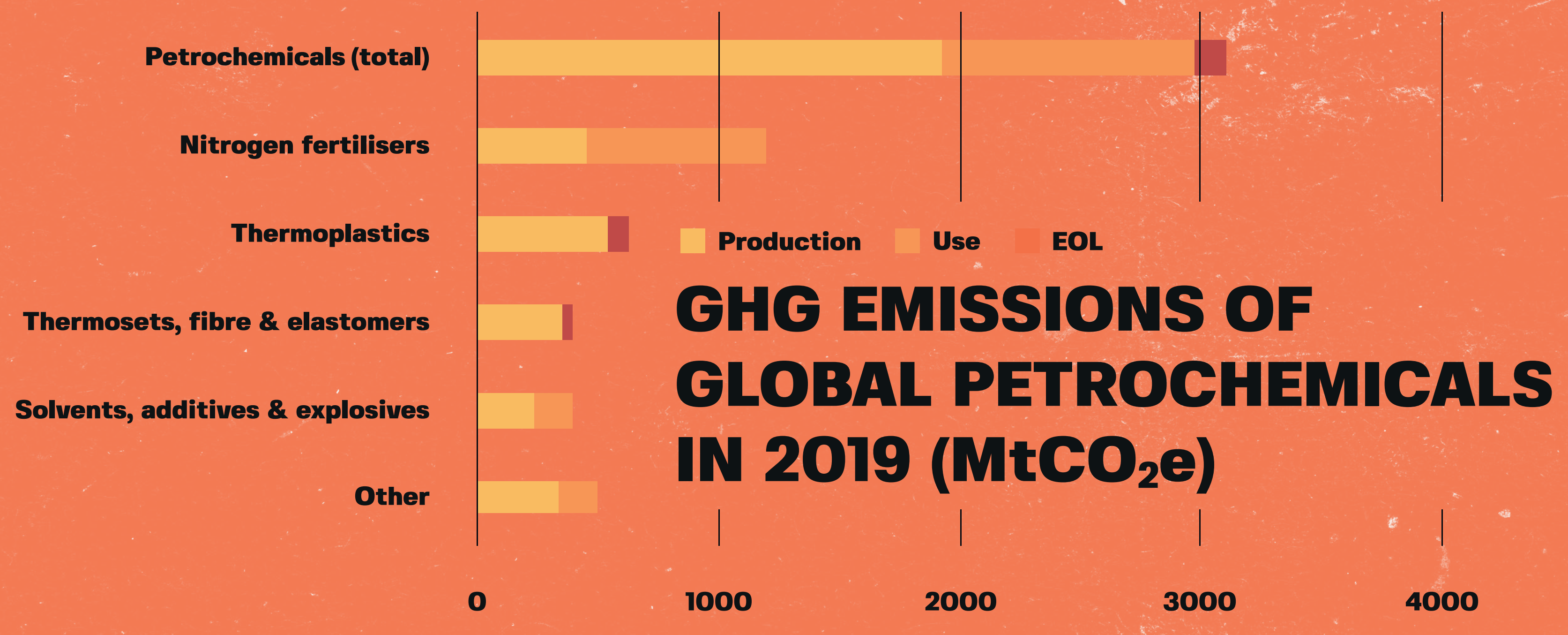


Figure 2-6a: GHG Emissions of Global Petrochemicals in 2019

The petrochemical sector is an energy- and emission-intensive industrial manufacturing sector which, the International Energy Agency (IEA) estimates, released approximately 1.5 billion tonnes of CO_2 to the atmosphere in 2015[1].

This chapter of the critical review describes the distinctive characteristics of the petrochemical sector and details the sources of emissions throughout the life cycle stages of the different groups of petrochemicals.

Section A

Section A describes what makes the petrochemical sector unique amongst other industrial sectors, highlighting:

- interchangeability of feedstocks, products, and energy, which is constrained by the laws of thermodynamics;
- increasing product and by-product complexity and variety down the production chain;
- interconnectivity within the sector.

For these reasons, emission mitigation options are less straightforward than in other industries, requiring a systems-wide approach. The sector is optimised for the current processes used, sharing by-products, waste heat and infrastructure between value chains. Therefore, mitigation solutions for one chemical's manufacture could affect hundreds of other processes involved in many other products' manufacture. To assess where interventions are required, allocation of emissions to specific materials and processes is required. This is challenging given the high interconnectivity of the sector.

Section B

Section B describes the emissions sources from each of the three life cycle stages: production (including extraction and refining of feedstocks and the conversions to products), product use, and EOL treatment. Emissions related to extraction and EOL are difficult to delineate by product and are not included in reported emissions by chemical firms. They are often overlooked by current sector emissions data, revealing incompleteness in the current picture of petrochemical emissions. Where the emissions are released within the life cycle varies depending on the products and the processes used in their respective life cycles.

Section C

Section C details the sources of emissions by the five types of petrochemical products: thermoplastics; thermosets; fibres and elastomers; nitrogen fertilisers; solvents, additives, and explosives; other chemicals. To understand sector emissions for mitigation options at a meaningful degree, emissions at the product level throughout their life cycles must be examined.

Figure 2-6a illustrates our preliminary estimation of emissions in the global petrochemical sector in 2019. We find for plastics, over 2/3 of emissions are from production and 1/3 from the EOL stage. For nitrogen fertilisers about 1/3 of emissions come from production and 2/3 from the use phase.

A. Distinctive characteristics

Key points:

The petrochemical industry is unlike other industrial and manufacturing sectors, with the result that it behaves and responds to changes and interventions in unanticipated ways, for the following reasons:

- **Raw materials, energy and products are often interchangeable**
- **It is constrained by fundamental laws of chemistry & thermodynamics:**
  - **There are limits to how far efficiency and yield can be pushed**
  - **Chemical equations must balance**
  - **A certain amount of energy consumption is unavoidable**
- **Product complexity and variety increases down the value chain**
- **By-products are inevitable**
- **Everything produced must go somewhere**
- **It is massively interconnected – it's impossible to isolate individual value chains**
- **Mitigation options require a system-wide approach:**
  - **Electrification will result in new by-products that will need to go somewhere**
  - **Allocation of emissions to specific materials is arbitrary (objectivity is only possible at a system-wide level)**
  - **Carbon is only problematic when emitted; maximising carbon retention within the product will be important.**

Figure 2-1 attempts to explain these key interactions and why mitigation options are less straightforward than in other industries.

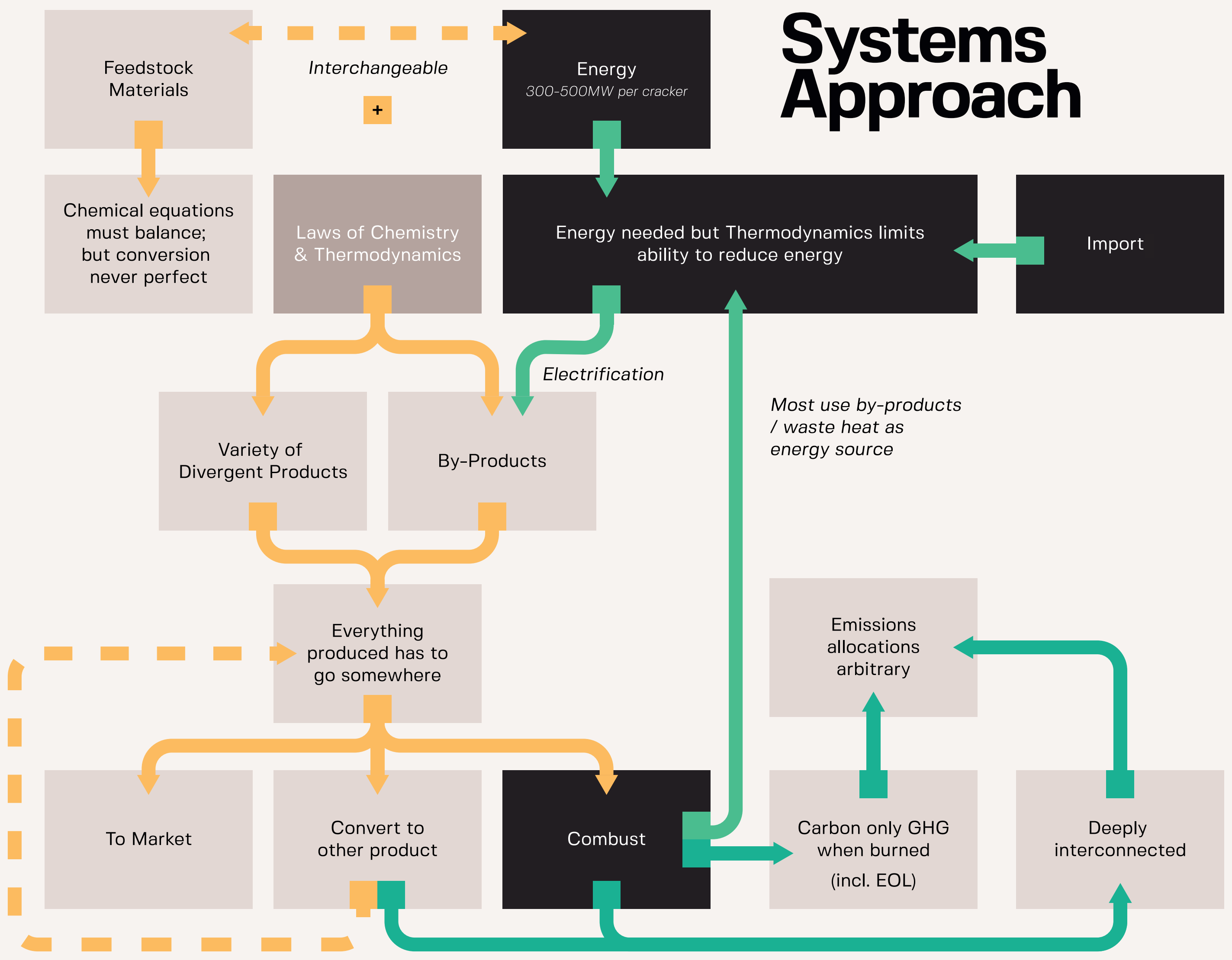


Figure 2-1: Why the petrochemical industry is unique

Raw materials, energy, and products are often interchangeable

In the petrochemical industry, particularly in the manufacture of commodity chemicals, there is significant potential interchangeability between materials used as feedstock or burned to generate energy. By-products and waste streams also have the potential to be used as internal fuels, rather than effluents or scrapped material. This interchangeability enables companies to be large energy consumers without imposing significant demands on external energy infrastructures, and for the value chain to evolve a structure that is as cost- and energy-efficient as possible.

Constrained by chemistry and thermodynamics

At a fundamental level the petrochemical industry is constrained by the laws of chemistry and thermodynamics. These set natural limits on how efficient a plant can be and the yield it can expect. Chemistry drives variety and a divergent value chain, and thermodynamics impose a significant energy requirement on the industry. The combination of these two results in a massively complex, interconnected and interdependent production system with profound implications for mitigation options.

The principle of conservation of matter means that the quantity of each element in a chemical reaction does not change and all chemical equations must balance.

At its most basic level this means that if there are 2 carbon atoms and 6 hydrogen atoms before a chemical reaction takes place, there must be the same number of carbon and hydrogen atoms afterwards, albeit in different configurations. If the petrochemical industry processed things one molecule at a time, it would be possible to be precise about what was produced. However, in practice, industrial-scale chemical processes involve millions of molecules simultaneously, significantly increasing the range of potential reactions that take place. Just two of the possible combinations are shown in Figure 2-2, illustrating one of the by-product routes that occur in an ethylene cracker.

Increasing product complexity and divergence

A typical manufacturing process, such as making a car, converges as you progress down the value chain. As illustrated by Figure 2-3, multiple individual components (which are produced from a huge variety of raw materials) are assembled into a single product.

In the chemicals industry the opposite occurs. From a handful of source materials an increasingly large number of products can be made. The sector produces thousands of different chemicals – some used as products directly, but many are inputs for other further manufacturing of a diverse range of items.

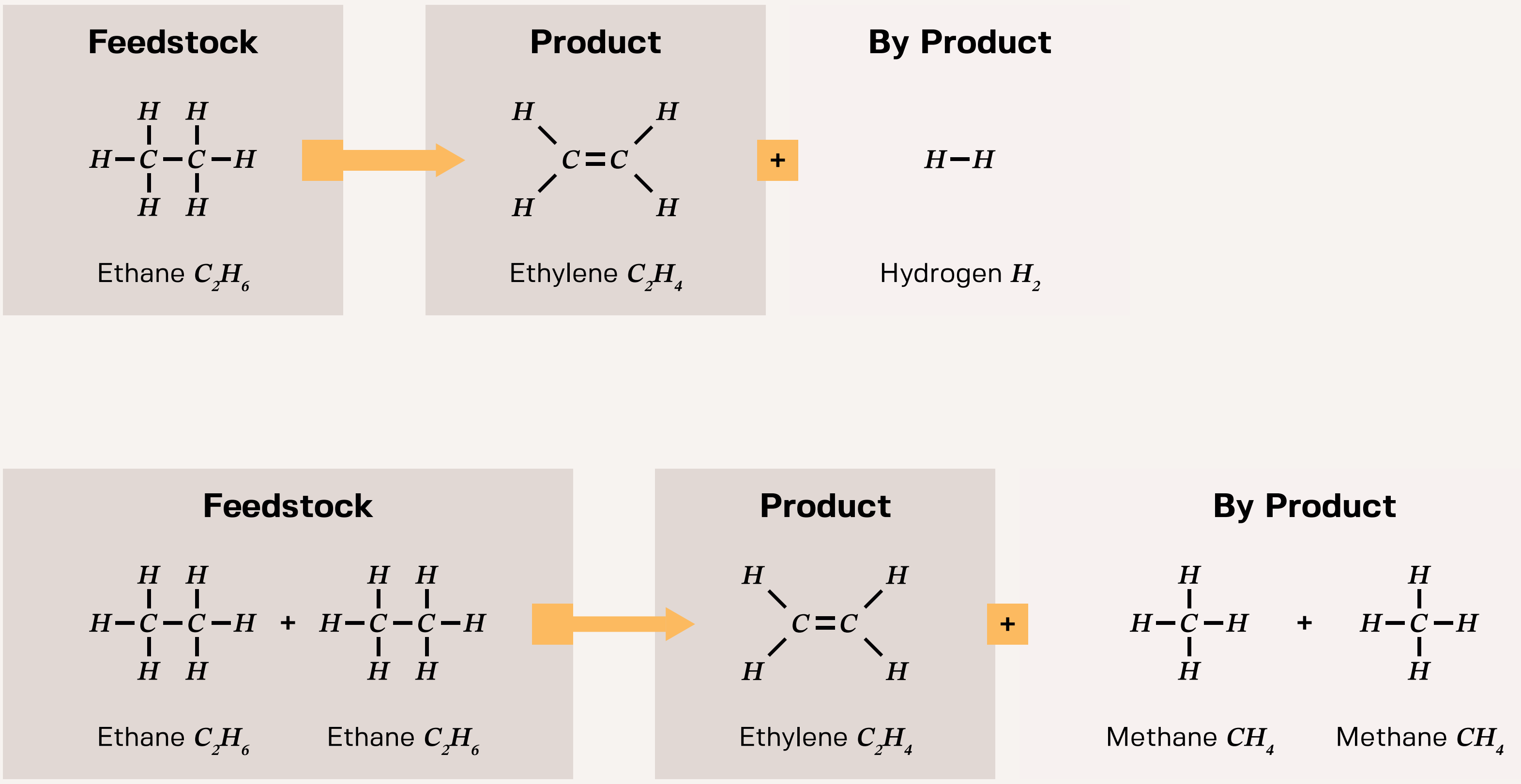


Figure 2-2: Chemical equations showing two of the many potential by-products of ethylene production

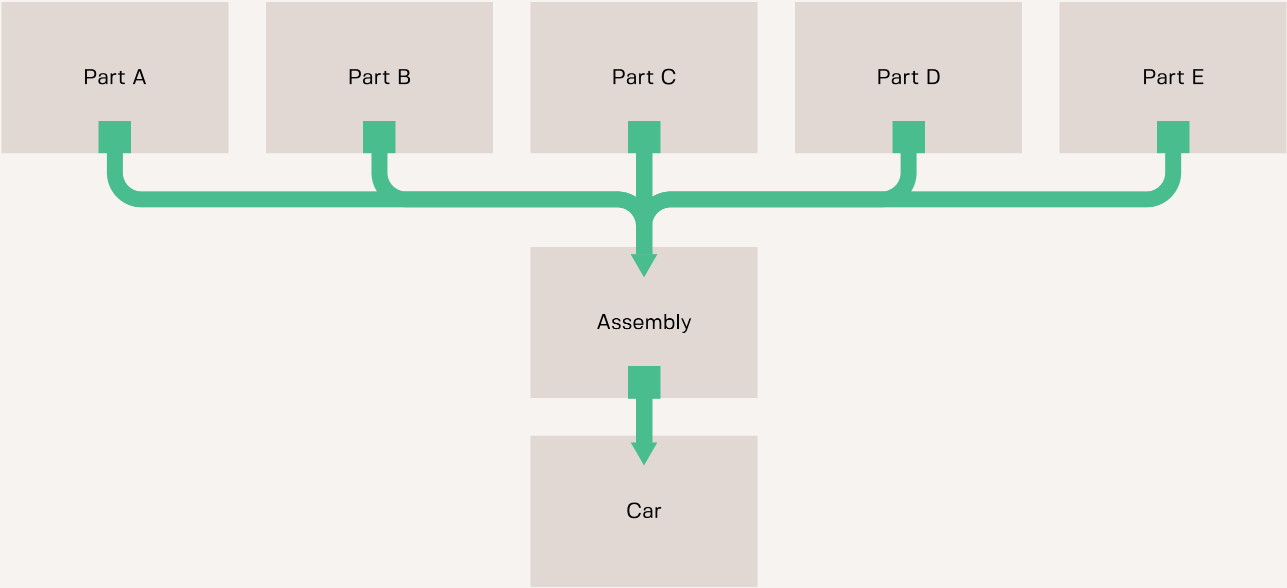


Figure 2-3: Generic car assembly process

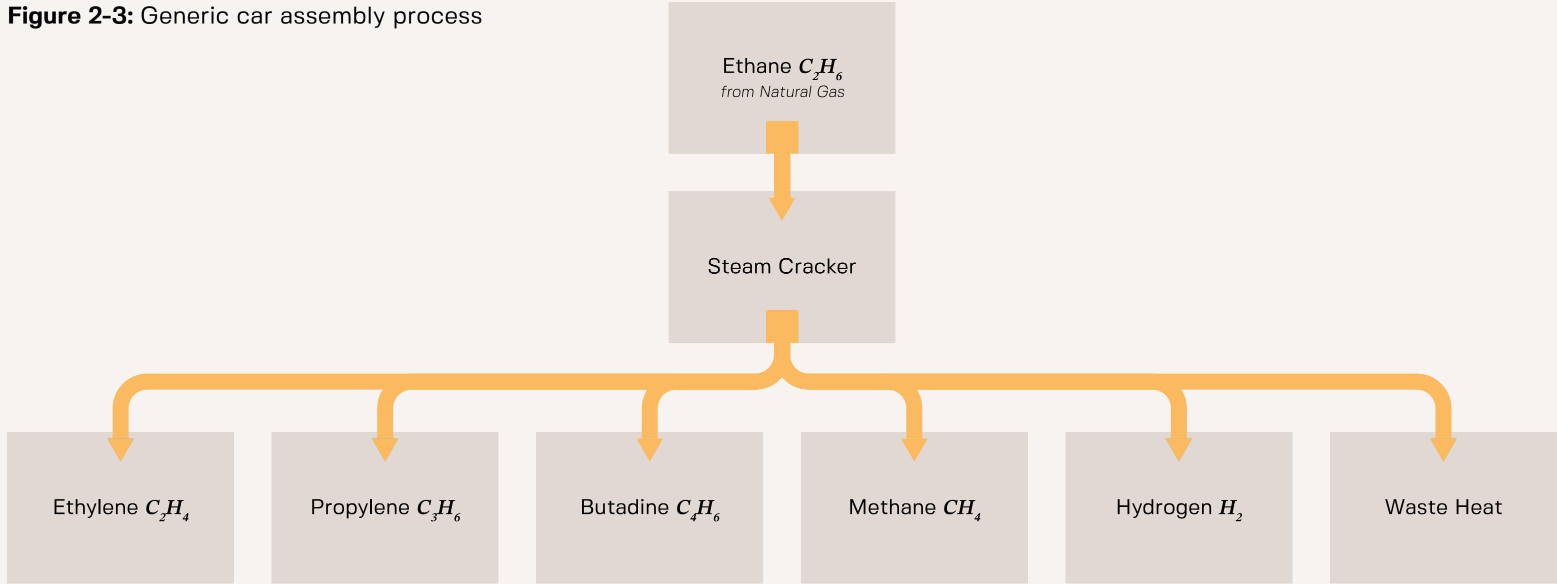


Figure 2-4: Ethylene production via natural gas showing diversity of by-products

By-products are inevitable

Alongside the desired and intended products, multiple by-products are inevitable and unavoidable. In other industries this rarely happens – generally a product is made, there may be waste material (e.g. remnants of cloth in clothing manufacture) but not the creation of a secondary product and waste energy which then require handling. You don't accidentally make Minis when you are trying to make BMWs, but you can't avoid making methane, hydrogen and propylene when you are trying to make ethylene.

Businesses work hard to optimise production levels to maximise the products they do want, but there will always be unwanted products that have to be dealt with. These cannot be treated as effluents or waste (because of the volumes, toxicity and danger that would be associated with doing so), so need to be put to some sort of productive use.

Everything has to go somewhere

Often a by-product can be and is utilised by other chemical companies as a feedstock for other production processes. They can also sometimes be used as a means of generating energy for use within the plant or by other companies within a cluster. For example, the methane produced as a by-product of ethylene production is usually burned to create energy which drives the reaction (chemical thermodynamics) and powers the refrigeration compressors on the plant. The butadiene by-product normally becomes the feedstocks for other processes that produce a variety of materials including rubber.

Thermodynamics

From an energy and thermodynamics perspective the petrochemical industry requires significant energy input to enable the chemical reactions to occur and to drive the separation and purification processes. A typical ethylene cracker requires 300-500MW of energy – equivalent to the amount generated at one of the largest offshore windfarms in the UK.

Burn or convert

For every molecule produced within a plant, there is a choice to sell, convert or burn it. This will depend on the molecule, its value to the company and its value to others. The economics of running the plant is a significant factor in deciding what happens. The decision for the primary product is simple, but by-products may be further converted within the business, burned to generate energy within the plant, or sold to other companies for use as feedstock or energy source. Waste heat can also be used internally to generate energy or sold to others.

In the case of an ethylene cracker, once it is up and running, this energy is provided from combustion of by-products or utilising waste heat from its own production processes. Generally speaking, the petrochemical industry has evolved to be largely self-sufficient in terms of satisfying its energy consumption needs – albeit different processes vary in the extent to which they are net energy consumers or producers. This re-use and recycling of materials is cost effective and means minimal additional energy input is required from the national energy infrastructure.

Profoundly interconnected

This shows why the petrochemical value chain is so interconnected - products from one plant become feedstock in others, by-products can be used as raw materials or burned, and waste energy from one plant can be used within it or sold on to others. These interconnections have encouraged the development of petrochemical clusters in many regions which are optimised to deal with all the products, by-products and waste energy streams generated. These interconnections must be considered when making changes to the system – removing one element may cause more problems than it resolves.

Mitigation options require a systems approach

With such an interconnected industry, mitigation options and adaptations have to be considered from a systems perspective to maximise impact. A change in one area is likely to also have an effect in another and this could be positive or negative. Understanding these interactions can improve the overall impact of mitigation actions and help avoid unintended consequences.

The complexity can be illustrated by considering some typical mitigation approaches, and the challenges these face within the petrochemical sector:

Electrification

Switching the energy source from hydrocarbon to electricity appears on the face of it to be a good solution. However, for the petrochemical industry this is less straightforward.

Currently, most plants utilise waste heat and by-products to generate energy to satisfy most of their process energy demands. This is cost effective and means that consumption from the national energy grid is relatively small.

Using electricity from external sources will place a significant additional burden on the grid. This would require massive scale up of renewable infrastructure to be able to meet these needs from green sources. It will also increase overall production costs for the company.

Whatever the source of energy utilised, by-products will still be produced and will still need to go somewhere. If they aren't needed for energy generation, something else will have to be done with them, which may require additional energy or result in more emissions.

Allocation of emissions

In many industries, it is possible to quantify the emissions associated with the production of a product. For example, in car manufacturing it is relatively straightforward to add up all the emissions from the production of the different components to estimate the embodied carbon in a vehicle. For chemical products it is less simple as there are products, by-products and waste heat and methods of attribution could be by mass, value or some other pro-rata basis. Equally the load could all be put onto the primary product with none associated with by-products but given many of these then become feedstock in other chemical manufacturing this approach is questionable. The difficulty of allocation also makes it problematic to claim emissions reductions related to particular chemicals and suggests that it is only really possible at a system-wide level.

Carbon is only problematic when emitted

It is important to remember that carbon only produces emissions such as CO_2 or methane when it is burned. While the carbon remains in the product it is not problematic from a GHG perspective.

The principle is that any production process that uses a hydrocarbon as a feedstock should be incentivised and encouraged to keep as much of the input carbon in the product as possible and discouraged or prohibited from allowing carbon leakage in effluent or fuel streams. The potential for mitigating GHG emissions from any production process can be measured by the proportion of carbon that is not retained within a product. This inevitably calls into question any production process using hydrocarbons as a raw material to produce a product with zero carbon content.

This highlights the importance of the C-THRU project to identify viable and realistic approaches that maximise the impact of mitigation options for the petrochemical industry *(See Chapter Four).*

B. Life cycle stage

Key points:

- Current data collection methods make it is extremely difficult to accurately and extensively account for all emissions across all life cycle stages for petrochemicals.
- Emissions can be found at each of the three life cycle stages: production (extraction and refining; conversion), use, and EOL. Emissions are often embedded and therefore more likely to be released at a different stage downstream.
- Significant emissions within petrochemicals' life cycles are produced at different stages depending on the petrochemicals and processes involved. For example, GHG emissions from nitrogen fertilisers predominantly arise from their use phase, whereas most plastics' GHG emissions are released during the production phase.

Petrochemical sector emissions consist of two main types: energy-related and process, accounting for 85% and 15% respectively. Energy-related emissions are released when fuel is combusted on-site to generate direct heat and steam (direct) or combusted upstream to generate electricity (indirect). Process emissions (0.2 GtCO_2 or 15%) result from the chemical reactions and reflect the difference in carbon content between ***feedstocks*** and products (e.g. natural gas feedstock ($CH_{3.951}$) ammonia product (NH_3))[1].

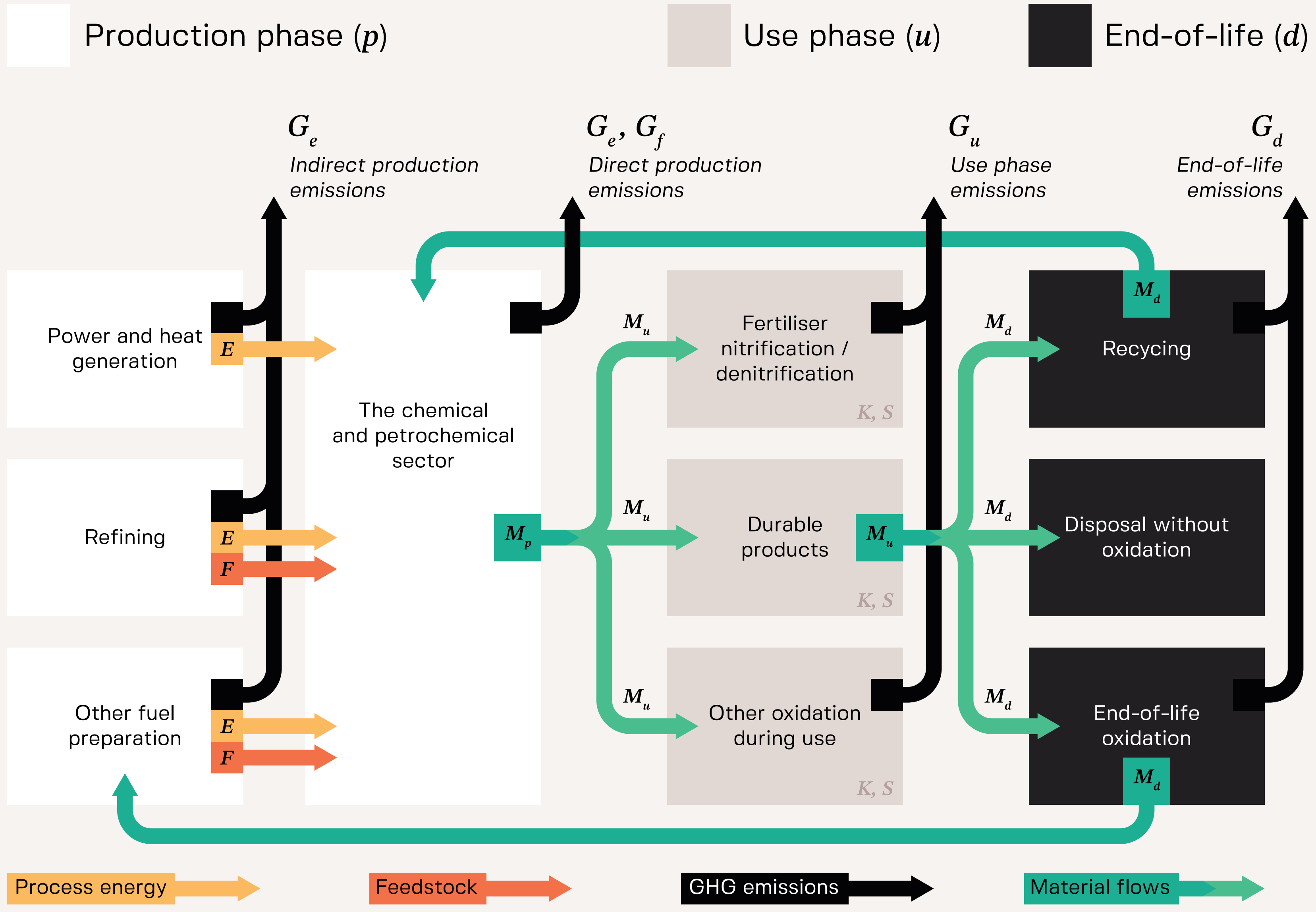


Figure 2-5: Representing emission sources throughout the life cycle of chemical products

Feedstocks

Feedstocks refers to raw material input to a process, which is converted into a chemical product. Feedstock materials are not combusted in the process, but can be chemically transformed. Petrochemical feedstocks include fossil fuels (oil, gas, coal, refinery products) and bio-materials.

Emission type	Emission source	Definition	GHGs
Energy-related emissions	Stationary Combustion	Emissions from fossil fuel combustion during oil refining and petrochemical raw material production	CO_2 CH_4 N_2O
	Mobile Combustion	Emissions generated in fuel combustion and evaporation from all mobile devices in transportation activities	
	Flares	Emissions from devices for flame spray combustion or incineration in the disposal of waste natural gas and hydrocarbon	
	Fugitive Emissions *(i.e. methane emissions)*	Emissions from the petroleum system, storage losses, pipeline breaks, etc	
	Emissions from the petroleum system, storage losses, pipeline breaks, etc	Emissions generated in power generation relevant to the net purchased electricity consumed by companies	
	Process heat/steam imports *(Indirect emissions)*	Emissions produced in heat generation relevant to the net purchased heat consumed by companies	
Industrial Process and Product Use Emissions	Petrochemical Manufacturing Process Emissions	Emissions generated in chemical interactions during the manufacturing processes of petrochemical products, for example cracked gases such as CO_2 generated during ethylene manufacturing by steam cracking and CO_2 emissions in hydrogen and oxidised asphalt manufacturing	CO_2 CH_4
	Catalytic Cracking & Catalytic Regeneration	Emissions generated in catalytic cracking & catalytic regeneration	CO_2 CH_4 N_2O
Waste Treatment Emissions	Waste Treatment and Disposal	Emissions from waste treatment in incinerator, bio-degradation plant or sewage treatment plant	CO_2 CH_4 N_2O

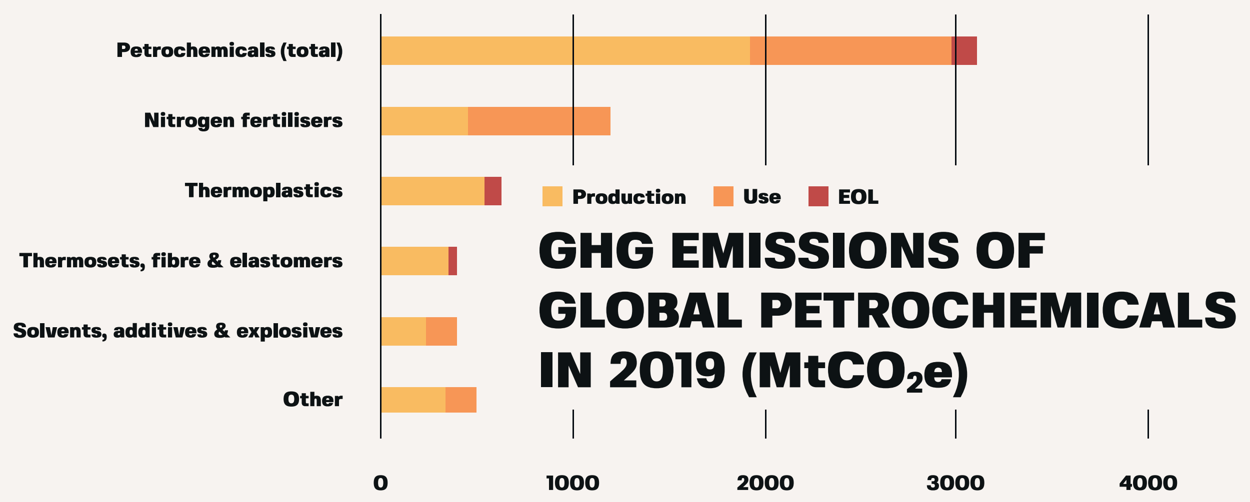
Table 2-1: Classification of GHG emission sources from the petrochemical industry

However, if we look across all life cycle stages of petrochemical products, we find additional GHG emissions from the extraction of feedstock chemicals and fuels, and in the use phase and the EOL treatment of petrochemical products. These related emissions are often overlooked because they are beyond the production boundary for chemical firms, and more difficult to delineate by chemical product. A more holistic view of emission sources across the sector is shown in Figure 2-5, with additional detail in Table 2-1.

Accurate emissions accounts that cover all life cycle stages, and the full range of chemical products, are challenging to compile because of how emissions data are currently collected and compiled. Emissions related to chemical production processes can be collated relatively simply from production facilities by product and aggregated for country level emissions accounts. However, fugitive emissions during extraction and emissions released in the use phase (i.e. emissions from the application of fertilisers) and EOL treatment emissions (i.e. from incineration and landfill emissions) are not well delineated, being reported as a single account, which makes it difficult to allocate these to specific chemical products.

There is currently an incomplete picture of where emissions occur.

Figure 2-6 illustrates our preliminary estimation of emissions in the global petrochemical sector in 2019. We find for nitrogen fertilisers about 1/3 of emissions come from production and 2/3 from use phase. For plastics, over 2/3 of emissions are from production and the remaining from the end of life. It should be noted that EOL emissions are those that occur during or after disposal of chemical products and only durable products (i.e. plastics) are considered to have emissions associated with their disposal.



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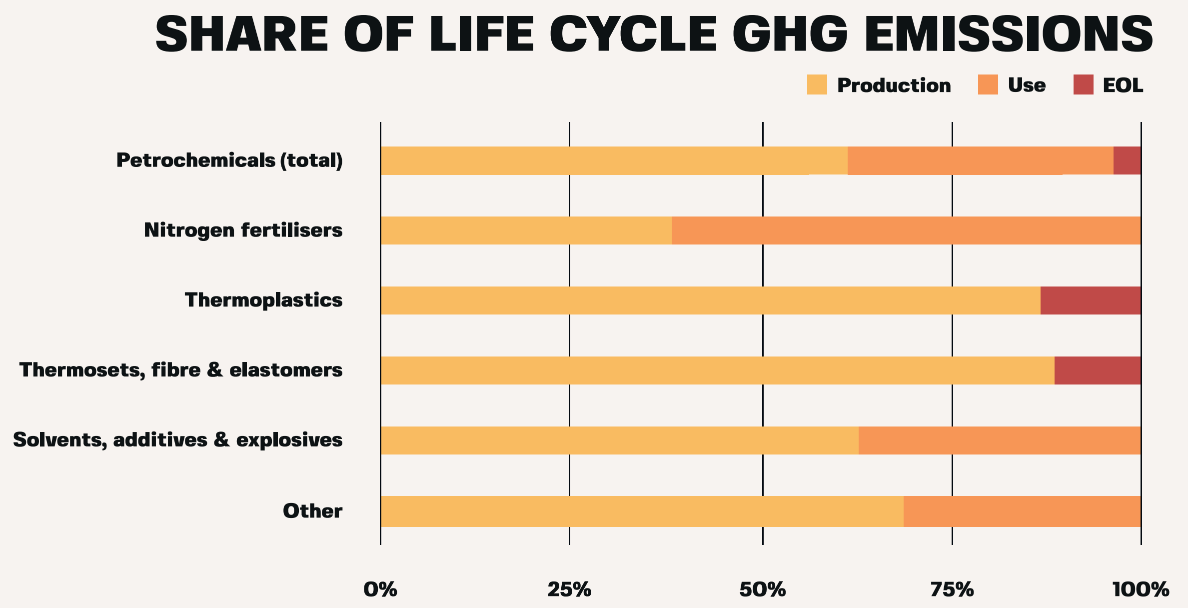

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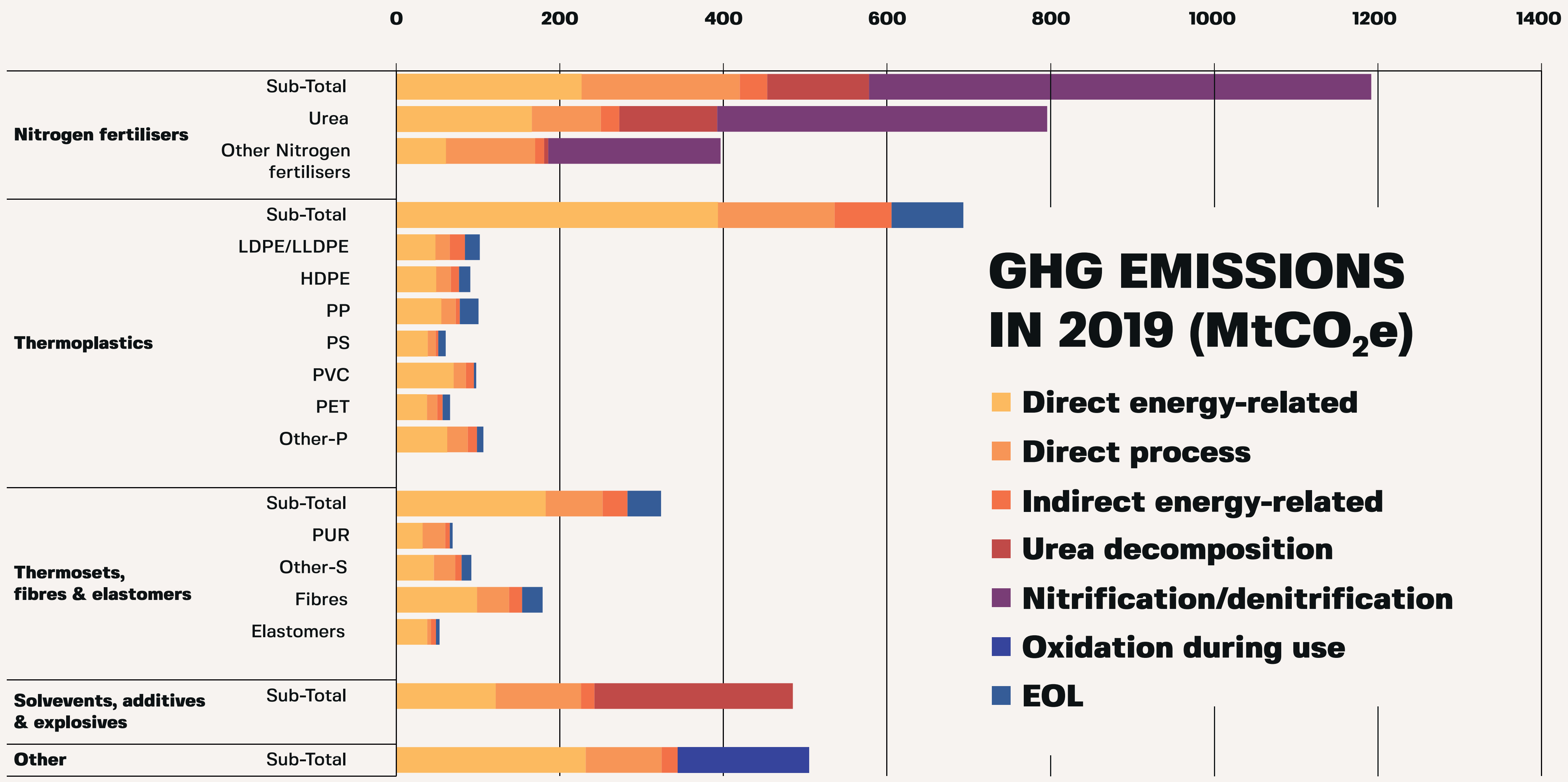

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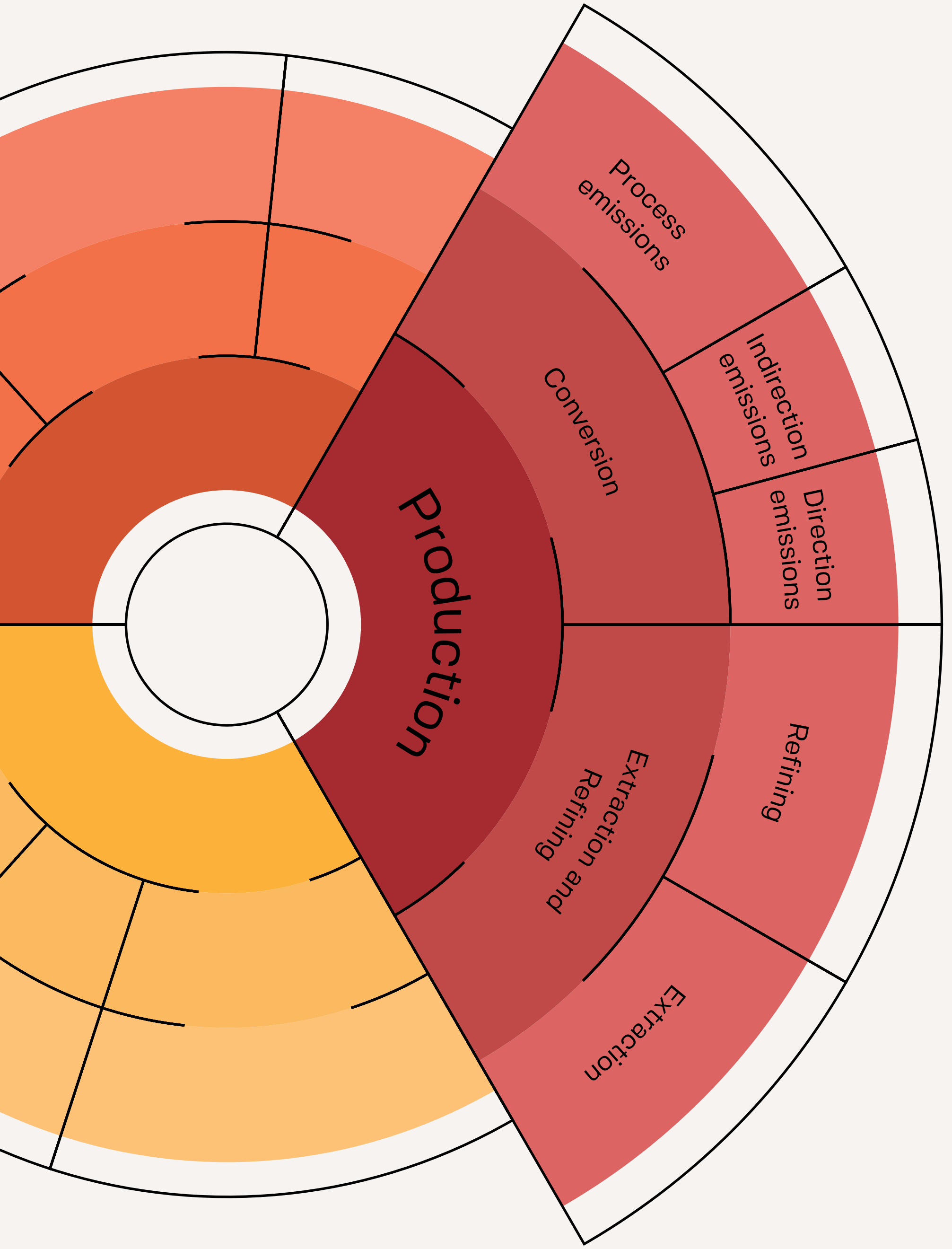
Figure 2–6: Estimation of emissions from the global petrochemical sector in 2019: a) absolute emissions, b) relative emissions, c) breakdown emissions. *Note: 1) Production emissions include extraction and refining, and conversion from process emissions, direct energy-related emissions and indirect energy-related emissions. 2) Use phase emissions for durable chemical products are assumed to be nil. They include urea decomposition, nitrification/denitrification, oxidation. 3) Only durable products (i.e. plastics) are considered to have emissions associated with their disposal. Durable product EOL emissions stem from recycling, incineration with/without energy recovery and landfill. Global average incineration (22%), recycling (10% collection rate and 51% yield rate) and landfill rates are used. No emissions resulting from landfill of durable chemical products are accounted. The assumed average efficiency of waste-to-energy plants (facilities producing electricity only are assumed for simplicity) is 21%. The average emissions intensity of grid electricity is 518 gCO_2e/kWh for production and energy recovery estimation.*



Production: extraction and refining emissions

The first GHG emitting phase in the life of a petrochemical product comes during resource extraction. During the extraction of petrochemical feedstocks (coal, oil and natural gas), fugitive emissions are released into the atmosphere. The Intergovernmental Panel on Climate Change (IPCC) indicates fugitive emissions from oil and gas activities may be attributed to the following primary types of sources:

- fugitive equipment leaks
- process venting
- evaporation losses
- disposal of waste gas streams (e.g. by venting or flaring)
- accidents and equipment failures

Fugitive emissions, which also occur downstream as oil and gas are moved, refined and used, are mostly methane. Methane is found in coal, oil and natural gas deposits and is released during the mining or extraction process.

In addition to fugitive emissions, resource extraction produces direct and indirect emissions through its energy intensive operations. Direct emissions occur when operators combust fuels to produce the energy for powering equipment. The chemical composition of direct emissions depends on the type of fuel, but the GHG component is mostly carbon dioxide. When operators rely on grid energy to power operations, indirect emissions are generated. As with direct emissions, the type of fuel used to generate the power determines the composition of emissions, with carbon dioxide representing the most significant GHG component.

In addition to methane and carbon dioxide, upstream resource extraction contributes to the greenhouse effect by emitting volatile organic compounds such as carbon monoxide and dinitrogen oxide. When considering the impact of petrochemical manufacturing it is important to consider the impact of these gases.

The refinery stage in the life cycle is the third largest global source of *stationary GHG emissions*,

accounting for 40% of emissions from the oil and gas supply chain and 6% of all industrial GHG emissions[2]. Refineries process natural gas and crude oils into petroleum naphtha, gasoline, diesel fuel, asphalt base, heating oil, kerosene, liquefied petroleum gas, jet fuel and fuel oils. Refineries produce emissions from venting, flares, and fugitive leaks. Thus, the composition of gases emitted from refineries often varies based on the crude input and refining process adopted.

Jing et al., (2020) categorises oil and gas refineries into four types: hydroskimming, medium conversion, deep conversion (coking) and deep conversion (hydrocracking) refineries, which are deployed in 37, 59, 34 and 8 countries and have global volume shares of 7%, 44%, 45% and 4%, respectively. Carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O) are important sources of GHG emissions from refining activities. Fugitive CH_4 emissions occur from process equipment leaks, asphalt blowing and blowdown systems. CO_2 is released during the flaring of methane often to alleviate safety concerns associated with equipment malfunction, gas purging to stop air entering the fuel gas system, and from the energy production processes required to power refineries. N_2O is also produced in combustion reactions occurring at refineries. On average, 95.6%, 4.0% and 0.4% of global refining ***global warming potential (GWP)*** is generated by CO_2, CH_4 and N_2O, respectively.

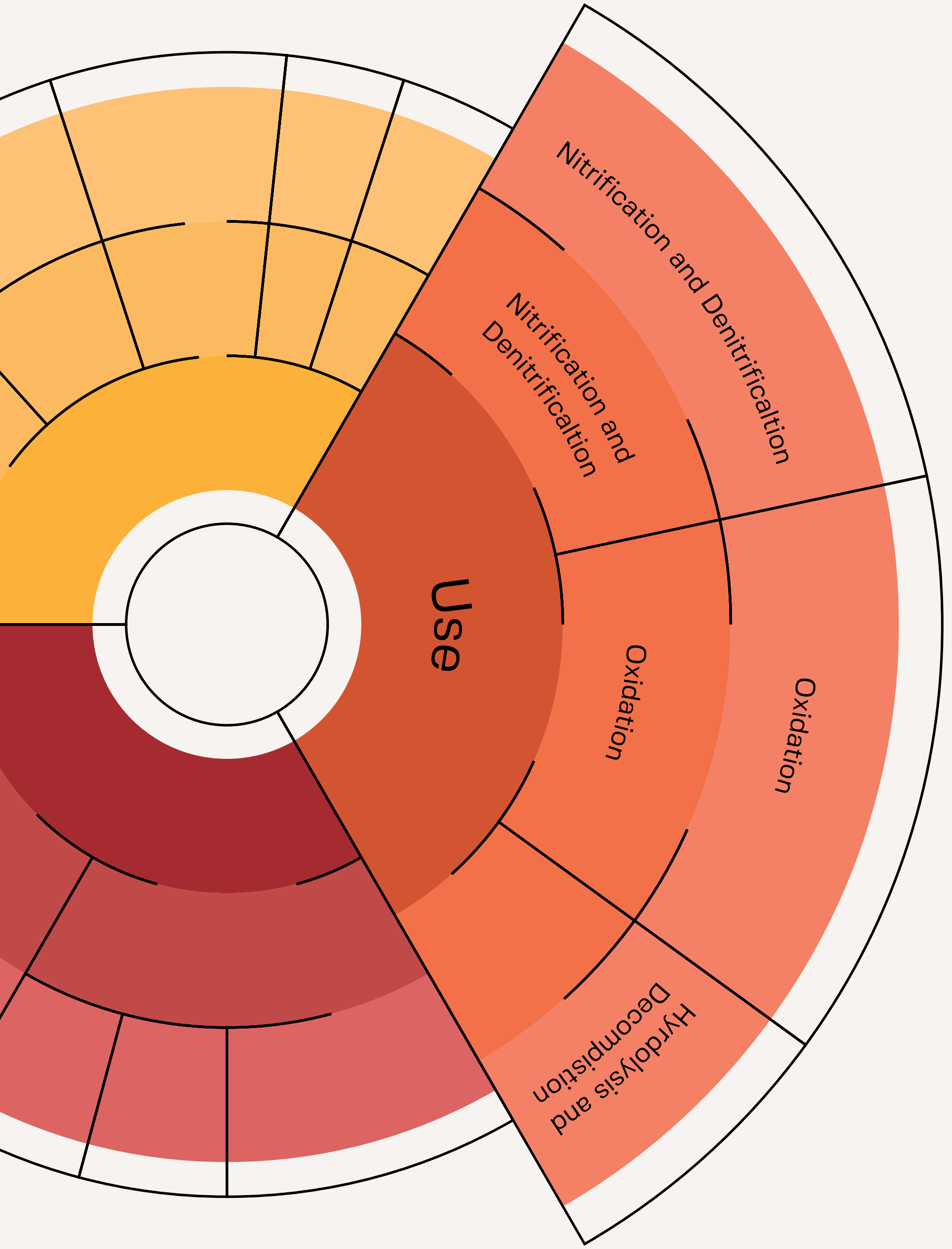
The proportional contribution from each gas changes from crude to crude and refinery to refinery.[3]

Stationary GHG emissions

Emissions from fossil fuel combustion during oil refining and petrochemical raw material production.

Global Warming Potential (GWP)

Global warming potential is a measure of how much energy the emissions of 1 tonne of a gas will absorb over a given period, relative to the emissions of 1 tonne of carbon dioxide (CO_2). Two time periods are commonly used for GWPs: 100 years and 20 years. Over 100 years, CO_2= 1 GWP, methane (CH_4)= 28 GWP, nitrous oxide (N_2O)= 265 GWP.



Production: conversion emissions

Conversion emissions result from the chemical processes which convert input materials and energy into chemical products. They are sometimes called production emissions or process emissions (confusingly). Conversion emissions are commonly divided into three categories: process emissions, direct energy-related emissions, and indirect energy-related emissions:

- Process emissions result from the chemical reactions in conversion processes, which convert reactants (input materials and energy) into products, by-products and losses. CO_2 is a common by-product/loss from chemical reactions, with CO_2 from ammonia manufacture being particularly significant. Process emissions are calculated by performing a carbon balance across the process, and multiplying the lost carbon by ~3.7 (molar mass difference of C and CO_2) following the IPCC's Tier 2 methodology.[4]
- Direct energy-related emissions stem from the combustion of fuels (i.e. natural gas, oil, naphtha, ethane, methane) to produce direct heat and steam used to drive chemical processes. Tables of emissions intensity for different fuels ($kgCO_2e$ /kJ) are used to calculate the emissions from fuel combustion.[5]
- Indirect energy-related emissions are produced in the upstream generation of electricity and refining of fuels, which are used in chemical production facilities. Emissions are estimated using country-based average emissions intensities for electricity ($kgCO_2$ /kWh) and various fuels ($kgCO_2$ /kJ fuel), or from measured data where electricity is generated on-site.

Use phase emissions

Significant portions of embedded feedstock are released during various chemical reactions, either in the use or EOL phases of a chemical product's life cycle. Other elements, mainly nitrogen but also sulphur and chlorine, enter the supply chain upstream and become temporarily embedded in products, leading to emissions downstream at a later stage.

There are three main reaction mechanisms that lead to GHG emissions during the use phase of the life cycle of chemical products:

- CO_2 emissions from the ***oxidation*** of chemical products during use. An example chemical might be an explosive, such as ammonium nitrate, or a fuel additive such as methyl tert-butyl ether.
- CO_2 emissions from the ***hydrolysis*** and decomposition of carbonaceous fertilisers. The CO_2 content of urea, for example, is released as it decomposes when it is applied to soils to deliver nitrogen.
- N_2O emissions from ***nitrification*** and ***denitrification*** of nitrogen fertilisers, occurring both directly and indirectly, from ***volatising*** and ***leaching***. This applies to all the fertilisers in this analysis, as they are all nitrogenous.

Oxidation

The process or result of oxidising or being oxidised. Chemical oxidation is a process involving the transfer of electrons from an oxidising reagent to the chemical species being oxidised.

Hydrolysis

The chemical breakdown of a compound due to reaction with water. Urea hydrolysis is a chemical reaction that occurs in soils, the human body, and in wastewater urine diversion systems. The reaction, which transforms the urea into ammonia and bicarbonate, results in ammonia volatilisation and mineral scaling in bathroom fixtures, piping, and storage tanks.
Urease: $(NH_2)2CO + H_2O \rightarrow CO_2 + 2NH_3$

Nitrification

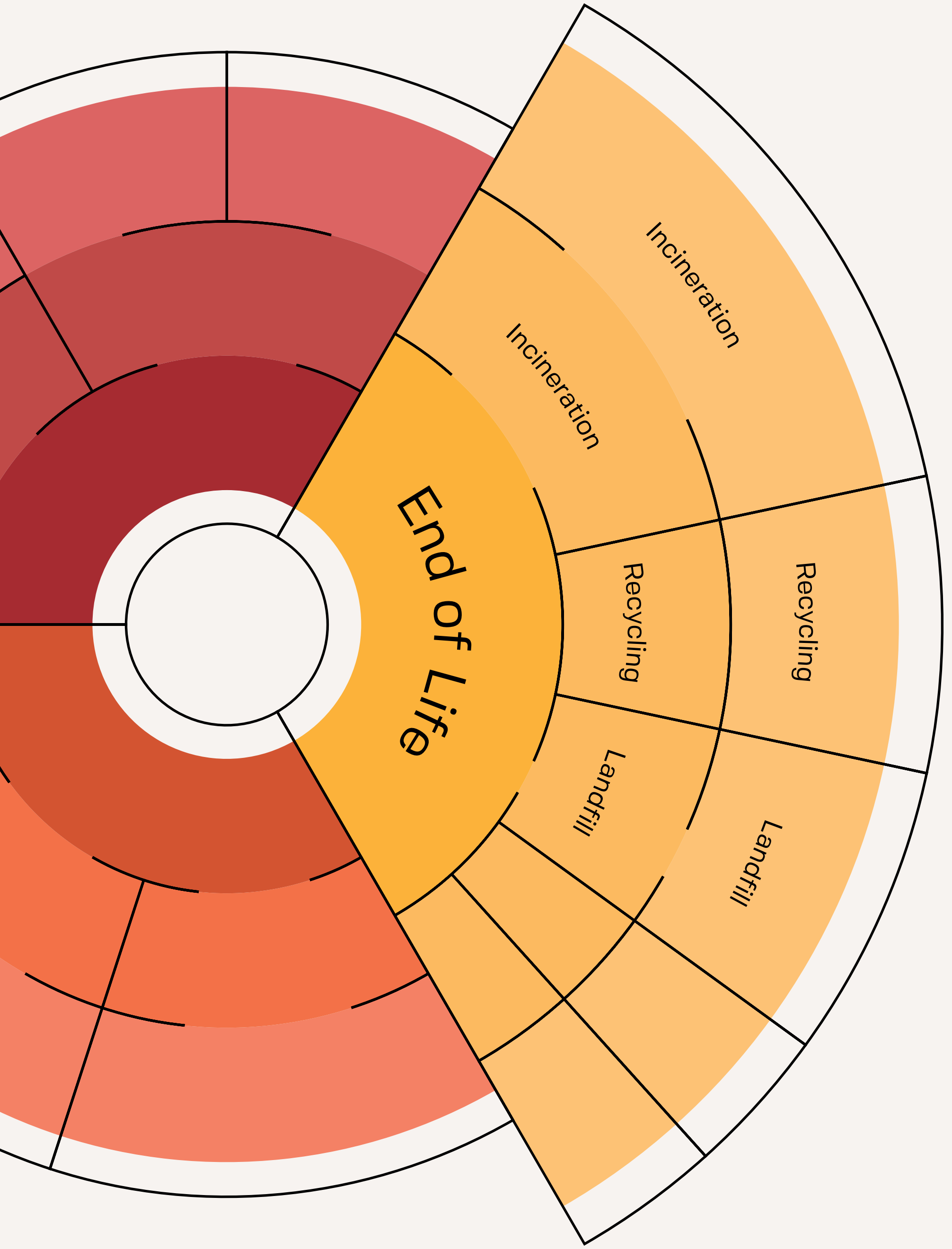
The process in which bacteria in the soil use oxygen to change compounds of nitrogen in dead plant material into nitrates which plants can then absorb as food. Denitrification is the anaerobic microbial reduction of nitrate to nitrogen gas (N_2).

Volatilising

Nitrogen is lost as ammonia (NH_3) *gas – this could either happen when ammonia is directly applied to the field as fertilisers, as a proportion "evaporates" instead of being absorbed by the soil, or when excess from other nitrogen fertilisers is transformed into gaseous ammonia through processes in the soil and released to the atmosphere. Refer to Figure 2-10*

Leaching

Soil does not retain nitrate particles well, as both are negatively charged. Consequently, nitrate moves easily with water and can be washed away by rainfall into nearby streams and rivers.



End-of-life emissions

End-of-life (EOL) emissions are those that occur during or after disposal of chemical products. The EOL treatment for most products is considered the responsibility of governments or municipalities, and often EOL treatment depends on the systems set in place by local municipalities and user behaviours. Only durable products are considered to have emissions associated with their disposal (as opposed to during production or use phase). Durable product EOL emissions stem from landfill, recycling, and incineration. Some EOL emission quantities may be net negative, meaning the disposal method results in emissions savings, primarily due to emissions avoided from energy (incineration with energy recovery) or virgin materials (recycling) replacement.

For some durable chemical products, such as inert, non-biodegradable plastics, landfill may offer a haven for the carbon embedded in the feedstock used to make them – a form of carbon capture and storage, perhaps. However, most carbon containing compounds oxidise eventually, and

there is the additional risk of chemical products decomposing anaerobically, leading to methane (CH_4) emissions that are 28 times more potent than CO_2.

C. Chemical products

Key points:

- **Production of primary chemicals (ammonia, methanol and HVCs) accounts for around two thirds of total energy consumption and around 60% of the total CO_2 emissions in the chemical industry.**
- **Plastics such as thermoplastics, thermosets, fibres, and elastomers mostly produce emissions during the production phase. In this phase, processes such as steam cracking are used. Steam cracking is the most energy consuming petrochemical process and the largest direct source of emissions in the plastic life cycle. At the EOL phase, all standard methods of disposal (incineration or landfills) or recycling are either energy intense or economically non-viable.**
- **About 2/3 of nitrogen fertilisers' emissions are from the use phase (738 Mt CO_2e in 2019). Indirect nitrogen fertilisers' emissions come from volatilisation and leaching.**
- **Solvents, additives, and explosives release most of their emissions during the production phase.**
- **Various production routes and technologies are implemented depending on the availability and cost of feedstocks in each region.**

Given the variety of materials and production methods used in the petrochemical sector, meaningful discussion of production emissions needs to occur at a material or product level. In this section, we explore in more detail the sources of emissions released in the petrochemical sector. The petrochemical sector can be divided into five categories of chemical products: thermoplastics; thermosets, fibres and elastomers; nitrogen fertilisers; solvents, additives and explosives; and other chemicals. The main chemical building blocks of the petrochemical industry, the precursors to these chemical products, include the following platform chemicals (also called primary chemicals): ammonia, methanol, ethylene, propylene, benzene, toluene and xylenes.

Primary chemicals for chemical products

Despite the diversity and complexity of the processing routes and products in chemical sector, seven large volume chemicals, i.e. ammonia, methanol, and high-value chemicals, HVCs (ethylene, propylene and the aromatics including benzene, toluene and xylene (BTX)), are the key building blocks for the sector's bulk products. For instance, ammonia is the key chemical in the production of all nitrogen-based fertilisers, while HVCs are processed for producing plastics, synthetic fibres, and rubber (with ethylene and propylene mainly for polyethylene and polypropylene production, and BTX for producing polymers like polystyrene, polyurethane, and polyesters). Producing these chemicals (as the most energy- and emission-intensive products) accounts for around two thirds of total energy consumption and around 60% of the total CO_2 emissions in the chemical industry[1]. As well as within the chemical sector, the energy and emission intensities of producing primary chemicals are considerably high compared to other heavy industrial sectors (Figure 2-7). Ammonia production has the highest contribution to emissions within the chemical sector, at 450 Mt CO_2 in 2020, while producing methanol and HVCs contributes for further 220 Mt CO_2 and 250 Mt CO_2, respectively.

To quantify the global energy use and greenhouse gas emissions associated with manufacturing these products, developing a unit process model library is one of the main objectives of this work to simulate their production pathways in different world regions and to be considered as a basis for identifying viable mitigation options. To this aim, understanding the current state of production technologies for major chemicals is a necessary first step. Accordingly, we mainly focus on reviewing current production technologies and feedstock types for the primary products in different regions.

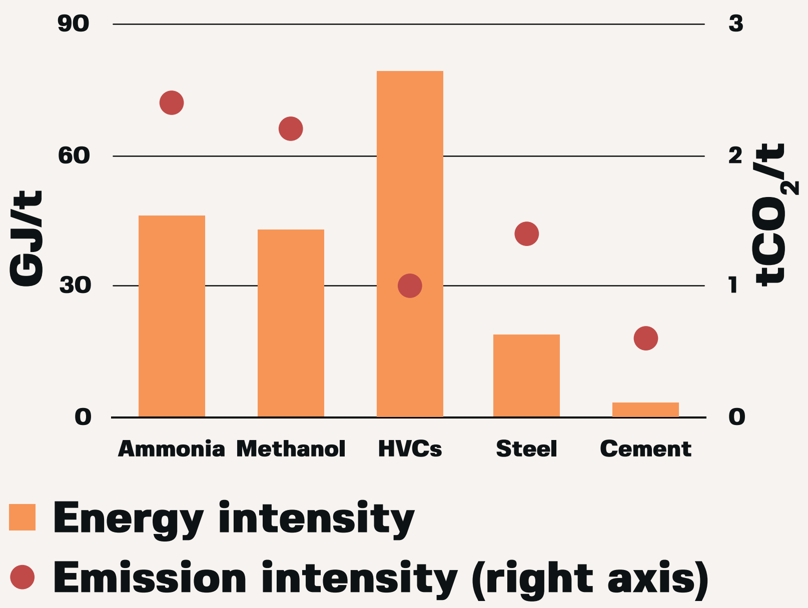


Figure 2-7: Comparative energy and emission intensities of primary chemicals production

Spatially, various feedstocks and technologies are implemented for these chemicals, which mainly depend on the availability and cost of feedstocks in each region. Chemical feedstocks, mainly fossil fuel-derived, account for more than half of the total energy inputs to the chemical sector globally. The input oil, mainly in the form of ethane or naphtha, is mostly (more than 90%) used for producing HVCs (ethylene, propylene and BTX), while minor amounts are used for methanol and ammonia production. Around a quarter of natural gas feedstock is used to produce methanol and the rest is used to produce ammonia. Coal feedstock is used for producing methanol and ammonia in approximately same proportions[1]. The main production routes for the primary chemicals are shown in Figure 2-8, and briefly explained as follows.

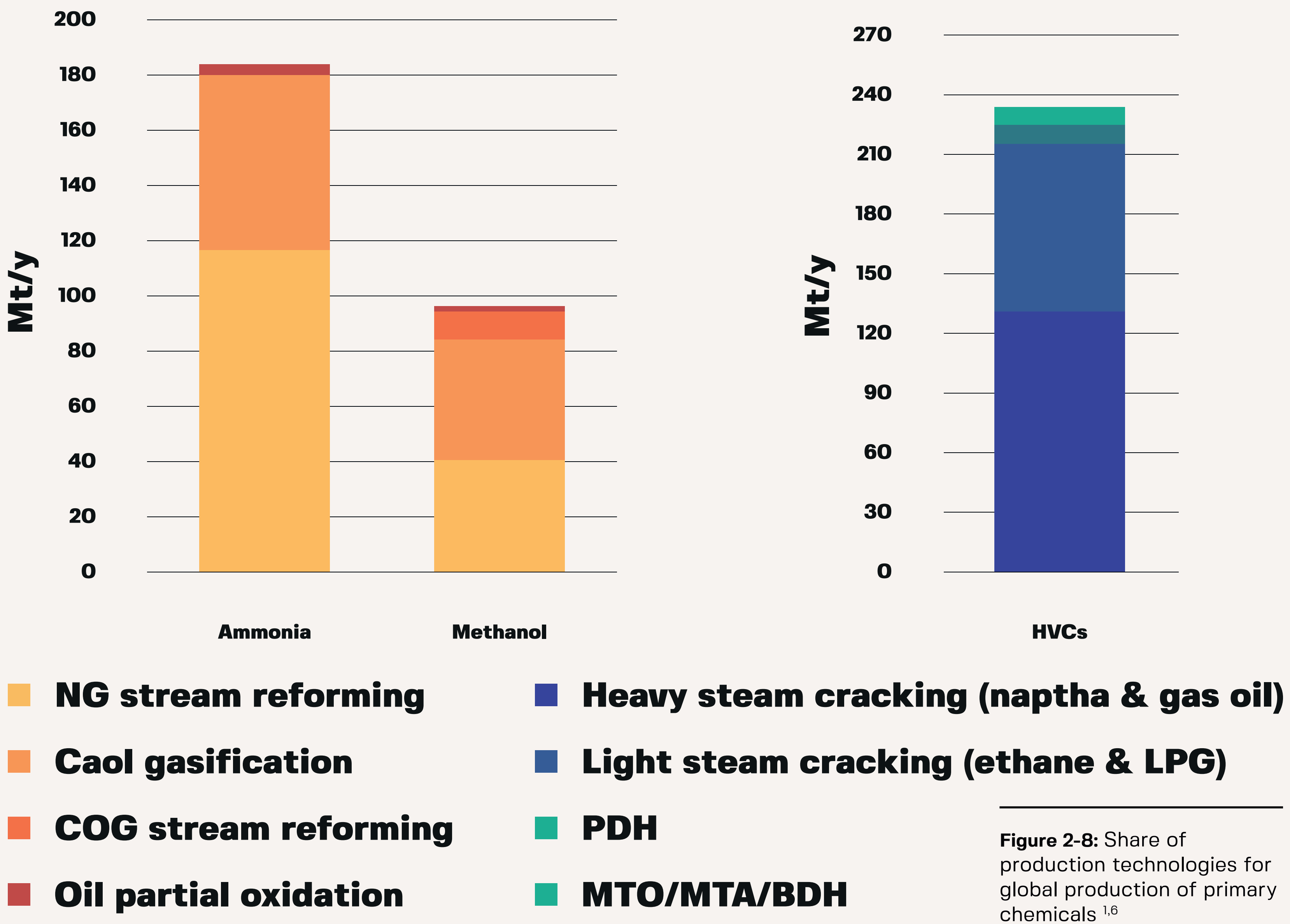


Figure 2-8: Share of production technologies for global production of primary chemicals [1,6]

Approximately 185 million tonnes of ammonia are produced globally per year (Mt/y), which are mainly utilised for producing fertilisers (e.g. urea). Among the various chemical products, ammonia is essentially decoupled from the rest of the petrochemical sector and is itself highly integrated due to the common petroleum feedstock. Regardless of the feedstock type, the process of ammonia production can be divided into sections to produce synthesis gas (syngas) containing hydrogen, carbon monoxide and carbon dioxide followed by the Haber-Bosch process for ammonia synthesis.[7] There are three key processes for producing ammonia synthesis gas:

- steam reforming of natural gas (with the highest share of production, 72%)
- coal gasification (26%)
- partial oxidation/steam reforming of oil feedstocks such as naphtha, LPG and fuel oil (2%)

North America, Europe and the Middle East favour natural gas steam reforming as the dominant ammonia production technology. Whilst China, which contributes to around 70% of Asia Pacific's ammonia production, produces its ammonia via the coal gasification technology due to its abundance of coal. Ammonia production is responsible for around 49% of total CO_2 emissions from primary chemicals production, in which the coal-based route has 2.5 times higher CO_2 intensity than the natural gas-based route. [1,8]

The process generally involves units for syngas generation, syngas purification and ammonia synthesis. Syngas generation units include reformers (for natural gas and lighter oil feedstocks) or gasifiers (for heavy oil and coal) to produce syngas ($xCO + yH_2 + zCO_2$), followed by water-gas shift (WGS) converters for increasing the hydrogen content of the syngas through CO conversion. The purification part involves units for removing CO_2 (mainly through chemical/physical absorption) and other impurities (e.g., by methanation or cryogenic purifiers). The required nitrogen is supplied by the process air input to the reformers (in steam reforming process), or from an air separation unit (in partial oxidation/gasification). [9] The ammonia synthesis includes units for purified syngas compression to high pressure (150-350 bar), ammonia conversion (hydrogen reacting with nitrogen on an iron catalyst) and ammonia separation (e.g., by an absorption refrigeration unit). Ammonia conversion is approximately 20-30% per pass requiring unreacted gases to be recycled within the synthesis loop for higher overall conversion. Within the whole process, the synthesis gas generation step requires the most energy (60-70% of total energy consumption). For this reason, the energy requirement of a specific technology mainly depends on the feedstock employed (e.g. syngas production with heavier and solid feedstocks like coal has higher process energy intensity due to the extra energy required for processing the feedstock).[10]

Methanol is a key compound for producing a variety of chemicals (e.g., plastics, plywood, paints, and textiles) and can be converted to other primary chemicals through methanol to olefins and methanol to aromatics processes (for longer chain hydrocarbon production). Global methanol production is approximately 100 Mt/y and the key processes for producing the required methanol synthesis gas are:

- steam reforming of natural gas (43%)
- coal gasification (45%)
- steam reforming of coke oven gas, COG (10%)
- partial oxidation of oil feedstocks (2%)

Analogously to ammonia, steam reforming of natural gas is the main technology for methanol production in North America, Europe, and the Middle East, while coal gasification is the dominant technology in China. Besides coal, China also uses COG (a by-product of coke oven plants) as the feedstock to produce about 20% of its methanol via COG steam reforming. Overall coal gasification and COG steam reforming technologies used in China account for around 90% of Asia Pacific's methanol production. Methanol production is responsible for ~24% of total CO_2 emissions from primary chemicals production, where the coal based route has almost five times higher CO_2 intensity than the natural gas-based route. [1,11]

Although the steam reforming and partial oxidation/gasification technologies are generally the same for methanol and ammonia (in terms of typical unit processes for syngas production and purification), the produced synthesis gas differs in the H_2:CO ratio in each case. For methanol, a stoichiometric H_2:CO ratio of 2 is required, whereas for ammonia only hydrogen is required from the syngas. Therefore, relevant steps (e.g. shift conversion reactions) are required to adjust the syngas to the ratio required for efficient methanol production. For methanol synthesis based on steam reforming, CO_2 is often co-fed into the process to adjust syngas composition. Thus the syngas purification step is not as energy demanding as it is for ammonia production. The methanol synthesis section involves units for syngas compression to high pressure, methanol conversion (with around 5% of conversion per pass), product separation (e.g. via distillation units) and recycling the unreacted gas within the synthesis loop. [9,12] It should be noted that besides identifying typical unit processes involved (and their operating conditions), the simulation of ammonia and methanol production routes requires addressing various factors including the level of process heat recovery (due to the high-level heat surplus usually available), the synthesis loop design, and typical conversion and energy efficiencies for each production technology.

Generally, besides fossil fuel-based feedstocks, ammonia and methanol can be also produced by water electrolysis powered by renewable electricity (to produce hydrogen) or by biomass gasification. Due to the higher energy intensity and production cost of these production routes, current production is mainly based on fossil fuel feedstocks, but efforts have been made to switch to such low carbon technologies. [1] Currently several projects for electrolysis-based production of ammonia have been planned [13–15], including the building of a solar-powered ammonia demonstration plant in Australia by Yara (completion planned for 2023). CF industries has started planning for green ammonia production through water electrolysis in Louisiana, US (be completed in 2023), and massive electrolysis-based ammonia complex has been also planned in Saudi Arabia by the industrial gas firm Air Products (start up in 2025). There are also demonstration plants and announced projects for electrolysis-based methanol production [16], such as a green methanol start-up project by Liquid Wind in Sweden (completion in 2024).

High-value chemicals (HVCs) which include light olefins (ethylene and propylene) and aromatics (BTX) have a global production of approximately 365 Mt/y (255 Mt/y light olefins and 110 Mt/y BTX), from which 234 Mt/y (213 Mt/y light olefins and 21 Mt/y BTX) are produced in the chemical sector while the rest (40% of propylene and majority of BTX) are sourced as by-products from refinery operations. HVC production is responsible for around 27% of total CO_2 emissions from primary chemical production in the chemical sector.

HVCs are produced through multiple or single product processes in the chemical sector via the following key processes:

- steam cracking of heavy hydrocarbons, naphtha, and gas oil (56%)
- steam cracking of light hydrocarbons, ethane, and LPG (36%)
- propane dehydrogenation, PDH (4%)
- methanol to olefins, MTO, methanol to aromatics, MTA, and bioethanol dehydration, BDH (4%)

Among these production routes steam cracking of light hydrocarbons is the dominant production technology in North America (~88% of production) and Middle East (~75% of production), while heavy hydrocarbons (mostly naphtha) are the main feedstocks of steam cracking to produce HVCs in Europe (~70% of production) and Asia Pacific (~83% of production). [1]

Steam cracking involves units for feedstock cracking into lower chain length (via steam in a furnace at 750-900 °C without any availability of oxygen), cracked gas quenching, compression, and processing for its separation (product fractionations). [17] The process and the obtained products generally depend on the feed composition, feed to steam ratio, cracking temperature, and the furnace residence time. Steam cracking processes with different feedstocks (light or heavy) differ in terms of obtained product yield (HVCs produced) and the diversity of products (ethylene, propylene and BTX). For example, steam cracking of ethane results in highest yield in HVCs production, but the obtained HVCs is mainly composed of ethylene (~80%). Steam cracking of naphtha gives a more balanced production of ethylene, propylene and BTX, however it has a lower yield of produced HVCs. Therefore, besides the feedstock availability, the level of demand for different HVCs can be an important factor for HVC production route selection. [1,18]

Although steam cracking of oil feedstocks is the major production technology which yields coproduction of HVCs, there are also other routes such as single-product processes for their on-purpose production. The on-purpose technologies can be implemented alongside steam cracking to adjust production of any specific HVC based on its demands at each region using locally available feedstocks. In this direction, propylene can be produced as a single product from propane through propane dehydrogenation (PDH) process and via olefin metathesis process as well, which produces propylene from a mixture of ethylene and butene. There is also a production route for ethylene production from bioenergy through bioethanol dehydration (BDH), in which ethylene is produced through removing water from ethanol. This production route could be promising in regions where low-cost bioethanol can be produced due to the sufficient availability of bio-based raw materials (e.g in Brazil with 50% of the world's bioethylene capacity). [1,6]

Besides single product production routes, olefins and aromatics can be produced from methanol using the methanol to olefins (MTO) process and methanol to aromatics (MTA) process. MTO and MTA are implemented only in China because of the abundance of coal feedstock and thus the high production capacity of coal-based methanol. Naphtha catalytic cracking (NCC) is also a promising technology for co-production which produces HVCs with higher selectivity than steam cracking process, but it is currently implemented only in one commercial plant operating in Korea with around 40 kt/y production capacity. [6,19] Overall, compared to steam cracking, production quantities from aforementioned production routes for HVCs are relatively very small and most of these technologies are still in early commercialisation phases or operating as pilot plants. [1]

Thermoplastics

Thermoplastics, or thermosoftening plastics, are a family of plastics that can be melted when heated and hardened when cooled. These characteristics, which lend the material its name, are reversible. That is, it can be reheated, reshaped and frozen repeatedly. When frozen, however, a thermoplastic becomes glass-like and subject to fracture. Thermoplastics are mechanically recyclable. Some of the most common types of thermoplastics are polypropylene, polyethylene, polyvinylchloride, polystyrene, polyethylene terephthalate and polycarbonate.

Almost all plastics, including resins, fibres, and additives, are derived from fossil fuels, with only tiny fractions being derived from bio-based materials. The molecules or monomers used to make plastic are derived from oil, gas, and coal. While not all fossil-fuel derived chemicals (petrochemicals) become plastic, nearly all plastic begins as fossil fuels.

The production of plastic is both energy and emissions intensive, producing significant emissions through the cracking of alkanes into alkenes, the polymerisation and plasticisation of olefins into plastic resins, and other chemical refining processes. We estimate that

About 540 Mt CO_2e emissions were released from the production of thermoplastics in 2019.

Ethylene and propylene are the most common intermediates for producing both thermoplastics and thermosets.[20,21] As mentioned previously, they are mainly produced using light and

	2015	2030
Global ethylene capacity *(million Mt per year)*	143.8	191.2-195.5
Feedstock mix	35% ethane, 47% naphtha, 18% other	38.5% ethane, 44% naphtha, 17.5% other
Feedstock-based emission factors *(Mt CO_2/Mt ethylene)*	1–1.2 (ethane) 1.6–1.8 (naphtha) 1 (other)*	
Estimated CO_2 emissions from global steam cracking *(Mt per year)*	184.3–213.0	241.7–286.2
Coal-plant equivalency	45–52	59-69

Table 2–2: Estimated Annual Global CO_2 Emissions from Steam Cracking, 2015–2030

	LHV (GJ/t)	% carbon
LLDPE	44.36	0.83
PE	45.27	0.86
PP	44.02	0.86
PS	37.98	0.92
PVC	18.00	0.38
PET	21.60	0.63
PUR	30.12	0.67
Other-P	34.48	0.74
Other-S	34.48	0.74
Fibres	35.34	0.72
Elastomers	41.36	0.72

Table 2–3: Lower heating value and carbon percentage in the chemicals

Thermoplastics

- Polyethylene *(PE)*
- Polypropylene *(PP)*
- Polyvinyl-chloride *(PVC)*
- Polyethylene Terephthalate *(PET)*
- Polystyrene *(PS)*
- Expanded polystyrene *(EPS)*
- ABS
- SAN
- Polyamides *(PA)*
- Polycarbonate *(PC)*
- Poly methyl methacrylate
- *(PMMA)*
- Thermoplastic elastomers *(TPE)*
- Polyarylsulfone *(PSU)*
- Fluoropolymers
- PEEK
- POM
- PBT
- EVOH
- Etc.

Thermosets

- Polyurethane *(PUR)*
- Unsaturated polyesters
- Epoxy resins
- Melamine resins
- Vinyl esters
- Silicone
- Phenol - formaldehyde resins
- Urea - formaldehyde resins
- Phenolic resins
- Acrylic resins
- Etc.

Fibres

- Polypropylene fibre *(PP fibre)*
- Polyethylene terephthalate
- fibre *(PET fibre)*
- Polyamide 6 fibre *(PA6 fibre)*
- Polyamide 66 fibre *(PA66 fibre)*
- Polyacrylonitrile
- Etc.

Elastomers

- Polybutadiene
- Styrene butadiene
- Nitrile butadiene
- Etc.

Free radicals

These are species with lone electrons.

heavy hydrocarbon feedstocks through the steam cracking process which is the most energy consuming petrochemical process and the largest direct source of emissions in the plastic life cycle. In steam crackers, a tonne of ethylene production emits about 1 to 1.6 tonnes of CO_2e .[21] This results in more than 260 Mt of CO_2 emissions per year (0.8% of the world's total carbon emissions).[22] Compared to the light hydrocarbons (e.g. ethane and propane) cracking, naphtha cracking is more energy intensive and thus more GHG emission intensive (naphtha cracking generates 1.8 to 2 tonne CO_2e per tonne ethylene or 1.6 to 1.8 tonne CO_2e per tonne HVCs). This is because it requires higher temperatures compared to ethane and propane, though the process generates more opportunities to recover steam which can be used as a heat source in other processes or recycled.

Figure 2-9 describes the reaction mechanism of steam cracking using ethane as a model molecule.[23] The reaction mechanism is a chain reaction which entails initiation, propagation, and termination. The initial step involves the cleavage of a C-C bond or a C-H bond leading to the formation of ***free radicals***. Propagation of the chain mechanism occurs by several different radical reactions which in turn produce radicals as products. The radicals can, at any time, react with each other to produce a non-radical product. These latter reactions, where radicals are consumed, are called termination steps because the products have no further reactivity with respect to chain initiation.

We assume that use phase emissions are negligible for thermoplastics and thermosets. However, there are several environmental challenges from GHG emissions associated with the improper disposal and management of plastics, particularly after they enter waste streams (EOL phase).

Conventional ways to deal with plastic waste are incineration and landfilling, both of which tend to be much cheaper than recycling, mostly because in incineration and landfill the plastics do not need to be separated from the other components of solid municipal waste streams. Despite the low cost, incinerators can cause local air pollution if not properly designed and maintained.

Incineration of plastic waste can be carried out with or without energy recovery. The former requires more capital investment but has the advantage of providing an energy source from waste. With or without energy recovery, to prevent pollution, sophisticated combustion and cleaning equipment, such as low-NO_x burners and flue-gas scrubbers, is needed to remove the toxic components of the exhaust gas to prevent local pollution.

Incineration of plastic waste with energy recovery should generally be avoided, but it persists today as an attractive option in jurisdictions that are land- and cost- constrained.

This is because the plastic portions of waste are highly calorific, with many resins containing an amount of embedded energy which is similar to that of crude oil, per unit of mass. Burning waste reduces its volume by roughly 90%, which reduces the amount of land required for landfill sites. However, unconstrained, this approach to incineration results in CO_2 emissions as the embedded carbon (see Table 2-3) is released as CO_2 by the ratio of the molar masses of C and CO_2 (~3.7) while wasting a potential source of energy (conversion efficiency loss).

Aside from incineration, landfill is the least favourable option for managing general waste as it causes pollution, especially when poorly managed. However, these emissions and environmental impacts are not caused by the plastic fraction in general waste, which is essentially inert in the soil, but instead the organic fractions (i.e. food, plant, paper, wood waste). If plastic waste is separated and cleaned, it could be stored in landfill, with almost no emissions or other environmental impacts. Discarded plastics could be stored indefinitely in 'land-storage' or 'plastic-caches', or until a practical and economic recycling options emerges.

Two main categories of plastic recycling options exist nowadays: mechanical and chemical recycling, with the former being much more widespread:

Mechanical recycling offers a simpler and generally lower cost source of secondary plastic production in which the chemical structure of the polymers remains intact.[24] Collected and sorted plastic waste is the feed material, where it is cleaned, cut up into chips, and re-melted ready for moulding. Some impurities often remain after cleaning, including various additives used in virgin plastics to yield certain properties. For instance, isophthalic acid is often used as an additive in PET bottles to reduce their ***crystallinity***, thereby improving the clarity and transparency. If the PET resin in the bottle is to be recycled and used for other purposes where this characteristic is no longer required, the additive – often deeply embedded in the chemical structure of the product – can become an inhibiting impurity, rather than helpful. These impurities can result in lower performance in recycled materials, relative to their virgin counterparts, sometimes called downcycling.

The colouring used in virgin plastics presents a further – but mainly aesthetic – challenge. Two plastics of the same chemical composition, but differing colours, are very difficult to separate using existing industrial sorting processes. In mixed waste streams, where thousands of colours of plastics are encountered, the consequence tends to be that resins of multiple colours are recycled together. This often limits the choice of the colour of the final product to black. This sounds trivial, but it has a significant impact on the extent to which recycled[25] material can displace virgin production.

Chemical recycling describes a group of processes in which the plastic waste is converted back to the chemical building blocks (monomers) from which the original virgin material was produced.[26] This involves chemical transformations, calling for complex industrial processing equipment, and is more capital-intensive than mechanical recycling. The key advantage of chemical recycling is that the quality obtained in secondary plastic production can be equal to that of virgin production, enabling the same product to be recycled many times. The difficulty, though, is the process economics and energy inputs to the process tend to be less favourable relative to the virgin production routes for the same plastic. As a result, this route is not yet followed at an industrial scale globally.

Initiation:

$$CH_3CH_3 \rightarrow CH_3^{\cdot} + CH_3^{\cdot}$$

Propagation:

$$CH_3CH_3 + CH_3^{\cdot} \rightarrow CH_4 + CH_3CH_2^{\cdot}$$
$$CH_3CH_2^{\cdot} \rightarrow CH_2 = CH_2 + H^{\cdot}$$
$$H + CH_3CH_3 \rightarrow H_2 + CH_3CH_2^{\cdot}$$

Termination:

$$2CH_3CH_2^{\cdot} \rightarrow CH_3CH_2CH_2CH_3$$
$$CH_3CH_2^{\cdot} + H^{\cdot} \rightarrow CH_3CH_3$$

Disproportionation:

$$CH_2 = CH_2 + CH_3CH_2^{\cdot} \rightarrow CH_3CH_2CH_2CH_2$$
$$2CH_3CH_2CH_2CH_2^{\cdot} \rightarrow CH_3CH_2CH = CH_2 + CH_3CH_2CH_2CH_3$$
$$CH_2 = CH_2 + CH_3^{\cdot} \rightarrow CH_3CH_2CH_2^{\cdot}$$
$$2CH_3CH_2CH_2^{\cdot} \rightarrow CH_3CH = CH_2 + CH_3CH_2CH_3$$

Figure 2–9: Steam cracking reaction mechanism

Crystallinity

Crystallinity is the degree of structural order in a material, where atoms or molecules are arranged in a more regular manner. Increased crystallinity results in harder and more dense plastics.

Thermosets, fibres, and elastomers

The global productions of thermosets, fibres and elastomers are estimated to release about 348 Mt CO_2e in 2019.

Broken down, this is 145 Mt CO_2e from thermosets, 154 Mt CO_2e from fibres and 49 Mt CO_2e from elastomers (Figure 2-6).

Thermosets are family of plastics which undergo an irreversible chemical change when heated, creating a three-dimensional network. Unlike thermoplastics, which melt when exposed to heat, thermosets have increased crosslinking between molecules which sets the polymer in a permanent form, delivering high heat resistance. After they are heated and formed these plastics cannot be re-melted and reformed; instead they keep their form and char upon heating. The family of materials known as thermosets includes many different material forms (polyester, epoxy, phenolic, vinyl ester, polyurethane, silicone, polyamide and polyamide-imide) and numerous applications (electrical components, insulators, circuit breakers, heat shields, building panels, agricultural feeding troughs, motor components, and disc brake pistons).

Synthetic fibres are made from synthesised polymers of small molecules. The compounds used to make these fibres come from raw materials such as petroleum-based chemicals or petrochemicals. These materials are polymerised into a chemical which bonds two adjacent carbon atoms. Differing chemical compounds are used to produce different types of synthetic fibres. Synthetic fibres are used as alternatives to natural fibres (i.e. cotton, wool), often exhibiting improved properties such as durability. The dominant synthetic fibres in production are nylon, polyester, acrylic and polyolefin, which are used across fibre and textile sectors for making products such as ropes, fabrics and clothing.

Synthetic elastomer, or synthetic rubber, is any rubbery material composed of long chainlike molecules or polymers which can recover their original shape after being stretched to great extents. They are made from various petroleum-based monomers and have viscoelasticity (i.e. both viscosity and elasticity) and weak intermolecular forces, generally low material stiffness (Young's modulus) and high failure strain compared with other materials. Synthetic elastomers include styrene-butadiene rubbers (SBR) derived from the copolymerisation of styrene and 1,3-butadiene, and nitrile butadiene. Synthetic elastomers are commonly used as alternatives to natural rubber, such as for car tires, seals for doors and windows, o-rings, gaskets, hoses, conveyor belts, and rubbery flooring.

Nitrogen fertilisers

Most nitrogen fertilisers are made from ammonia (NH_3) produced by the Haber-Bosch process. It is an energy intensive process that requires a source of hydrogen (mainly from fossil fuels) and a source of nitrogen (from air). It is estimated that about 1/3 of nitrogen fertiliser emissions come from the production phase (454 Mt CO_2e out of a total 1,192 Mt in 2019).

Ammonia-based fertilisers include urea ($CO(NH_2)_2$) and ammonium phosphate ($(NH_4)_3PO_4$) / sulphate ($(NH_4)_2SO_4$) / nitrate (NH_4NO_3). Urea is the most common nitrogen fertiliser with a tonne of urea requiring a minimum of 0.73 tonnes of CO_2 and a chemical reactant in the process. In rare cases CO_2 is manufactured or sourced from naturally occurring underground deposits, but in most cases, it is provided by an adjacent ammonia plant. It is estimated that nearly half of all process CO_2 generated during ammonia production globally is used in this way as a raw material input for urea production. The characterisation of the process stoichiometry reveals the source of CO_2 emissions in ammonia production:

For natural gas

$$CH_n + 2\,H_2O + \left(\frac{n}{3}\right)N_2 \rightarrow \left(\frac{2n}{3}\right)NH_3 + CO_2$$

where n=3.951 for gas

For oil and coal

$$2CH_n + 2\,H_2O + O_2 + \left(\frac{n+2}{2}\right)N_2 \rightarrow \left(\frac{2n}{3}\right)NH_3 + CO$$

where n=1.829 for oil and n=0.456 for coal.

Types of nitrogen fertilisers are listed as below (nitrogen content refers to total nitrogen)[27]:

- Ammonium fertilisers
  - ammonia (82% N), ammonium sulfate (21% N), ammonium bicarbonate (17% N), all moderately quick-acting. Uptake by plants can be retarded by addition of nitrification inhibitors.
- Nitrate fertilisers
  - calcium nitrate (16% N), sodium nitrate (16% N), Chilean nitrate, all quick-acting and increasing soil pH.
- Ammonium nitrate fertilisers
  - ammonium nitrate (about 34% N), calcium ammonium nitrate which is a combination of ammonium nitrate and calcium carbonate (21-27% N), ammonium sulfate nitrate (26-30% N).
- Amide fertilisers
  - urea (45-46% N), calcium cyanamide (20% N).
- Solutions containing more than one form of N
  - urea ammonium nitrate solution (28-32% N).
- Slow- and controlled-release fertilisers
  - either derivatives of urea with N in large molecules, or granular water-soluble nitrogen fertilisers;
  - controlled-release urea (encapsulated in thin polymer film, slow- or very slow-acting according to type of polymer or thickness of film);
  - often includes a quick-acting component;
  - or other means of slow-release, e.g. sulfur coated urea (SCU);
- Multi-nutrient fertilisers containing N
  - NP: Nitrophosphate (20-23% N, 20-23% P2O5); Monoammonium phosphate (11% N, 52% P2O5); Diammonium phosphate (18% N, 46% P2O5); Liquid ammonium polyphosphates (e.g. 12% N, 40% P2O5);
  - NK: fertilisers containing both N and K (e.g. potassium nitrate);
  - NPK: fertilisers containing N, P, and K.

Liming

Liming is the treatment of soils with lime (calcium and magnesium carbonates) to reduce acidity and improve fertility.

Nitrogen fertilisers can also be produced using ammonium sulphate or ammonium phosphate as intermediaries. There are no direct emissions from the chemical reactions required for producing these intermediaries, which result from exothermic reactions. Notably, the process does not require CO_2 as a reactant and so often the carbon footprint of the ammonia used in producing nitrogen fertilisers with ammonium sulphate or ammonium phosphate will be higher than in the production of nitrogen fertilisers using urea.

The primary purpose of a nitrogen fertiliser is to deliver nitrogen to the root of plants and crops. This is achieved by applying the nitrogen fertiliser to the soil. However, several chemical reactions that result in the production of GHG emissions take place in this stage. One example is the CO_2 embedded in the fertiliser, which is released into the soil and, following decomposition, into the atmosphere.

About 2/3 of nitrogen fertilisers emissions are generated during the use phase (738 Mt CO_2e in 2019).

Fertiliser use-related emissions can be from the following pathways:

- Direct N_2O emissions (nitrification, denitrification)
- CO_2 from urea hydrolysis: $(NH_2)_2CO$
- Indirect N_2O via NH_3 and fraction of volatilisation
- Indirect N_2O via NO_3- and fraction of leaching
- CO_2 from ***liming***

Direct nitrous oxide (N_2O) emissions from synthetic nitrogen fertiliser application result from two main mechanisms present in the nitrogen cycle. Both mechanisms are essential in facilitating the uptake of nitrogen by plants, but the addition of synthetic nitrogen fertilisers can exacerbate imbalances between a plant's rate of uptake and the rate of fertiliser application.[28] N_2O is a gaseous intermediate in the reaction sequence of denitrification and a by-product of nitrification that leaks from microbial cells into the soil and ultimately into the atmosphere. One of the main controlling factors in this reaction is the availability of inorganic nitrogen in the soil. The IPCC provides methodology to estimate N_2O emissions using human-induced net nitrogen additions to soils (e.g. synthetic or organic fertilisers, deposited manure, crop residues, sewage sludge), or of mineralisation of nitrogen in soil organic matter following drainage/management of organic soils, or cultivation/land-use change on mineral soils (e.g. forest land/grassland/settlements converted to cropland).

(2.1)

$$\text{Nitrification } NH_4^+ \rightarrow NH_3O \rightarrow NO_2^- \rightarrow NO_3^-$$

(2.2)

$$\text{Denitrification } NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2$$

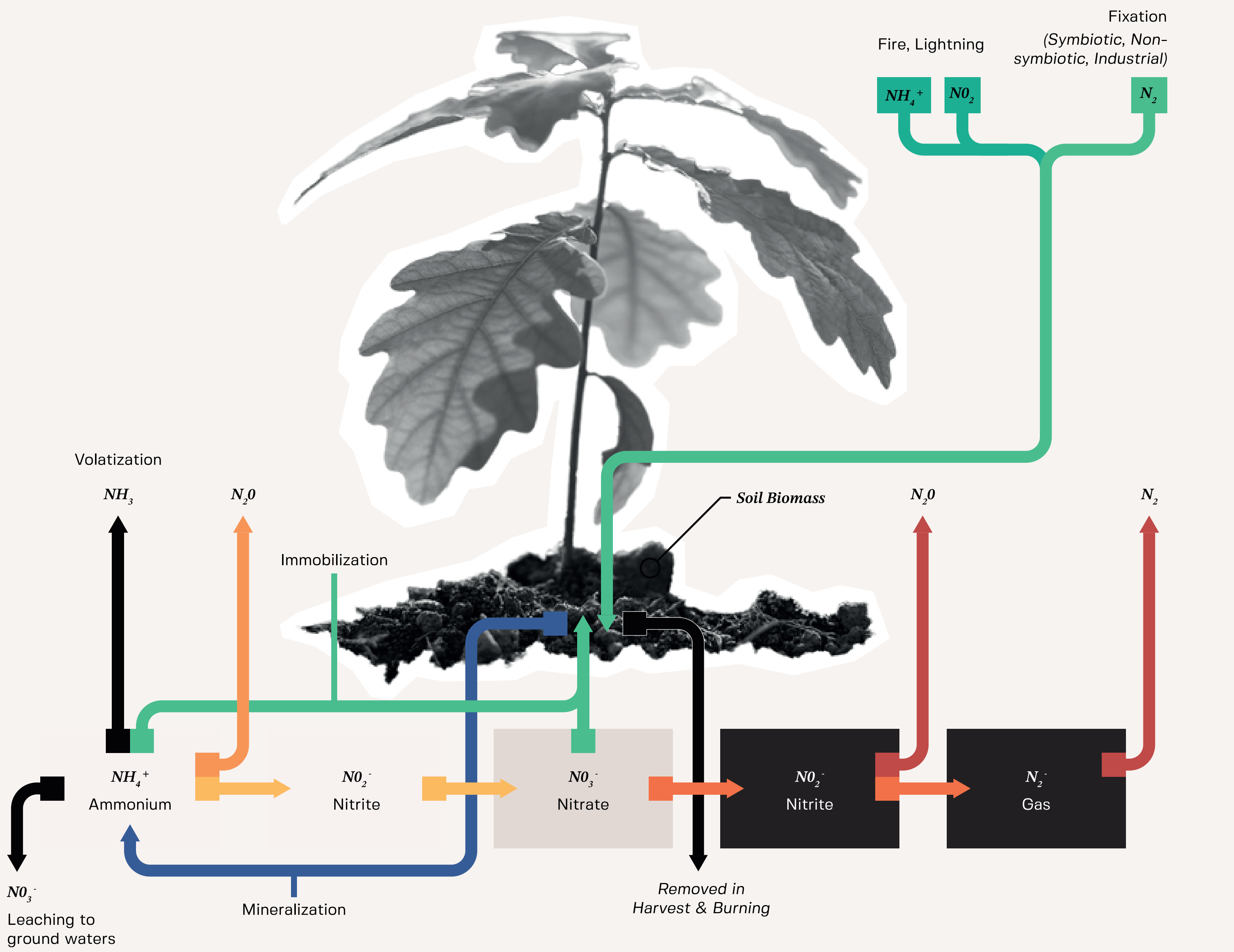


Figure 2–10: Schematic diagram illustrating the sources and pathways of N that result in direct and indirect N_2O emissions from fertiliser use [27]

Urea hydrolysis emissions occur either when urea or urea ammonium nitrate are used. These fertilisers contain carbon that is released as CO_2 when applied to soils. The CO_2 that is used in the manufacture of urea forms a carbonyl group, to which 2 mols of ammonia (NH_3) are affixed. When the urea (CH_4N_2O) is applied to soils and hydrolysed, it decomposes to re-form ammonia and a CO_2 by-product, via the intermediate carbamic acid (CH_3NO_2). This simplified urea life cycle is summarised in equations (2.3) and (2.4) below. The same principle applies to the urea component of urea ammonium nitrate. The ammonium nitrate contains no carbon, so has no relevance in terms of carbonaceous fertiliser emissions, although it does contribute to N_2O emissions from nitrogen fertilisers.

(2.3)

Urea manufacture $2NH_3 + CO_2 \rightarrow CH_4N_2O + H_2O$

(2.4)

Urea hydrolysis and decomposition
$CH_4N_2O + H_2O \rightarrow NH_3 + CH_3NO_2 \rightarrow 2NH_3 + CO_2$

Indirect N_2O emissions stem from two further mechanisms: volatilisation and leaching:

Volatilisation can occur when ammonia gas (NH_3) present in the soil reaches the surface, where it can then be oxidised in the atmosphere to produce nitrous oxide (NO_x). This ammonia gas stems from the over-application of fertiliser, which leads to the availability of ammonium in the soil surpassing the quantity able to be taken up by plants. Volatilisation also stems from fossil fuel combustion and biomass burning, and the subsequent redeposition of these gases and their products NH_4+ and NO_3- to soils and water.

Leaching occurs when an excess of fertiliser is present along with water transport, such as groundwater, rain or irrigation. This water transport moves fertiliser available for plant uptake (ammonium and nitrate) away from the roots of plants to non-agricultural soils and water courses where it may form nitrous oxides. There are other environmental impacts, such as hypertrophication from excess nitrogen compounds in water courses, although these do not have direct GHG emissions consequences, so are not considered in this analysis. The principal pathways are illustrated in Figure 2-10.

The disproportionate contribution of fertilisers to overall emissions levels is mainly due to the large contribution of use phase (urea decomposition, nitrification/denitrification mechanisms) emissions from this product category, compared with plastics, which have negligible use phase emissions.

Solvents, additives, explosives, and other chemicals

Solvents come in three types: oxygenated solvents (e.g. alcohols, ketones and esters), hydrocarbon solvents (paraffinic, aliphatic and aromatic hydrocarbons), and halogenated solvents (usually chlorinated hydrocarbon solvents). All solvents apart from alcohols and water are manufactured from the building blocks of the petrochemical industry (syngas, ethylene, propylene, butenes, butadiene, benzene, toluene and xylenes), and are produced from crude oil and natural gas. However, only a small amount of oil is required for solvent production – only 1-2% of the world's oil use goes towards solvent production.

About 2/3 of life cycle emissions for solvents, additives and explosives are from the production phase (242 Mt CO2e in 2019) and 1/3 from the use phase (147 Mt CO2e in 2019).

Carbon black, a common chemical additive for the production of tires and pigments, is made by combusting a hydrocarbon feedstock such as oil or natural gas with a limited supply of air between 1320°C to 1540°C. This can be achieved by either the 'oil furnace' process, in which an aromatic feedstock is continuously injected into a natural gas-fired furnace, or the 'thermal' process, a cyclic process in which natural gas is decomposed into carbon particles, with the ***offgas*** being recycled and burned in the next furnace to provide heat for cracking. Although emissions from both processes include carbon monoxide (CO), nitrous oxides (NO_x) and sulfur compounds, although emissions are significantly lower for the thermal process due to the recycling of the offgas. Gaseous emissions can be controlled with carbon monoxide boilers, incinerators, or flares.

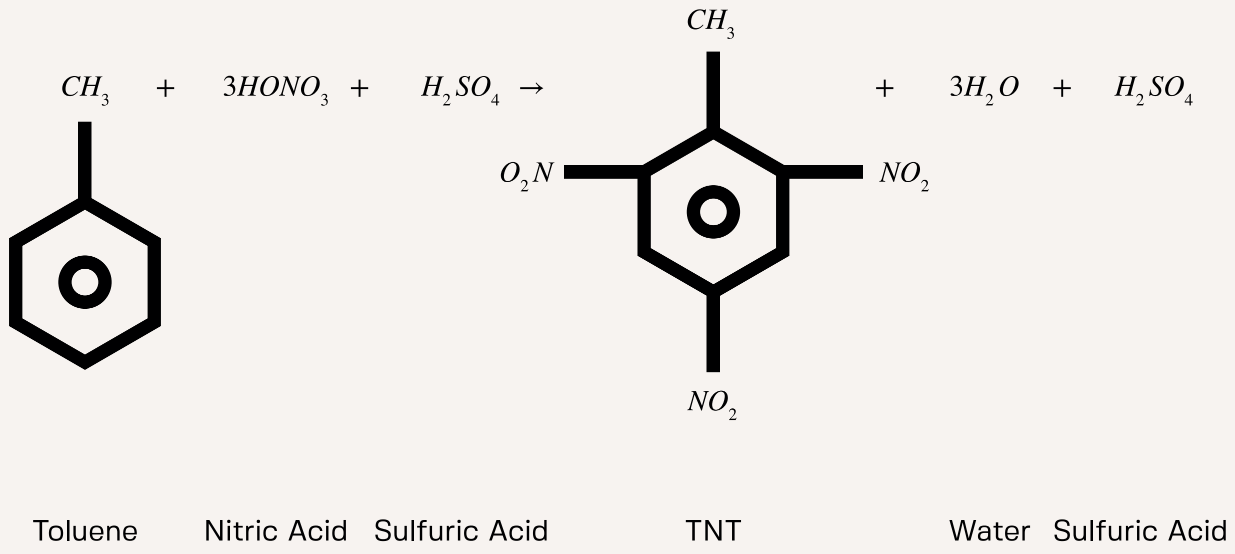
Acetic acid, a widely used chemical solvent, is mainly synthesised by methanol carbonylation – the reaction between methanol and carbon monoxide under a metal catalyst (usually rhodium complex) at 150-200°C and 35-65 atm:

$$CH3 - OH + CO \rightarrow CH_3 - COOH$$

Offgas

Offgas is a gas released as part of a chemical process.

Acetic acid can theoretically be produced by a sustainable process as the raw materials are available from renewable feedstock (biomass or biogas). The GHG emissions from the production of acetic acid combine the amounts of CO_2 and equivalent GHGs produced, as well as those released from the production of heat, electricity, and cooling water. There are two major categories of explosives: high (e.g. TNT) and low (e.g. nitrocellulose). TNT is prepared using sulfuric acid, nitric acid and toluene as raw materials.



Nitrocellulose (NC) is prepared by the nitration of cellulose in acid, followed by centrifugation of the crude nitrocellulose followed by washing and boiling with water to purify the product.

$$\left(C_6H_7O_2(OH)_3\right)_x + 3HONO_2 + H_2SO_4 \rightarrow \left(C_6H_7O_2(ONO_2)_3\right)_x + 3H_2O + H_2SO4$$

NOx and SOx gases are the major emissions from the manufacture and concentration of the acids used for explosive production. The production of nitric acid generates nitrous oxide (N_2O) as a by-product of the catalytic oxidation of ammonia at high temperatures, and involves three chemical reactions:

$$4NH_3 + 5O_2 \rightarrow 4NO + 6N_2O$$

$$2NO + O_2 \rightarrow 2NO_2$$

$$3NO_2 + H_2O \rightarrow 2HNO_3 + NO$$

Associated with the production of nitric acid are, of course, the emissions involved in producing ammonia, which are discussed earlier, so that the overall emissions comprise those from both the ammonia and nitric acid production processes.

The use phase and EOL phase of explosives are treated as the same (detonation). As in most combustion processes, a deficiency of oxygen favours the production of carbon monoxide (the pollutant formed in greatest quantities from the use of explosives) during detonation. TNT (Trinitrotoluene or 2,4,6-trinitrotoluene), with the formula $C_6H_2(NO_2)_3CH_3$, due to being oxygen-deficient, produces more CO than oxygen-balanced dynamites (see below). The use phase emissions from explosives depend on many factors including explosive composition, length of charge and confinement.

$$2C_7H_5N_3O_6 \rightarrow 3N_2 + 5H_2 + 12CO + 2C$$

Incineration and recycling are the two EOL practices which allow material or energy recovery from solvents, though sometimes other waste transfer protocols are followed to manage hazardous substances, or solvents may be discharged into municipal sewage treatment plants.

There are many thousands of chemical products, all of which cannot be covered here in this report. However, we explore some examples of important ‘other chemicals’ below.

Nitric acid and ammonia, whose production emissions are discussed above, are key chemicals as they are precursors to many products including fertilisers, additives and explosives.

Titanium dioxide is commonly used as a white pigment in the manufacture of paints, paper and plastics (among other applications), and can be manufactured either by the chloride process or the sulphate process. The former creates process-related CO_2 emissions from the use of petroleum and chlorine as raw materials, whilst the sulphate process does not emit any direct production GHGs.

Soda ash (sodium carbonate) is used in many industries for the production of glass (mainly), paper, pulp and soaps. It is produced from the mining of trona ore, followed by its calcination according to the following reaction:

$$2Na_2CO_3 \cdot NaHCO_3 \cdot 2H_2O(Trona) \rightarrow 3Na_2CO_3(Soda\ ash) + 5H_2O + CO_2$$

GHG emissions are due both directly to the stoichiometric CO_2 released in the above reaction, but also indirectly from the fuel used in the ore crushers and driers, industrial boilers, and other industrial equipment.

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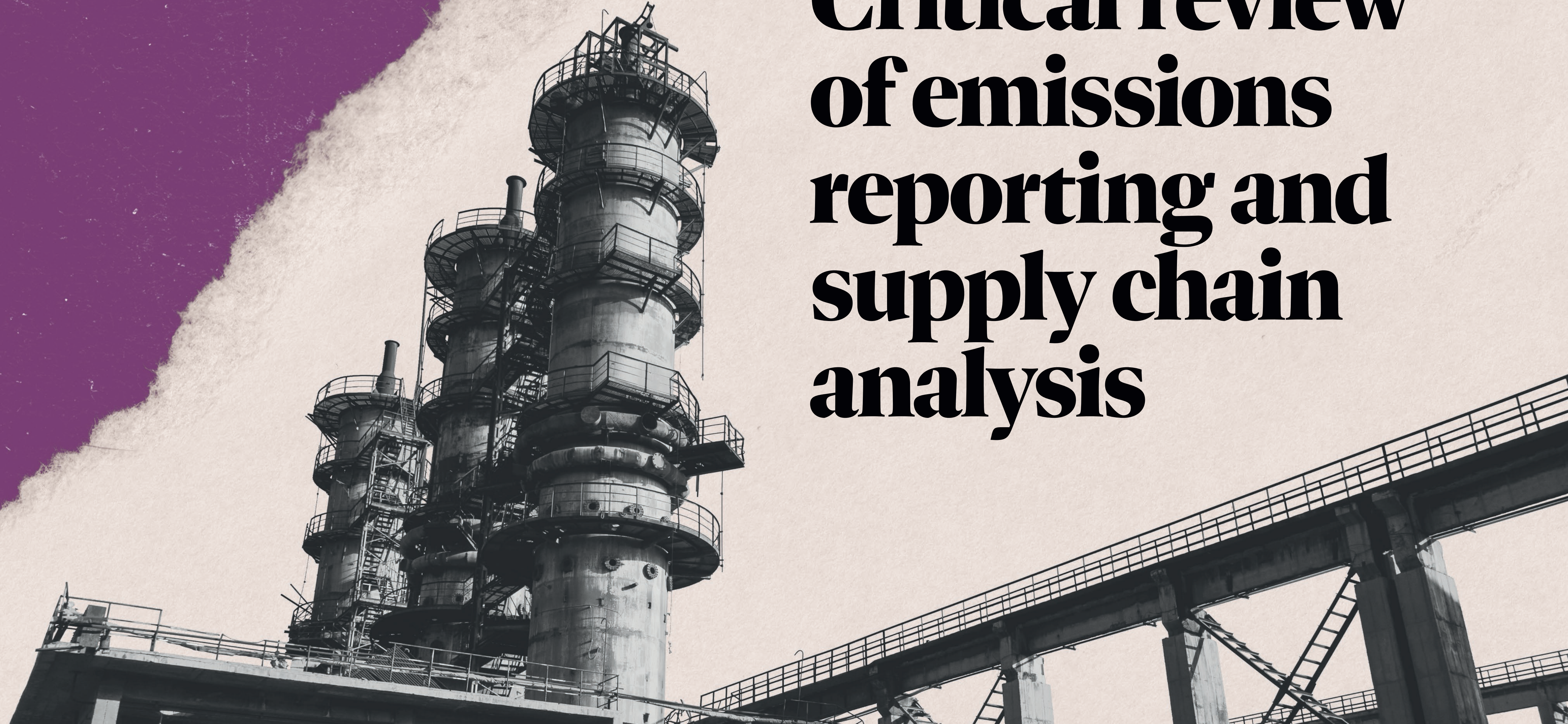
3

Chapter Three:

Critical review of emissions reporting and supply chain analysis



Chapter Summary

There is currently no reliable, comprehensive picture of GHG emissions or energy, mass, and trade flows of the petrochemical sector due to its complexity. The petrochemical sector produces thousands of materials and products using thousands of chemical processes. This chapter examines how GHG emissions are reported, how supply chains are analysed, and how uncertainties in these data are managed.

Our critical review of GHG emissions data has revealed that current top-down methods for collecting and reporting emissions data for the petrochemical sector lack the integration, transparency, and robustness to answer the types of questions currently being asked in the public realm, such as:

- Can the plastic waste problem be solved with recycling or biodegradable plastics?
- Do bans on plastic carrier bags lead to less plastic use and reduced carbon footprint?
- Can we decarbonise fertilisers while still feeding the 7.7billion people in the world?
- Which country produces the most plastic waste and related emissions?

32 emissions databases and 20 key studies were analysed to understand the breadth of coverage and level of detail provided by each. We found that the following issues are obscuring the petrochemical emissions picture:

- Some countries only report as the sector in total.
- The emissions at extraction and end of life (EOL) stages are not disaggregated at the product level.
- There are inconsistencies in the methodologies used for aggregating emissions, leading to inconsistent data.
- Significant data quality and coverage issues were found across six dimensions: products, life cycle stages, countries/regions, GHG emissions, time series, and uncertainty.
- Primary data and monitoring standards for the petrochemical sector are lacking, especially for developing countries.
- There is a scarcity of data on material flows through the highly interconnected supply chain.

A significant issue revealed is a lack of reported uncertainties on the data. Only a minority of data sources explicitly consider uncertainty. Quantifying uncertainty is critical in moving forward with emissions data collection and calculation to gauge the reliability of the modelling results and conclusions. This critical review catalogued the data, their uncertainty sources, and uncertainty handling methods.

No open, reliable, and comprehensive framework exists for analysing GHG emissions across the full life cycle of petrochemical products, at the national or global level. To measure emissions across the whole sector consistent measurement methods should be used for every process and product. Both direct (top-down) and derived (bottom-up) measurement methods should be utilised.

The petrochemical supply chain involves multiple stakeholders spanning many sectors and industrial facilities from across the globe. This makes collating GHG emissions data for the petrochemical industry a very challenging task.

Currently there are two methods for counting GHG emissions from the chemical sector. These are Direct Measurement and Derived Measurement. A top-down accounting approach collates Direct Measurements of emissions released. It requires the assessment of fossil fuel inputs to chemical plants, used for reactions and process heat which release emissions, and multiplying these by emissions intensity factors to calculate the emissions burden. Emission accounts are reported by chemical plants, often annually, to national and regional statistical bodies for verification and collation. Separate accounts are reported for fossil fuel extraction emissions and EOL treatment emissions.

There are concerns around the accuracy of directly measured top-down reports of GHG emissions. An alternative approach is to use derived measurement, where resource flows and production volumes (which are accurately measured for financial and accounting purposes) are combined with the underlying reaction and thermodynamic principles, which are largely untouched, to model GHG emissions. This bottom-up approach involves process-level energy and mass balancing of input feedstocks, materials, energy, and emissions across the life cycle of chemical products. There is a growing interest to characterise the material flows and product stocks of petrochemical products at the global, regional, national, and urban scales, and to use material maps to infer bottom-up GHG emissions accounts. This requires the collection and reconciliation of multiple data sources.

In this chapter, we review the direct measurement and accounting methods for GHG emissions related to the chemical sector. We focus on the life cycle stages where emissions are released and the emissions profiles of the key chemical products. We aim to document how chemical emissions are measured and reported and identify data quality issues and gaps. We also review the chemical databases and key peer-reviewed studies which report material flow data or use derived data of material flows for the petrochemical supply chain analysis.

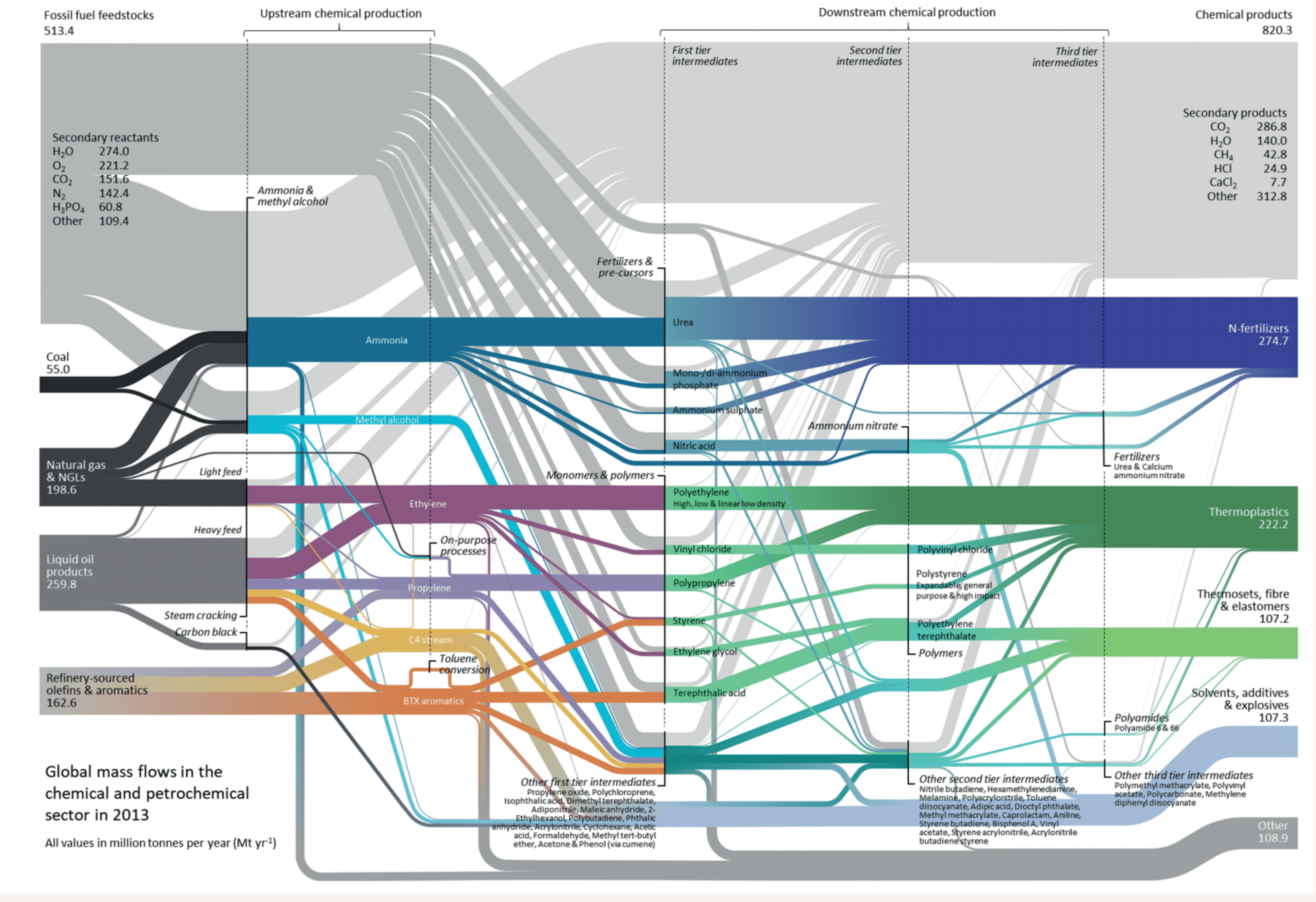


Figure 3-1 Levi & Cullen (2018) Sankey diagram showing 2013 material flows in the chemical sector [1]

A. How are GHG emissions reported?

Key points:

- Measurement of emissions involves multiplying fossil fuel inputs by emissions intensity for each process.
- It is difficult to measure and compile emissions records because the petrochemical sector produces thousands of products, yet many countries report emissions as a single chemical sector. This limits a product- and process- specific approach to investigating emissions and mitigation strategies.
- There is significant variation in the methodologies used for aggregating emissions, leading to data inconsistencies.
- EDGAR and UNFCCC databases use the IPCC framework to report emissions data by sector. These are the main databases, though other smaller databases are detailed in this chapter and Appendix A that are industry- or region-specific.

The measurement of emissions from a single chemical process is relatively simple. It involves tallying the fossil fuel inputs to the process and multiplying by emissions intensity figures. What is more challenging, is that the petrochemical sector produces thousands of materials and hundreds of thousands of products. Producing accurate emissions accounts requires applying consistent measurement methods across every process and collating emissions data from multiple stakeholders and operators across the whole sector.

Such an undertaking, if applied consistently, would allow production emissions to be attributed to the main chemical products. Yet, many countries only report chemical emissions as a single sector, limiting the product specific view. Furthermore, emissions data from other life cycle stages, including extraction and mining (e.g. fugitive emissions) and EOL treatment (e.g. incineration), is not disaggregated at the product level, further obscuring the emissions picture.

The lack of data completeness for these country and life cycle stages is amplified by more general data inconsistencies across the whole collection process.

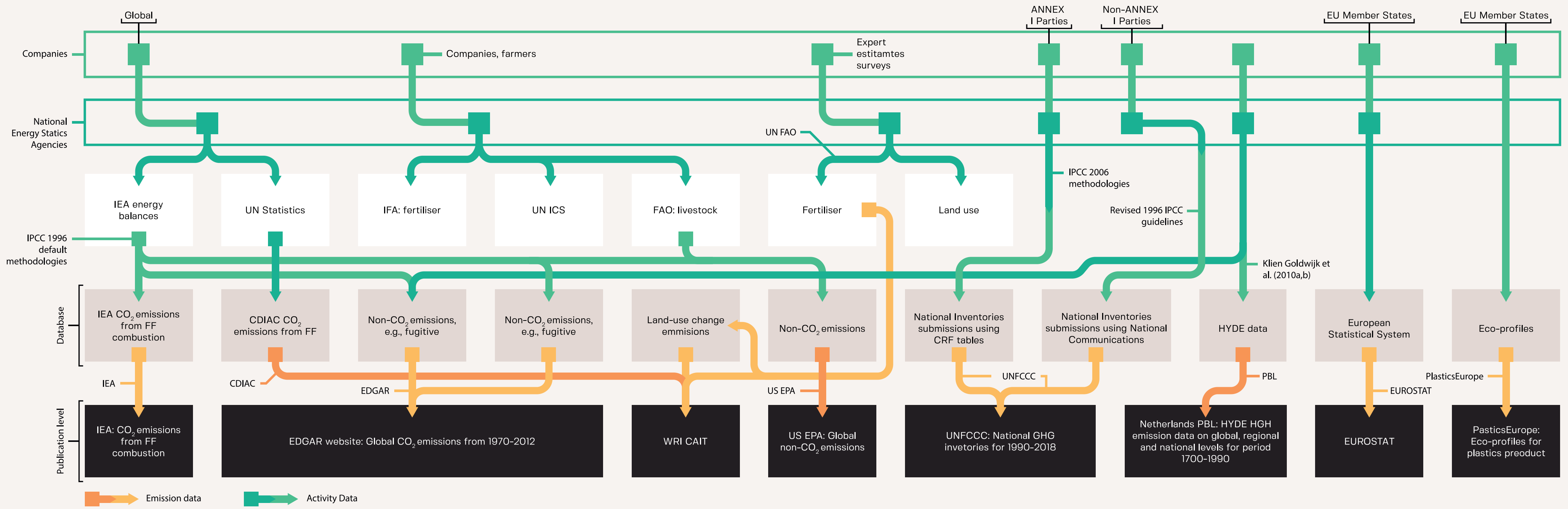


Figure 3–2: Accumulation of emissions data

Top-down reporting

This generally refers to breaking down a sector to gain insight into its compositional sub-sectors in a reverse engineering fashion. In top-down reporting, an overview of the sector is formulated, specifying, but not detailing, any first-level subsectors. Each subsector is then refined in yet greater detail, sometimes in many additional subsector levels, until the entire specification is reduced to base elements. Top-down is commonly associated with the word "macro".

Bottom-up reporting

This focuses on specific characteristics and "micro" attributes of an individual subsector. Generally, the individual base elements of the system are first specified in great detail. These elements are then linked together to form larger subsectors, which then in turn are linked, sometimes in many levels, until a complete top-level sector is formed.

Figure 3-2 provides an overview of how emissions data, from primary sources, is collected and accumulated, and eventually feeds into global databases of emissions data. Yet, variations are found for emissions data between country, regional and global level databases[2]. In most cases, the original data is collected from the same companies, expert estimates, and surveys[3]. This leads to the conclusion that the variation in emissions accounts comes from the different methodologies used for aggregating emissions.

In this section we detail how GHG emissions from the petrochemical sector are measured, collated and reported today. We identify where data coverage is limited and where data inconsistencies can be found, which lead to inaccuracies in emissions accounts for the chemical sector and creates challenges in providing answers to the many questions being raised in the public domain.

GHG emissions databases

The two preeminent global accounts of GHGs emitted are the Emissions Database for Global Atmospheric Research (EDGAR) and the United Nations Framework Convention on Climate Change (UNFCCC). Both databases make use of the IPCC framework for global emission accounts, for organising and reports emissions data. This framework divides emissions into agreed sectors and subsectors, including disaggregating industrial emissions by sectors.

Figure 3-3 shows how emissions released in the production of petrochemical products are spread across the defined IPCC sectors and subsectors. It illustrates the challenge of totalling emissions for a specific petrochemical material (i.e. thermoplastics) from across several different sector accounts, each with their own measurement guidelines and level of detail recorded.

The UNFCCC and EDGAR databases report by industrial sector at country level. This is not always the most detailed data available from industry, but it is comprehensive and covers global petrochemical GHG emissions, across nations. Some specific issues which exist in the data are:

- Countries collect data differently and therefore estimate GHG emission data differently.
- Some methods lack accuracy, are not comprehensive and/or use unreliable data sources.
- ***Bottom-up emission accounting*** is not used for many petrochemical industries.

More detailed accounts of global petrochemical GHG emissions

are found in various industry-specific databases. For instance, the International Association of Oil and Gas Producers (IOGP, formerly OGP) report GHG emissions annually for the upstream oil and gas sector[4], collecting emissions data directly from producers. These detailed, 'bottom-up' oil and gas industry-specific inventory methods provide much more granular and realistic estimates than national scale estimates under the IPCC inventory methods[5].

Life cycle inventories (LCIs), such as those provided by ecoinvent[6], PlasticsEurope[7], the United States Argonne National Laboratory (ANL)[8] and National Renewable Energy Laboratory[9] contain information on material input requirements and emissions for industrial processes. The components of the information stored in LCIs are less susceptible to the boundary issues that afflict product-specific life cycle assessment.

Table A1 found in Appendix A provides a list of data sources which report on emissions from the petrochemical sector, including details of the price, database type, geographical and product coverage, and time series. Although this list likely omits some specific data sources, we have attempted to document and review the most used data sources.

Appendix A provides further information on some of the emission data sources for the petrochemical sector.

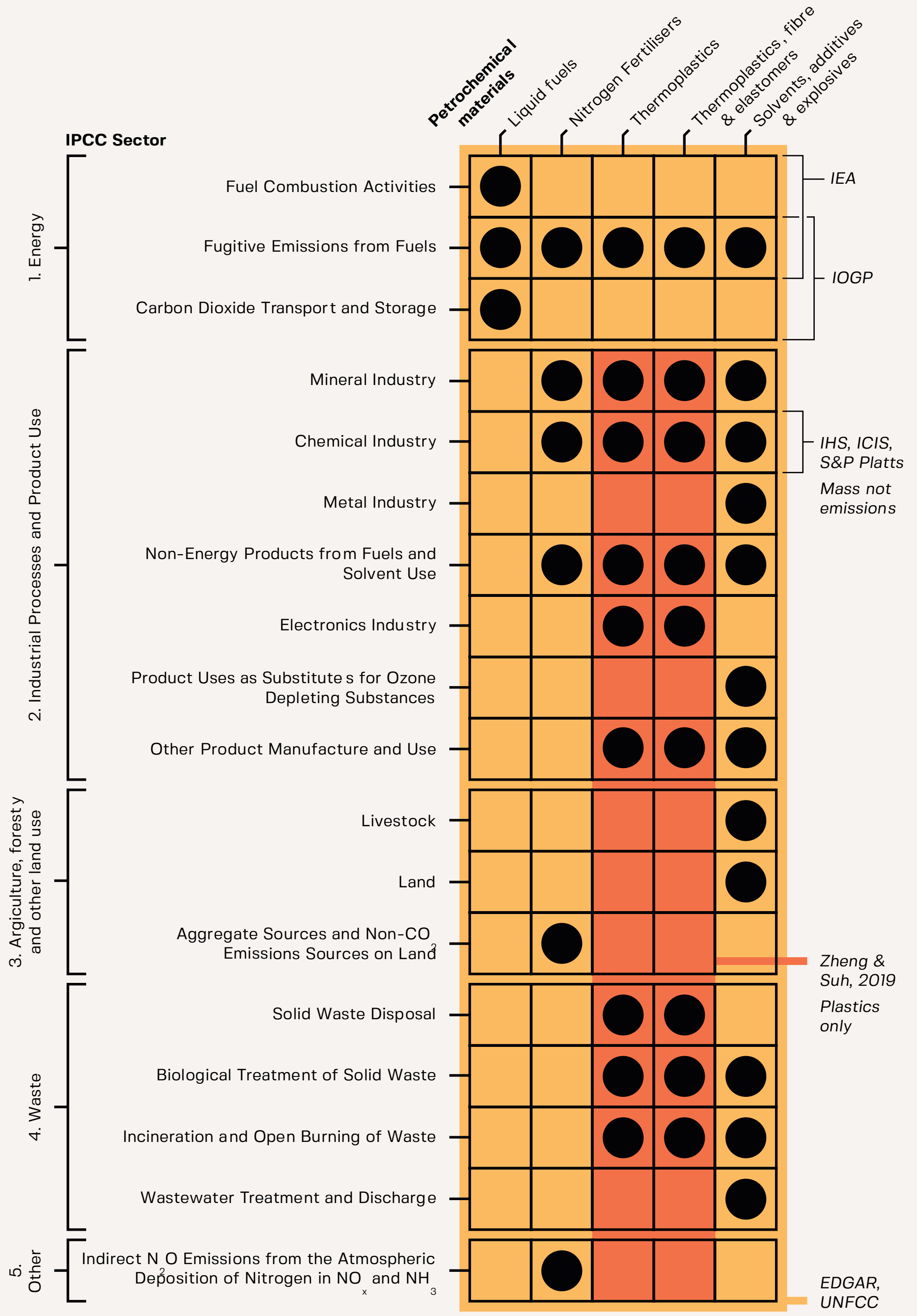


Figure 3–3: Petrochemical emissions in different IPCC sectors (black dots indicate that the petrochemical product contributes to emissions in the IPCC sector)

Studies reporting on emissions

Alongside the emissions data stored in various databases, several academic studies have used emissions data and modelling techniques to provide more granular data for aspects of the petrochemical sector. In this chapter, we identify the key studies of the petrochemical sector which take a holistic or system view across some groups of chemical products or life cycle stage for petrochemicals, at least a country level or higher. Thus, we avoid the numerous papers which focus on a single petrochemical product or processing stage and include only systemic analyses. We conducted a search of Scopus/Web of Science using the keywords "petrochemical"/ "chemical" AND "carbon dioxide"/"CO_2" OR "greenhouse gas emission"/"GHG" AND/OR "Material flow analysis"/"Accounting" from titles of peer-reviewed journal articles in English as of 24 May, 2021. The results were further refined by the research area "environmental science" and "environmental studies". We then review the titles and abstracts of the resulting publications to identify systemic studies on petrochemical emissions.

Our search highlights 20 salient peer-reviewed studies on petrochemical flows and emissions.

While the earliest data for petrochemical emissions were published in 2002, 15 of these 20 studies were published after 2010, reflecting the increasing public attention on plastic waste after 2010. These studies focus on petrochemical flows and emissions, for plastics in particular, at multiple spatial scales: global, regional (mostly Europe) and national (mostly European and Asian countries).

Table A2 found in Appendix A shows the time series, geographic region, product, life cycle stages and GHG emission types covered by each study, including single-year studies, historical analysis over many years, and future dynamic predictions for the petrochemical sector. The studies are ordered by publication year. In the remaining sections, we discuss the data gaps from five dimensions in these studies.

Neelis et al.(2005) [10] constructed a NEAT (non-energy emissions accounting table) model to compile CO_2 emission estimates associated with non-energy use flows. The NEAT model was employed to compile national non-energy emissions inventories for the Republic of Korea [11], Italy [12], Germany [13] and The Netherlands [14]. By better describing the degree to which non-energy consuming products are oxidised during or after use, the model allows the authors to improve emissions inventories relative to those compiled with the IPCC reference approach available at the time. [15] The model requires production and trade data for 77 organic and 18 inorganic chemicals, which the authors acknowledge is an extensive data requirement. The country level studies prove it is possible, but only with close cooperation from national statistical offices or consultancies. No intermediate mapping data are presented in the country level studies.

At the global scale, Geyer et al. (2017) [16] examined the production, use, and fate of eight types of plastics from 1950 to 2015. It constitutes the most comprehensive and recent study of plastic material flows available in the literature. The authors use the relatively few data that are publicly available on production, consumption and waste volumes for key regions (Europe, United States, China and India) to make estimates of global plastic flows. The polynomial curve-fit methodology they employ helps to fill the multiple gaps in available statistics during the period they examine (1950 to 2050), but it does result in conflicts with certain periods that do have statistical coverage. It is estimated that, in 2015, approximately 6,300 million metric tonnes of plastic waste had been generated, around 9% of which was recycled, 12% was incinerated, and 79% was accumulated in landfills or the natural environment. The first-ever estimation of global plastic stocks and flows has been widely cited in later papers including Zheng and Suh (2019) and Nicholson et al (2021) [17,18]. Zheng and Suh (2019) evaluated strategies to mitigate the life cycle GHG emissions of plastics on a global scale. The results showed that the global life cycle GHG emissions of conventional plastics were 1.7 Gt of CO_2 equivalent (CO_2e) in 2015, which would grow to 6.5 Gt CO_2e by 2050 under the current trajectory. However, aggressive application of renewable energy, recycling and demand-management strategies, in concert, has the potential to keep 2050 emissions comparable to 2015 levels. Nicholson et al. (2021) estimated the supply chain energy requirements and GHG emissions associated with US-based plastics consumption. Major commodity polymers, each of which has a global consumption of at least 1 Mt per year, account for an estimated annual 104 Mt CO_2e of GHG emissions in the US alone.

For individual countries, Zhu et al [19] and Zhou et al [20] estimated CO_2 emissions and reduction potential in China's chemical/ammonia industry, Talaei et al [21] assessed the impacts of process-level energy efficiency improvement on GHG mitigation potential in the Canada petroleum refining sector.

Masnadi et al. (2018a) [5], Masnadi et al. (2018b) [22] and Jing et al. (2020) [23] provide comprehensive life cycle inventory data for one stage of the life cycle for petrochemicals: the crude oil extraction and refining at the global and national level. Masnadi et al. (2018a) used their developed open-source oil-sector CI modelling tools-OPGEE [24] to model well-to-refinery CI of all major active oil fields globally. Using renewable solar energy could result in sector-wide emissions reduction about 5 kg CO_2e per billion barrels of oil (~1.7 CO_2e per MJ) [25]. Previously, Masnadi et al. (2018b) used a per-barrel well-to-refinery life cycle analysis model with data derived from hundreds of public and commercial sources to model the Chinese crude mix and the upstream carbon intensities and energetic productivity of China's crude supply. They generated a carbon-denominated supply curve representing Chinese crude oil supply from 146 oilfields in 20 countries. The selected fields are estimated to emit between ~1.5 and 46.9 g CO_2e per MJ of oil, with volume-weighted average emissions of 8.4 g CO_2e per MJ. Jing et al. (2020) used bottom-up engineering-based refinery modelling on crude oils representing 93% of 2015 global refining throughput. They reported the global refining carbon intensity at country level and crude level as 13.9 to 62.1 kg CO_2e per barrel and 10.1 to 72.1 kg CO_2e per barrel, respectively, with a volume-weighted average of 40.7 kg CO_2e per barrel (equivalent to 7.3 g CO_2e per MJ) (Table 3-1). Based on projected oil consumption under 2 °C scenarios, the industry could save 56 to 79 Gt CO_2e to 2100 by targeting primary emission sources. These reported data can be fed into the bottom-up model to be developed in the C-THRU petrochemical emission model. Most recently, Rutherford et al. [26] developed a new inventory-based model for CH_4 emissions using bootstrap resampling that allows for isolation of differences between the inventory and the GHG inventory at the equipment-level.

Source Country/ Region	Volume Produced *(M bbl d-1)*	Source Country Refining Carbon Intensity kg *(kg CO_2e bbl-1)*	Source Country Refining Carbon Intensity kg *(g CO_2e MJ-1)*	Source Country Upstream Carbon Intensity kg *(g CO_2e MJ-1)*	Source Country Upstream and Refining Combined Carbon Intensity *(g CO_2e MJ-1)*
Australia	0.28	32.1	5.9	9.1	15
Austria	0.02	49.6	8.8	7.6	16.4
Chile	0.00	44.6	7.9	11.2	19.1
China	3.22	50.9	9.0	7.0	16
Congo	0.16	54.7	9.6	10.6	20.2
Democratic Republic of Congo	0.01	34.3	6.2	29.2	35.4
Denmark	0.15	22.7	4.1	3.3	7.4
United Arab Emirates	2.82	35.7	6.5	7.1	13.6
United Kingdom	0.78	39.3	7.1	7.9	15
United States	9.28	41.4	7.4	11.3	18.7
Global Averages		**40.73**	**7.28**	**10.28**	**17.56**

Table 3-1: Daily volume of crude oil refined, volume-weighted-average crude oil upstream and refining carbon intensity by selected source countries (10 of the 66 countries) in 2015 [23]

B. How are chemical supply chains analysed?

Key points:

- Chemical databases provide insight into mass, energy and trade flows involved in petrochemical processes. This section reviews the databases, which range from short- to long-term outlooks on global and regional scales.
- Some databases are specific to certain products, such as plastics, fertilisers and packaging, which provide more detailed data on a sector level.
- Many of the databases available are commercial and keep data behind paywalls.

The chemical supply chain involves multiple stakeholders spanning many sectors and industries across the globe. Mapping global chemicals flows and accurately forecasting future demand of petrochemicals is difficult given the scarcity of data on the sector's material flows, and the highly intertwined nature of its complex supply chains. Moreover, the model needs access to market intelligence to help provide informed views on the market. In this section, we search for and review chemical databases which provide insight into the mass and energy flows, trade flows, and conversion processes involved in petrochemical process.

Chemical databases

Existing chemical supply databases such as ICIS Supply and Demand Database, IHS Chemical Economic Handbook, and S&P Global Platts Petrochemicals provide an end-to-end perspective of the global petrochemical markets. These chemical databases provide production (varies at the plant, country, regional and global level), trading and consumption data. With such material stock and flow data, one can account and identify patterns of material consumption, predict the generation of waste, and evaluate the potential of recycling. The databases also provide detailed plant-level data, e.g. products, process technologies and locations in current and predicted years across different regions.

IHS Markit has two related chemical databases: the Chemical Economics Handbook (CEH) and PEP Yearbook. CEH provides five-year outlooks and extensive market data on more than 300 industrial chemicals covering North America, Europe, China, Japan (Economic database covering 200+ countries). There is information on supply, demand, manufacturing processes, price and trade information for individual chemicals or these major chemical groups with global and regional supply/demand and five-year forecast. CEH includes detailed information on and analysis of the history, status and projected market trends for the industry's major products in most commercial chemical markets. The PEP Yearbook database includes process recipe information (i.e. mass, energy). This includes 1500 production processes, on a per kilogram basis, with regional values for energy inputs, process yields, etc. It also includes operating and capital costs estimates by regions.

The ICIS Supply and Demand Data Service provides a long-term view of the rapidly changing petrochemical markets. It offers end-to-end perspectives across the global petrochemical supply chain, including refineries. It provides quick access to data on import and export volumes, plant capacities, production, and product trade flows covering 160 countries and over 100 products.

Valpak produces biannual datasets of plastic packaging placed on market by their members, covering almost all plastic packaging placed on market in the UK. Although this dataset only covers data about UK packaging practices, it provides a very detailed level of granularity, which could enable the assessment of opportunities for polymer substitution, replacement, reuse, or elimination for all packaging uses.

These databases will serve as the basis for C-THRU's development of spatially resolved mass flows and product stocks of the chemical industry. Appendix B provides further information on the chemical databases reviewed in this chapter.

Supply chain approaches

Derived data approaches are used in several peer-reviewed studies, to understand the material flows in the chemical industry and model environmental impacts from processes. The mapping of material flows, using MFA (material flow analyses) also allows emissions reduction actions to be computed and compared from across different life cycle stages of chemical products.

In this section, a search of Scopus/Web of Science was conducted using the keywords “petrochemical”/ “chemical” AND/OR “Material flow analysis” from titles of peer-reviewed journal articles in English as of 24 May, 2021. The results were further refined by the research area “environmental science” and “environmental studies”. We then review the titles and abstracts of the resulting publications to identify systemic studies on petrochemical material flows. We find and review 35 key papers which provide insight from derived data. Table B8 in Appendix B presents a list of these studies, including details on their publication year, data type, life cycle stages covered, geographical region, product breakdown and year of analysis.

Common challenges are identified by existing databases and literatures on material flows and product stocks of petrochemical products. The challenges include the complexity of data due to complex petrochemical supply chain with a wide range of chemical reaction processes, many of which overlap and intertwine. Primary data and monitoring standards are also lacking especially for developing countries which are both main product and waste producers. All these result in data uncertainty and inconsistent data structure for the global petrochemical sector.

Many of the existing databases miss data for specific countries or regions, certain periods of time, or particular types of petrochemicals, products, or waste. This makes it difficult to collate material flow into emissions data across the entire global sector, as a single account.

Current supply chain data are compiled with different purposes for different life cycle stages. At the production phase, data are collected by types of chemicals as a whole, such as IHS, ICIS, but not linked between extraction and refining stage and conversion stage. At the use stages, data are collected mainly by products that contain petrochemicals rather than by their types (Valpak documents data on the type of packaging, its purpose, the polymer composition, sector and mass in UK Grocery/Clothing/Wholesale sector). Production and consumption data for nitrogen fertilisers are well documented in IFA and UN FAO. However, material production for thermoplastics and thermosets are not well recorded for the major production countries and regions. Data on additives are not covered by any databases. At the EOL stage, petrochemical waste (mainly durable products - plastics) is not specifically tracked and managed. Currently the global recycling rate for plastics is estimated to be only 9%. Furthermore, many of these chemical databases are commercial, with data sitting behind paywalls, particularly for country, company and facility level data and thus not reproducible at granular level.

C. How is data uncertainty managed?

Key points:

- Quantifying the uncertainty present in data sources is valuable for the development of improved data collection and calculation methods, as well as to gauge the reliability of modelling results from the petrochemical industry.
- When uncertainty exists, it does not necessarily prevent conclusions being drawn or actions taken; it simply better shows the robustness of conclusions.
- Only a minority of petrochemical GHG and supply chain data sources explicitly consider uncertainty.
- A key source of uncertainty is simply a lack of reported data. When data is available, there is often significant uncertainty about the value. Uncertainty also arises from the ambiguity of different classifications and definitions for what is being reported.
- Most analyses use a probability-based approach to uncertainty, using Monte Carlo analysis or analytical error-propagation methods. Alternative methods could bring benefits for dealing with imprecise expert knowledge.

Why is it important to consider uncertainty?

A definition of uncertainty [27] from the fifth assessment report of the IPCC is “a cognitive state of incomplete knowledge that results from a lack of information and/or from disagreement about what is known or even knowable.” Quantifying the uncertainty in assessing GHG emissions [28] is crucial as it could affect our conclusions about the current scale of the problem, and about the true trend of reducing or increasing emissions. There are three main benefits of dealing with uncertainty. One is to help researchers to identify potential opportunities for developments or improvements in data measurement and collection, calculation theory, and software. The second is to prioritise resources to establish a reasonable and robust foundation on which to support policymakers to make effective decisions to reduce future emissions. Without uncertainty analysis, resources cannot be targeted towards improving data about the specific emissions most in need of better knowledge. Finally, results can be better communicated together with an estimate of their variation or uncertainty.

This is not to say that any conclusions about petrochemical GHG emissions will be subject to such a high degree of uncertainty as to be worthless. Quite the opposite: a proper understanding of data uncertainties allows the robustness of conclusions to be more transparently judged and acted upon.

Sources of uncertainty in petrochemical emissions data

Some uncertainty is associated with the specific numeric values reported by a particular source, while further uncertainty arises when multiple datasets are combined to estimate emissions of a wider system, or to cross-check estimates from different sources.

Within a single dataset, uncertainty arises from different sources [29] such as statistical variation, variability, inherent randomness and unpredictability, subjective judgment of belief, disagreement, linguistic imprecision, and approximation. Some of these uncertainties are due to statistical variation and randomness, known as ***aleatory uncertainty***. These can be understood in principle through repeated measurement and statistical analysis. Other uncertainties are due to a lack of knowledge about exactly what has been measured and whether it should be believed, known as ***epistemic uncertainty***. These uncertainties are difficult to quantify exactly, but in the context of petrochemical emissions data, are often the more significant. Aleatory uncertainty cannot be reduced, while epistemic uncertainty can be reduced by gathering more data or by refining models.

Epistemic uncertainties can be related to the five data dimensions introduced previously: time, region, GHG, petrochemical product, and life cycle stage. For example, if an ambiguous definition of the GHGs that are included in the data is used, there is epistemic uncertainty about how much CO_2 specifically has been reported. Or if information is needed on emissions from a specific country, but only regional data is reported, there is epistemic uncertainty about how much of the regional data should be attributed to the specific country.

When combining multiple datasets to model or estimate the emissions of a wider system, further uncertainties arise related to the consistency and clarity of definitions and boundaries used by different datasets. For example, different datasets use slightly different definitions of the “chemical sector”, leading to uncertainty about whether the data from another dataset can be directly compared. Similar issues arise with definitions of processes, materials, products, time periods, and regions. Finally, it is important to keep track of the ***provenance of the data***. The same figures are often re-quoted in other datasets, and it is important to recognise when this happens to avoid treating the repeated figures as independent corroboration of the data.

Aleatory uncertainty

It is an inherent and irreducible variation associated with a parameter or a system. For example, variability in emission parameters due to measurement error.

Epistemic uncertainty

It is a subjective and reducible uncertainty that arises from lack of knowledge or ignorance. For example, insufficient data to precisely characterise a probability distribution of a coefficient in an emissions model.

Provenance of data

This is where the data originally came from and how it has been processed.

Methods for representing and analysing uncertainty

According to the availability of data samples, approaches of uncertainty analysis can be classed into three types: probability approaches, non-probability approaches, and hybrid/mixed approaches. Probability-based uncertainty analysis has been widely used in estimating emissions results, while there are few studies on non-probability approaches and hybrid/mixed approaches.

The Revised 1996 IPCC Guidelines [15] specify the following probability-based approach: "Where there is sufficient information to define the underlying probability distribution for conventional statistical analysis, a 95 percent confidence interval should be calculated as a definition of the range. Uncertainty ranges can be estimated using classical analysis or the Monte Carlo technique. Otherwise, the range will have to be assessed by national experts." And 2000 IPCC Guidelines [30] specify the following "the range of an uncertain quantity within an inventory should be expressed such that: (i) there is a 95% probability that the actual value of the quantity estimated is within the interval defined by the confidence limits, and (ii) it is equally likely that the actual value, should it be outside the range quoted, lies above or below it."

The IPCC guidance [31] provides two approaches for analysing uncertainty described by these probability distributions, Taylor series expansion-based error propagation and Monte Carlo simulation. These methods can be used for combining uncertain input data and parameters into an uncertainty estimate for emissions. Error propagation is simple, but it is difficult to deal with correlations and large uncertainty. Monte Carlo simulation is more complex and needs initial probability density distributions, but it is suitable where uncertainties are large, and where correlations and non-normal distribution exist.

These guidelines do not answer the question of how to determine the underlying probability distributions. One approach is a "pedigree matrix" [32], which can be useful to describe and manage data quality and uncertainty resulting from the data limitations. It consists of data quality indicators to assess data quality under uncertainty, and gives a basis for improving data collection.

Apart from the above approaches based on probability distributions, there are other uncertainty analysis strategies. Compared to the probability-based uncertainty analysis approach, a fuzzy set [33] is often less dependent on data sample size and assumptions. It is suitable for expressing expert judgment based on imprecise information. Interval analysis [34], which is one typical kind of non-probability approach, has been successfully applied to deal with uncertainty in practical engineering such as reliability analysis and optimisation design. It is particularly well suited to expressing expert judgment because only lower- and upper-bound values are needed to form an interval. Hybrid approaches that combined probability and non-probability can be suitable for dealing with multi-type or multi-source uncertainties with less dependence on assumptions. The advantage and disadvantages of the above six approaches are summarised in Table 3-2.

Approach	Advantage	Disadvantage
Error propagation	Suitable for small uncertainty Normal probability density distribution	No correlations between data Same uncertainty for different years
Monte Carlo	Suitable for the small or large uncertainty Any probability density distribution Data can be correlated Uncertainties can vary between years	The high number of simulations May underestimate uncertainty Lack of running the Monte Carlo from start to finish of the petrochemical life cycle Lack of clarity in guidance on how to effectively apply the Monte Carlo to estimate petrochemical emissions
Pedigree matrix	Assessment of data quality Useful for uncertainty resulting from lack of data	May underestimate uncertainty
Fuzzy set	Suitable for large uncertainty or imprecise information Suited to express expert judgment Less dependent on assumptions	Lack of petrochemical emissions studies on fuzzy set theory
Interval analysis	Suitable for small uncertainty or imprecise information Suited to express expert judgment Less dependent on assumptions	Lack of clarity in guidance on how to effectively apply the interval analysis to estimate petrochemical emissions
Hybrid approach	Suitable for the small or large uncertainty or imprecise information Multi-type or multi-source uncertainties and correlations Less dependent on assumptions	No petrochemical emissions studies on the hybrid approach The theory and implementation of the hybrid approach may be complex

Table 3-2: Evaluation of approaches to deal with uncertainty in petrochemical emissions

Parameter uncertainty

Uncertainty about the correct values of model parameters. For example, the carbon emitted per tonne of chemical produced is a parameter in a bottom-up emissions model, but the precise true value for this parameter may not be known.

Model uncertainty

Uncertainty about the assumptions and modelling choices made, rather than the specific parameter values chosen. For example, a control equation in a bottom-up emissions model could be different in different (linear or non-linear, etc.) assumptions.

How is uncertainty currently reported in petrochemical GHG and supply chain data?

Although the issues of uncertainty are well known, in practice data is frequently reported as simple point values with no assessment of uncertainty. While comparison [35] studies of major petroleum life cycle models and databases have been reported, the way that uncertainty is reported for petrochemical emissions data has not been directly reviewed. The key data sources discussed in Section 3B have been reviewed to summarise whether and how they discuss and report uncertainty. Since the data sources vary in scope and coverage, their relevance to the aims of the C-THRU project was also estimated, based on the coverage of emissions data, and whether the information was reproduced from elsewhere. Full details are given in Appendix A and B.

Figure 3-4 shows that data from around 60% of sources do not appear to give any consideration of uncertainty. While nearly 40% have guidelines to follow to quantify uncertainty.

Focusing on the 39% of data sources which do discuss uncertainty, Table 3-5 summarises how they describe the sources of uncertainty and methods for handling uncertainty. A dominant cause of uncertainty in assessing petrochemical emissions is the lack of knowledge about the system and data because limitations of information are unavoidable. ***Parameter uncertainty*** in input data is commonly considered as a main source of uncertainty, while Ecoinvent, PRELIM, United Nations Environment Programme (UNEP) Global Environment Outlook (GEO) and World Resources Institute point out that ***model uncertainty*** is another major source of uncertainty.

In terms of how the uncertainty is represented in practice, probability distributions such as normal or lognormal distribution are usually used. For example, UNFCCC National Atmospheric Emissions Inventory, United States Environmental Protection Agency (USEPA), and Netherlands Environmental Assessment Agency, etc. mainly follow the IPCC guidance that possible values can be characterised as a probability density function (PDF). Ecoinvent includes detailed lognormal distribution to describe variable uncertainty that could be caused by data, completeness, aggregation level, geography, modelling, and forecasting. The GREET model has some parameters with default probability distributions and allows users to add specific distributions to perform stochastic simulations. It is important to point out that data sources such as EUROSTAT and Food and Agriculture Organisation (FAO) do report uncertainty, however, it is not clear how to directly manage uncertainty in the petrochemical emission data.

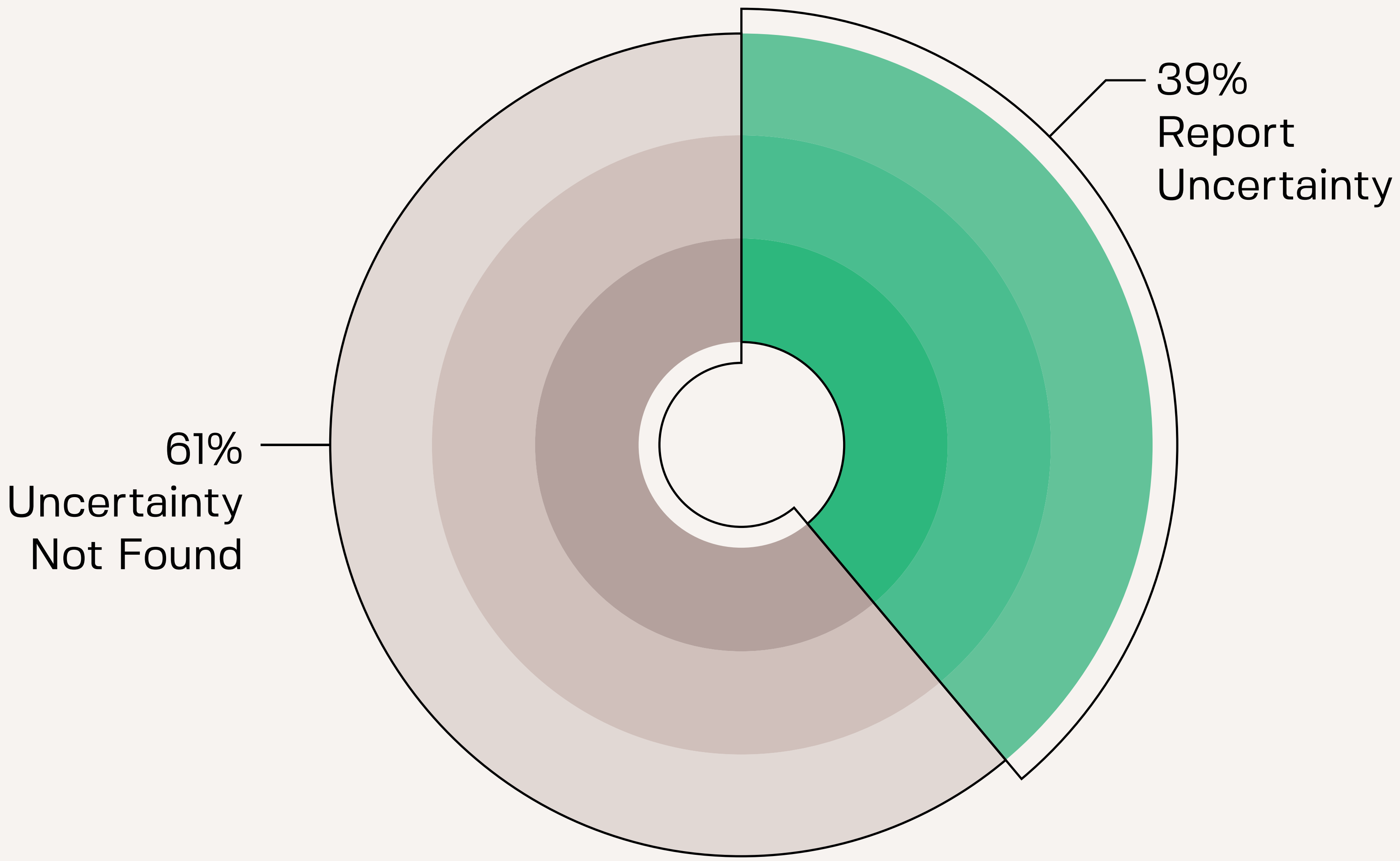


Figure 3-4: How many data sources account for uncertainty

No.	Sources of data	Sources of uncertainty	How uncertainty was handled
1	United Nations Framework Convention on Climate Change (UNFCCC) GHG Data Interface	Lack of knowledge of the true value of a variable	• A PDF to characterise the range and likelihood of possible values • Uncertainty is quoted as the 2.5 and 97.5 percentile i.e. bounds around a 95% confidence interval • Two approaches are recommended Error Propagation and Monte Carlo
2	Ecoinvent	• Data • Completeness • Aggregation level • Geography • Modelling • Forecasting	The lognormal is the most common distribution chosen to describe the uncertainty in ecoinvent. It has the advantage of not being defined in the negative domain, so credits do not accidentally happen during a Monte Carlo simulation.
3	US ANL GREET model (LCA data, excel)	Not found	The GREET model has some parameters with default distributions and allows users to add other parameters, specify distributions, and perform different types of stochastic simulations.
4	PRELIM	Uncertainty may come from the modeling structures and data sources	Uncertainty range: A Kw factor of 11.5 (as opposed to Kw factor of 12 in PRELIM v1.1) is assumed for the delayed coking gas oil product, the range narrows down to 11.38 to 12.44.
5	United Nations Environment Programme (UNEP) Global Environment Outlook (GEO)	• Linguistic uncertainty (Imprecise meanings of words) • Stochastic uncertainty (Inherently unpredictable systems) • Scientific uncertainty (Limits of methods and data) • Decision uncertainty (Differences in understanding of the world)	• The four-box model for the qualitative communication of confidence • Likelihood scale for the quantitative communication of the probability of an outcome occurring
6	United States Environmental Protection Agency (USEPA)	Lack of knowledge of the true value of a quantity	• Uncertainties are often expressed in the form of a probability distribution • Follow the IPCC guidance
7	World Resources Institute (WRI), Climate Watch (CAIT): Country Greenhouse Gas Emissions Data	• Parameter uncertainty • Model uncertainty	• For parameter uncertainty: sensitivity analysis and Monte Carlo analysis • For model uncertainty: examining a range of models or run a model with different parameters
8	Netherlands Environmental Assessment Agency (PBL)	Part of the uncertainty is due to an inherent lack of knowledge concerning the sources. Another part, however, can be attributed to elements of the inventory whose uncertainty could be reduced over time by dedicated research initiated by either the NIE or other researchers.	Mainly follow the IPCC guidance
9	Food and Agriculture Organisation (FAO), Fertilisers by Nutrient	• Sampling • Pre-treatment • Method bias • Variation in conditions • Changes in a sample matrix • Imprecision in estimating Method or laboratory bias	Not found
10	Oil Production Greenhouse Gas Emissions Estimator (OPGEE)	Missing data	Using defaults to fill missing information
11	California Air Resources Board	• Random error (precision uncertainty) • Systematic error (bias uncertainty	• Objective method: normal and lognormal distributions • Subjective method: Need to check

Table 3-3: Uncertainties in the selected petrochemical emissions data sources and how they were handled

D. What are the emerging data quality issues?

Key points:

- There is currently no reliable and comprehensive picture of GHG emissions from the petrochemical sector due to a lack of consistency in protocols used to collect data by companies and countries, and patchy data in less developed regions.
- EDGAR and UNFCCC databases are too generic for product-specific emissions models – the UNFCCC only covers eight different groups
- We detail the inconsistencies and gaps in GHG emissions data across six dimensions: products, life cycle stages, country/region, GHG emissions, time series and uncertainty.
- There is no coverage of GHG emissions for individual products, but relatively good coverage for the process of crude oil extraction and the refining processes in the petrochemical sector.
- GHG emissions are divided into CO_2, CH_4 and N_2O emissions. The reduction of non CO_2 emissions could be critical as it may be less costly and more rapidly financially rewarding.

Our review of databases for chemicals and systemic studies across parts of the petrochemical sector reveals that an open, reliable and comprehensive picture of GHG emissions from the petrochemical sector does not exist. Across the petrochemical databases, coverage is traded against the level of product detail, countries collect chemical data using different protocols, and emissions data across the life cycle stages is patchy at best. Furthermore, the process of collecting and accumulating emissions data into national-level accounts introduces future data inconsistencies. It is also noted that most studies reveal that the numbers are higher than standard inventories report [36,37]. If these numbers are correct, this has real implications for the carbon footprint of these categories, e.g. the discrepancies are likely significant

The overall result is a collection of emissions accounts and more specific studies, each of which can only address limited questions about the emissions impact of petrochemicals. Although useful for providing answers to specific questions, these data sources lack the integration, transparency and robustness needed to respond to the breadth of questions asked in the public realm.

To provide more context around these data issues, we summarise the data quality and coverage gaps across five dimensions: products, life cycle stages, country/region, GHG emissions, and time series.

Products

Emissions accounts at the global level fail to provide disaggregated emissions data for individual petrochemical products. EDGAR and the UNFCCC account for emissions across the life cycle of some petrochemical products but are too generic to inform product specific emission models. For example, the UNFCCC emissions database only reports the GHG emissions for eight product groups: ammonia, methanol, ethylene, ethylene dichloride and vinyl chloride monomer, ethylene oxide, acrylonitrile, and carbon black.

Table 3-4 highlights those emission databases and key papers that provide emissions data for specific petrochemical products[1], across the life cycle stages.

The table shows that coverage of emissions from extraction and refining, use and EOL are non-existent for single chemical products.

Even at the conversion stage, where production data is routinely collected by industrial companies and collated by countries, the coverage of products is inconsistent.

Chemical group	Chemical	Ext/Ref	Conv	Use	EOL	Total
Primary chemicals						
	Propylene		27			
	Ethylene		1,27			
	Butene		27			
	Butadiene		27			
	Benzene		27,			
	Xylene		27,			
	Toluene		27			
	Carbon black		1			
	Syngas					
	Ammonia		1,27			
	Methanol		1			
Inorganic chemicals						
	Soda ash		1			
	Chlorine		27			
	Nitric acid		1			
Organic chemicals						
	Ethylene glycol					
	Terephthalic acid					
	Vinyl chloride		27			
	Styrene		27			
	Acetone		27,			
	Phenol		27,			
	Acrylonitrile		1,27			
	Other Intermediate Organic Chemicals					
	Cyclohexane					
	Adiponitrile					

	Acetic acid					
	Methyl Methacrylate (MMA)		27			
	Adipic acid		1,			
	Caprolactam					
	Vinyl acetate					
	Bisphenol A		27,			
	Hexamethylenediamine					
Nitrogen fertilisers						h
	Ammonia		1,29,f	29		,g
	Diammonium phosphate		29	29		
	Monoammonium phosphate		29	29		
	Ammonium sulphate		29	29		
	Urea		29	29		
	Ammonium nitrate		29	29		
	Calcium ammonium nitrate		29	29		
	Urea ammonium nitrate		29	29		
	Other ammonium based fertilisers					
	Other ammonia based fertilisers					
	Other mixed fertilisers					
Plastics						l,o,t
Thermoplastics	High density polyethylene (HDPE)		o	38	o	
Thermoplastics	Low density polyethylene (LDPE)		o	38	o	
Thermoplastics	Linear low density polyethylene (LLDPE)			38		
Thermoplastics	Polypropylene (PP)		o,t	38	o	
Thermoplastics	Isophthalic acid			38		
Thermoplastics	Polyvinyl chloride (PVC)		o,t	38	o	
Thermoplastics	Polystyrene (PS)		o,t	38	o	
Thermoplastics	Expandable polystyrene (EPS)		o,t	38	o	
Thermoplastics	General purpose polystyrene (GPS)		o,t	38	o	

Thermoplastics	High impact polystyrene (HIPS)	o,t	38	o
Thermoplastics	Polyethylene terephthalate (PET)	o,t	38	
Thermoplastics	Acrylonitrile butadiene styrene (ABS)	o		o
Thermoplastics	Dioctyl phthalate	o		o
Thermoplastics	Methyl methacrylate (MMA)			
Thermoplastics	Styrene acrylonitrile (SAN)	o,t	38	o
Thermoplastics	Polyamide 6 (PA6)	o,t	38	o
Thermoplastics	Polyamide 66 (PA66)	t	38	
Thermoplastics	Polycarbonate		38	
Thermoplastics	Polymethyl methacrylate (PMMA)		38	
Thermoplastics	Polyvinyl acetate (PVA)	29		
Thermosets, fibre & elastomers	Polypropylene fibre (PP fibre)	o		o
Thermosets, fibre & elastomers	Acetone			
Thermosets, fibre & elastomers	Formaldehyde			
Thermosets, fibre & elastomers	Isophthalic acid			
Thermosets, fibre & elastomers	Maleic anhydride			
Thermosets, fibre & elastomers	Phenol			
Thermosets, fibre & elastomers	Phthalic anhydride			
Thermosets, fibre & elastomers	Polybutadiene			
Thermosets, fibre & elastomers	Polychloroprene			
Thermosets, fibre & elastomers	Propylene oxide			
Thermosets, fibre & elastomers	Polyethylene terephthalate fibre (PET fibre)			
Thermosets, fibre & elastomers	Epoxy resin			
Thermosets, fibre & elastomers	Melamine			
Thermosets, fibre & elastomers	Nitrile butadiene			
Thermosets, fibre & elastomers	Polyacrylonitrile			
Thermosets, fibre & elastomers	Styrene butadiene			
Thermosets, fibre & elastomers	Toluene diisocyanate	35		
Thermosets, fibre & elastomers	Polyamide 6 fibre (PA6 fibre)	35		

Thermosets, fibre & elastomers	Polyamide 66 fibre (PA66 fibre)
Thermosets, fibre & elastomers	Methylene diphenyl diisocyanate
Solvents, additives & explosives	Methyl alcohol
	Carbon black
	Butene 1
	Butene 2
	Isobutene
	Toluene
	Acetic acid
	Cyclohexane
	Methyl tert-butyl ether
	Ammonium nitrate
Other chemicals	
	Lubricants
	Other rubber products
	Agricultural chemicals
	Special industrial chemicals
	Basic pharmaceuticals
	Glues, additives, sealants
	Paints, water-based
	Paints, solvent-based
	Pigments, glazes
	Inks

Table 3-4: Current available emission data coverage for petrochemical product group and life cycle stages coverage in primary data sources and selected studies. *Ext=Extraction, Ref=Refining, Conv=Conversion, EOL= End of life*

Life cycle stages

The IPCC framework for collating and reporting emissions data, used by the UNFCCC and EDGAR databases, has some coverage of the life cycle stages of chemical products [38]. Table 3-5 shows the breadth of IPCC guidance, divided across many different sections which relate to the life cycle stages. This makes linking the different accounts across the life cycle of a specific chemical product challenging.

Fairly good data coverage for crude oil extraction [5] and the refining sector [23] of petrochemicals' life cycle has been reported. The proliferation of new technologies in the petrochemical sector has exacerbated variation in carbon intensity for these life cycle stages. Masnadi et al. (2018) [5] analysed emission data from 8,966 different oil fields in 90 countries. They show that carbon intensity is heterogenous across global crudes with fields in the highest 5th percentile emitting more than twice as many emissions per unit mass as the median field. This study also finds significant variation in carbon intensity at a national level. Similar findings were reported in Jing et al (2020) [23] investigating carbon intensity variation in upstream crude oil extraction and refining stage. For instance, carbon intensity for some crudes range from 12.1 to 49.2 kg CO_2e bbl^{-1} at the country level (35 countries) and from 12.2 to 60.8 kg CO_2e bbl^{-1} at the refinery level.

There is less published data describing regional variation in carbon intensity for downstream production, use and EOL treatment in the petrochemical sector. Based on Geyer et al.'s [16] first-ever estimation of global plastics stocks and flows, Zheng et al. [17] compiled a dataset covering ten conventional and five bio-based plastics and their life cycle GHG emissions on a global scale. Results showed that the global life cycle GHG emissions of conventional plastics were 1.7 Gt of CO_2e in 2015, which would grow to 6.5 Gt CO_2e by 2050 under the current trajectory. The life cycle GHG emissions were also evaluated under various mitigation strategies.[16]

Life cycle assessment methods are widely adopted to estimate the whole supply chain emissions for individual petrochemical products. However, summing these up to national or global level emissions accounts for products can be complex. Notably, given the evidence for regional variation in the carbon intensity of national electricity grids and heat network and variation in petrochemical product recycling rates, it is highly likely that regional variation in carbon intensity will be present for production, use and EOL treatment.

Life cycle stage	Processes	IPCC Guidance	IPCC Section
Raw material extraction	Crude oil extraction	4.2 Fugitive emissions from oil and natural gas systems (Vol 2)	1B2, 1A1
	Natural gas extraction and processing	4.2 Fugitive emissions from oil and natural gas systems (Vol 2)	1B2, 1A1
Chemical production	Oil refining	3.9 Petrochemical & carbon black production (Vol 3)	2B8
	Steam Cracking	3.9 Petrochemical & carbon black production (Vol 3)	2B8
	Catalytic reforming	3.9 Petrochemical & carbon black production (Vol 3)	2B8
	Steam reforming	3.9 Petrochemical & carbon black production (Vol 3)	2B8
	Ammonia Production		2.B.1
	Nitric Acid Production		2.B.2
	Adipic Acid Production		2.B.3
	Caprolactam, Glyoxal and Glyoxylic Acid Production		2.B.4
	Carbide Production		2.B.5
	Titanium Dioxide Production		2.B.6
	Soda Ash Production		2.B.7
	Petrochemical and Carbon Black Production		2.B.8
	Methanol	3.9 Petrochemical & carbon black production (Vol 3)	2.B.8.a
	Ethylene	3.9 Petrochemical & carbon black production (Vol 3)	2.B.8.b
	Ethylene Dichloride and Vinyl Chloride Monomer	3.9 Petrochemical & carbon black production (Vol 3)	2.B.8.c
	Ethylene Oxide		2.B.8.d
	Acrylonitrile	3.9 Petrochemical & carbon black production (Vol 3)	2.B.8.e
	Carbon Black	3.9 Petrochemical & carbon black production (Vol 3)	2.B.8.f
	Fluorochemical Production		2.B.9
	By product emissions		2.B.9.a
	Fugitive Emissions		2.B.9.b
	Other (Please specify)		2.B.10
	Combustion emissions	2 Stationary combustion (Vol 2)	1A2
Product Manufacture			
Use	Urea fertilisation		3C3
	Solvents		2F5
EOL treatment	Landfill	3 Solid Waste Disposal (vol 5)	4A
	Incinerate, Thermal recycling	5 Incineration and open burning of waste (Vol 5)	4C

Table 3-5: IPCC guidance related to chemical sectors across life cycle stages

Countries/ regions

The coverage and quality of emissions data varies between countries and regions. The UNFCC emissions reporting obligations are different for Annex I and non-Annex I countries, with the least developed countries and small islands states having the most discretion over the level of detail reported. At the global scale, GHG emission data for Annex I parties are generally complete while those for non-Annex I parties are less well documented. Among non-Annex I parties, countries in the Asia-Pacific, Latin American and Caribbean regions have moderately complete data compared to those in Africa.

Figure 3-5 shows the classification of Parties to the UNFCCC by colour.

- Annex I: There are 43 Parties to the UNFCCC listed in Annex I of the convention, including the European Union. These Parties are classified as industrialised (developed) countries and "economies in transition" (EITs). The 14 EITs are the former centrally planned (Soviet) economies of Russia and Eastern Europe. Annex I countries have absolute targets in the Paris Accord.
- Annex II: Of the Parties listed in Annex I of the convention, 24 are also listed in Annex II of the convention, including the European Union. These Parties are made up of members of the Organisation for Economic Co-operation and Development (OECD): these Parties consist of the members of the OECD in 1992, minus Turkey, plus the EU. Annex II Parties are required to provide financial and technical support to the EITs and developing countries to assist them in reducing their GHG emissions (climate change mitigation) and manage the impacts of climate change (climate change adaptation).
- Annex B: Parties listed in Annex B of the Kyoto Protocol are Annex I Parties with first- or second-round Kyoto GHG emissions targets (see Kyoto Protocol for details). The first-round targets apply over the years 2008–2012. As part of the 2012 Doha climate change talks, an amendment to Annex B was agreed upon containing with a list of Annex I Parties who have second-round Kyoto targets, which apply from 2013 to 2020. The amendments have not entered into force.
- Least-developed countries (LDCs): 49 Parties are LDCs and are given special status under the treaty in view of their limited capacity to adapt to the effects of climate change.
- Non-Annex I: Parties to the UNFCCC not listed in Annex I of the convention are mostly low-income developing countries. Developing countries may volunteer to become Annex I countries when they are sufficiently developed. Non-Annex I countries have relative targets in the Paris Accord so petrochemical industries can increase emissions when based in non-Annex I countries.

Figure 3-6 and Figure 3-7 show how the per capita emissions from the chemical sector have changed between 2005 and 2013, for different countries in the world. It is noted that many countries do not report even a total emissions account for the chemical sector. The emissions accounting gaps are found primarily in the non-Annex I countries.

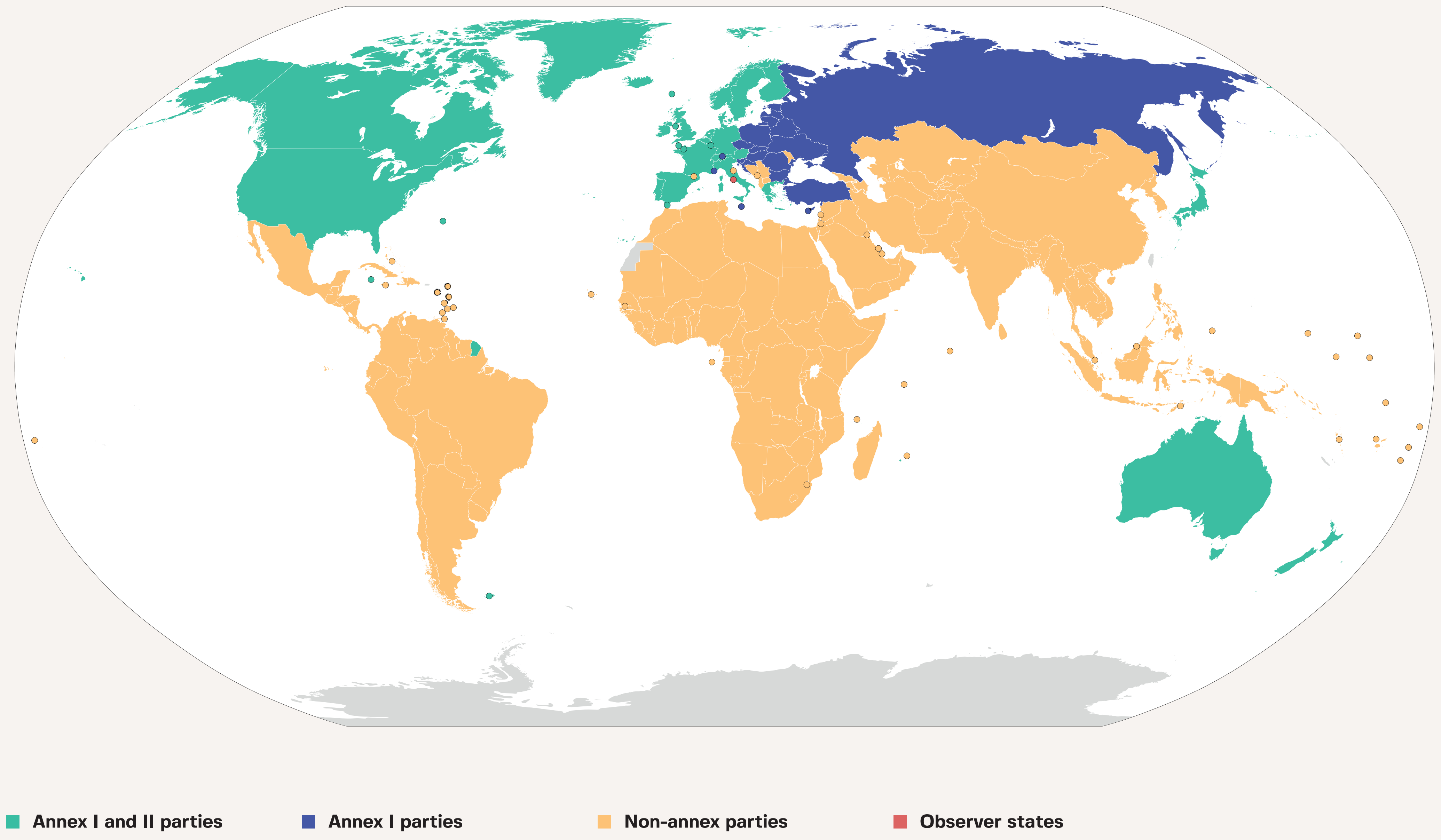


Figure 3-5: Parties to the UNFCCC *Annex I and II parties | Annex I parties | Non-annex parties | Observer states*

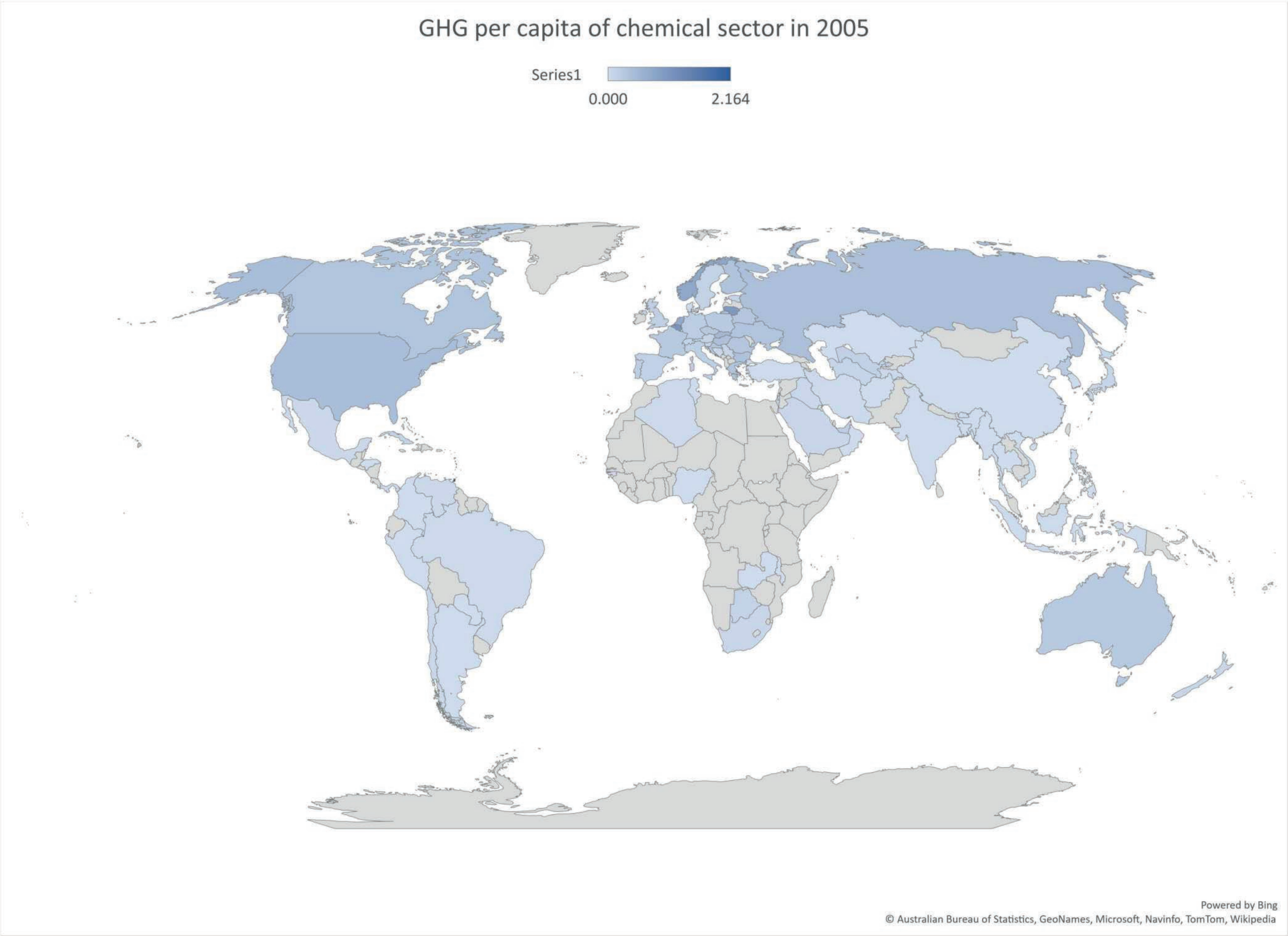


Figure 3-6: GHG emissions per capita of chemical sector (tonne CO_2 per capita) in 2005. Grey colour indicates no data available. Data from UNFCCC

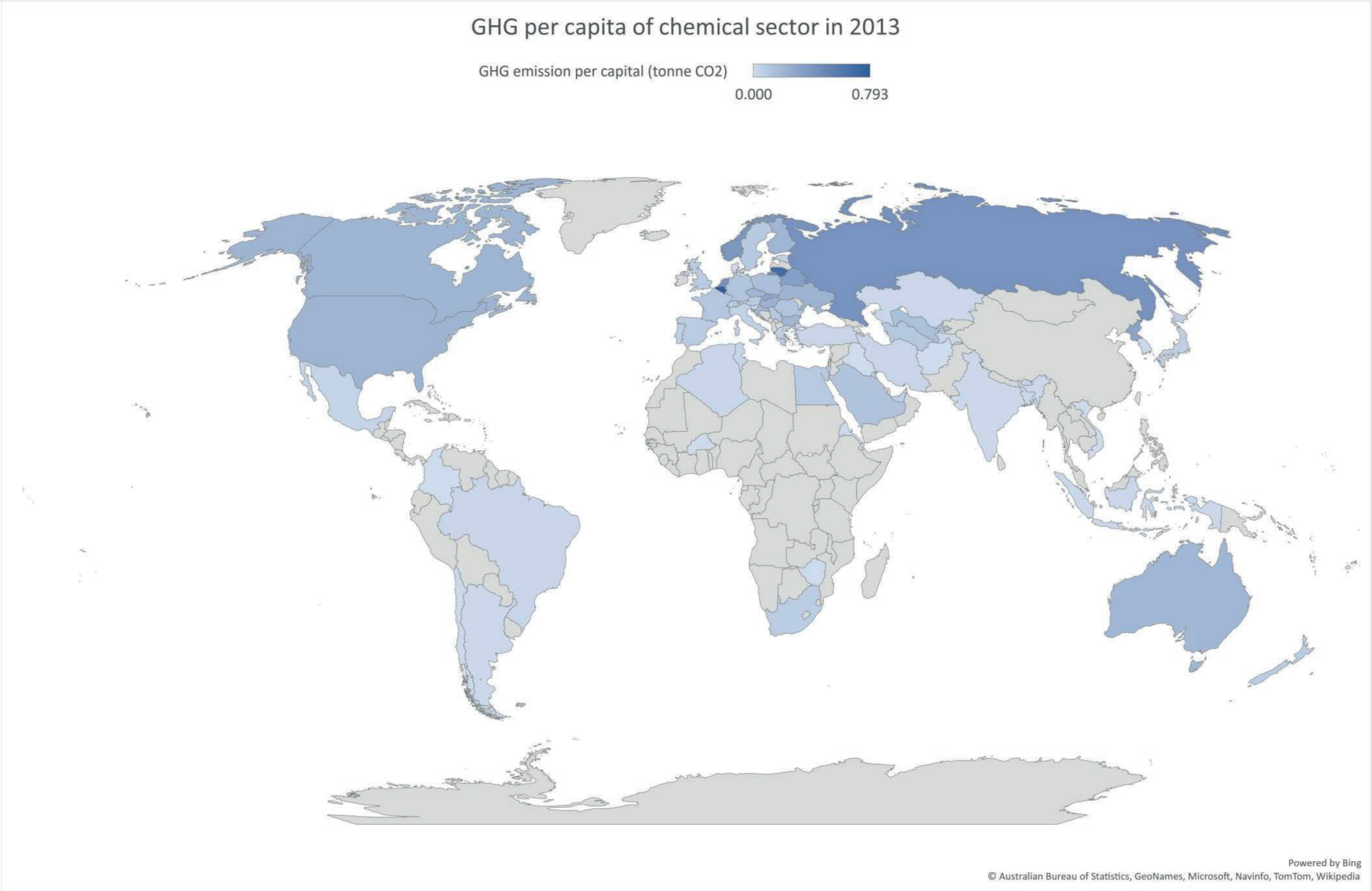


Figure 3-7: GHG emissions per capita of chemical sector (tonne CO_2 per capita) in 2013. Grey colour indicates no data available. Data from UNFCCC

F-gases

Fluorinated gases (F-gases) are a family of man-made gases used in a range of industrial applications. F-gases are often used as substitutes for ozone-depleting substances because they do not damage the atmospheric ozone layer. However, F-gases are powerful GHGs, with a global warming effect up to 23 000 times greater than carbon dioxide (CO_2), and their emissions are rising strongly.

GHG emissions

Carbon dioxide (CO_2) emissions are significantly higher than methane (CH_4) or nitrous oxide (N_2O) emissions by mass in the current chemical industry (see Figure 3-8). However, non-CO_2 GHGs, such as methane, nitrous oxide and fluorinated gases, trap more heat within the atmosphere than CO_2. These gases are emitted from a broad range of sectors and sources as follows: CH_4 is mostly emitted from extraction, distribution and combustion of fossil fuel, industrial processes, enteric fermentation, rice cultivation, manure management, other agricultural sources, and the waste sector; N_2O is mostly emitted from industrial processes, agricultural soils, manure management and wastewater; and ***F-gases*** are mostly emitted from industrial processes. Moreover, the emission composition across the production process can vary significantly, e.g. carbon dioxide and methane can contribute on average 65% and 34% of total field-level CO_2e emissions for crude oil production, respectively [5].

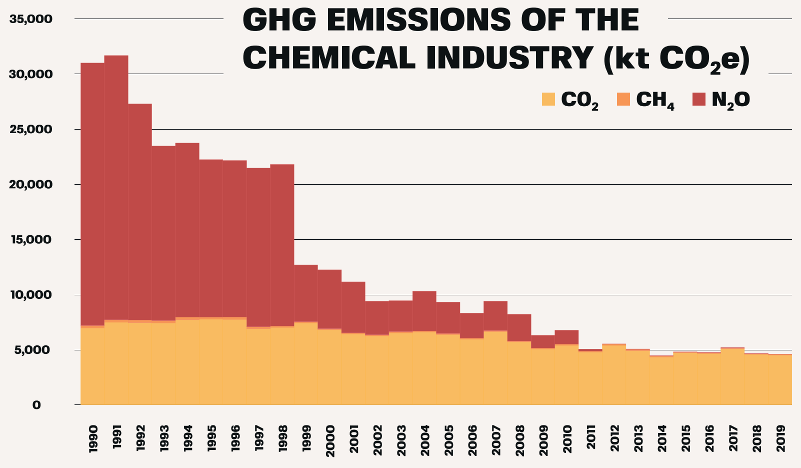
Mitigation of these emissions is an important and relatively inexpensive supplement to CO_2-only mitigation strategies. For example, the United States Environmental Protection Agency estimates that

2.7 Gt CO_2e of non-CO_2 emissions could be mitigated by 2020 at a cost below USD50/t CO_2e

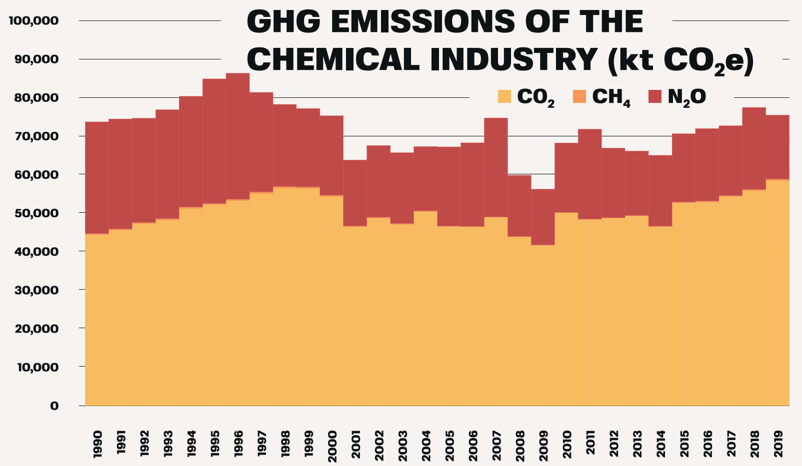
and a substantial portion of these reductions could generate an immediate financial return [39]. However, it shall be noted that petrochemical industry to a large extend has been exempt from European Union Emissions Trading System (EU-ETS); and that plastics often account for a small part of the overall product value.

The coverage of UNFCCC reported GHG emissions, across different sectors, is shown Table 3-6 (reported GHG is shaded).

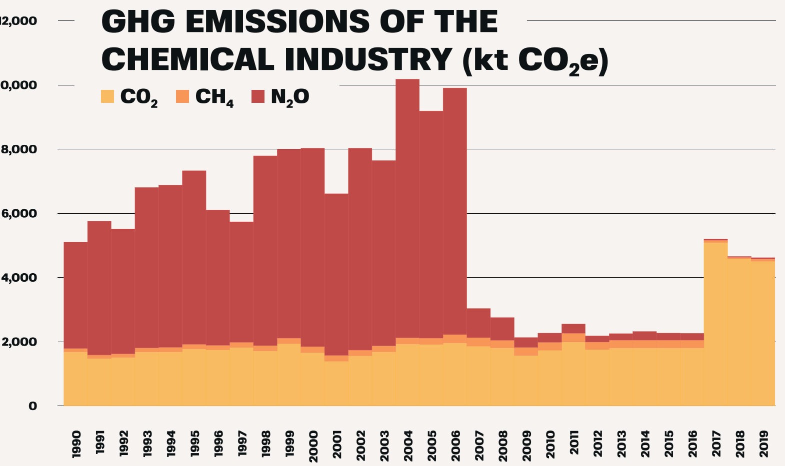
Figure 3-8: Examples of GHG emissions of the chemical industry by emission types as reported by UNFCCC: a) UK, b) USA, c) Brazil, d) China, e) Annex I countries



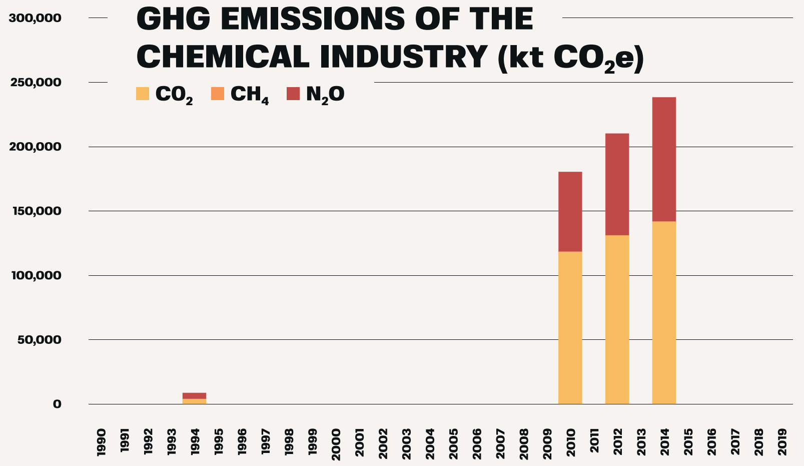
a



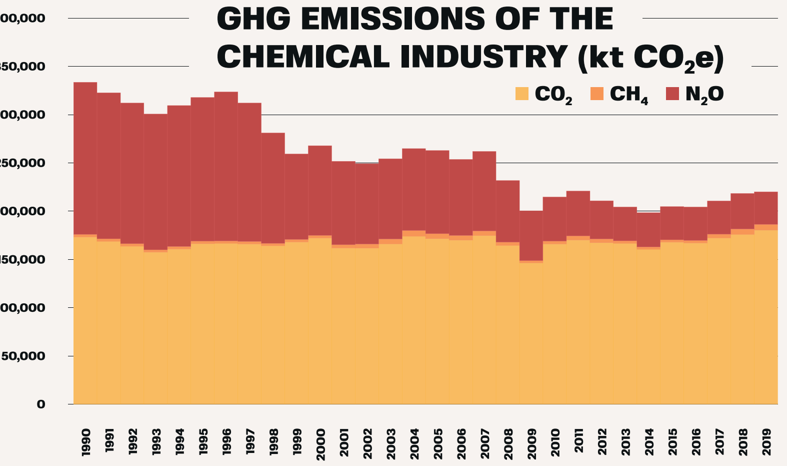
b



c



d



e

Categories	Net CO_2 (1) (2)	CH_4	N_2O	HFCs	PFCs	SF_6	Other halogenated gases with CO_2 equivalent conversion factors (3)	Other halogenated gases without CO_2 equivalent conversion factors (4)	NO_x	CO	NMVOCs	SO_2
	(Gg)			CO_2 equivalent (Gg)				(Gg)				
1A Fuel Combustion Activities												
1A1 Energy Industries												
1A2 Manufacturing Industries and Construction												
1A3 Transport												
1A4 Other Sectors												
1A5 Non-Specified												
1B Fugutive Emissions and Fuels												
1B1 Solid Fuels												
1B2 Oil and Natural Gas												
1B3 Other Emissions from Energy Production												
2B Chemical Industry												
2B1 Ammonia Production												
2B2 Nitric Acid Production												
2B3 Adipic Acid Production												
2B4 Caprolactam, Glyoxal and Glyoxylic Acid Production												
2B5 Carbide Production												
2B6 Titanium Dioxide Production												
2B7 Soda Ash Production												
2B8 Petrochemical and Carbon Black Production												
2B9 Fluorochemical Production												
2B10 Other (please specify)												

Table 3-6: Coverage of GHGs across emissions account categories. *[1] CO_2 net emissions (emissions minus removals) — [2] Total amount of CO_2 captured for long-term storage is to be reported separately for domestic storage and for export in the documentation box — [3] The other halogenated gases for which the CO_2 equivalent conversion factor is not available should not be included in this column. Such gases should be reported in the column 'Other halogenated gases without CO_2 equivalent conversion factors' — [4] When this column is used, gases should be listed separately and the name of the gas in the documentation box.*

Time series

Time series data is available for Annex I countries for total GHG emissions by petrochemical sector. However, the coverage of time series data varies, with some national series updated regularly, while others are well out of date. In Figures 3-9 and 3-10 we have illustrated the span of years covered by the database or study. This includes single-year studies, historical analysis over many years, and future dynamic predictions for the petrochemical sector. Geyer et al [16] provided the first estimation of plastics stocks and flows at the global level from 1950 to 2015. Masnadi et al [5] and Jing et al [23] released historical analysis and future dynamic predictions of emissions of US crude oil and global/national refining sector, respectively until 2100. However, no single study has reported the time series GHG emission data of across all petrochemical products and life cycle stages.

At the global scale, GHG emission time series data for Annex I parties are generally complete from their base year to the calendar year minus 2 (currently 1990 – 2018). However, GHG emission data for some non-Annex I parties, such as North Korea and China, are poorly documented; information is only submitted periodically and for selected years, following UNFCCC guidelines. Figure 3-9 shows the inconsistency in reporting across different countries, with gaps in the times series and less comprehensive product lists, shown for North Korea and China.

Uncertainty

Although uncertainty in reported data is often expected to be significant, in the majority of data sources reviewed it is not explicitly dealt with. Despite this, some of the major data sources do tackle the issue, such as the UNFCC reported data, and databases such as Ecoinvent. When primary data on uncertainties are not available, uncertainty is either neglected, or left to the estimation of those doing the analysis. Alternative non-probabilistic uncertainty analysis methods may be valuable in this situation.

Since there is no single data source that can map global petrochemical emissions in detail, a full understanding of these emissions must involve combining and reconciling multiple sources of data. Beyond any uncertainty about the values reported in these individual datasets, further uncertainty arises when definitions and terminology is unclear or conflicting.

Further errors can arise when converting data between different forms. Statistics are also often published in PDFs, either as the tables of data or as tables and figures within reports. This is often given as context for the data but is difficult to extract and use further. The formats of data across the data sources reviewed here vary widely. To integrate the data into one large, detailed picture of global petrochemical industry emissions, the data must be combined and one format adopted for all data.

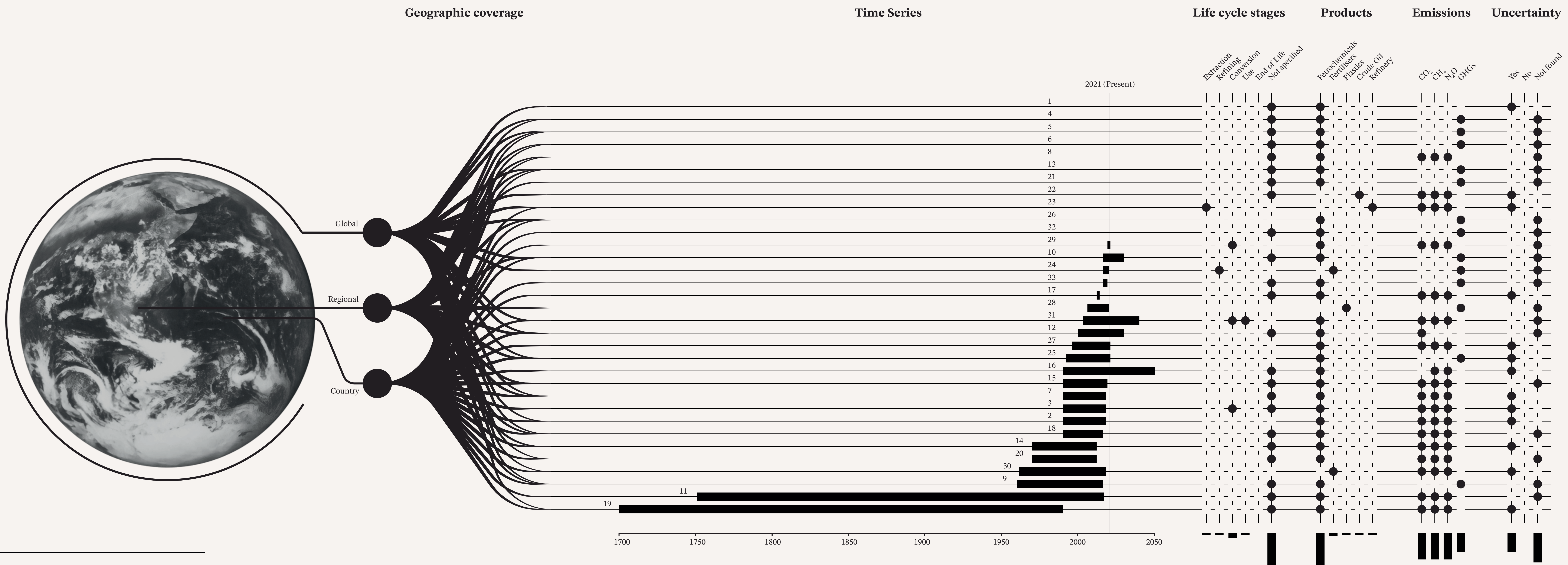


Figure 3-9: Time series reported in the primary data sources

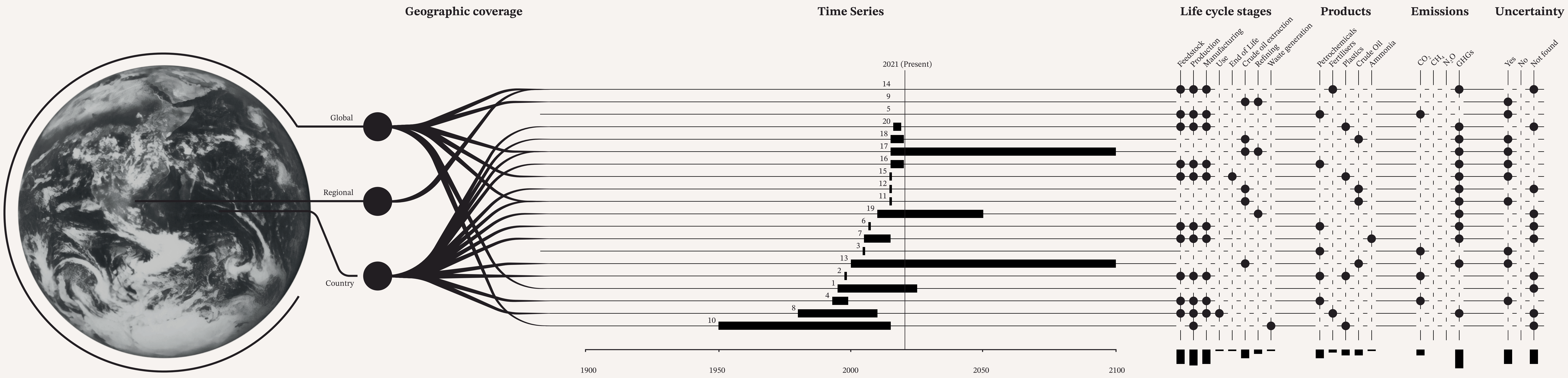


Figure 3-10: Time series reported in the selected studies

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4

Chapter Four:

C-THRU Carbon clarity in the global petrochemical supply chain

Chapter Summary

We have reviewed GHG emissions literature and data from the petrochemical sector and identified knowledge gaps. In C-THRU, we will provide an accessible and reliable repository of global resource flows, emissions data, and mitigation options for the petrochemical sector, accounting explicitly for uncertainty. We will create accurate and verifiable accounts of current GHG emissions and environmental impacts (by chemical product, life cycle stage, sector, and region) and validate the accuracy of existing top-down GHG emissions accounts. Based on these accounts, we will catalogue and model supply-side mitigation options (e.g. new process route, efficiencies, and technologies), demand-side mitigation options (e.g. materials efficiency, recycling, and recovery), and their potential impacts on future pathways and emissions reductions outcomes. Additionally, we will explore the petrochemical sector's influence on environmental policy, considering the implications of economic, legal, business, governance, regulation, and policy contexts. We will support an international response to climate change and co-create active stakeholder networks, by delivering an unbiased, open, and rigorous approach to reducing GHG emissions from the petrochemical sector. In this chapter, we discuss the details of our project plan to achieve these aims and present focus studies of current work in each of three research channels: materials flow and emissions accounting (Section A); mitigation options and pathways (Section B); and wider societal contexts (Section C).

Section A

In this section, we summarise the approaches C-THRU is taking to account, catalogue, and calculate resource flows and GHG emissions. The various modelling frameworks we utilise are described. We draw attention to our aims of mutual exclusivity and collective exhaustivity of the data; mass and energy balancing; and accounting for the heterogeneity across the sector. The focus study in Section A presents an inspection of direct emissions from chemical manufacturing in the United States.

Section B

Section B gives a review of supply- and demand-side emissions mitigation options for the petrochemical industry including process technologies, mitigation interventions, and recycling processes. The TIMES platform, the energy technology systems model used by the IEA for petrochemicals analysis, is the model we will use for decarbonisation scenario analysis. A focus study of our review work of decarbonisation pathway models is presented, summarising model characteristics and scenario designs.

Section C

In Section C, we introduce the business landscape and economic environment of the petrochemical sector. A focus study describes the HARMONEY economic model and explains how it will be extended for C-THRU to cover multiple natural resource types and include the efficiency of energy conversion into work. We discuss the complexity of the petrochemical industry and the diversity of companies and other actors within it. A second focus study of our work to date on the petrochemical business landscape presents our archetypal model.

Section D

We will conclude this Year 1 report in Section D with a round-up of our work to date, our plans for the next two years, and information about how to engage with the project and its researchers.

A. Resource flows and emissions acounting

Key points:

- In our accounting we aim to:
    - Be holistic, conducting a whole system integration for mutual exclusivity and collective exhaustivity of the data.
    - Respect mass and energy balancing in supply-chain modelling and consider uncertainty at every stage.
    - Account for heterogeneity across different chemical products, life cycle stages, sectors, and regions.
- Data uncertainty and the lack of whole-system models for the petrochemical sector affect not only the assessment of today's GHG emissions, but also the evaluation of the accuracy of emissions projections and future mitigation options.
- Levi and Cullen have developed the most comprehensive whole-system analysis of material flows to date, providing the key link between supply- and demand- side mitigation options[1].
- A small number of GHG intensive processes, used to produce large quantities of chemicals, dominate gate to gate GHG emissions in the chemical manufacturing sector.
- The project will address the complexity of supply chains and processes in the petrochemical sector by developing an integrated model that combines life cycle analysis with material flow analysis.

Until recently, no suitable framework for mapping chemicals from their raw materials to their end-use products existed in the public realm. The paucity of publicly available information on petrochemical material flows was identified as a key barrier to a robust examination of potential mitigation options in the sector. This has made reliable and transparent assessments of GHG emissions accounts and mitigation options, across the whole life cycle of chemical products, very difficult. It has also led to

an overreliance on supply-side GHG mitigation options in the models that do exist

supplied with data sourced primarily from the industry itself and including mitigation options that are susceptible to overly optimistic assumptions about their parameters and potentials. The missing component is an open and reliable bottom-up framework for mapping resources, processes, life cycle emissions, and exploring supply- and demand-side mitigation options.

To address this knowledge gap Levi and Cullen (PI for C-THRU) undertook a bottom-up assessment of key material flows from fossil fuel feedstocks to chemical products. The analysis traces 77 chemicals through 65 core production processes using 2013 data, resulting in the most comprehensive global assessment of its type. The results, shown in Figure 3-1, involved consulting more than one hundred data sources across academic and grey literature to minimise the need for estimation and interpolation.
The resulting dataset is built upon extensive engineering analysis, with consideration of the stoichiometry and mass/energy balancing for every chemical process. In addition, the entire dataset is published openly, resulting in the first comprehensive and freely available transparent model of the whole petrochemical sector. This modelling framework and extensive data collection activity were instrumental in the publication of the IEA's 2018 report The Future of Petrochemicals: Towards More Sustainable Plastics and Fertilisers[2] for which Levi was a lead author. This level of rigor, consistency, and transparency constitutes an important step forward in both the quality and quantity of information available on the petrochemical sector and will be a hallmark of the C-THRU project, as well.

A holistic approach: whole system integration for mutual exclusivity and collective exhaustivity

C-THRU brings together several of the current, most rigorous modelling efforts that are focused on analysing the environmental impacts of the petrochemical sector to produce a holistic account of the sector flows and impacts. This whole system view allows for the identification of data gaps and double counting issues to ensure mutual exclusivity and collective exhaustivity of the analysis. Each modelling activity uses different tools, to address various research questions, through life cycle stages, across geographical areas, and over time spans. These models are:

- The global model of key material flows in the petrochemical sector, from fossil fuel feedstocks to chemical products, co-developed by Cullen (PI) at Cambridge University.
- The iterative Bayesian framework for explicitly characterising uncertainty in material and energy flows systems, co-developed by Lupton (Co-I) at Cambridge and Bath Universities.
- Process engineering models and decarbonisation scenario analysis (TIMES) for analysing energy and emissions from the US chemical industry, co-developed by Masanet (Co-I) at Northwestern and UC Santa Barbara.
- A dynamic material flow analysis framework for anticipating material demand and product stocks and discards, co-developed by Serrenho (Co-I) at Cambridge University for UK vehicle [3] and housing stocks.
- Spatial and process models of the US chemical industry, including analysis of methane leakage and disruptive events co-developed by Allen (Co-I) at University of Texas at Austin.

We require our supply-chain modelling to be respectful of mass and energy balancing

Levi and Cullen's global map of chemicals flows[1] provides the crucial missing link between supply-side and demand-side GHG mitigation options. This is shown in the identity equation below, where the mitigation levers are clustered within two groups: supply-side options (green) and demand-side options (red). Highlighted orange terms show the material flow links.

$$G_t = S \cdot \left\{ \left(\frac{G_e}{E} \cdot \frac{E}{M_p} + \frac{G_f}{F} \cdot \frac{F}{M_p} \right) \cdot \frac{M_p}{K} + \frac{G_u}{M_u} \cdot \frac{M_u}{K} + \frac{G_d}{M_d} \cdot \frac{M_d}{K} \right\} \cdot \frac{K}{S}$$

Supply-side options Demand-side options Link: material flows

Notes: G_t is the sum of all emissions directly attributable to chemical products, including those relating to process energy G_e, G_f, use G_u, and disposal G_d; S is the aggregated final service demand met by chemical products; G_e/E is the process energy emissions intensity; E/M_p is the process energy intensity; G_f/F is the feedstock emissions intensity; F/M_p is the feedstock intensity; M_p/K is the material production required to maintain the stock of all chemical products; G_u/M_u is the emissions intensity of products in the; M_u/K is the material in use while maintaining the stock; G_d/M_d is the emissions intensity of product disposal; M_d/K is the material disposed in maintaining the stock; K/S is the stock required per unit of final service

In C-THRU, we will develop a systems supply-chain model structure capturing material and energy flows, stocks in use, emissions, and environmental impacts. We use different types of models, appropriate to different parts of the life cycle, the integrative model will abstract a common structure. The mathematical structure combines the flow and emissions modelling of Life Cycle Analysis with the dynamic stock modelling of Material Flow Analysis. We will:

- Establish an integration process to bring together results from each model to calibrate the integrative model structure, and feedback to the modes for data improvement priorities and potential inconsistencies.
- Compile industry data to quantify production quantities, plant capacities [4], plant vintages, feedstock types, typical technologies [5,6], and trade flows [7] at the regional and global levels.
- Output results from the model in a consistent format[8] (i.e. dynamic Sankey diagrams of mass, energy, and emissions, using the FloWeaver tool developed by Co-I Lupton)[9] for further analysis and data visualisation, acting as a toolkit for others to extract relevant evidence from the model.
- Assess and characterise data uncertainties and propagate these through the model using Monte Carlo simulations in a Bayesian framework, as previously developed by Lupton (Co-I) for material and energy flows.
- Present uncertain results in the context of decisions or questions and use sensitivity analysis to explore the areas of the model most in need of improved characterisation of uncertainty or improved data quality, driving an iterative improvement cycle.

We account for heterogeneity – flows in the petrochemical sector are different given five variables

There are five aspects of particular interest in our study: time, region, GHG, petrochemical product and life cycle stage. As they vary through the sector, the picture of petrochemical energy, mass, and emission flows changes, i.e. the petrochemical sector is not homogeneous. The first three variables, time, region and GHG, are present in some capacity in each data source. These three concepts are all interrelated and each is considered as the 'source of emissions'. The petrochemical product, life cycle stage, or the process which produces the emissions may also be listed in the data. These five variables must be used in conjunction and with awareness of data uncertainty, to allow datasets to be integrated, and a full picture of the petrochemical sector generated.

Next, we present a focus study of the work we are doing on direct emissions from chemical manufacturing in the USA.

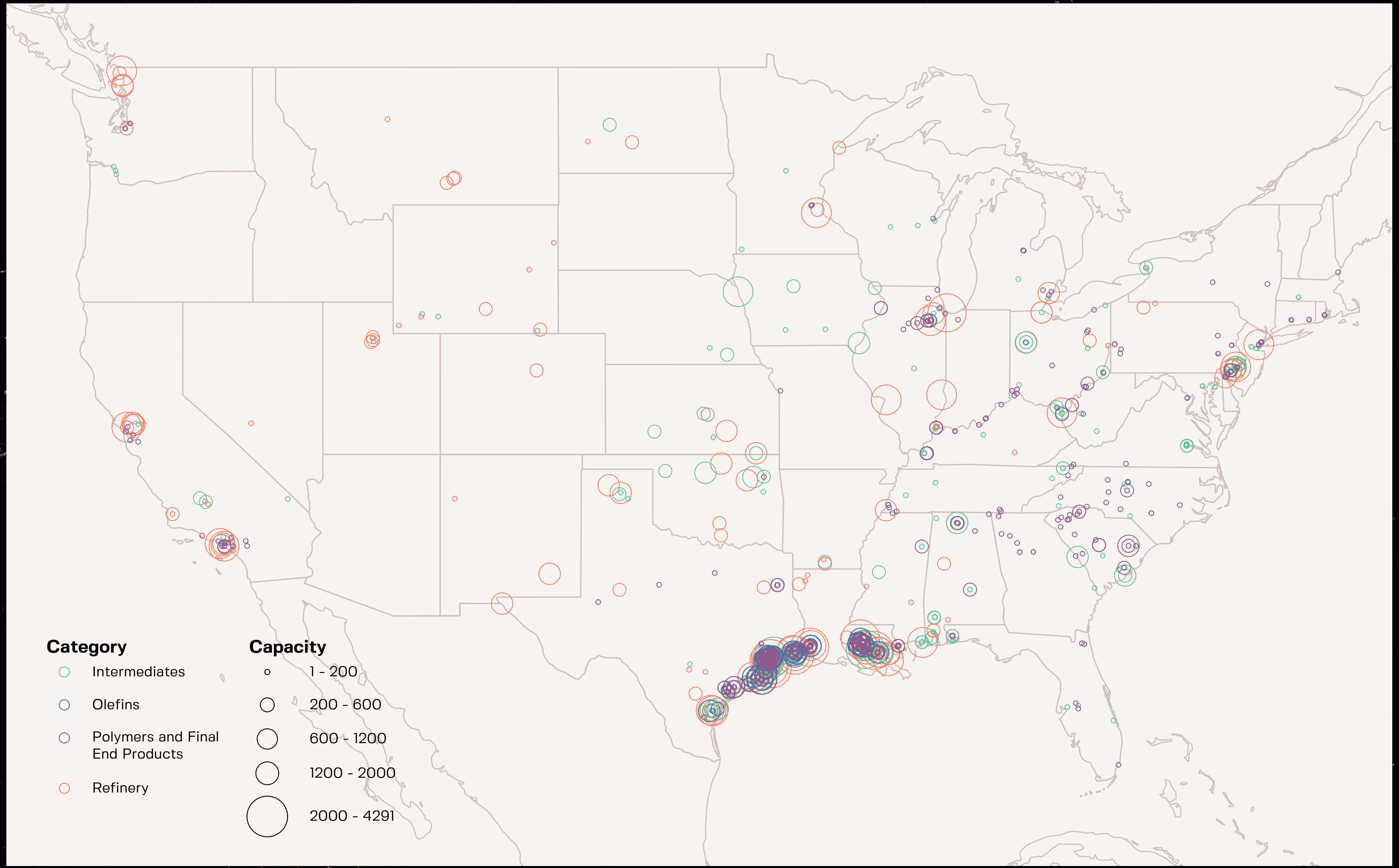


Figure 4-1: Chemical manufacturing facilities represented in the review of greenhouse gas emissions from chemical manufacturing in the United States[10]

Focus study: Annual GHG emissions in the USA per tonne of product

The chemical manufacturing industry is one of the most energy intensive manufacturing sectors, making it a significant source of GHG. Direct and indirect GHG emissions from chemical manufacturing processes can be assessed in a variety of ways, including analysis of process flowsheets and emission reporting and measurement. Our initial work, compares process-based estimates of GHG emissions to reports made through measurements and governmental reporting and identifies the distribution of GHG emission sources by process and by source type (process heat, electricity consumption).

Process based GHG emissions estimation was based on the models of the US chemical industry described by DeRosa et al. (2015) [11,10]. These models represent the US chemical industry in 2017 and map the interconnections of chemical processes that produce hundreds of commodity chemicals and intermediates. Locations of production facilities are spatially resolved and include production capacity information. Figure 4-1 maps the locations of manufacturing facilities represented in the model.

GHG emissions associated with each of the processes was based on stoichiometric and utility usage data from the 2012 IHS 2012 Process Economics Program Yearbook, and capacity data were derived from the 2017 ICIS Supply and Demand Database. GHG emissions were assessed for a total of 135 processes. Direct emissions of processes (gate to

Emission types	Indirect emissions (upstream) kg CO_2e/MMBTU	Direct emissions (combustion/consumption) kg CO_2e/MMBTU	Total emissions kg CO_2e/MMBT
Natural Gas	11.2	59.6	70.8
Fuel oil	4.8	85.6	90.4
Electrcity	131.6	0	131.6

Table 4-1: Emission factors for fuel and electricity use

gate emissions) and direct emissions coupled with indirect emissions were assessed. Direct emissions include process utility usage, and emissions from chemical reactions. Utility requirements separately tracked combustion of natural gas on-site as an energy source, combustion of fuel oil on-site as an energy source, and use of electricity. Indirect emissions included upstream emissions for fuel and electricity (e.g. emissions associated with the production of fuels and electricity used in the processes). National average emission factors are summarised in Table 4-1. All emissions are assigned to the main product of the process and are reported as emissions per unit mass of the primary product, and emissions per process per year, multiplying the emissions per unit mass of product by the production capacity in the United States.

Figure 4-2 shows the gate-to-gate GHG emissions per pound of product for the 135 processes that were evaluated. Figure 4-2 shows the large variation, over approximately 3 orders of magnitude, in GHG emissions per unit mass of primary product for the 135 processes that were evaluated. The 5 most GHG intensive processes are listed in Figure 4-2. Some of these GHG intensive processes produce small volumes of product, while others, such as ethylene production are used to produce large quantities of commodity chemicals. Figure 4-3 shows the emissions per unit mass of product multiplied by production capacity. A small number of chemicals dominate. Ethylene production alone contributes approximately half of total gate to gate GHG emissions of the 135 chemical processes evaluated. Chlorine and ammonia manufacturing are also significant.

The emission estimated based on process models were compared, where possible to facility-level emissions reported by the US Environmental Protection Agency Greenhouse Gas Reporting Program (GHGRP, ghgdata.epa.gov/ghgp), using ammonia production as a test case. Ammonia production was selected because ammonia is frequently produced in facilities dedicated to ammonia production, rather than in highly integrated facilities producing multiple products. This allows the facility level GHGRP emissions reporting to be compared to the process level data, a comparison that is very difficult in integrated facilities. Figure 4-4 shows the mapping of ammonia facilities considered in this work and the ammonia facilities reported to the GHGRP based in 2017. A total of 31 ammonia plants emit 28.4 Mt CO$_2$e emissions as estimated in this work, while a total of 29 ammonia plants emit 33.1 Mt CO$_2$e in 2017 as reported by GHGRP. Although the total amount of greenhouse gas emissions from ammonia manufacturing estimated in this work are in reasonable agreement with the emissions reported by GHGRP, emissions estimated for individual facilities might be different due differences in utility sources, emission factors, and the inclusion of processes such as nitric acid and phosphoric acid production.

GHG emissions associated with feedstock production (upstream emissions)

We are currently evaluating the GHG emissions associated with producing the feedstocks for chemical manufacturing in the United States. The goal of this work is to assess the relative importance of feedstock production and chemical manufacturing emissions in total well to product manufacture GHG emissions. The emissions associated with ethane production will be used to illustrate the framework and the preliminary results that are emerging. Ethane is the primary feedstock for ethylene and polyethylene manufacturing and is broadly representative of light alkane feedstocks which are currently the dominant hydrocarbons used as chemical manufacturing feedstocks in the United States.

Ethane is co-produced along with oil and/or natural gas, in most oil and gas production regions in the United States. We have reviewed the literature on these emissions and have synthesised data on emission sources and magnitudes. A few key points emerge:

- GHG emissions per kg of ethane produced varies significantly, depending on the production region from which the ethane is sourced.
- Variability in methane emissions is the dominant cause of the emission differences.
- The importance of upstream emissions is highly dependent on whether near-term or long-term climate impacts are the focus of mitigation because the short term climate impacts of methane (over time periods of 1-20 years) are 3-4 times the impacts integrated over 100 years.

To provide a specific example, in the Eagle Ford Shale region in south central Texas, one of the larger production regions in the United States, our team conducted a detailed analysis of GHG emissions, assembling emission estimates site by site for ~17,000 sites in the region.[10] Upstream emissions per pound of ethane produced are approximately 30-40% of the emissions associated with manufacturing ethylene from the ethane feedstock if the climate impacts of methane emissions are integrated over a 100-year period. On the other hand, if the climate impacts of methane are evaluated over a 20-year period, the climate impacts of ethane production are approximately equal to the impacts of ethylene production for feedstock sourced in the Eagle Ford. If the feedstock is sourced from the Permian Basin, where methane emissions are roughly three times those in the Eagle Ford, feedstock emissions can dominate.

These preliminary results from the C-THRU project suggest that minimising methane emissions during feedstock extraction may be a more effective level for reducing emissions as addressing the chemical conversion process. However, feedstock emissions vary greatly across facility and region, and further analysis is required.

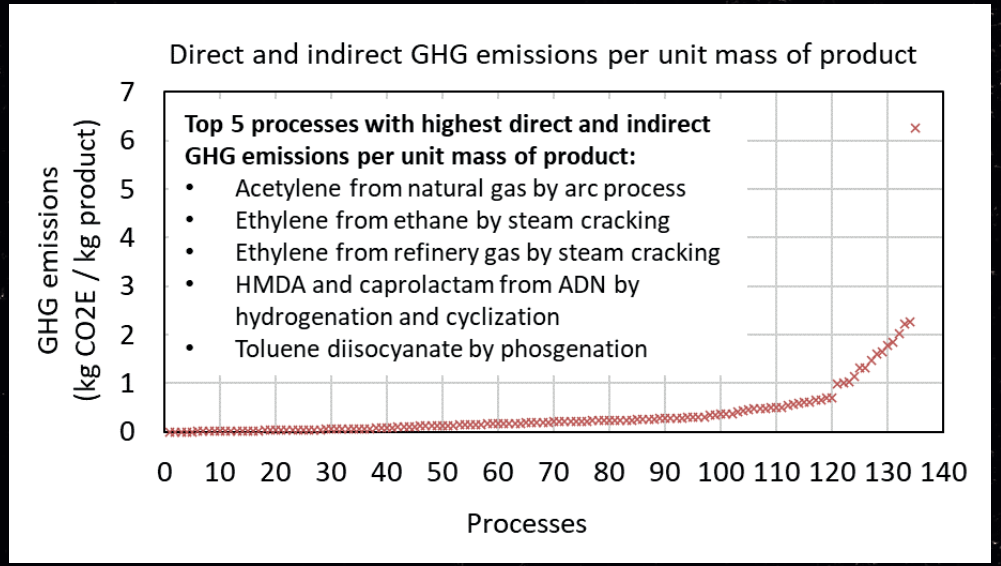


Figure 4-2: GHG emissions per unit mass of primary product direct and indirect emissions

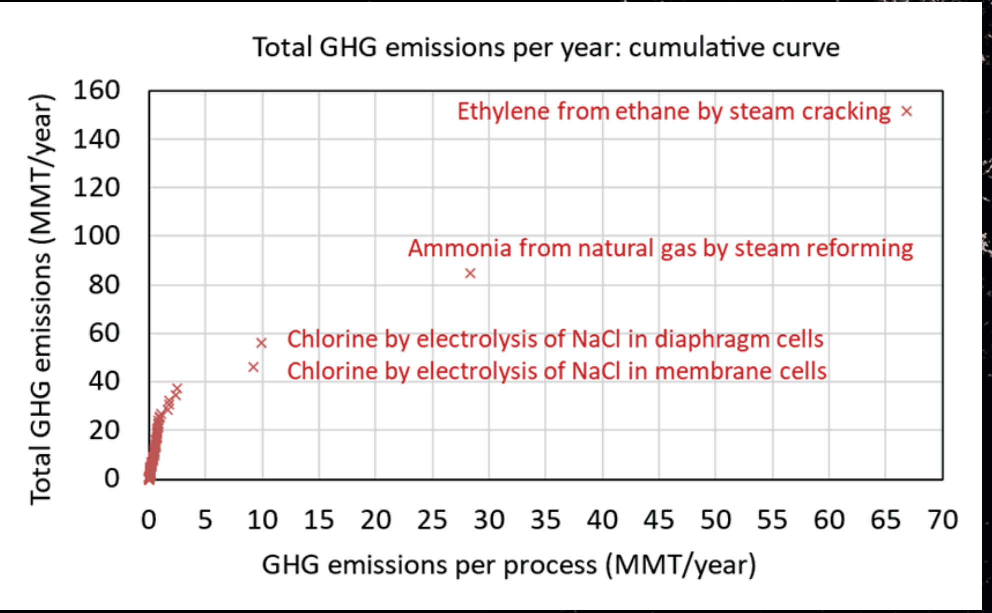


Figure 4-3: Emissions per unit mass of product multiplied by US production capacity

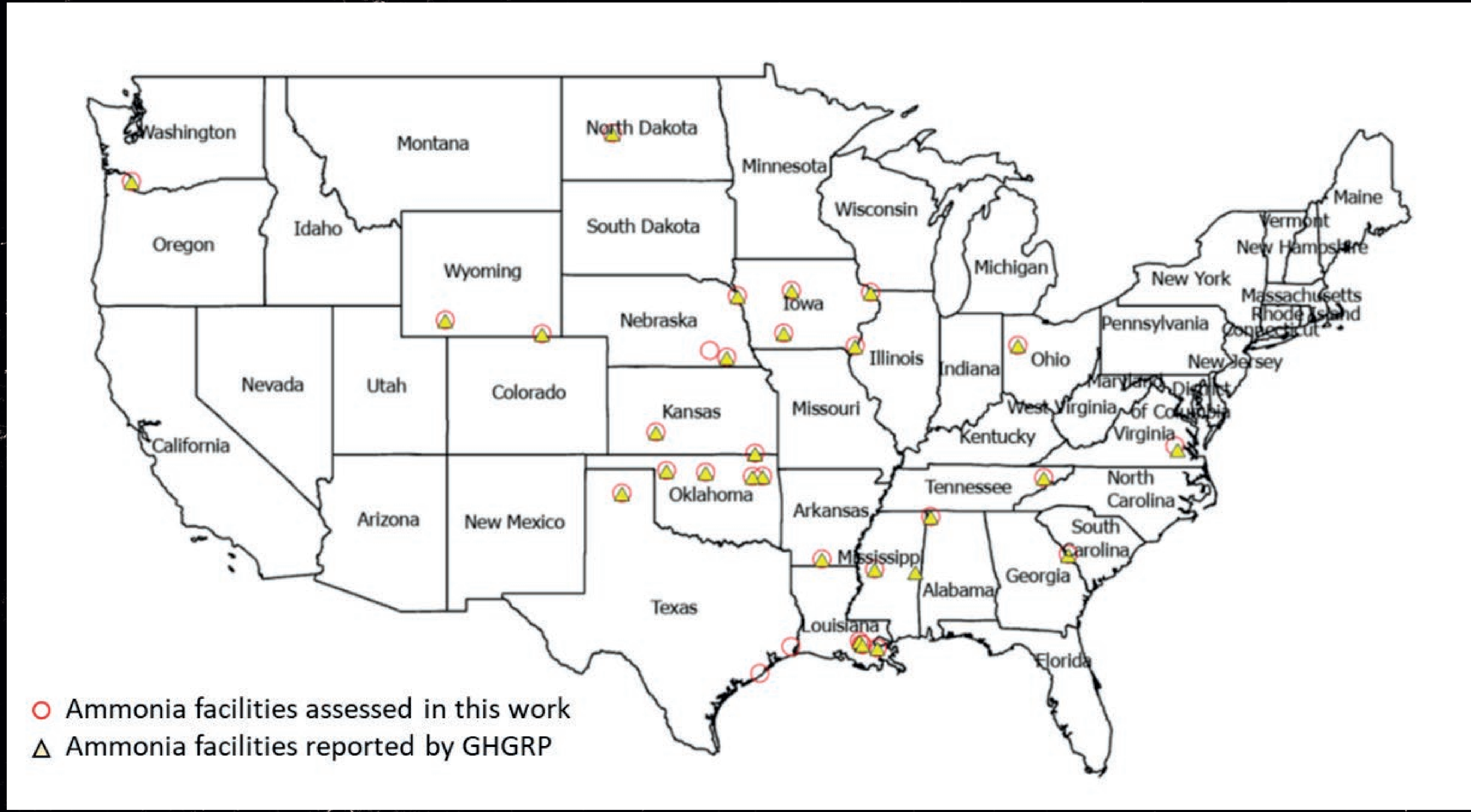


Figure 4-4: Mapping of ammonia facilities assessed in this work and reported by GHGRP based in 2017

B. Cataloguing mitigation options and modelling decarbonisation pathways

Key points:

- This project will create an open-source database on decarbonisation technologies that will be instrumental in documenting the technical viability, environmental impact, and economic performance of different decarbonisation scenarios, providing insights into the most effective decarbonisation pathways.
- Existing de-polymerisation processes could lead to substantial GHG emission reductions if focused on avoiding the most impactful feedstocks and manufacturing processes.
- The main decarbonisation options for the chemical manufacturing processes include switching feedstocks and fuels from oil/gas to hydrogen and other non-petroleum-based chemicals, improving both energy and material efficiencies, and carbon capture and storage/utilisation.
- Current decarbonisation technologies are not yet able to compete economically with fossil fuel technologies for large-scale implementation.
- Datasets for decarbonisation technologies with statistics on process energy consumption, carbon emissions, Technology readiness level (TRL), and economic costs are needed to analyse the potential decarbonisation pathways.
- Relevant scenario narratives provide insightful principles to design the potential decarbonisation pathway scenarios for the chemical industry based on technological characteristics and relevant assumptions (e.g., carbon intensity of electricity and carbon price).

Data uncertainty and the lack of whole system models for the petrochemical sector affect not only the assessment of today's GHG emissions, but also the evaluation of future mitigation options and the accuracy of emissions projections.

Mitigation options in the petrochemical sector can be broadly divided into supply-side options and demand-side options.

Supply-side options are those employed upstream in the supply chain, primarily within the producer's remit, and focus on technological engineering solutions. Key examples include improving production energy efficiencies, using lower carbon feedstocks, and carbon capture for sequestration or subsequent utilisation. Demand-side options concern the use of chemical products, the curtailment of which can yield indirect emissions savings upstream. Options include aspects of material efficiency, such as life extension, repeated or more intensive use, light-weighting and material recovery or recycling [12]. They reduce the required production, use and end-of-life (EOL) treatment emissions, while sufficiently maintaining stocks of chemical products.

Mitigation options occur across the entire life cycle of chemicals and assessing the emissions reduction potential of supply- and demand-side options requires the physical mapping of resources and unit process technologies.

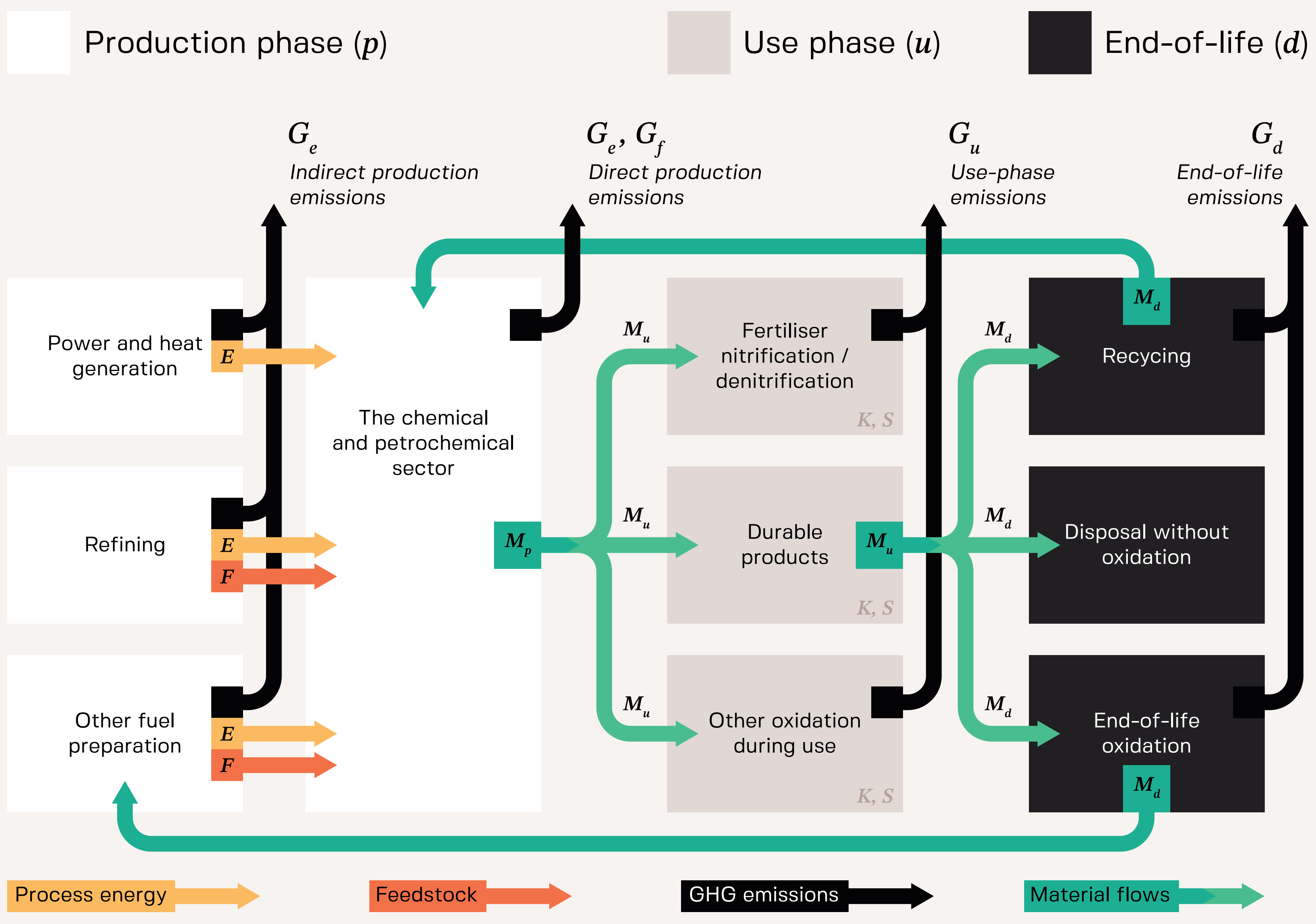


Figure 4-5: Systems view of energy, materials, technologies and emissions in the petrochemical sector

C-THRU's framework will add new insight into supply- and demand-side mitigation solutions.

This deep-dive analysis of process technologies, mitigation interventions, and recycling processes (represented in Figure 4-5) will generate comprehensive accounts of both life cycle emissions and regional emissions for High Value Chemicals (light olefins, BTX, aromatics), ammonia, methanol, and other chemicals (as defined by the UN Statistics Division International Standard Industrial Classification (ISIC)). The analysis will initially focus on four plastic products: polypropylene (PP), polyethylene (LDPE, LLDPE, HDPE), polyethylene terephthalate (PET) and polyvinyl chloride (PVC), which together make up nearly two-thirds of global plastic production and cover the range of dominant production routes and recycling processes.

Following the baseline energy and emissions analysis, the decarbonisation scenario analysis will consist of:

- compiling and deriving technology performance and economic data for promising low-carbon process technologies (i.e. electrification technologies, advanced energy-efficient processes, biomass and hydrogen feedstocks, solar thermal heating, and CCSU);
- integrating baseline process archetype models and process technology options into a plant-level simulation framework;
- using the simulation framework to identify viable decarbonisation pathways, quantifying the energy, resource input, and GHG and non-GHG emissions implications of each scenario at the global and regional levels;
- and interpreting these results considering wider modelling literature on climate change impacts.

Methods for decarbonisation scenario analysis

The decarbonisation scenario analysis will use the TIMES platform [13], the energy technology systems model used by the IEA for petrochemicals analysis (previously overseen by Co-I Masanet), which will enable exploration of different low-carbon pathways for meeting future chemicals demand in different regions. TIMES models are developed by and shared among a global community of energy analysts [14] which will enable the project to contribute directly to the broader climate community and leverage data developed by other TIMES research groups.

To populate the model, a comprehensive dataset of low-carbon technology options will be generated, inclusive of mass and energy balances, technology readiness levels and economic data. Options will include process electrification (e.g. mechanical separations, heat pumps, and resistive heaters), bio-based feedstock processing [15], hydrogen feedstock pathways (e.g. renewable electricity with electrolysis, methane pyrolysis), advanced energy efficiency practices (e.g. process intensification) [16], use of recycled feedstocks, solar process heating [17], and carbon capture, sequestration, and utilisation [18]. These data will be based on a comprehensive review of process innovations from scientific literature, technology roadmaps, and pilot and start-up plants [2,19].

C-THRU's account of global flows in the petrochemical sector will be used to build a dynamic model of product stocks.

This model will test the impact of alternative interventions along the chemicals supply chain in future demand, waste generation and global life cycle emissions.

The mitigation options assessed fall into three categories:

- Recycling technologies
- Available and emerging low-carbon technologies
- Demand reduction strategies

Technology	Scale of operation (at present)	Temperature (°C) (in process)	Sensitivity (to feedstock quality)	Polymer breakdown (affecting yield and material recovery)	TRL
Conventional pyrolysis	Commercial	300 – 700	High	Moderate	9
Plasma pyrolysis	Laboratory	1800 – 10000	Low	Very detailed	4
Microwave assisted pyrolysis	Laboratory	Up to 1000	Medium	Detailed	4
Catalytic cracking	Commercial	450 – 550	High	Moderate	9
Hydrocracking	Pilot	375 – 500	High	Detailed	7
Conventional gasification	Commercial	700 – 1200	Medium	Detailed	9
Plasma gasification	Commercial in decomposing hazardous waste	1200 – 15000	Low	Very detailed	8
Pyrolysis with in-line reforming	Pilot	500 – 900	Medium	Detailed	4

Table 4-2: Example summary of technologies for chemical de-polymerisation [20]

What recycling technologies are available?

Potential depolymerisation recycling pathways for polystyrene and polyethylene

Our initial literature reviews have revealed that feedstock production and manufacturing chemical intermediates (e.g. ethylene) can be major contributors to the GHG emissions associated with the life cycles of plastics. These findings have allowed us to focus more attention on reviewing the literature on plastics recycling to processes that have the potential to lead to significant GHG emission reductions. Thermal and catalytic cracking of plastics to produce olefins is an example of the types of de-polymerisation processes that could lead to substantial GHG emission reductions. A brief summary of the types of information being assembled in our review is shown in Table 4-2.

What are the available and emerging low-carbon technologies?

Decarbonising the chemical sector will require a combination of energy efficiency improvements of heating processes, the utilisation of alternative carbon feedstocks (e.g., bio-based raw materials and captured CO_2), carbon capture technologies, and electrification processes that benefit from the emerging low-carbon power sector [21,22]. Figure 4-6 adapted from Pires da Mata Costa et al. (2021) [23] illustrates how decarbonisation technologies can be integrated in the production stages of the plastic chain.

Key decarbonisation options for the chemical sector and include:

- **Feedstock substitution:** The feedstock for chemical production is dominated by oil and gas, making up about 90% of the raw materials [24]. Biomass can be used as a feedstock to produce chemicals with a minimal or negative carbon footprint when carbon capture and storage (CCS) is implemented. Hydrogen generated from water electrolysis, rather than the steam cracking of natural gas, has been used as the feedstock for ammonia synthesis. However, such non-petroleum based chemical synthesis approaches minimally contribute to overall global production. It should be noted that massive integration in the petrochemical industry must be considered at a system level to understand the impact of feedstock replacement on broad industry carbon emissions.

- **Fuel switching:** Energy consumption and emissions from fossil fuel combustion can be reduced via fuel substitution. Owing to its carbon neutrality, biogas (e.g. biomethane) has been used as a replacement for fossil fuels in the chemical industry. For example, natural gas boilers can be replaced with biomethane boilers. Moreover, hydrogen can potentially be used in place of natural gas for process heating. However, non-upgraded biogas and hydrogen would require retrofits and may not be cost effective solutions. Electrification of the conventional heating and combustion equipment provides another decarbonisation pathway for the chemical industry and requires low or zero-carbon electricity generated from renewable energy.

- **Carbon capture and storage, or utilisation (CCS or CCU):** Industrial carbon capture and storage (CCS) can play an important role in reducing emissions, for instance in fertilizer production plants, hydrogen production, and refining. CCS is a technically viable option for most large combustion industrial facilities globally without requiring existing process configurations to be retrofitted [56,26]. These CCS technologies are classified into three routes: oxyfuel combustion, pre-combustion, and post-combustion. Instead of sequestering captured carbon as in CCS system, Carbon capture and utilisation (CCU) system can capture and convert carbon dioxide into a chemical product (such as synthetic fuels, plastics, building materials, etc.).[27]

The current decarbonisation technologies (excluding CCS or CCU) that can be applied to each processing stage for different chemicals are listed in Table 4-3. For example, ammonia is one of the primary chemicals with the largest

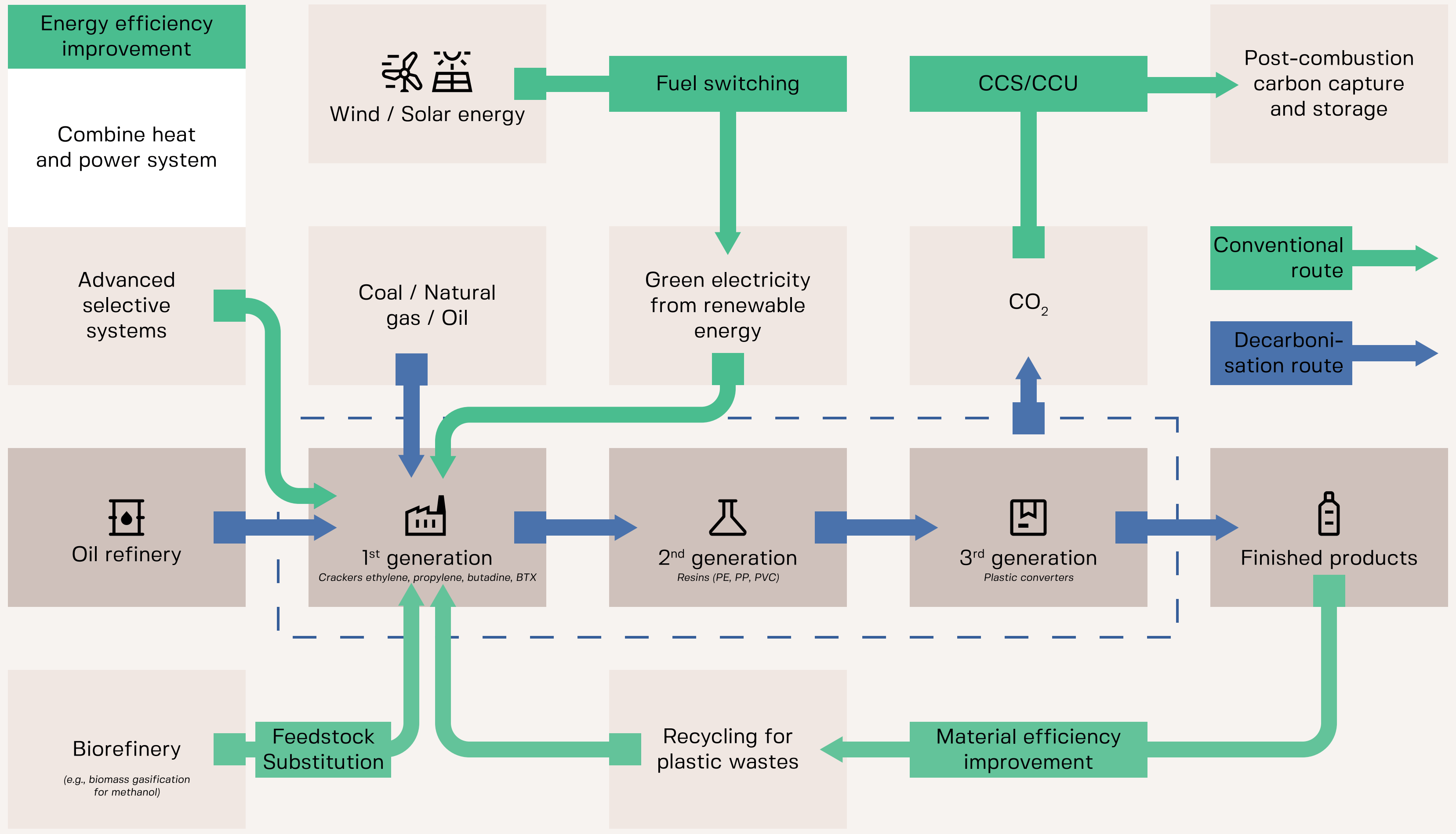


Figure 4-6: Schematic representation of decarbonisation technology integration for a typical fossil-based plastic chain [23]

annual production rate globally. One promising way of decarbonising ammonia production is to use hydrogen generated from water electrolysis as the hydrogen feedstock to replace fossil fuel-derived methane. However, the implementation of these technologies faces huge challenges and uncertainties, such as availability of low carbon electricity, and investments in new assets. Lange (2021) [28] concluded that the investment cost of large-scale hydrogen electrolyser units (about 5 MW) is estimated to be more than $500/kW or $1800 per Nm3/h of H_2. A technology report from DECHEMA implied that the production costs for ammonia, methanol, olefins and BTX (aromatics) would be two to five times higher than their fossil alternatives under current conditions [21]. Technologies that switch feedstock to biomass are not able to economically compete with conventional fuels for large-scale implementation. Moreover, the large-scale application of electrification for high-temperature crackers and other heating units will present new challenges in terms of equipment design, process control, and system integration.[29]

CCS and CCU techniques (see Table 4-4 and 4-5) can have additional energy consumption and costs (e.g. oxygen cost for oxy-firing). An open-source database on decarbonisation technologies for different chemicals is needed to document the information related to the technical viability, environmental benefit, and economic performance. Such a database could provide useful insights into the utilisation of decarbonisation technologies (in terms of economic cost, TRL, carbon emissions, etc.) and could be used to define the decarbonisation scenario and model the decarbonisation pathways.

Product	Process stages: FEEDSTOCK	REFORMATION	SYNTHESIS	TRL	Low carbon technology category	Cost $ in 2020 {CAPEX + OPEX}	Specific energy use	Carbon reduction {tCO2/t product}	Conventional technology
Ammonia	Renewable H2 from water electrolysis and N_2		Haber Bosch process	7-9	Feedstock substitution	$305-465/t	38.9 GJ/ t NH3	1.12-1.29	H2 from natural gas reforming
	N2 and water		Electrochemical synthesis	1-3	Feedstock & fuel switching		730-1500 GJ/t NH3	-19.8- -8.48	Natural gas reforming
Methanol	Biomass	Gasification & WGS (water gas shift)	MeOH synthesis	4	Feedstock substitution	$192-1126/t	14.6 GJ/t MeOH	1.57	Reforming of natural gas
	Captured CO2 & renewable H2		MeOH synthesis	7	Feedstock substitution	$347-535/t	11.02MWh/t MeOH	1.53	
Ethanol	Biomass		Fermentation	7-9	Feedstock substitution	$750/t ($0.66-0.77/L)	38-47.7 GJ/t EtOH	1.94-2.54	
Ethylene	Ethane/LPG	Electric stream cracker		4	Feedstock/fuel switching				Steam cracking with naphtha
	Ethane & O2		Oxidative dehydrogenation	6-7	Feedstock/fuel switching				
	Bioethanol		Catalytic dehydration	5-9	Feedstock substitution	$2694-3353/t	85.5GJ/t	1.95	
Propylene	Naphtha	Electric stream cracker		3-4	Fuel switching				Steam cracking with naphtha
		New catalysts		9	Energy efficiency				
	Methanol		MTP (methanol to propylene)	8-9	Feedstock substitution	$814-1736/t	26.6MWh/t	1.89	
	Bio-methanol		MTP	6-7	Feedstock substitution		95.5GJ/t	-0.23	
Hydrogen	H2O		Alkaline electrolysis	7-9	Feedstock substitution & fuel switching	$10.3/kg		9.44	H2 from natural gas reforming
			PEM electrolysis	7-8	Feedstock substitution & fuel switching				
BTX	Methanol (H2 based)		Methanol-to-aromatics (MTA)	7	Feedstock substitution	$1552-3342/t	176GJ/t BTX	1.7	Steam cracking with naphtha
	Biomass	WGS	MeOH synthesis and MTA	6-7	Feedstock substitution	>$3581/t	72 GJ/t BTX	0.7	

Table 4-3: Characteristics of decarbonisation technologies for major upstream chemicals [21,29–31]

CSS Technology	Flue gas source	Carbon capture route	TRL	Specific energy use	Decarbonisation rate	Cost $ in 2020 ($/t CO_2)	Reference
MDEA (Methyl-DiEthanol-Amine)	Electricity from coal power plant	Post combustion	8-10		0.9	49-60	32
	Steel					89	
	Cement					106	
	Petroleum				0.5	68.7	26
Calcium looping	Electricity from coal power plant	Post-combustion	6-8	200kw/t O_2	0.9	38-39	32
	Steel					84	
	Cement					71	
MEA (monoethanolamine) capture	Petrochemical	Post-combustion	8-10	1420-2340 kJ/t CO_2 captured	0.9	27-46/68	33
Ammonia solution	Petrochemical	Post-combustion	7-9			182-250	26
	Electricity from coal power plant					20-45	34
High pure CO_2 source	Ammonia	Pre-combustion	8-10			3.9-45.3	26
	Hydrogen		8-10			35.9	
	Natural gas processing		8-10			10.25	
	Ethanol production		8-10			12.3	
	Ethylene oxide production		8-10			15.4	

Table 4-4: Characteristics of CCS technologies

CCU pathway	Chemical produced	TRL	Specific energy use	CO_2 avoided	Reference
$9\ CO_2 + 27\ H_2 \rightarrow C_6H_6 + 18\ H_2O + 3\ CH_4$ (with Fe/Fe_3O_4 nanoparticles as catalyst)	Benzene	6-7		0.9	35
$2\ CO_2 + 6\ H_2 \rightarrow C_2H_4 + 4\ H_2O$ (Catalytic CO_2 hydrogenation)	Ethylene	6-7			
$2\ CO_2 + 2\ CH_4 \rightarrow C_2H_4 + 2\ CO + 2\ H_2O$	Ethylene	6-7			
$C_2H_4 + CO_2 \rightarrow C_2H_4O + CO$	Ethylene oxide	6-7	45.2 Nm3/kg EtO and 1.3kWh/kg EtO	2.82 kg/kg EtO	36
$CO_2 + 4\ H_2 \rightarrow CH_4 + 2\ H_2O$ (Sabatier reaction)	Methane	6-7	14.4 kWh/Nm^3 natural gas		37
$CO_2 + 3\ H_2 \rightarrow CH_3OH + H_2O$ (direct hydrogenation of CO2)	Methanol	6-7	12 kWh/kg MeOH	0.6 kg/kg MeOH	38
$3\ CO_2 + 9\ H_2 \rightarrow C_3H_6 + 6\ H_2O$ (Catalytic CO_2 hydrogenation)	Propylene	6-7			35
$9\ CO_2 + 26\ H_2 \rightarrow C_7H_8 + 18\ H_2O + 2\ CH_4$ (with Fe/Fe_3O_4 nanoparticles as catalyst)	Toluene	6-7			
$9\ CO_2 + 25\ H_2 \rightarrow C_8H_{10} + 18\ H_2O + CH_4$ (with Fe/Fe_3O_4 nanoparticles as catalyst)	Xylene	6-7			

Table 4-5: Characteristics of CCU technologies

Demand reduction options

Demand reduction has been demonstrated to be a powerful decarbonisation strategy for various materials and sectors.

Since end-use products are the last of all stages of material production and manufacturing, they embody the highest GHG emissions of any other stage of the supply chain.

For this reason, any reduction in demand has a disproportionate large effect in reducing impacts, as these are propagated throughout all upstream stages of supply chains[39].

Many studies have explored the potential to reduce demand across various sectors. For steel and cement, various demand reduction interventions have been identified with the potential of reducing demand without compromising the levels of service provided by these materials. Examples include:

- Energy efficiency: Improving the efficiency of heating will substantially reduce carbon emissions because heating accounts for a significant share of the total energy consumption of chemical production. For instance, residual heat, particularly from PTA production, can be recovered and reused to decrease the overall energy demand[40]. Combined heat and power (CHP) systems have helped to reduce substantial energy use in bulk chemical plants.
- The optimisation of product design: Avoiding overuse of materials, and the extension of product lifetimes to reduce the pace of product replacement and thus material production[12,41].
- Material efficiency: Increasing the recycled content of chemical-based production (e.g. plastics) and reusing secondary materials could help to reduce the emissions upstream and downstream in the value chain. Changing the product design and using alternative materials could also potentially contribute to these emission savings, both directly in the process and in other parts of the supply chain.

Product design optimisation is particularly effective when applied to long-lasting and material-intensive products, such as cars and buildings. For buildings, the elimination of overdesign of structures could lead to a reduction of demand for structural steel of up to 50%[42], and the deployment of opportunities to reuse structural steel could further reduce future demand[43,44]. For cars, weight reduction plays a key role in reducing not only the emissions associated with car manufacturing, but also substantially reduces the emissions produced when driving them[3].

Demand and impacts in petrochemicals are dominated by two families of products: plastics and fertilizers, which together account for 70% of total chemicals.

For plastics, we have demonstrated that halving packaging in the UK by 2050 could reduce UK plastic emissions by up to 20%[45]. But further reductions could be achieved indirectly — e.g. eliminating food waste could result in a 20% reduction in plastic film and 5% reduction in plastic bottles. However, these are just examples of the scale of impacts that could be explored globally to keep enjoying the benefits of plastic use, while reducing its demand. This is what we will explore in C-THRU by quantifying the global potential of various demand reduction interventions, their viability and impact in reducing emissions.

For fertilizers, most GHG emissions are produced during the use of fertilizers in the soil. Unfortunately, this problem is amplified because more nitrogen fertilizers are used than the nitrogen requirements of crops[46]. When fertilizers are decomposed in the soil, the nitrogen not absorbed by crops partially leads to the formation of N_2O, a powerful GHG. For this reason, strategies for demand reduction of fertilizers have a powerful impact in the reduction of emissions. Existing evidence suggests that there is a vast potential for demand reduction in fertilizers, with one study for the Netherlands concluding that fertilizer use could be almost halved without loss in productivity[47]. By developing the first global map of fertilizer use and emissions, we are quantifying the global potential of all opportunities and revealing the main challenges to reduce fertilizer emissions.

In C-THRU we will explore the global potential of demand reduction options for petrochemicals

and how this strategy can be combined with other interventions along supply chains. For this purpose, we are developing modelling tools that allow us to test the impact of various alternative mitigation interventions in reducing future waste and emissions. This involves a detailed consideration across various world regions of consumption patterns, existing stocks of products in service, and projections of population growth and waste availability.

Putting the options into action

Many studies have developed system models for analysing the decarbonisation pathways for the chemical sector. In this focus study, we present a review of decarbonisation pathway literature.

Focus Study: A review of decarbonisation pathway models

The latest net-zero emission by 2050 report [48] from the International Energy Agency (IEA) quantified the carbon emission of 65 million tonnes for the global chemical sector to achieve the net-zero emission goal by 2050. CCS/CCU and hydrogen-based technologies play key roles for decarbonising the chemical sector in the IEA net-zero emission scenario. Meys et al. (2021) [49] projected a net-zero pathway by 2050 for the global plastic industry with technologies of optimal plastic waste recycling, CCU, and biomass feedstock switching. This study points out that only when the carbon density of electricity is low as 8.6 g CO_2 eq/kWh, the CCU technology is favourable for plastic manufacturing.

Besides different emerging technologies of decarbonisation, there are some patterns and variations in the modelling frameworks that show how the deployment of decarbonisation technologies can achieve carbon reduction whilst meeting the demand for chemical products in different scenarios. The common time horizon of the net-zero carbon emissions climate goal for the global chemical industry decarbonisation scenarios is in the year of 2050, in line with the year proposed in the Paris Agreement [28,50]. The timing of the carbon reduction target affects the final quantity of carbon reduction derived from the utilisation of decarbonisation technologies. [51–55] Some commercial decarbonisation technologies (e.g. renewable hydrogen production and CCS commercial for the ammonia production) with substantial infrastructure requirements can be considered in the near future to begin to lower carbon emissions in a large scale for the chemical industry. However, decarbonisation technologies with low TRLs have more uncertainties around when they may be deployed in the timeline of decarbonisation. The degrees of carbon reduction resulting from different decarbonisation technologies depend on the demand for various chemical product activities and the required time scales for significant market penetration. Therefore, it is necessary to have a comprehensive understanding of the feasibility of decarbonisation technologies for various production processes of each chemical product.

In terms of economic performance under decarbonisation scenarios, only a few studies evaluated the potential costs for the implementation of these technologies in the chemical industry. For instance, Gielen (2021) [56] estimated that a total investment of $4.3 trillion needed for achieving a net-zero emission pathway with low-carbon technologies between 2018 and 2050 in the global chemical sector, but $1.8 trillion investment in the fossil fuel based production capacity can be saved compared to the reference case which is a slow decarbonisation scenario.. The IEA Energy Technology Perspectives 2020 [57] indicates that ammonia production with electrolytic hydrogen generation can compete with the conventional production route equipped with CCS/CCU (ammonia production cost is around $375 – 650/t depending on the price of natural gas) at electricity prices of $ 10-60/MWh. Future studies should address the economic viability of different decarbonisation technologies in terms of capital investment cost, fixed and operational cost, and labour cost.

Decarbonisation scenarios defined in the previous modelling research usually vary with increasing levels of ambition in decarbonisation by policy implementation, ranging from "business-as-usual" (BAU) (no deployment of low carbon options nor energy efficiency measures) up to "maximum" (theoretical potential with full implementation of low-carbon technologies including CCUS) [21]. Assumptions under different decarbonisation scenarios also play an important role in modelling the decarbonisation pathways in the chemical industry. For example, a common technical assumption of low or zero CO_2 emissions for grid electricity in 2050 is considered under decarbonisation scenarios in many studies, especially in the case of electrification in heating processes [58,59]. Moreover, Bataille et al. (2018). [60] discussed that policy commitment and design could play an important role in facilitating the commercialisation and penetration of decarbonisation technologies in the chemical and other industrial sectors. Policy supports are often assumed to be the drivers of the implementation of new low-carbon technologies and the utilisation of renewable energy (e.g. wind, solar, and biomass)[61] for achieving a net-zero emission pathway in the chemical sector. Some studies considered carbon prices with small subsidies for electricity-based process heating and full subsidies for investment in decarbonisation technologies for the chemical industry. There will be regulations that ban fossil-based technologies and no newly built steam generation installations consuming fossil fuels in the Germany chemical plants from 2025 [52]. Policy analysis for subsidy and incentive assumptions for the chemical industry can provide solutions to the economic barriers of decarbonisation technologies and insights for policymakers to plan the best strategies for improving decarbonisation pathways.

A decarbonisation pathway towards to the net zero-emission climate target for the global or regional chemical industry relies heavily [57] on low-carbon technologies that are not ready or near-commercial today. Many studies have analysed the potential decarbonisation pathways for the energy and industrial sectors, quantifying the final energy demand and GHG emission reduction in a variety of scopes [48,57,62]. Table 4-6 summarises decarbonisation scenarios for the regional chemical industry modelled by previous studies. The decarbonisation pathways under different decarbonisation scenarios for the chemical industry provide useful estimates of energy consumption and carbon reduction associated with the utilisation of low-carbon technologies. Moreover, emerging decarbonisation technologies are still in their early stages and there are large uncertainties surrounding availability, energy efficiency, and production cost of these technologies. In this project, we will create an open-source database for existing and emerging decarbonisation technologies of major chemical production streams that can be updated over time. This database will include data for low-carbon technologies on a process level for different chemicals in various regions, such as energy efficiency, TRL, production cost, carbon emissions, and regional availability. Furthermore, we will use this database to better define various decarbonisation scenarios and analyse the decarbonisation pathways on different regional scales.

Literature	Model characteristics	Scenario definitions
Bazzanella et al., 2017 [21]	Time horizon:2050 Region: EU Chemical subsectors: Ammonia, chlorine, urea, methanol, ethylene, propylene, and benzene/toluene/xylene (BTX) Low-carbon technology categories: All Scenario considered: BAU, intermediate, and maximum scenarios	BAU: no deployment of low carbon options nor energy efficiency measures Intermediate:30% share of H_2-based methanol, olefins and BTX plants; 35% of plant replacement rate; 70% of electric steam generation Maximum: 85% share of H_2-based methanol, olefins and BTX plants; 100% of plant replacement rate; 70% of electric steam generation
Lechtenböhmer et al., 2016 [52]	Time horizon: 2050 and 2060-2070 Region: EU Chemical subsectors: HVC, chlorine, and ammonia Low-carbon technology categories: Fuel switch (electrification) Scenario considered: 100% electrification for basic chemicals	100% shift to electrification: For 2050 it is assumed that the analysed energy intensive production will be based completely on renewable electricity (zero emissions) and hydrogen and syngas/FT-naphtha. 67 million tons of chemicals in 2050
Palm et al., 2016 [53]	Time horizon: 2050 Region: EU Chemical subsectors: Plastics-polyethylene (PE), polypropylene (PP), and polyethylene Low-carbon technology categories: Feedstock switch and fuel switch (electrification) Scenario considered: 100% shift to electricity-based plastic production.	100% shift to electrification: EU plastic production (57 million tons/year) remains constant, but is completely electricity-based
Barrett et al., 2018 [63]	Time horizon: 2050 Region: UK Chemical subsectors: Ammonia and lower olefins Low-carbon technology categories: Fuel switch (electrification), energy efficiency, and CCS Scenario considered: Low action, reasonable actions with/without CCS	Low action: slight improvements and no investments in low-carbon technologies. Reasonable action: All identified low-carbon technologies are installed by 2025, and retired plants are replaced with best practice ones by 2030. Additional scenario with CCS is investigated
Rehfeldt et al., 2020 [64]	Time horizon:2030 Region: Germany Chemical subsectors: Ammonia, chlorine, ethylene, methanol, oxygen, polypropylene, soda ash, etc. Low-carbon technology categories: Fuel switch (electrification) and energy efficiency Scenario considered: Base, investment, replacement, regulation	Base: slow growth in production activity and carbon price is 25 EUR/tCO_2 in 2020, linear growth to 50 EUR/tCO_2 in 2030 Investment: 100% investment grant for low-carbon technologies Replacement: 75% of technical lifetime 2025–2030 Regulation: Besides replacement scenario, fossil ban on new installation after 2025
Wang & Chen, 2019 [62]	Time horizon: 2050 Region: Western EU, China, and India Chemical subsectors: not specified Low-carbon technology categories: Fuel switch (electrification) and energy efficiency Scenario considered: reference scenario and 2-degree constraint scenario	Reference: no specific carbon constraints. Five trajectories of socio-economic development are investigated to drive the energy system and mitigation pathways. 2-degree: global carbon budget for 2010–2050 is 1095 Gt
Fleiter et al., 2019 [55]	Time horizon: 2050 Region: Globe Chemical subsectors: Ethylene, ammonia, and methanol Low-carbon technologies: All Scenario considered: reference, best available technology (BAT), and decarbonisation scenarios	Reference: annual growth rate of gross added value in chemical sector is 1.1%. CO_2 price is 25€/tCO_2 in 2030, 50€/tCO_2 in 2040 and 85€/tCO_2 in 2050. No additional efforts in terms of material efficiency and substitution occur. BAT: this scenario is more ambitious concerning recycling and assumes higher shares of secondary production compared to the reference scenario. No additional efforts in terms of material efficiency and substitution Decarbonisation scenarios: Scenarios with CCS, hydrogen-based production technologies, and shift to biomass feedstock are investigated
International Energy Agency, 2018 [2]	Time horizon: 2050 Region: Globe Chemical subsectors: HVC, methanol, and ammonia Low-carbon technologies: All Scenario considered: reference technology scenario (RTS) and clean technology scenario (CTS)	Reference: following the historical trends of energy price and chemical demand informed by the range of existing and announced policies and by established behavioural and other exogenous considerations CTS: besides RTS, direct CO_2 emissions to be reduced by 45% by 2050, compared to the levels in 2017
IEA ETP, 2020 [57]	Time horizon: 2070 Region: Globe Chemical subsectors: Methanol, ammonia, ethylene, BTX Low-carbon technologies: Fuel and feedstock switch, energy and material efficiency improvement, CCS&CCU Scenario considered: Sustainable Development Scenario (SDS) to achieve net zero emissions in 2070	For the chemical sector, CCUS-equipped routes expand rapidly, accounting for 50% of chemicals production weight basis by 2070, with hydrogen- and bioenergy-based routes accounting for a further 16% and 4% respectively. Ammonia demand declines and 50% of total ammonia production in 2070 are electrolytic hydrogen-based.
Saygin and Gielen, 2021 [56]	Time horizon: 2050 Region: Globe Chemical subsectors: Ethylene, propylene, BTX, carbon black, methanol, ammonia, and plastics Low-carbon technologies: Fuel and feedstock switch, energy and material efficiency improvement, CCS&CCU Scenario considered: Planned Energy Scenario (PES) and net zero pathway (1.5 ℃ case)	PES: 2.5-fold increase in global plastic demand in 2050 compared to that in 2017; a 2.5- and 2-fold growth in ammonia and methanol demand, respectively. No alternative low-carbon technologies are deployed 1.5 °C: one-third reduce in plastic demand compared to PES, but higher demand for ammonia and methanol due to new market segments emerge for chemical building blocks, shipping fuels and power generation

Table 4-6: Summary of scenario definitions for reviewed models

C. Exploring wider societal contexts

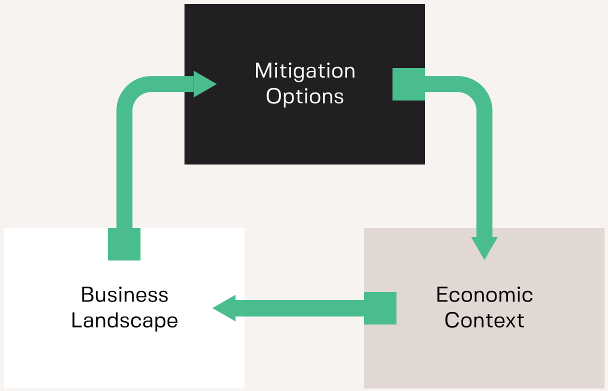
Key points:

- The analysis will be global in nature, providing clarity about both the impacts of the global petrochemical industry on GHG emissions, but also disaggregated down to the regional level to reveal the business and economic contexts of mitigation decisions in each area.
- Established economic modelling approaches can be improved as they currently don't account for time, debt, or natural resources.
- HARMONEY model has incorporated these elements and will be extended for C-THRU to cover multiple natural resource types and include the efficiency of energy conversion into work.
- The macroeconomic modelling of the economy consistently tracks the accumulations (stocks) and flows of mass, energy, and money. this enables a consistent view of how changes to the investment and operation of the petrochemical sector (e.g., recycling, energy efficiency, lower GHG emissions) feedback to economic growth.
- We will also analyse the business ramifications of future changes to petrochemical supply chains to understand the economic context and add confidence to the decision-making process for businesses.
- Understanding the influence and interactions of geography, human agency and transition pathways are critical to generating effective mitigation options.
- Developing an archetype model of the industry helps to characterise how the different business types will respond to different mitigation options including circularity and recycling technologies.
- Value chain disconnects have been identified as important in determining where future production of specific chemicals is likely to occur, and hence which mitigation steps might be appropriate.

The petrochemical industry is a complex network of actors, all with differing business structures, drivers, constraints, and value chain positions. The mitigation options and approaches to decarbonisation discussed in the previous section (4B) are important, but they will only be effective if it is understood how to achieve them. This requires knowledge of:

- The economic environment – both in terms of macro-economic impact of these changes, and an appreciation of the financial costs of implementation.
- The complexity of the petrochemical industry and the diversity of companies and other actors within it.

The business landscape, economic environment and mitigation options are all influenced by, and impact, each other.



Surrounding the modelling activities, we will conduct exploratory research to evaluate the wider business landscape, assessing regional production capacities and the restraining effects of sunk costs, and the economic context, including trends in per capita demand for petrochemical products. The analysis will be global in nature, providing clarity about both the impacts of the global petrochemical industry on GHG emissions, but also disaggregated down to the regional level to reveal the business and economic contexts of mitigation decisions in each area.

We will create a high-level macroeconomic model of how the plastics supply chain, including recycling and capturing of GHG emissions (e.g. from industrial facilities) integrates within a large economy.

The purpose is to model the dynamics and feedbacks of carbon mitigation efforts, including petrochemical production and recycling to explore feedbacks from a circular economy. Information from the material flows and emissions accounting will be applied in a macroeconomic model for the United States and serve as a template for other economic regions. This US model will be informative as the U.S. economy is large and complex, with few imports of energy and petrochemical feedstocks.

We will also analyse the business ramifications of future changes to petrochemical supply chains.

These possible future interventions will have profound impacts on stakeholders from across the life cycle stages of chemical products.

This analysis of the business landscape will work to understand the economic context, and add confidence to the decision-making process for businesses.

A primary objective will be the creation of a comprehensive model of commercial activity in oil and gas production and petrochemicals and plastics manufacturing to provide insight into the system-wide impact of specific changes. This will include:

- developing a baseline understanding of the current business landscape and the interactions between companies, sites and production facilities;
- reviewing how firms have reacted historically to emissions and sustainability related pressures, to inform future business strategy and provide a view of the overall future shape of the industry;
- building from the mitigation analyses our material flows and emissions accounting, we will explore the influence of current businesses in the petrochemical industry on overall GHG emissions, and how this varies by company type;
- and developing an understanding of the global business strategy, including how supply-side actors will respond to future reductions in demand for transport fuels, and feeding this insight into the integrated model and the future scenarios.

How is the economy impacted by technologies and mitigation options?

The C-THRU project takes a heterodox approach to understanding the role of physical resources and debt in the macroeconomy. This approach includes the dynamic accounting of stocks and flows for energy, materials, and money. We do this by recognising limitations in the usual methods and theory of neoclassical growth theory. Because most economics faculties focus on teaching neoclassical theory to their students, the numbers of economists using this theory, and thus interpreting the economy under its worldview, far outweighs those using other worldviews. A quote from 2018 Nobel Laureate Paul Romer's 2016 [65] paper, "The Trouble with Macroeconomics," sums up the frustration:

"The trouble is not so much that macroeconomists say things that are inconsistent with the facts. The real trouble is that other economists do not care that the macroeconomists do not care about the facts. An indifferent tolerance of obvious error is even more corrosive to science than committed advocacy of error."

The so-called neoclassical approach is the most common approach to economic growth modelling. The problem with neoclassical growth models is that in they are not accurate in accounting for mass and energy flows, aren't consistent with data, and don't accurately enough describe how the economy works in at least three important facets [66–69]

These facets are important to the petrochemical industry for at least two reasons: (1) because it uses long-lived capital and its business is almost entirely focused on taking in mass and energy (e.g., hydrocarbons) to transform the input feedstocks into new chemical forms by using processes that are best characterised by engineering-type efficiencies rather than "labour productivity", and (2) the demand for its products are affected by the state (e.g., rate of growth) of the global economy.

First, there is no role for time. Everything happens over some unspecified time to come to equilibrium, or agreement, on prices and quantities. Because there is no time, it becomes almost impossible to discuss an energy or low-carbon transition.

The second facet is the role of money as credit (loans, debt) in the modern economy. This is less important for global petrochemical firms since they might be able to fund most investment from profits and for some regions which have state-owned companies where private debt is not relevant. However, during a rapid low-carbon transition, there could be a larger need for loans in the petrochemical sector. Demand for products (fertilizers, plastics, etc.) is affected by the debt status of customers. Neoclassical economists don't consider debt as a fundamental influence in the economy since the borrowed money changing hands nets to a $0 change in the overall economy. This, combined with the lack of consideration of time means that interest payments on debt, paid over time by debtors to creditors, have little to no effect on the economy.

The third facet is the physical operation of the economy that is based on extracting and using natural resources from the environment. This is the basic starting assumption for ecological and biophysical economics [70,71]. We use natural resources for two major reasons: (1) as fuel in machines that perform thermodynamic work (e.g. moving cars, heating, lighting) at some specific conversion efficiency that is limited by the second law of thermodynamics, and (2) to rearrange and refine raw natural resources into more highly refined and structured forms (e.g. plastics, alloy metals) including the building of engineering structures (machines, roads, buildings). Thus, if the resources in the environment take too much energy to extract and refine, this feeds back to higher costs and hinders economic growth. Neoclassical economics usually assumes no negative feedback on growth that is related to the physical (i.e. energetic) cost of using natural resources, and thus this cost is not reflected in macroeconomic models based on this paradigm. In effect, prices are assumed to be derived solely in the heads of buyers and sellers coming to an "equilibrium" of supply and demand, neither of which are influenced by the physical environment. Neoclassical growth theories do consider technological progress, but in ways that are too abstract for considering the necessary actions to transform to a low-carbon economy. So-called "exogenous" growth theory, derived in the 1950s by Robert Solow, assumes that the economic growth is a function of inputs of capital (machines) and labour (workers). This describes about half of observed economic growth, and thus the other half is assumed to occur "exogenously", or independent of any changes in the model with no concrete explanation as to why that is. Another often-used alternative neoclassical growth model is "endogenous" growth theory, but it usually focuses on human knowledge (or human capital) increases from education as the driver of economic growth [72–74]. This concept is still devoid of a separate characterisation of natural resources from some description of our ability to use resources (e.g. power plant conversion efficiency of fuel to electricity). Knowledge is important, but out of the context of the use of natural resources, it has little meaning.

In the context of the three facets summarised above, many citizens of both industrialised and developing nations have become disillusioned with politicians' and economists' explanations for the economic outcomes since the 1970s.

The following focus study outlines the work we are doing around the economic environment of the petrochemical sector and describes the economic growth model we are using.

Focus study: Exergy, GDP, the HARMONEY model, and C-THRU

The C-THRU workstream "Economic Context" builds upon research that considers that a more accurate description of "technological progress" is that of increases in exergy conversion efficiency of final exergy in fuels (e.g. gasoline, electricity) to "useful work", "useful exergy", or thermodynamic work [75-77]. In essence: useful work = (fuel exergy input) × (efficiency of conversion to work)

Here, note that exergy is a more specific term than energy. Energy is conserved, but exergy is not conserved. Exergy is not conserved because it considers the second law of thermodynamics and thus imparts some practical limitations in energy efficiency of converting natural resources into work and structures (materials, machines, etc.). Further, project PI Jonathan Cullen's previous research has used the concept of exergy and exergy efficiencies to characterise various industrial processes, and we will incorporate these methods and insights into macroeconomic modelling [78,79].

The reason that energy (or exergy) and conversion efficiencies are important is that useful work has been shown to be a much more accurate way to estimate country level GDP than using the standard neoclassical growth approaches [77].

Useful work scales linearly with GDP such that 10% more useful work relates to 10% more GDP, or more succinctly:

GDP ≈ a × (useful work) = a × (fuel exergy input) × (efficiency of conversion to work)

(where a is a scaling constant)

This linear scaling is not the case for global primary energy consumption since the 1970s when energy constraints, mainly from oil, impacted the global economy. Since 1970, 10% more GDP has been associated with about 7% more primary energy [80,81,69]. Thus, the size of the economy is best measured not by how much energy it consumes, but how much work it performs. Thus, more useful work and more GDP can be performed with either or both of (i) more fuel consumption and (ii) higher efficiency of converting fuel to work [82]. The corollary is that lowering efficiency of conversion to work has a negative effect on GDP (i.e. reduces GDP) [83]. Making plastics and petrochemicals is considered the performing of work (e.g., making materials and structures) [78].

The C-THRU workstream "Economic Context" builds on heterodox macroeconomic and energy systems research linking time, debt, natural resources, and efficiency of energy conversion into work into a consistent macroeconomic framework.

This is achieved by adding features to PI King's Human And Resources with MONEY (HARMONEY) economic growth model [84,82] (see Figure 4-7). The model has the following basic characteristics:

- Continuous time dynamics -- thus it is not constrained to solve prices by equating supply and demand in an "equilibrium" condition.
- It uses what is known as a "stock and flow consistent" post-Keynesian approach. This means that there are entities that accumulate and store "stocks" of money (banks, firms, governments, households) and there are "flows" of money among these entities.
- Natural resources (e.g. wind, solar, oil, gas) are explicitly defined in terms of their size and requisite work to extract them (e.g. how much energy and capital does it take to extract the next bit of resource) such that we can influence how their cost of extraction feeds back to the economy.
- Both the government and private sector can create money.
- Governments that control their own currency can create money by spending it on incentives (e.g., carbon taxes) and other programs (i.e. per Modern Monetary Theory [85]).
- Private banks can create money by lending to firms and households.
- The interplay between these forms of money creation affects income inequality (e.g. by differently affecting wages, profits, and interest payments) and inflation (inflation in assets versus commodities is partially determined by to whom newly created money flows).

Completed work in Year 1 of the project has added the government sectors and a central bank to the King (2020) [84] HARMONEY model with a single natural resource. Work to be performed in Year 2 of the project will add multiple natural resources (e.g. wind, solar, oil, gas, coal) to enable exploration of a shift to low-carbon energy. Included will be definitions of energy efficiency conversions to useful work in the economy. Year 2 will also begin work on defining a petrochemical sector that uses capital (machines) to take hydrocarbon inputs (petroleum, natural gas) and convert them to various products (plastics, fertilizers, etc.) and refined fuels (e.g. gasoline, diesel). This task includes specifying the mass (e.g. carbon) of fossil fuels that act as both feedstocks that become plastics and a source of energy required in the petrochemical facilities. The Business Landscape (Workstream 7) informs many of the economic parameters in the model to understand the influence and situations of different regions of the world (e.g., U.S., E.U, Asia) that have different types of industrial plants and economic systems. Year 3 of the project can explore technological pathways for recycling plastics (e.g. using existing plastics as inputs to make new plastics) including the provision of heat and electricity required to run the processes. The recycling is represented in the centre* of Figure 4-7 indicating that outputs of the consumer goods sector (e.g. end use plastics) can be input back as feedstocks into the machines that perform industrial production within the economy.

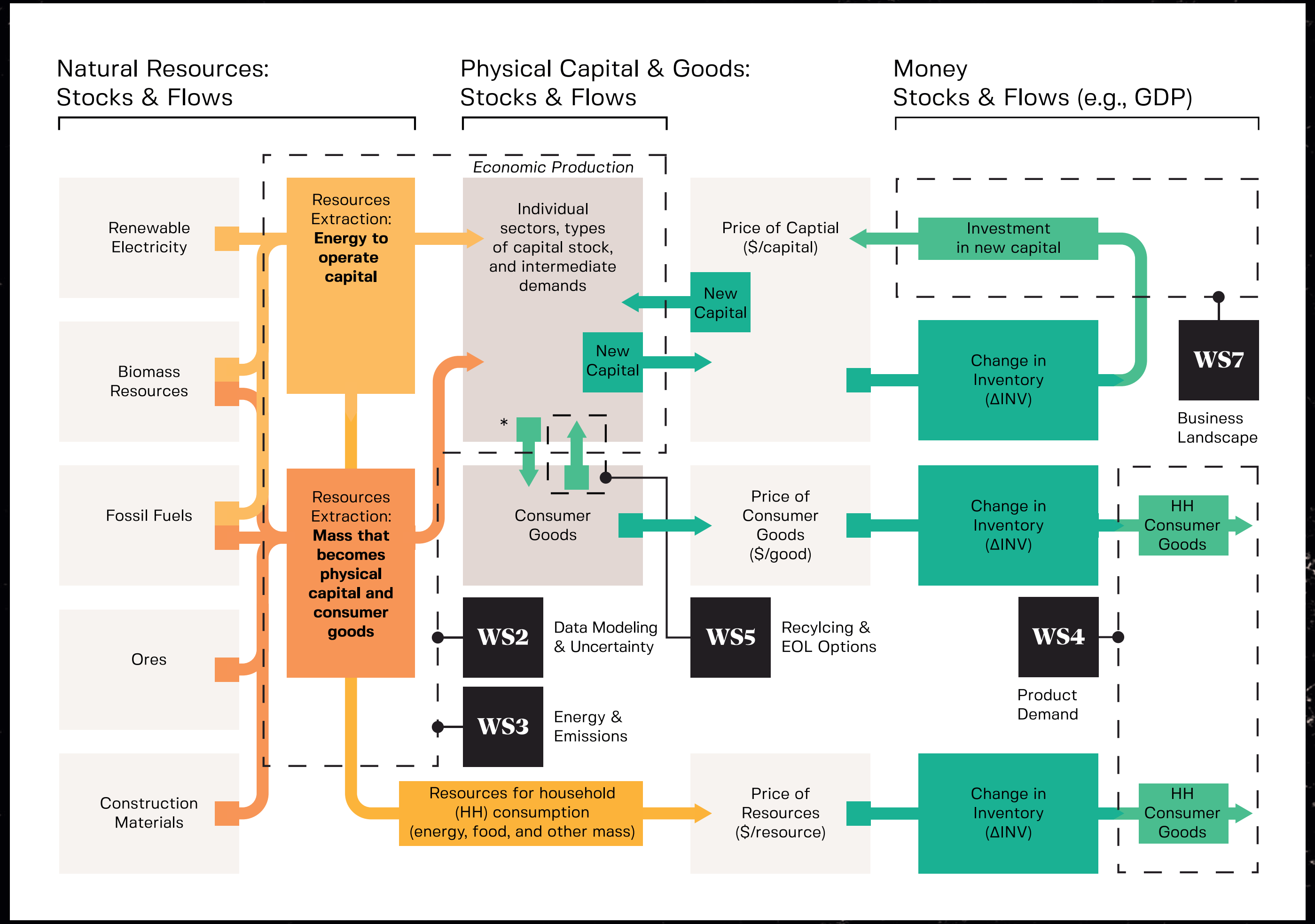


Figure 4-7: The macroeconomic framework to model scenarios associated with changes to the petrochemical sector. The model is informed by data and findings from the other workstreams

How is the business landscape prepared for future mitigation options?

Understanding the technology and mitigation options available to the petrochemical sector is important in identifying potential routes to reducing emissions and combatting climate change. However, it is also critical to understand the nature of the business landscape itself to determine how a company will respond to the risks and opportunities presented by the adaptation and mitigation proposals, and which options will have the biggest impact in a particular circumstance.

As already discussed in Chapter Two, the petrochemical industry is unique.

The diverse and divergent nature of the sector means that different businesses will respond to mitigation options in different ways

This depends on the environments in which they operate and their core drivers.

The sector is inherently dynamic with pressures exerted upstream, downstream and from within the companies themselves. The reduced demand for hydrocarbons for fuel production will create a glut of oil and gas if current levels of extraction continue. Given the forecasted increased demand for plastics, the expectation is that the excess will be used in petrochemical production in the plastics chains. This is in sharp contrast to the simultaneous pressure building from consumers and investors to reducing the use of plastics – primarily single use plastics – and pushing for more recycling and circularity.

The petrochemical business landscape is not well understood.

In the policy and academic environments in depth understanding of the global petrochemical sector is scarce, and there is a tendency to consider the industry as homogeneous or equate it to the oil and gas industry. A review of academic literature reinforced this scarcity of knowledge about the sector. There were some country specific studies [86–90] focusing on governance or emissions in relation to oil and gas or petrochemicals. Whilst these provide insight into the dynamics of the industry in Indonesia, Thailand and Saudi Arabia respectively, the scopes are too narrow to apply globally.

There are also regional studies that shed light on the development of petrochemicals in particular areas. The work on how the industry developed in East Asia [91] despite scarcely any oil extraction locally is informative from a historical perspective but less helpful in forecasting future developments, as the industry is no longer viewed as the stepping stone to economic development it once was.

Other petrochemicals-focused literature looked to apply network analysis to the sector [92] or focused on single elements of the industry such as ownership [93–95]. However, whilst providing interesting insights and ideas, none of these generate a complete picture of the industry. The grey literature provided more petrochemicals-specific reports that segment the industry in different ways, with the majority focused on ownership, products or operating models [96–99].

These are simplified classifications which look at whether a company is upstream or downstream, private or public, single site or large multi-national operating across many sites. This adds some detail but is largely generic.

The paucity of current research reinforces the need for a new model that establishes the characteristics of the petrochemical landscape which can be used to predict the future development of the industry.

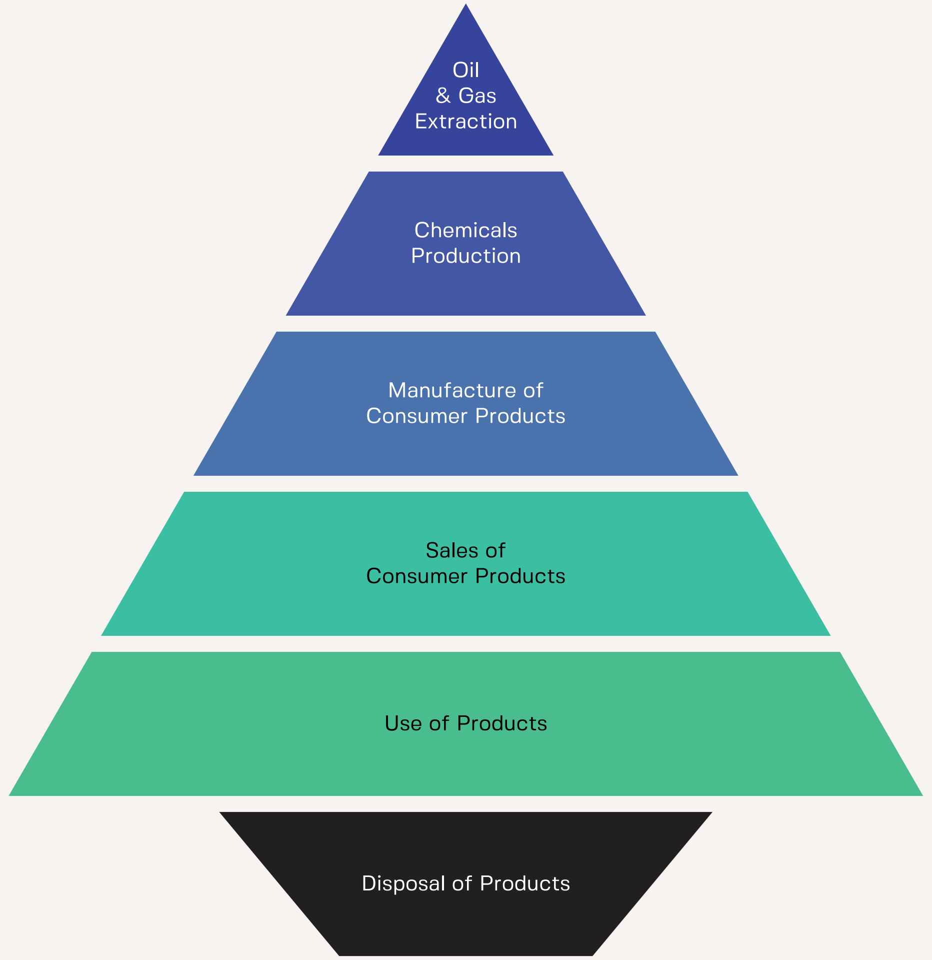


Figure 4-8: Schematic of the pyramid of participants in the petrochemical industry

Important factors

The response of the industry players to external and internal pressures depends on their positions in the value chain, the environments in which they operate and their ownership structure. Three factors are particularly important:

- Geography
- Human Agency
- Transition Pathways

Geography

Raw materials extraction, chemicals production, and end use consumption of the chemicals by manufacturers rarely happen in the same location which adds complexity to the sector. The numbers of countries and companies that participate in the chemicals value chain increases the further down the chain (see Figure 4-8) – only a handful of countries have significant oil and gas reserves, but all countries have consumers that use products containing chemicals. The number of end-of-life companies providing recycling solutions or waste management related to those products are then insufficient for the capacities involved.

The impact of economic and regional groupings also needs to be understood as these influence potential solutions. Mitigation options for an entire region may be different to those for a specific country, and those linked by pipelines may be more amenable to particular solutions due to this interconnectivity.

Human Agency

Human agency helps to explain how and why the industry responds and reacts as it does, but most models fail to account for this, implicitly characterising the sector as a collection of homogeneous actors. The importance of ownership and the impact this has on the drivers and business aims of companies cannot be underestimated - public companies have shareholder expectations to manage, whereas a state-owned enterprise often serves a broader purpose in the economy.

The petrochemical sector can be seen as a complex self-organising network which tends to adjust to nullify external actions.

The relevance of this to mitigation options is that to change behaviours in such a network you need to work from within. Therefore, acknowledging and supporting people in the sector to instigate the change will improve the impact.

The petrochemical industry is often perceived as comprising inhuman conglomerates that operate with no regard for their impact. However, the reality is that the sector comprises multiple networks, and many individuals are working within the system to make reduce emissions in their own companies and supply chains, which will be instrumental in achieving the changes required but require support to do so.

Transition Pathways

Many goals and targets have been set to achieve reductions in emissions with the expectation that a particular technology will enable these to happen. However, the viable transition paths to move from current state to the desired result are often poorly defined. The practicality of applying new technology to a chemical plant at scale and understanding its impact on by-products or feedstock requirements is seldom addressed. The interconnectedness of the petrochemical sector makes these pathways more complicated. Changing one thing in one plant may have unintended consequences further down the chain or switching to a more environmentally component may not be possible in older plants without a complete rebuild. A radical new technology may attract new companies to the sector without displacing existing ones, potentially increasing emissions if both plants continue to operate.

These factors all illustrate the need for taking a systems approach to looking at the petrochemical industry and the risks and opportunities presented by the adaptation and mitigation options available.

Focus study: An archetypal model of the petrochemical industry

In this first year of C-THRU, the focus has been to develop an archetypal model of the industry to help inform the project and wider community of key differentiating factors in the petrochemical sector.

In complexity theory, archetypes are used to describe extreme representations of characters, values, issues or situations. They are different from stereotypes in that an archetype is a caricature that is not a description of a real person or situation. The archetypes will be specific to the petrochemical sector and grounded in that industry and will provide a common understanding and language for the project. They can also be used to investigate the complexities of emissions reduction adaptations and mitigations with their associated likely impacts.

Following considerable research and deliberation on the dimensions and factors that influence the sector, three geographic dimensions were identified as particularly dominant and causal:

1. Openness of the economy in which the company operated in
2. Extent of hydrocarbon self-sufficiency
3. Growth in petrochemical demand from manufacturing

The three factors combine to influence the type of petrochemical company that operates within a country and its focus. From these, seven archetypal industry structures have been identified that represent the extremes of the model and these will be validated with real world data during Year 2 of the project.

Value chain disconnects

Our observations on geography and its importance to the petrochemical industry are most clearly illustrated by disconnects in the petrochemical value chain. These geographical disconnects are inevitable because hydrocarbon feedstocks are rarely located in regions with high levels of petrochemical consumption and demand, so breaks appear where a chemical is exported and imported. Certain chemicals will be manufactured close to feedstock sources, whilst others make more sense to produce nearer to the end use customers. The volume, volatility and toxicity of the chemicals being transported, together with transportation viability and costs, are likely determining factors in the location of such disconnects.

By identifying where the breakpoints are for each production chain, it should be possible to predict how far down that chain a particular country is likely to operate. For example, Saudi Arabia is a significant producer of oil and gas. Much of its crude oil is exported, whilst the natural gas is utilised for energy and for chemicals production. However, chemicals production is largely at the monomer or primary polymer level with polyethylene and polypropylene accounting for 42% of the value of its $42.9B of chemicals exports in 2018 [100] and China being the recipient of more than a quarter of Saudi Arabia's chemicals exports. Although the country aspires to move further downstream in their production it is unlikely to progress into small batch specialty chemicals due to transportability, cost and logistics issues unless the market locally (or regionally) grows sufficiently to justify the investments.

We are developing a new version of the petrochemical value chain that identifies these key disconnects. This will help us understand the viability and impact of different mitigation options.

How the archetypes will add value

The disconnects model and our archetypal industry structures work will be used to inform predictions of the efficacy of different mitigation options. To illustrate how this can add value to existing knowledge we have considered what the model can tell us about the most relevant recycling approach in different geographies and archetypes.

Taking the Closed Loop Partners diagram [101] of where recycled materials feed back into the value chain as a starting point, we can then use the disconnects and archetypes model to explain which circular systems approaches are likely to have the biggest impact in which locations. For example, a country exhibiting ArtisanLand or FactoryState characteristics that usually imports most of its feedstocks will be more interested in recycling back to polymers to reduce the need for imports. Factoring in geography and ownership to the value chain shows the complexity of circularity and how there is no 'one size fits all' solution.

These initial predictions and observations will be explored and tested over the next few months, along with consideration of any differences in approach based on the openness of the economy.

The final model will be used to help the C-THRU project understand and predict how the sector will respond to the various mitigation options being considered.

Archetypal structure	Openness of economy	Hydrocarbon self-sufficiency	Petrochemicals demand growth
Oilopia	High	High	Low
Petrostate	Low	High	Low
Cornucopia	High	High	High
State Incorporated	Low	High	High
ArtisanLand	High	Low	High
FactoryState	Low	Low	High
Black Hole	Low/High	Low	Low

Table 4-7: The archetypal model archetypes and their properties

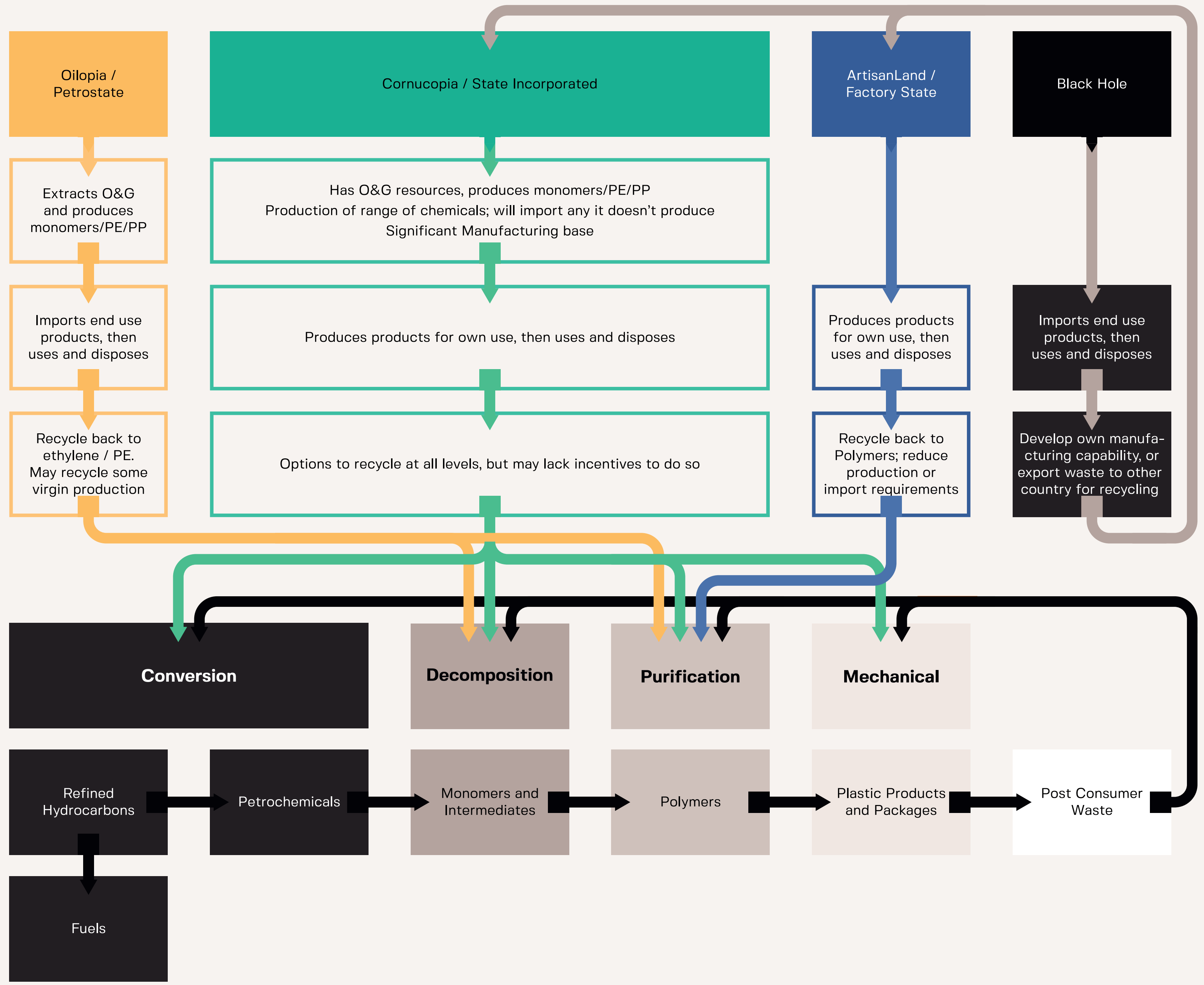


Figure 4-9: How the industry archetypes map onto the value chain and recycling technologies

D. Conclusion to Year 1

The bold ambition of C-THRU is to deliver foresight on the future interventions and innovation opportunities in the petrochemical sector required to minimise GHG emissions. This will be achieved by delivering the world's most comprehensive, reliable, and transparent account of current and future emissions for the global petrochemical sector. This Year 1 Report is the first deliverable of the C-THRU project and has presented a critical review of GHG emissions reporting of the petrochemical sector. We laid out the motivations behind the project in Chapter One before presenting the work we have completed so far. Chapter Two gave a comprehensive overview of the petrochemical sector, including products, processes, emissions, and life cycle stages. Chapter Three presented our literature and data reviews, highlighting the gaps in the literature and the problems with data accounting in other models and databases of the sector. There is currently no reliable, comprehensive picture of GHG emissions or energy, mass, and trade flows of the petrochemical sector due to its complexity. Finally, in Chapter Four, we have presented our approach to create an extended framework which incorporates process energy inputs and emissions; demand for chemical products; process and end-of-life mitigation options; and economic and business contexts. We have described the models, processes and frameworks which will be applied to create the framework. Through the focus studies, we have given insight into some specific work we have completed thus far.

In Years 2 and 3, we will continue to build on the models and datasets to create our extended framework. We will use this framework, derived from bottom-up measurements to validate current direct top-down GHG emissions accounts and add new insight into mitigation solutions. Our analysis will be truly global in nature, providing clarity about both the impacts of the global petrochemical industry on GHG emissions, but also disaggregated down to the regional level to reveal the business and economic contexts for mitigation decisions in each area. We will continue to develop decarbonisation scenarios and investigate how these will interact with the business landscape and economic environment. We will also explore the petrochemical sector's influence on environmental policy, considering the implications of economic, legal, business, governance, regulation, and policy contexts.

To close this report, we would like to invite you to interact with and follow the progress of the project through our website or by getting in touch with us.

CARBON CLARITY IN THE GLOBAL PETROCHEMICAL SUPPLY CHAIN

Get in touch

- c-thru.org
- c-thru.org/contact
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- @CTHRUproject

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Appendix A

Data sources: How GHG emissions are reported

GHG emissions databases

No.	Database name	Data type	Price	Database type	Geographical coverage	Product	Time series	Uncertainty
1	Intergovernmental Panel on Climate Change (IPCC)	Reporting Framework	Free	International	Global	Petrochemicals	n/a	Y
2	United Nations Framework Convention on Climate Change (UNFCCC)	Emission	Free	International	Global, country	Petrochemicals	1990-2018	Y
3	National Atmospheric Emissions Inventory	Emission	Free	Government	UK	Petrochemicals	1990-2018	Y
4	United Nations Statistics Division	Emission	Free	International	By country, by region, global	Petrochemicals	-	Not found
5	Millennium Development Goals Indicators	Emission	Free	International	By country, by region, global	Petrochemicals	-	Not found
6	United Nations (UN) Data	Emission	Free	International	By country, by region	Petrochemicals	-	Not found
7	United Nations Environment Programme (UNEP) Global Environment Outlook (GEO)	Emission	Free	International	By country, by region, global	Petrochemicals	1990-2018	Y
8	United Nations Environment Programme/ Global Resource Information Database (UNEP/GRID) Arendal	Emission	Free	International	Annex I Parties By country	Petrochemicals	-	Not found
9	The World Bank – World Development Indicators (WDI) Online Database	Emission	Free	International	By country, by region, global	Petrochemicals	1960-2016	Not found
10	The World Meteorological Organization (WMO)	Emission	Free	International	By country, by region, global	Petrochemicals	2016-2030	Not found
11	Carbon Dioxide Information Analysis Center (CDIAC)	Emission	Free	International	CO2 emissions by country	Petrochemicals	1751-2017	Not found

No.	Database name	Data type	Price	Database type	Geographical coverage	Product	Time series	Uncertainty
12	International Energy Agency (IEA)	Emission	Free	International	By country, by region, global	Petrochemicals	2000-2030	Not found
13	Organisation for Economic Co-operation and Development (OECD)	Emission	Free	International	By country. by group (e.g. OECD), global	Petrochemicals	-	Not found
14	Statistical Office of the European Communities (EUROSTAT)	Emission	Free	International	By country, by group	Petrochemicals	1970-2012	Y
15	European Environment Agency	Emission	Free	International	By country, by group	Petrochemicals	1990-2019	Not found
16	United States Environmental Protection Agency (USEPA)	Emission	Free	International	By country	Petrochemicals	1990-2050	Y
17	World Resources Institute (WRI)	Emission	Free	International	By country	Petrochemicals	2013	Y
18	World Resources Institute (WRI) Climate Analysis Indicators Tool	Emission	Free	International	By country, by region, global	Petrochemicals	1990-2016	Not found
19	Netherlands Environmental Assessment Agency (PBL)	Emission	Free	International	By country, global	Petrochemicals	1700–1990	Y
20	EDGAR- (European Commission - Joint Research Centre (EC-JRC)	Emission	Free	International	By country, global	Petrochemicals	1970-2012	Not found
21	European Chemicals Agency	Emission	Free	International	EU	Petrochemicals	-	Not found
22	Carnegie_Oil Climate Index	Emission	Free	Academic paper	Global	Crude oil	-	Y
23	PRELIM	Emission	Free	Academic paper	Global, country	Refinery	-	Y
24	Yara International ASA	Emission	Free	International	Global	Fertiliser	2016-2020	Not found
25	Ecoinvent	Emission	Price	Commercial	Global, Europe, Rest of World, country	Petrochemicals	1992-2021	Y
26	GaBi database	Emission	Price	Commercial	Global, Europe, Rest of World, country	Petrochemicals	-	Not found
27	US ANL GREET model (LCA data, excel)	Emission	Free	International	US average	Petrochemicals	1996-2021	Y
28	PlasticsEurope	Emission	Free	International	EU	Plastics	2006-2020	Not found
29	US Federal LCA Commons	Emission	Free	International	US average	Petrochemicals	2020	Not found
30	FAO, Fertilisers by Nutrient	Mass, Emission	Free	International	Global, country	Fertiliser	1961-2018	Y
31	Statista	Mass, Emission	Price	Commercial	Global, country	Petrochemicals	2003-2040	Not found
32	Statistical Database, National Bureau of Statistics of China	Mass, Emission	Free	Government	China	Petrochemicals	-	Not found
33	US NREL MFI tool	Mass, Emission	Free	International	US average	Petrochemicals	2016-2019	Not found

Table A–1: List of emission data sources for the petrochemical sector

Intergovernmental Panel on Climate Change (IPCC)

ipcc.ch

The Intergovernmental Panel on Climate Change (IPCC) is an intergovernmental body of the United Nations established in 1988 that provides the world with scientific information relevant to understanding the risk of human-induced climate change, its natural, political and economic impacts and risks, and possible response options.

The 2006 IPCC Guidelines for National Greenhouse Gas Inventories (2006 IPCC Guidelines)[1] provide methodologies for estimating national inventories of anthropogenic emissions by sources and removals by sinks of greenhouse gases. See Figure A-1 for an overview of the key sources and sinks.
The 2006 IPCC Guidelines were prepared in response to an invitation by the Parties to the UNFCCC. They may assist Parties in fulfilling their commitments under the UNFCCC to report on inventories of anthropogenic emissions by sources and removals by sinks of greenhouse gases not controlled by the Montreal Protocol, as agreed by the Parties. The 2006 IPCC Guidelines are in five volumes:

Volume 1 (General Guidance and Reporting) describes the basic steps in inventory development and offers general guidance in greenhouse gas emissions and removals estimates based on the authors' understanding of accumulated experiences of countries over the period since the late 1980s, when national greenhouse gas inventories started to appear in significant numbers.

Volumes 2 to 5 offer guidance for measuring emissions in different sectors of economy

The IPCC has developed the Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories 1 (1996 IPCC Guidelines). The IPCC Methodology Report, titled the 2019 Refinement to the 2006 IPCC Guidelines for National Greenhouse Gas Inventories (2019 Refinement), was published in 2019[2] to refine the 2006 IPCC Guidelines with the aim to provide an updated and sound scientific basis for supporting the preparation and continuous improvement of national greenhouse gas inventories.

United Nations Framework Convention on Climate Change (UNFCCC)

unfccc.int

The United Nations Framework Convention on Climate Change is an international environmental treaty addressing climate change. The Convention has near universal membership (197 Parties) and is the parent treaty of the 2015 Paris Agreement and the 1997 Kyoto Protocol.

The UNFCCC publishes guidelines to create transparency in global GHG emission accounting. Near universal ratification of the Paris Accord sees adherence to the IPCC guidelines for reporting emissions. The UNFCCC maintains the GHG data interface, which is an online database publicly accessible on the secretariat website **di.unfccc.int** where users can access GHG data for all Parties. The flexible queries module of the GHG data interface contains the most detailed level of data and allows users to make complex queries for multiple sectors and gases, and then export the query result.

The original submissions (the source of GHG data in the Data Interface) from Annex I Parties are accessible as Common Reporting Format (CRF) tables. The CRF tables of each Party contain detailed data on GHG emissions for the whole time series for all sectors including activity data and implied emission factors. For Non-Annex I Parties, the source of data are their national reports, namely National Communication and Biennial Update Reports.

Under the UNFCCC process, the reporting requirements for Annex I and Non-Annex I Parties differ both in terms of the methodologies used (Annex I Parties use the 2006 IPCC guidelines while Non-Annex I Parties are recommended to use the Revised 1996 IPCC guidelines) and in the frequency they submit GHG emissions information. Annex I Parties submit annually a complete time series from their base year to the current calendar year less 2 years (currently 1990 to 2018), whereas Non-Annex I Parties submit information periodically, and only for selected years.

World Resources Institute (WRI)

EarthTrends, an initiative of the WRI [3], is an online collection of information providing statistical, graphic, and analytical data on environmental, social and economic trends. To facilitate the comparison of data from different sources, EarthTrends supplements its content with detailed metadata that report on research methodologies and evaluate the reliability of information. Emissions data for CO_2 are sourced from the IEA, CDIAC sources and WRI's own analyses (e.g. calculation of cumulative emissions, carbon intensity of economy), and from EDGAR for non-CO_2 gases.

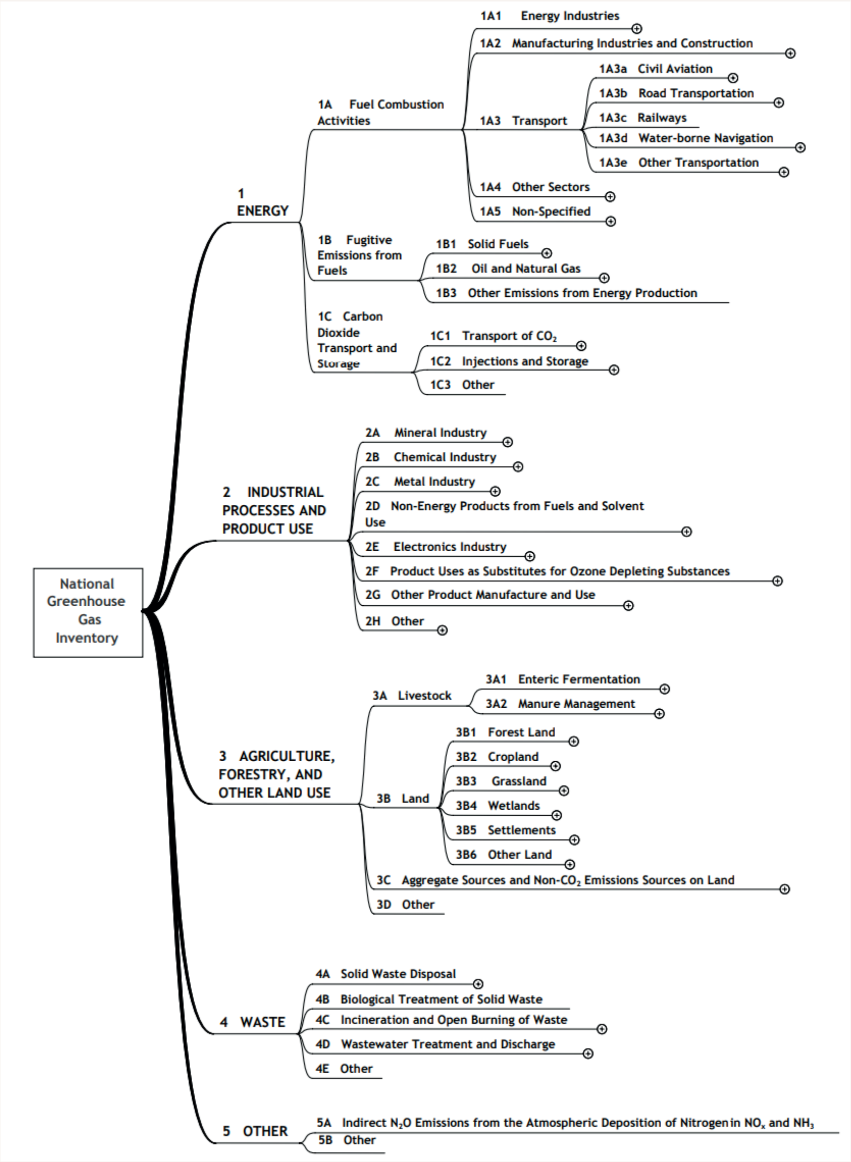

Figure A-1: Main categories of emissions by sources and removals by sink. Reprinted with permission. Copyright 2022 IPCC[1]

International Energy Agency (IEA)

iea.org

The IEA provides data and information on energy consumption, products, prices and taxes. Energy-related statistical data include coal, oil, gas, electricity and heat statistics, energy balances, prices and emissions. The IEA calculates and publishes CO_2 emissions from fuel combustion from its energy data. The data are originally collected by official bodies (often national statistical offices) in OECD member countries from firms, government agencies and industry organizations. The data for non-OECD-member countries are collected directly from government and industry contacts and from national publications. CO_2 emissions are calculated by the IEA.

Carbon Dioxide Information Analysis Center (CDIAC)

The Carbon Dioxide Information Analysis Center (CDIAC) [4] is the primary climate-change data and information analysis centre of the U.S. Department of Energy (DOE). The CDIAC closed on September 30, 2017, with data distributed to several different repositories, primarily the U.S. Department of Energy's (DOE) Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) archive.

The CDIAC's data holdings include records of the concentrations of CO_2, CH_4, SF_6, and HFC-23 in the atmosphere; emissions of CO_2 from fuel combustion; emissions of CH_4; and long-term climate trends. Data records are presented in multipage formats, each dealing with a specific site, region, or emissions species. The data records include tables; graphs; discussions of methods for collecting, measuring, and reporting the data; trends in the data, and references to literature providing further information. CDIAC's data is available in Trends Online: A Compendium of Data on Global Change which provides synopses of frequently used time series of global-change data, including estimates of global, regional, and national CO_2 emissions from the combustion of fossil fuels, gas flaring, and the production of cement:

- historical and modern records (from ice cores and current monitoring stations) of atmospheric concentrations of CO_2
- atmospheric concentrations of methane
- isotopic measurements atmospheric greenhouse gases
- estimates of global, regional, and national CO_2 emissions from the combustion of fossil fuels, gas flaring, and the production of cement
- global emissions estimated for methane (CH_4)
- carbon flux from land-cover change
- long-term temperature records, whose spatial coverage ranges from individual sites to the entire globe and from the Earth's surface to the lower stratosphere total cloud over China
- ecosystems (area and carbon content)

EDGAR (European Commission - Joint Research Centre (EC-JRC))

The JRC provides the Emissions Database for Global Atmospheric Research (EDGAR) [5] with open access to anthropogenic emissions data. EDGAR is a multipurpose, independent, global database of anthropogenic emissions of greenhouse gases and air pollution on Earth. EDGAR provides independent emission estimates compared to those reported by European Member States or by Parties under the United Nations Framework Convention on Climate Change (UNFCCC), using international statistics and a consistent IPCC methodology. EDGAR provides both emissions as national totals and grid maps at 0.1 x 0.1 degree resolution at global level under the format of historic time series (1970-2012), with yearly, monthly and up to hourly data. The chemical substances include all Kyoto Protocol greenhouse gases (CO_2, CH_4, N_2O, HFCs, PFCs and SF6), and all air pollutants and aerosols of the Convention for Long Range Transboundary Air Pollution (CO, NOX, NMVOC, SO_2, NH_3, PM_{10}, $PM_{2.5}$, BC, OC and Hg). Data sources include statistical offices at the country level and own calculations.

Netherlands Environmental Assessment Agency (PBL)

The Netherlands Environmental Assessment Agency (Dutch: Planbureau voor de Leefomgeving - abbr. PBL) [6] is a research institute that advises the Dutch government on environmental policy and regional planning issues. Its research fields include sustainable development, energy and climate change, biodiversity, transport, land use, and air quality. The PBL produces several different databases:

IMAGE is an integrated assessment modelling framework that simulates the environmental consequences of human activities worldwide [7], such as for Integrated Environment Assessment and the Global Environmental Outlook. It represents interactions between society, the biosphere and the climate system to assess sustainability issues such as climate change, biodiversity and human well-being. The model can be used to explore the long-term pathways for future environmental and sustainable development problems as well as possible response strategies. The IMAGE modelling framework has been developed by the IMAGE team under the authority of PBL Netherlands Environmental Assessment Agency. IMAGE has several downloadable data items available.

HYDE (History Database on the Global Environment) database consists of statistical as well as geo-referenced historical data sets (e.g. population, land use, GDP, livestock, value added, energy consumption, emission of greenhouse gases) on global, regional, and national levels for the period 1700 to 1990.

GEIA: Global Emissions Inventories on NMVOC Compound Groups, Ammonia (NH_3) and Carbon Monoxide (CO) reside; data sets at RIVM. These datasets have been constructed in line with the corresponding EDGAR inventories. The PBL website of the Global Emissions Inventory Activity 'GEIA' is no longer online but is still available in archive [8].

NH_3 emission inventory: New global inventory of ammonia emissions from application of fertilisers and animal manure to agricultural fields based on a Residual Maximum Likelihood model.

N_2O/NO emission inventory: New global inventory of N_2O / NO emissions from agricultural fields based on a Residual Maximum Likelihood model.

Data sources are statistical offices at the country level and own calculations.

United States Environmental Protection Agency (USEPA)

epa.gov

The USEPA has published emissions and projections of non-CO_2 greenhouse gas emissions from developing countries (CH_4 and N_2O) and from developed countries (CH_4, N_2O, HFCs, PFCS and SF_6). The data sources come from USEPA's calculations. The non-carbon dioxide (non-CO_2) greenhouse gas (GHG) assessments were released in two reports in 2012 and 2019.

The report Global Non-CO_2 GHG Emissions: 1990-2030 was published in 2012 and provided projections of non-CO_2 emissions globally through 2030 [9]. The report data annex includes all emission data tables in excel format.

The report Global Non-CO_2 Greenhouse Gas Emission Projections & Mitigation Potential: 2015-2050 provides emissions projections and estimates of mitigation potential for non-CO_2 GHGs through a comprehensive global analysis [10]. It provides a consistent and comprehensive set of historical and projected estimates of emissions and technical and economic mitigation estimates of non-CO_2 GHGs from anthropogenic sources for 195 countries. The analysis provides information that can be used to understand national contributions of GHG emissions, historical progress on reductions, and mitigation opportunities. The report data annex includes all emission projections and mitigation data tables in excel format.

The accompanying data sets to this report are also available through the Non-CO_2 Greenhouse Gas Data Tool [11]. This is a data exploration tool for querying and visualizing the non-CO_2 GHG projections and mitigation assessments compiled in the report.

European Environment Agency

The European Environment Agency (EEA) [12] is an agency of the European Union which provides environmental data and indicator sets, assessments, and thematic analyses that forms the basis for environmental policies in the EU and Member countries. At the time of writing, the EEA has 30 member countries (i.e. the 27 EU Member States together with Iceland, Liechtenstein, and Norway). The European environment information and observation network (Eionet) is a partnership network of the EEA and the countries. The information provided by the EEA comes from a wide range of sources. These include a network of national environmental bodies involving more than 300 institutions in Europe, as well as European and international organisations (eg. Eurostat, the Joint Research Centre (JRC) of the European Commission, OECD, UNEP, FAO and WHO.

Statistical Office of the European Communities

EUROSTAT [13] provides the European Union with statistics at European level that enable comparisons between countries and regions. As part of the European Statistical System (ESS), it focuses on EU policy areas, but, with the extension of EU policies, harmonization has been extended to nearly all statistical fields. The ESS also coordinates its work with international organizations such as OECD, the United Nations, the International Monetary Fund and the World Bank.

The data is collected by member States. The EEA compiles an annual greenhouse gas inventory report on behalf of the EU. Estimates of greenhouse gas emissions are produced for a number of sources which are delineated in sectors primarily according to the technological source of emissions, as devised by the Intergovernmental Panel on Climate Change (IPCC).

The five main emission source sectors include:

- energy (fuel combustion and fugitive emissions from fuels) — which also includes transport;
- industrial processes and product use;
- agriculture;
- land use, land use change and forestry; and
- waste management.

Eurostat presents three perspectives of greenhouse gas (GHG) emissions statistics:

Perspective	Statistical framework	Purpose	Ref.
GHG emissions classified by economic activities	Air Emissions Accounts (AEA) by Eurostat	Tailored for integrated environmental-economic analyses	14
GHG emissions classified by technical processes	GHG emission inventories by UN	Official international reporting framework for international climate policies (UNFCCC, EU MMR)	15
'footprints' = GHG emissions classified by final use of products	Modelling results published by Eurostat	One particular analytical application of AEA	16

Table A-2: Three perspectives of greenhouse gas (GHG) emission statistics

Location	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019
European Union - 27 countries	363,979.88	363,333.19	350,362.05	348,243.02	354,884.91	347,797.15	349,288.46	357,481.29	349,143.21	339,781.38
European Union - 28 countries	397,072.4	394,853.92	382,541.03	382,608.65	388,998.57	381,441.97	380.776.87	389,536.62	379,928.64	369,877.72
European Union - 28 countries	395,053.5	392,923.64	380,529.66	380,554.29	386,959.44	379,336.8	378,690.43	387,419.5	377,819.8	367,767.04
Belgium	22,095.73	21,474.85	19,724.02	20,406.19	20,716.47	20,815.92	21,343.73	21,333.84	21,571.13	20,178.21
Bulgaria	4,441.45	5,017.02	4,780.23	4,754.8	5,115.35	5,764.56	6,114.23	6,407.9	6,526.04	6,359.87
Czechia	15,054.51	15,292.52	15,061.6	14,908.97	15,703.82	15,359.83	15,621.18	15,697.59	16,283.63	15,522.92
Denmark	1,913.39	2,055.63	2,091.69	2,055.03	2,010.35	1,835,45	2,044,45	2,028.54	2,048.45	1,840.09
Germany (until 1990 former	62,598.98	62,530.33	61,621.69	61,386.98	61,258.88	60,288.8	62,144.36	66,115.46	63,254.17	61,355.88
Estonia	538.46	662.19	907.42	998.69	711.29	515.77	502.26	638.55	626	618.42
Ireland	2,594.7	2,482.63	2,686.83	2,639.93	3,057.79	3,246.35	3,474.68	3,488.35	3,235,98	3,184.03
Greece	11,759.57	10,423.91	11,245.63	11,966.8	12,329.99	11,998.07	12,506.82	12,795.12	12,399.23	11,688.04
Spain	40,545.54	37,659.79	36,015.27	34,830.24	36,661.93	31,056.08	30,577.08	28,311.19	27,860.35	26,109.64
France	54,129.96	53,720.52	51,641.79	53,227.73	52,915.89	51,384.36	51,299.05	52,661.08	49,919.94	47,676.72
Croatia	3,356.1	3,201.83	2,924.69	2,671.48	2,794.52	2,866.61	2,532.76	2,783.81	2,638	2.735.07
Italy	37,000.49	37,319.84	34,573.45	33,600.3	33,209.58	33,232.31	33,426.77	33,817.48	34,569.82	33,937.08
Cyprus	831.35	842.15	807.28	1,057.51	1,288.02	1,199.14	1,221.19	1,277.12	1,220.97	1,181.39
Latvia	749.42	846.9	905.1	848.74	863.37	791.24	690.97	768.36	893.93	890.87
Lithuania	2,234.4	3,714.51	3,560.91	2,999.19	3,185.54	3,509.22	3,332.53	3,650.2	3,184,26	3,410.13
Luxembourg	658.31	670.07	639.37	622.17	632.63	624.02	646.32	656.72	657.31	675.07
Hungary	6,394.8	6,559.28	6,266.1	5,670.48	6,487.53	6,936.54	6,647.43	7,423.03	7,703.8	7,665.81

cont.

Location	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019
Malta	155.37	182.61	212.68	235.79	248.06	261.74	272.27	278.27	271.2	263.7
Netherlands	10,750.65	10,409.57	9,957.22	10,314.23	9,782.15	9,795.15	9,267.43	9,758.11	9,925.42	9,794.6
Austria	15,692.55	15,864.25	15,476.67	15,791.74	15,903.97	16,552.01	16,301.56	17,113.73	15,471.13	16,383.02
Poland	23,889.72	26,704.9	25,702.68	25,361.01	27,021.65	26,208.83	25,155.57	25,693.35	24,438.84	24,129.15
Portugal	7,545.97	6,952.23	6,683.21	7,164,45	7,647.01	7,715.74	7,160.26	7,631.59	7,277.73	7,653.81
Romania	14,032.27	14,663.76	13,343.92	11,584.84	12,290.57	12,468.85	12,679.17	12,922.64	13,226.37	13,113.98
Slovenia	1,015.53	1,030.94	1,058.7	1,123.51	1,162.84	1,145.77	1,144.97	1,191.13	1,214.37	1,260.96
Slovakia	9,423.49	9,024.28	8,954.84	8,665.63	8,880.59	9,084.87	9,292.4	9,574.07	9,553.64	8,689.12
Finland	6,159.57	6,109.68	5,956.58	5,850.03	5,612.68	5,792.36	6,000.26	5,826.17	5,844.32	5,514.6
Sweden	8,417.59	7,916.97	7,562.45	7,506.55	7,392.44	7,347.58	7,888.76	7,637.91	7,322.18	7,949.2
Iceland	1,910.71	1,831.98	1,907.14	1,947.41	1,931.54	1,998.36	1,986.58	2,024.05	2,022.53	2.024.37
United Kingdom	31,073.62	29,590,45	30,167.61	32,311.27	32,074,53	31,539.65	29,401.98	29,938.21	28,676.59	27,985.66

Table A-3: Example greenhouse gas emissions by source sector [17]

United Nations Environment Programme/ Global Resource Information Database (UNEP/GRID) Arendal

The United Nations Environment Programme (UNEP) is the leading global environmental authority that sets the global environmental agenda, promotes the coherent implementation of the environmental dimension of sustainable development within the United Nations system, and serves as an authoritative advocate for the global environment [18].

The Global Resource Information Database [18] includes graphical representations of greenhouse gas emissions produced in preparation for the Conference of the Parties at its seventh session. The graphs feature actual (1990–1999) and projected (2000, 2010) emissions of six greenhouse gases: CO_2, CH_4, N_2O, HFCs, PFCs and SF_6. The emissions data are aggregated and represented as CO_2 equivalents. The Data, covering Annex I Parties and by country, are taken from several UNFCCC documents compiling data from submissions by Annex I Parties, including first and second national communications, and annual national inventory data. Additional sources include updated reports from individual countries.

United Nations Environment Programme (UNEP) Global Environment Outlook (GEO)

Global Environment Outlook (GEO)[19] data are from sets used by UNEP and partners in the Global Environment Outlook Project – mainly the United Nations and other international organizations as well as national data centres. The online database holds more than 400 different variables as national, subregional, regional and global statistics or as geospatial data sets (maps), covering themes such as freshwater, population, forests, emissions (CO_2, N_2O, CH_4, aggregated HFCs, PFCs, SF_6), climate, disasters, health and GDP. These data, provided by UNFCCC, OECD/IEA, CDIAC, RIVM, can be displayed in tabular or graphic format.

United Nations Statistics Division

The United Nations Statistics Division [20] compiles statistics from many international sources and produces global updates, including the Statistical Yearbook, World Statistics Pocketbook and yearbooks in specialized fields of statistics. It also provides to countries specifications of the best methods of compiling information so that data from different sources can be readily compared. The original data sources include FAO, OECD, UNICEF, UNFCCC (carbon dioxide), World Bank and others.

PLASTICS EUROPE

PlasticsEurope

plasticseurope.org

PlasticsEurope is a leading pan-European association and represents plastics manufacturers active in the European plastics industry. The plastics industry in Europe is a vibrant sector that helps improve the quality of life by enabling innovation, facilitating resource efficiency and enhancing climate protection. In addition to the plastics manufacturers, the plastics industry includes converters, represented by European Plastics Converters (EuPC), recyclers, represented by Plastics Recyclers Europe (PRE), and machine manufacturers, represented by European Plastics and Rubber Machinery (EUROMAP).

PlasticsEurope networks with European and national plastics associations and has more than 100 member companies, who are responsible for producing more than 90% of all polymers across the 27 member states of the European Union, plus Norway, Switzerland, Turkey and UK. On a global level, PlasticsEurope actively supports the World Plastics Council (WPC) and the Global Plastics Alliance (GPA).

PlasticsEurope was the first industry organisation to assemble and publish detailed environmental data on the processes operated by its member companies. The first Eco-profile reports were published in 1993. Since then, reports have been added and continuously updated, so that there are now more than 70 Eco-profile reports freely available.

Eco-profiles[21] are reports on product-specific environmental impacts. Based on European industry averages of the respective polymer production technologies, they include detailed environmental datasets – the so-called Life Cycle Inventory (LCI) – and environmental key performance indicators. An example of PlasticsEurope's Eco-profiles can be found in Figure A-2. Their scope is from cradle (extraction of raw materials) to gate (uncompounded precursors or resins). They cover the high volume, bulk polymers, some of the more widely used engineering plastics, and several common plastics conversion processes. While the inventory consists of all relevant material and energy inputs as well as emissions and waste outputs associated with the production, the key performance indicators contained in the associated Environmental Product Declaration (EPD) provide impact metrics, such as the carbon footprint and many others. While the detailed data are used by life cycle experts, the EPD is suitable for business-to-business communication with downstream users of plastics. The Eco-profile methodology is aligned with ISO standards 14040–44, 14025 and the ILCD Handbook of the European Commission's Joint Research Centre. Widely acknowledged among life cycle practitioners and other stakeholders worldwide as representative datasets, they have been included in various commercial life cycle databases as well as in the publicly available European Life Cycle Database (ELCD).

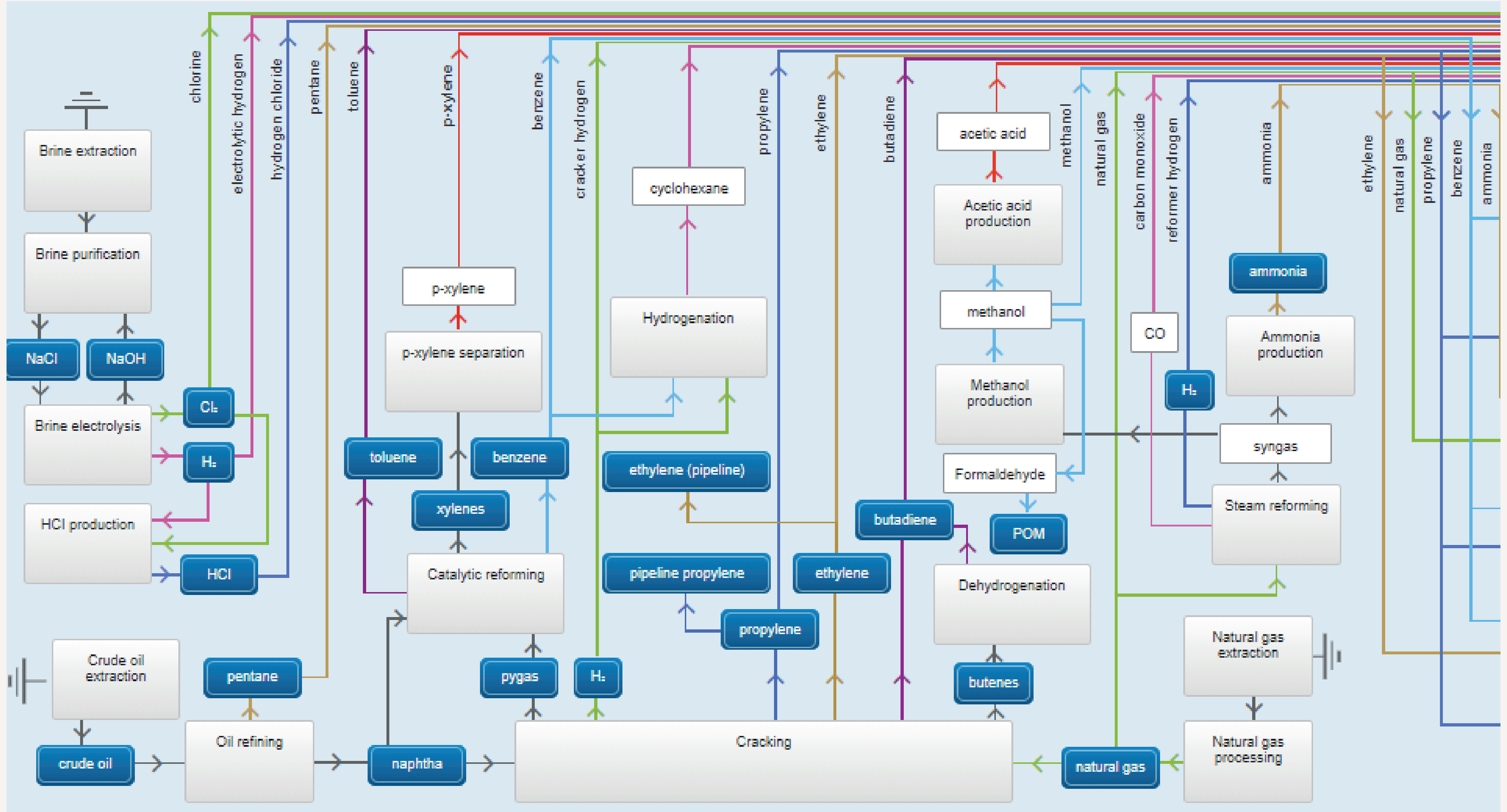

Figure A-2: Flowchart of PlasticsEurope's Eco-profiles[28]

ecoinvent

ecoinvent is a not-for-profit association dedicated to promoting and supporting the availability of environmental data worldwide. It publishes the ecoinvent database [22], which provides well documented process data for thousands of products. With around 18,000 LCI datasets in many areas such as energy supply, agriculture, transport, biofuels and biomaterials, bulk and specialty chemicals, construction materials, wood, and waste treatment, ecoinvent version 3 is the most comprehensive, transparent, international LCI database. A system model describes how activity datasets are linked to form product systems. The ecoinvent version 3 database offers three system models to choose from (see Table A-4).

ecoinvent is used in a broad range of environmental studies including Life Cycle Assessment (LCA), Environmental Product Declaration (EPD), Design for Environmental or Carbon Footprinting, and allows studies to be conducted with different levels of detail: from screenings for basic inventory analysis, initial answers to extensive studies such as peer-reviewed, ISO-compliant studies.

Cut-Off System Model	APOS System Model	Consequential System Model
The system model Allocation, cut-off by classification, or cut-off system model in short, is based on the recycled content, or cut-off, approach. The underlying philosophy is that a producer is fully responsible for the disposal of its wastes, and that he does not receive any credit for the provision of any recyclable materials.	The system model Allocation at the point of substitution is also simply know as APOS system model. The APOS system model follows the attributional approach in which burdens are attributed proportionally to specific processes.	The system model substitution, consequential, long-term is also known as consequential system model. The consequential system model uses different basic assumptions to assess the consequences of a change in an existing system.

Table A-4: System models in ecoinvent 3

US Federal LCA Commons

The US Federal LCA Commons [23] is an interagency community of practice for life cycle assessment research methods. The Federal LCA Commons collaborates to share expertise and methods to move toward common federal data modelling conventions and make federal data sets freely available through a web-based data repository.

The US Federal LCA Commons Life Cycle Inventory Unit Process Template is a multi-sheet Excel template for life cycle inventory data, metadata and other documentation. The template comes as a package that consists of three parts: (1) the main template itself for life cycle inventory (2) a 'validator' that consists of a VBA macro that can be run to validate data entered into a completed template against openLCA and Federal LCA commons requirements and guidelines, and (3) a compiled Java archive (.jar) that can be dropped into a users' openLCA program files to provide a plugin to import this template into openLCA. The template was developed by the USDA National Agricultural Library and the US EPA Life Cycle Center of Excellence through their collaboration as leading parties in the Technical Working Group on US Federal LCA Data Interoperability.

Food and Agriculture Organization (FAO) of the United Nations

The FAOSTAT database [24] provides the ratio between the totals by nutrient of agricultural use of chemical or mineral fertilisers, reported in the FAOSTAT domain "Inputs/Fertilisers by Nutrient" for nitrogen (N), phosphorus (expressed as P_2O_5) and potassium (expressed as K_2O), and the area of cropland (sum of arable land and permanent crops) reported in the FAOSTAT domain "Inputs/Land Use". The data are provided at national, regional, and global level over the time series 1961-present.

The FAOSTAT emissions database is computed following Tier 1 IPCC 2006 Guidelines for National GHG Inventories **ipcc-nggip.iges.or.jp/public/2006gl/index**. GHG emissions are provided by country, regions and special groups, with global coverage, relative to the period 1961 to present (with annual updates) and with projections for 2030 and 2050, expressed as Gg CO_2 and CO_2eq (from CH_4 and N_2O), by agricultural emission sub-domain and by aggregate. GHG emissions from synthetic fertilisers consist of nitrous oxide gas from synthetic nitrogen additions to managed soils. Specifically, N_2O is produced by microbial processes of nitrification and de-nitrification taking place on the addition site (direct emissions), and after volatilization/re-deposition and leaching processes (indirect emissions). The FAOSTAT emissions database is computed following Tier 1 IPCC 2006 Guidelines for National GHG Inventories vol. 4, ch 11 **ipcc-nggip.iges.or.jp/public/2006gl/vol4**. The FAOSTAT domain Synthetic Fertilisers disseminates information on the amount of nitrogen in chemical and mineral fertilisers applied to agricultural soils (kg of nutrients); and the associated direct and indirect N_2O emissions (kilotonnes N_2O). Data are available by country, for standard FAOSTAT regional aggregations, including for Annex I and non-Annex I groups. The 2019 values for this update are computed from the average of two most recent years. This domain also disseminates the activity data and emissions data reported by countries to the United Nations Framework Convention on Climate Change (UNFCCC) for the category Inorganic N fertilisers applied to managed soils. Activity data are sourced from the most recently available GHG National Inventories (NGHGI) or from National Communications. Emission data are sourced directly from the UNFCCC data portal or from Biennial Update Reports (BURs). UNFCCC data are disseminated in FAOSTAT with permission, formalized via a FAO-UNFCCC Memorandum of Understanding.

The Fertilisers by Product dataset contains information on the Production, Trade and Agriculture Use of inorganic (chemical or mineral) fertilisers products, over the time series 2002 to present. The fertiliser statistics data are for a set of 23 product categories. Both straight and compound fertilisers are included.

The Fertilisers by Nutrient dataset contains information on the totals in nutrients for Production, Trade and Agriculture Use of inorganic (chemical or mineral) fertilisers, over the time series 1961 to present. The data are provided for the three primary plant nutrients: nitrogen (N), phosphorus (expressed as P_2O_5) and potassium (expressed as K_2O). Both straight and compound fertilisers are included.

CEFIC – European Chemical Industry Council

cefic.org

The European Chemical Industry Council (CEFIC) is the main European trade association for the chemical industry. It was founded in 1972 and serves its Members and the European chemical industry by generating and aggregating scientific knowledge that fosters the purpose of the Association in critical areas and by offering needs-oriented services and expertise to its Members. It releases facts and figures annually [25], which includes the most recent data and analysis of the latest trends in the EU chemical industry, and chemical quarterly report. CEFIC report is significant to explore the impact, opportunities and risks of various energy and technology development scenarios for the European chemical industry by 2050.

Statista

Statista is a German company specializing in market and consumer data [26]. According to the company, its platform contains more than 1,000,000 statistics on more than 80,000 topics from more than 22,500 sources and 170 different industries. Statista provides information on the key metrics by which these industries are measured: reserves, production, and consumption (supply and demand), as well as prices, M&A activity, and other economic indicators for the wide array of chemical products and resource commodities covered.

European Chemicals Agency (ECHA)

echa.europa.eu

The European Chemicals Agency is an agency of the European Union which manages the technical and administrative aspects of the implementation of the European Union regulation called Registration, Evaluation, Authorisation and Restriction of Chemicals [27]. The ECHA keeps an inventory of commercially manufactured chemicals with over 100,000 entries. It includes a range of chemicals from fertiliser precursors produced on the 1011 kg scale, such as ammonia, to powerful analgesics administered in dosages on the 10-6 kg scale, such as fentanyl.

Studies reporting on emissions

	Reference	Publication year	Data type	Life cycle stages	Geographic region	Petrochemical products *(plastics, fertiliser, etc)*	GHGs *(CO_2, CH_4, N_2O, fugitive emission)*	Time series	Uncertainty
a	Gielen et al[28]	2002	Emissions		Global			1995-2025	Not found
b	Gielen et al[29]	2002	Mass, Emission	Feedstock, production, manufacturing	Japan	Petrochemicals, plastics	CO_2	1998	Not found
c	Neelis et al[30]	2005	Emissions	-	-	Petrochemicals	CO_2	-	Uncertainty ranges for 77 commodities are given
d	Neelis et al[31]	2005	Emissions	Feedstock, production, manufacturing	Netherlands	Petrochemicals	CO_2	1993–1999	Using standard error propagation rules to calculate the 95% confidence intervals for the consumption of ODU and NODU products
e	Ren et al[32]	2009	Emission	Feedstock, production, manufacturing	-	Petrochemicals	CO_2	-	The only significant uncertainty introduced is the assumed energy efficiency in electricity co-generation, 55%.
f	Zhu et al[33]	2010	Emissions	Feedstock, production, manufacturing	China	Petrochemicals (coal-based ammonia, calcium carbide, caustic soda, coal-based methanol, sodium carbonate, and yellow phosphorus)	GHGs	2007	Not found
g	Zhou et al[34]	2010	Emissions	Feedstock, production, manufacturing	China	Ammonia	GHGs	2005-2015	Not found
h	Zhang et al[35]	2013	Emissions	Feedstock, production, manufacturing, use	China	Fertiliser	GHGs	1980-2010	Not found
i	Wang et al[36]	2017	Emissions	Crude oil extraction, refinery	Global				Uncertainty range is a factor of 2 in each direction from the central estimate (i.e., from 0.5 to 2 times the central estimate)
j	Geyer et al[37]	2017	Mass flow	Production and waste generation	Global	Plastics (PE, PP, PS, PVC, PET, PUR, PP&A fibers, other, additives)	-	1950-2015	Not found
k	Masnadi et al[38]	2018	Emissions	Crude oil extraction	Global, 90 countries	Crude oil	GHGs	2015	Using probabilistic uncertainty analysis for the missing input data
l	Masnadi et al[39]	2018	Emissions	Crude oil extraction	China	Crude oil	GHGs	2015	Not found
m	Brandt et al[40]	2018	Emissions	Crude oil extraction	US	Crude oil	GHGs	2000-2100	Each observation is drawn from a normal distribution
n	Hoxha et al[41]	2018	Emissions	Feedstock, production, manufacturing	Global, regional, countries	Fertiliser	GHGs	-	Not found
o	Zheng et al[42]	2019	Emission	Feedstock, production, manufacturing, EOL	Global	General plastics	GHGs	2015	Making various assumptions to simplify the processes involved in a plastic's life cycle
p	Zhang et al[43]	2019	Emissions	Feedstock, production, manufacturing	China	Petrochemicals	GHGs	2015, 2020	Parameters are provided with uniform distribution. Uncertainty is analyzed using Monte Carlo simulation
q	Jing et al[44]	2020	Emission	Crude oil, refining	Global, 343 crude oils, 478 refineries	-	GHGs	2015-2100	Probability distribution for parameter uncertainty
r	Rutherford et al[45]	2020	Emissions	Crude oil extraction	US	Crude oil	GHGs	2015, 2020	Estimating uncertainty by using Monte Carlo method
s	Talaei et al[46]	2020	Emissions	Refining	Canada		GHGs	2010-2050	Not found
t	Nicholson et al[47]	2021	Mass, emission, cost	Feedstock, production, manufacturing	US	Plastics (PET, PE, PP, PVC, PS, Rubber, PU, Acrylics, Vinyl Acetates, Nylons, UPE, ABS, PC, Polyglycols, Epoxy, Alkyd Coatings, Polyacetals, PBT)	GHGs	2016-2019	Not found

Table A–5: Peer-reviewed studies on petrochemical emissions reviewed in this study

Appendix B

Data sources: How chemical supply chains are analysed

Chemical databases

No.	Database name	Data type	Price	Database type	Geographical coverage	Product	Time series	Uncertainty
1	IHS Markit	Mass, cost	For quote	Commercial	Global and regional, country	Petrochemicals	1965-2020	No access
2	ICIS	Mass, cost	For quote	Commercial	Global, regional, country	Petrochemicals	1978-2040	Not found
3	International Fertiliser Society (IFA)	Mass	Free	International	Global, country	Fertiliser	N/A	No access
4	Food and Agriculture Organization (FAO) of the United Nations	Mass, Emission	Free	International	Global, country	Fertiliser	1961-2018	Yes
5	International Fertiliser Society (IFS)	Mass	Free	International	Global, country	Fertiliser	N/A	No access
6	UN Comtrade Database	Mass	Free	International	Global, country	Petrochemicals	1962-2021	Not found
7	Prodcom Eurostat	Mass	Free	International	EU, country	Petrochemicals	2008-2019	Not found
8	American Chemistry Council (ACC)	Mass	$300/ report	Commercial	US	Plastics	2009-2019	Not found
9	Petrochemicals Europe	Mass	Free	International	EU, country	Petrochemicals	N/A	Not found
10	The Fiber Year GmbH	Mass	750 CHF/ report	Commercial	Global, country	Fiber	2005-2024	No access
11	Valpak	Mass	For quote	Commercial	UK	Plastics	2015-2019	Not found
12	Japan Plastics Industry Federation (JPIF)	Mass	Free	International	Japan	Plastics	N/A	Not found

Table B–1: List of mass flow data sources for petrochemical sector

Products covered in CEH

Inorganics
Mining Materials
Industrial Gases
Fertilisers
Fibres
Films
Polymers
Elastomers
Renewables
Nutrition Chemicals
Resins
Coatings
Solvents
Surfactants
Petrochemicals

Table B-2: Summary of products covered in CEH

IHS Markit

The Chemical Economics Handbook (CEH) of IHS Markit [48] provides five-year outlooks and extensive market data on more than 300 industrial chemicals covering North America, Europe, China, Japan (Economic database covering 200+ countries). There is information on supply, demand, manufacturing processes, price and trade information for individual chemicals or these major chemical groups with global and regional supply/demand and five-year forecast. CEH includes detailed information on and analysis of the history, status and projected market trends for the industry's major products in most commercial chemical markets.

- Supply—producers, plant locations, annual capacities, capacity utilisation, and production volumes,
- Demand—market size, end-use applications, consumption trends, and competing materials,
- Manufacturing processes—commercial processes and basic chemistry,
- Trade—import/export data, countries of origin and destination, and shipment values,
- Price—histories, unit sales volumes, and factors affecting prices.

The Process Economic Program (PEP) yearbook [49] provides in-depth, independent technical and economic evaluations of more than 1,500 commercial and emerging technologies used to manufacture over 600 chemicals. PEP reports can be used to evaluate the impact of changes in processes, feedstocks, energy prices, and government regulations on chemical and fuel production economics. The PEP yearbook provides provides in-depth, independent technical and economic evaluations of more than 1,500 commercial and emerging technologies used to manufacture over 600 chemicals.

- Compare capital and production costs for competing process technologies based on technoeconomic analysis
- Cover production economics and capital costs for 1,900 + processes
- Cover 600+ chemicals, biochemical, and refinery products
- Provide economics for 6 regions of the world

ICIS

The ICIS Supply and Demand Data Service [50] provides a long-term view of the rapidly changing petrochemical markets. It offers end-to-end perspectives across the global petrochemical supply chain, including refineries. It provides quick access to data on import and export volumes, plant capacities, production, and product trade flows covering 160 countries and over 100 products.

Data includes:

- Historical and forecast data (1978-2040)
- Petrochemical trade flows and patterns
- Import, export and consumption volumes
- Plant capacity, production and operating status
- Upcoming plants, including speculative and announced projects
- Key information on over 12,000 refinery units, and 18,500 petrochemical plants

ICIS helps senior management, strategists, business planners, analysts and risk managers to:

- Identify, evaluate and optimise opportunities,
- Identify and manage financial or investment risks,
- Validate commercial and growth strategies.

Name	ICIS supply and demand database
Product coverage	Up to 103 petrochemical products; 28 product families
Geographical coverage	Global - broken down by country Over 160 countries listed Searchable by single or multiple countries, by region or for global overview
Historical + forecast data	From 1978 to 2040
Import and export volumes by product	Searchable by single or multiple products; or by product family Map out data against the importing and exporting countries or region Available in multiple volume denomination Data may be viewed in table, chart, graph Data is downloadable in multiple formats
Capacity and production volumes by product	Searchable by single or multiple products; or by product family Plant capacity, production and utilisation rate by company, country and region Populate producer's list by country or region Plant details - operating status, technology, site location, licensor, downstream integration Available in multiple volume denomination Data may be viewed in table, chart, graph Data is downloadable in multiple formats
Consumption volume per product	Searchable by single or multiple products; or by product family Consumption per company, country and region Data may be plotted with import, export, production and capacity data Available in multiple volume denomination Data may be viewed in table, chart, graph Data is downloadable in multiple formats
Product trading patterns and trade statistics	Searchable by single or multiple products Shows historical and forecasted importing/exporting countries and the volumes per product Historical average trading price in USD/mt Create own data set or choose from pre-set data segments: product flows, product derivatives, net trade balance, and more
Plants and refineries	Covers 12,700 refinery streams and 11,500 petrochemical plants Details on plant capacities, company names, site location, downstream integration, ownership, process route, technology, licensor
Plant operating status	Indicates: start-ups, expansions, output reductions, placed on standby, shutdown, speculative and announced projects
Monomer-derivative	Balance analyses for world, region country site and company
Company ownership	10,300 companies covered. Provides details on company structure, subsidiaries and affiliates
Econometrics	Country's GDP, population and consumer price index

Table B-3: Summary of ICIS Supply & demand database

International Fertiliser Association (IFA)

IFASTAT [51] is the leading source of fertiliser and raw materials statistics in the world. IFA considers 10 regions:

- West Europe
- Central Europe
- Eastern Europe & Central Asia
- North America
- Latin America
- Africa
- West Asia
- South Asia
- East Asia
- Oceania

Compiled by IFA's Market Intelligence team, IFASTAT is a one-stop-shop for the most comprehensive statistical information on fertilisers and raw materials supply and fertiliser consumption. Production and trade statistics are essentially collected from manufacturing companies. Export data are provided by exporting companies. In a few cases, trade statistics are collected from national customs statistics and trade statistics providers. The differences between IFASTAT fertiliser statistics and FAOSTAT fertiliser statistics are listed in Table B-4.

The scope of the Supply and Consumption Data sets are compared in Table B-5. The Supply Database looks at fertiliser raw materials, intermediates and finished products, for all uses (plant nutrition, animal feed and industrial uses). It is updated on a regular basis according to the following publication schedule. Production statistics comprise gross production in all forms and for all uses (plant nutrition, animal feed and industrial uses). Trade statistics compile import and export tonnages for all uses. They do not differentiate between plant nutrition, animal feed and industrial end-uses. Apparent consumption for all uses is calculated as follows: Production + Imports – Exports.

The Consumption Databases focuses on fertiliser products, for plant nutrition uses only (applications to crops, pastures, forests, fishponds, turf, ornamentals). It is updated once a year, usually in September. The Consumption Database provides estimates of fertiliser consumption by product, by country and by year. These consumption statistics reflect plant nutrition uses only. The consumption estimates provided in the Consumption Database relate, to the extent possible, to real consumption. When real consumption is not available, apparent consumption figures (calculated as follows: Production + Import – Export) are provided.

	IFASTAT - Supply Database	IFASTAT - Consumption Database	FAO DATA
Coverage	All uses (agricultural and industrial)	Plant nutrition uses only (applications to crops, pastures, forests, fish ponds, turf, ornamentals).	Production, Import and Export include all uses (agricultural and industrial). Total Use is split into "Agricultural use" and "Other uses". - "Agricultural use" covers fertilisers used in agriculture (crops, livestock, fisheries and aquaculture; excluding use for animal feed).- "Other uses" covers fertilisers not included under agricultural use. (i.e. Total use minus Agricultural Use).
Treatment of technical use	Included.	Excluded.	See above.
Period of study	Calendar year Quarterly reports (selected products) Half year reports (MOP)	Consumption statistics: mix of calendar and fertiliser years. Production, imports and exports: mainly calendar years.	Calendar year (otherwise, country note provided).
Sources of data	IFA members mostly; Contributors, Fert association Consultants	Consumption statistics are collected primarily from IFA correspondents: fertiliser associations, fertiliser companies, researchers, consultants. Consumption statistics for EU countries come from Fertiliser Europe. In a few cases, consumption statistics are collected from national agencies. Consumption figures are finalized after consultation with partner organizations. Production and trade statistics are derived from correspondents, IFA Supply statistics and trade statistics providers.	Main data source is national data collected via the FAO Fertilisers Questionnaire sent to FAO focal points in national governments. Additional data sources may include: official national publications, official national websites, publications related to groups of countries, country project reports, studies available in other FAO Divisions, economic journals, and country trade data received from custom departments and industry experts. The source of trade data is the United Nations Statistics Division, COMTRADE database.
Estimation of consumption	Apparent consumption (production + imports - exports)	The consumption estimates provided in the Consumption Database relate, to the extent possible, to real consumption. When real consumption is not available, apparent consumption figures (calculated as follows: production + import – export) are provided.	Country data received from questionnaires are given priority; otherwise additional data sources are used, if available, or apparent consumption is calculated.
Treatment of bulk blends	Excluded	Excluded (exception: China where blends are included).	Included as products, but they are excluded from 'totals in nutrients' (to avoid double counting of nutrients) if it can be inferred that their nutrients were already accounted under the primary products.

Table B-4: Comparison table between IFASTAT fertiliser statistics and FAOSTAT fertiliser statistics [51]

	Supply	Consumption
Products	Fertiliser raw materials, intermediates and finished products	Fertiliser products only
Uses	All uses (plant nutrition, animal feed and industrial uses)	Plant nutrition uses only (applications to crops, pastures, forests, fishponds, turf, ornamentals)
Focus activity	Production and trade (export and import trade matrix by country)	Consumption (nutrient totals only for production and trade)
Timeseries	Yearly and quarterly data since 2002	Yearly data starting in 1961, with breakdown by product from 1973
Units	In both product weight and nutrient (N, P2O5 and K2O) volumes	In nutrient (N, P2O5 and K2O) volumes only
Reference years	Calendar years only	Mix of calendar and fertiliser years
Access	Country data restricted to IFA members	Fully publicly available
Format	Data extracted from database in Excel format	Data extracted from database in Excel format

Table B-5: Comparative Scope of the Supply and Consumption Data sets

Food and Agriculture Organization (FAO) of the United Nations

The FAOSTAT database [24] provides the ratio between the totals by nutrient of agricultural use of chemical or mineral fertilisers, reported in the FAOSTAT domain "Inputs/Fertilisers by Nutrient" for nitrogen (N), phosphorus (expressed as P_2O_5) and potassium (expressed as K_2O), and the area of cropland (sum of arable land and permanent crops) reported in the FAOSTAT domain "Inputs/Land Use". Data are provided at national, regional, and global levels over the time series 1961-present.

International Fertiliser Society (IFS)

The International Fertiliser Society [52] was founded in 1947 as a learned society for individuals who have a professional interest in any aspect of fertiliser production, marketing and use. The scientific and technical papers presented at IFS Conferences and Meetings are published as the Proceedings of the International Fertiliser Society (ISSN 1466-1314) and now number more than 820 in total. The published Proceedings of the Society Meetings are one of the major publicly available sources of information on fertiliser production and use, and on crop nutrition. The subjects covered range from raw material mining and shipping, through fertiliser plant design, production techniques, safety, distribution and marketing, to fertiliser usage, crop production and environmental management.

UN Comtrade Database

UN Comtrade [53] is a repository of official international trade statistics and relevant analytical tables. Detailed and up-to-date plastics trade data is accessible through API. However, polymer-specific data on traded plastics waste are only available for PET, PS, and PVC, while trade data for other types of polymer waste are aggregated. In addition, trade data for specific polymers, plastics products, or plastics waste for some countries or regions are not available in weight, rather in other physical units. Some historical data is only available in specific classification systems in the UN Comtrade data.

Prodcom Eurostat

Prodcom [54] provides statistics on the production of manufactured goods carried out by enterprises on the national territory of the reporting countries. The term comes from the French "PRODuction COMmunautaire" (Community Production). Prodcom covers mining, quarrying and manufacturing: sections B and C of the Statistical Classification of Economy Activity in the European Union (NACE 2). Prodcom statistics aim at providing a full picture at EU level of developments in industrial production for a given product or for an industry in a comparable manner across countries.

Prodcom statistics may be used to answer such questions as:

- Which countries are specialised in the production of a given product?
- How productive is a particular industry in terms of physical volume and the value of production sold during a year?
- Which country has the lowest or the highest value per unit for the production of a certain product?
- Is there a shift or a trend in the manufacture of a group of products over the years?

American Chemistry Council (ACC)

The Resin Review 2020 [55] edition contains detailed resin data tables from 2009-2019 on domestic production, sales and captive (internal) use by end-use application, sales distribution by major market, industry capacities, and capacity utilization rates. Data reported for the following resins only: Polyethylene (LDPE/LLDPE/HDPE), Polypropylene, PVC, Polystyrene, Expandable Polystyrene (EPS), Epoxy, Isocyanates, and Polyether Polyols.

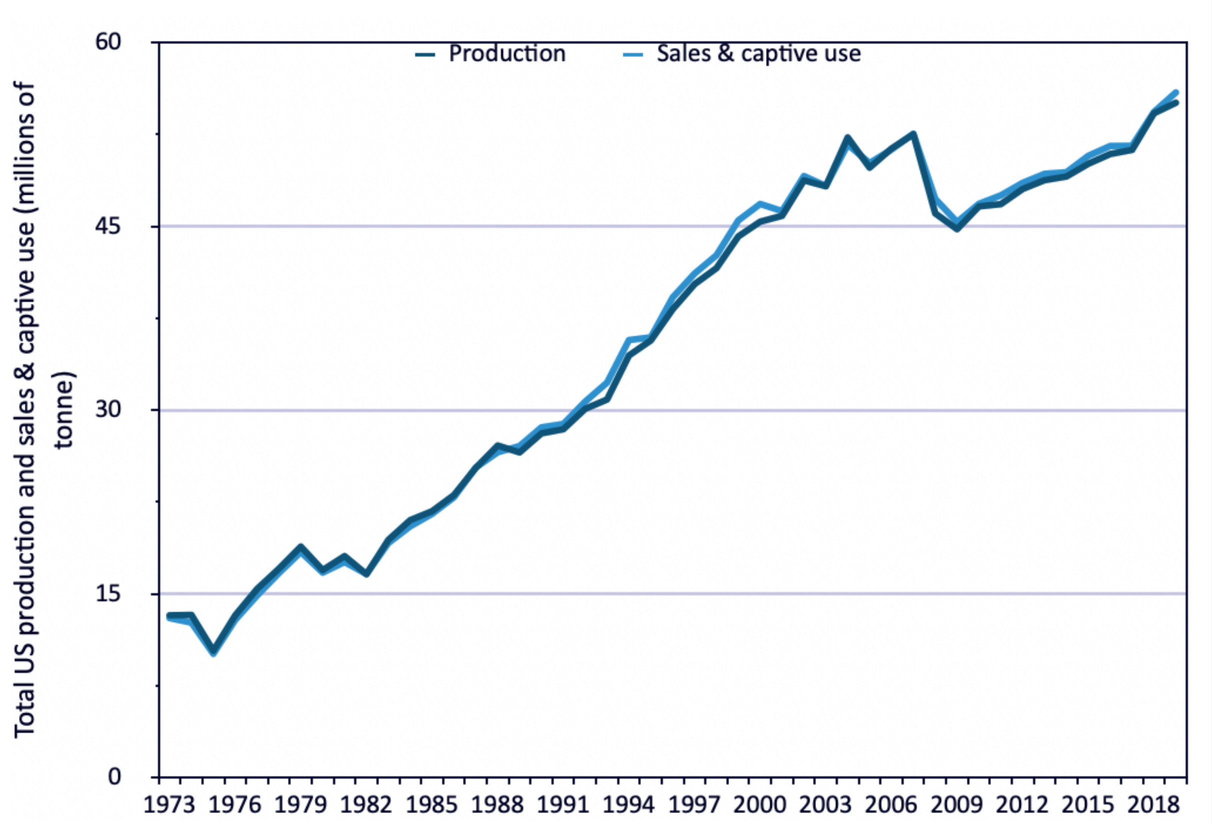

Figure B-1: US Plastic resins: total production and sales and captive use during 1973-2019[55]

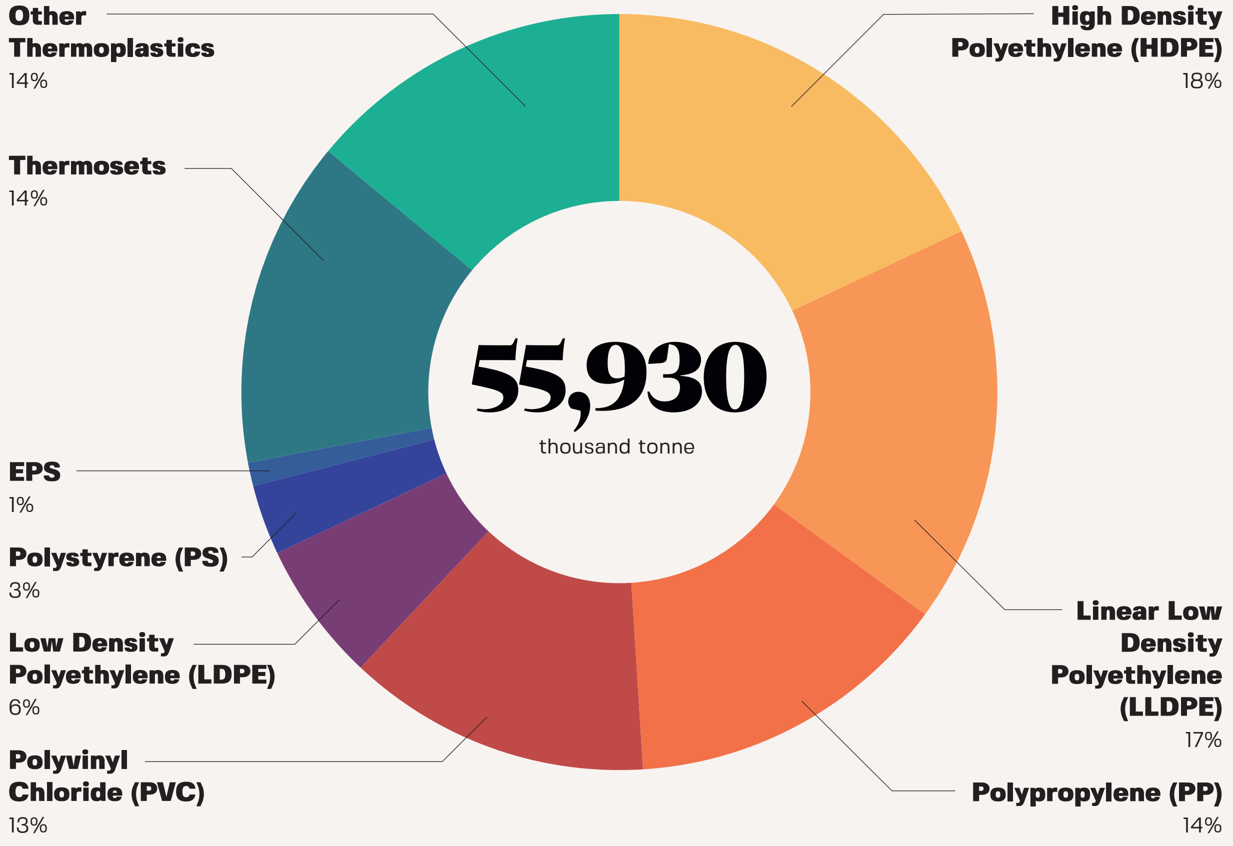

Figure B-2: 2019 percentage distribution of plastic resins sales and captive use by material in US

Petrochemicals Europe

petrochemistry.eu

Petrochemicals Europe is an industry sector of CEFIC, the European Chemical Industry council, representing about 29,000 large, medium and small chemical companies that account for nearly 17% of the world's chemical production. Petrochemicals Europe brings together companies manufacturing ethylene and propylene from steam cracking and/or other olefins, and/or aromatics for chemical use, and/or major first stage petrochemical derivatives (excluding polymers). These are the raw materials of the petrochemical industry, which turns them into products used in the manufacture of a wide range of consumer goods. The Petrochemicals Europe flowchart traces the main steps between raw materials and feedstocks through to building blocks, derivatives and everyday products (see Figure B-3). They also provide facts and figures and a review of the market situation for ethylene, propylene and benzene, as well as an analysis of the competitiveness of the European petrochemical industry [56,57]

Location	Operator	Capacity *Kt ethylene per year (2019)*
AUSTRIA		
Schwechat	OMV	500
BENELUX		
Antwerp	TOA	550
Antwerp	TOA	610
Antwerp	BASF	1,080
Geleen	Sabic Europe	1.31
Moerdijk	Shell	910
Terneuzen	Dow	565
Terneuzen	Dow	580
Terneuzen	Dow	680
CZECH REPUBLIC		
Litvinov	Unipetrol	544
FINLAND		
Porvoo	Borealis	400
FRANCE		
Berre (Aubette)	LyondellBasell	470
Dunkerque	Versalis	380
Feyzin	A.P. Feyzin	250
Gonfreville	Total	525
Lavera	Naphtachimie	740
NDG	ExxonMobil	425
GERMANY		
Boehlen	Dow	565
Burghausen	OMV	450
Gelsenkirchen	BP	1,073
Heide	Klesch	110
K-Worringen	Ineos Olefins	946
Ludwigshafen	BASF	220
Ludwigshafen	BASF	400
Munchmunster	LyondellBasell	400
Wesseling	LyondellBasell	305
Wesseling	LyondellBasell	735
Wesseling	Shell	310
HUNGARY		
Tiszaújváros	MOL	380
Tiszaújváros	MOL	300
ITALY		
Brindisi	Versalis	440
Priolo	Versalis	530
Porto Marghera	Versalis	490
NORWAY		
Rafnes	Ineos Olefins	560
POLAND		
Plock	PKN Orlen	700
PORTUGAL		
Sines	Repsol	410
TURKEY		
Aliaga	Petkim	588
SLOVAKIA		
Bratislava	MOL	225
SPAIN		
Puertollano	Repsol	102
Tarragona	Repsol	702
Tarragona	Dow	675
SWEDEN		
Stenungsund	Borealis	625
UK		
Grangemouth	Ineos Olefins	700
Fife	ExxonMobil / Shell	770
Wilton	Sabic UK	786
TOTAL		23,468

Table B-6: Cracker capacity in Europe [56]

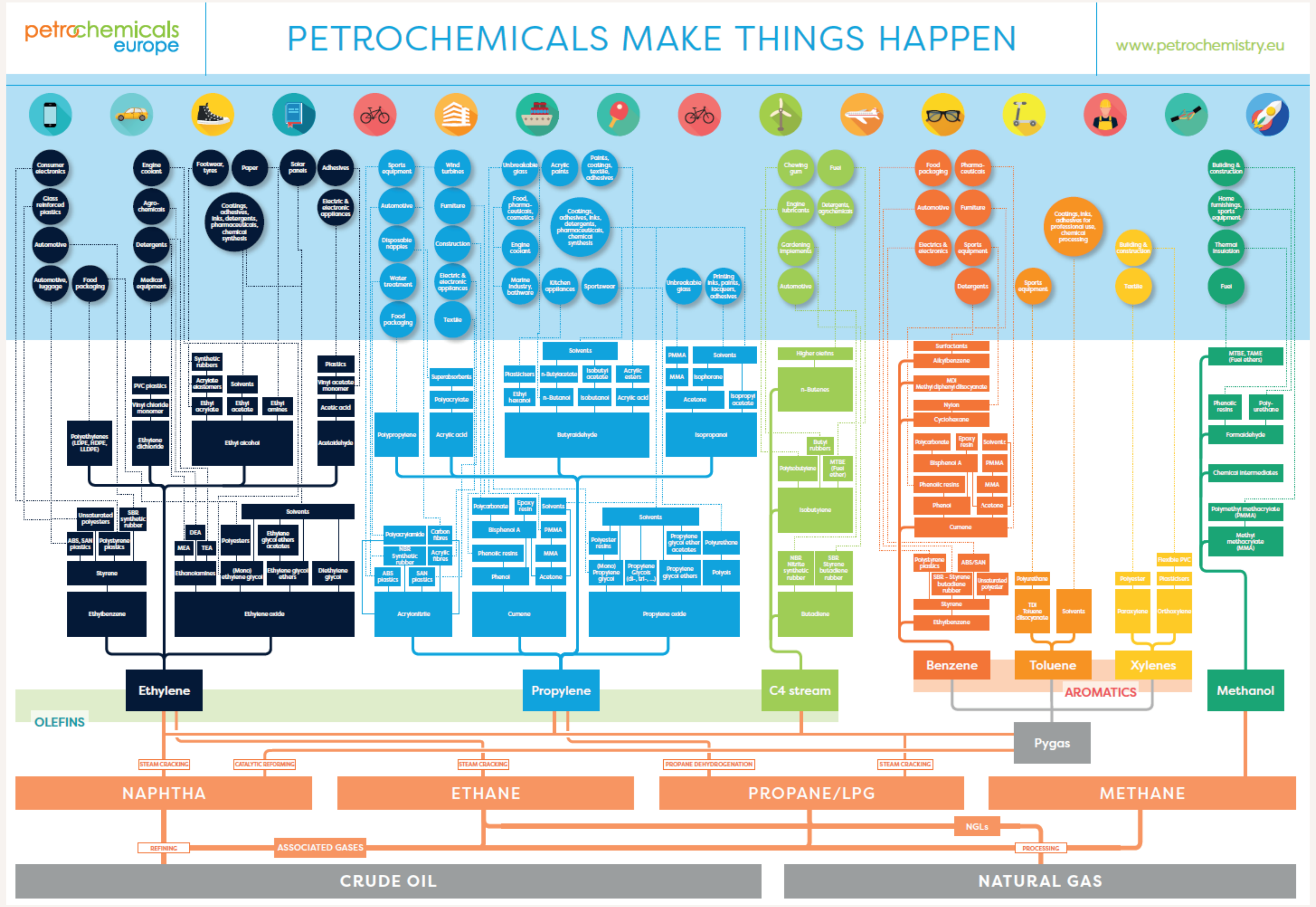

Figure B-3: Flowchart for a general view of the uses and benefits of the petrochemical industry [56]

The Fiber Year GmbH

The Fiber Year GmbH[58] was founded end of 2010 to provide international expertise, analyses, strategy consulting and customized solutions to the international textile industry. The Fiber Year report provides statistics in upstream feedstock industry, staple fibres, yarns, other manmade fibres, and the associated supply and demand data on the global and country level.

Valpak

Valpak [59] holds a detailed dataset on all types of packaging for the UK, which includes resolution on the type of packaging, its purpose, the polymer composition, sector and mass. The dataset covers four sectors (i.e. Grocery/DIY/Clothing/Wholesale) across three different years (i.e. 2015/2017/2019). They can be used to explore alternatives to current packaging to facilitate plastics recycling and emissions savings.

Japan Plastics Industry Federation (JPIF)

The Japan Plastics Industry Federation (JPIF) [60] is an organization representing the Japanese plastics industry engages actively in various aspects including raw material resins, moulding/fabrication and management of used products both at home and abroad. JPIF pursues the overall advance and development of the plastics industry, to promote the common interests in the business of the member companies and to contribute to the development of the Japanese industry. Specifically, JPIF carries out the following major activities, while addressing domestic and international changes in the business environment surrounding the plastics industry:

- Statistics compilation, investigation, and information collection and provision
- International information exchanges and public relations
- Activities relating to environment preservation and safety
- Activities relating to the Containers and Packaging Recycling Law and the Effective Resources Utilization Promotion Law
- Activities relating to domestic ISO examinations and work as a leading ISO country
- Activities relating to safety of electrical appliances

Two JPIF Groups, namely, the Administration/Environment and Standards Groups, are responsible for the above activities. For example, the collection and analysis of statistical information on the plastics industry includes:

- Monthly and yearly statistics of plastics material production (Table B-7 for example), sales and inventory (provisional and final).
- Monthly and yearly indexes of wholesale trade on plastics materials products and related chemicals.
- Monthly and yearly statistics of import/export of plastics materials and products.

Commodity		Total (unit: tonne)
Phenol-formaldehyde resins	*Sub Total*	258,409
	Molding materials	22,505
	Laminates	12,524
	For lumber manufacturing adhesives	127,706
	For others	95,674
Urea-formaldehyde resins		49,251
Melamine-formaldehyde resins	*Sub Total*	65,326
	For decorative laminating	1,978
	For coating	17,365
	For adhesives	35,319
	For others	10,664
Unsaturated polyester resins	*Sub Total*	107,734
	For fiber glass reinforced plastics	69,553
	For others	38,181
Alkyd resins		56,668
Epoxy resins		107,728
Polyurethane foam	*Sub Total*	174,916
	Flexible foam	113,377
	Rigid foam	61,539
Thermosetting Resin (Total)		820,032
Polyethylene	*Sub Total*	2,246,009
	Low-density	1,330,831
	Hight-density	738,545
	Ethylene-vinyl acetate copolymers	176,633
Polystyrene	*Sub Total*	723,848
	Molding materials	616,297
	Foamed polystyrene	107,551
Styrene-acrylonitrile		54,164
Acrylonitrile-butadiene-styrene		279,204
Polypropylene		2,246,815
Petroleum resins		105,887
Methacrylic resins	*Sub Total*	129,345
	Molding materials	81,481
	For others	47,864
Polyvinyl alcohol		177,940
Polyvinyl chloride	*Sub Total*	1,626,549
	Polymer	1,412,783
	Copolymer	83,052
	Paste resin	130,714
Polyamide resins		178,549
Fluorocarbon resins		25,066
Polycarbonate		269,660
Polyacetal resins		89,683
Polyethylene terephthalate	*Sub Total*	342,495
	For bottle	-
	For others	-
Polybutyene terephtalate		96,836
Polyphenylene Sulfide		34,055
Thermoplastic resin (Total)		8,626,105
Other resins		193,082
Grand total		9,639,219

Table B-7: Annual production of Plastics Materials in Japan in 2020

Supply chain approaches

No.	Study	Publication year	Life cycle stages	Geographic region	Petrochemical products (plastics, fertiliser, etc)	Year	Uncertainty
a	Wang et al, 2021	2021					Normal distributions of the lifespan of plastics products
b	Pete Levi, 2018	2018	Feedstock, production, Manufacturing	Global	Petrochemicals, plastics, fertilisers,	2013	Take four steps to mitigate the impacts of uncertainty in the source data
c	Heller et al., 2020	2020	Production, Manufacturing, use, waste management and trade	US	LDPE, LLDPE,HDPE, PP, PS, EPS, PVC, PET, polyester fiber, ABS, polycarbonates, other thermoplastics, and styrene butadiene rubber	2017	Not found
d	Eriksen et al, 2020	2020	Production, manufacturing, use and source-separation, wastemanagement, recycled material	Europe	Plastics (PET, PE, PP)	2016-2066	The major sources of uncertainties are related to the model: (1) data on how the waste management system handles individual product flows were often scarce and based on data for individual countries rather than Europe, (2) limited data quality for nonpackaging products, and (3) uncertainties related to quantification of the consequences from quality reductions, such as cascading pathways and maximum recycled content ultimately affecting the potential for market saturation.
e	Hsu et al, 2021	2021	Production, Manufacturing, Use, waste management	EU28	Plastics (PET, PE, PVC, PP, PS, other thermoplastics, thermosets, man-made fibres)	2016	Quantitative uncertainties within different sensitivity levels for different indicators (Laner et al., 2015).
f	Di et al, 2021	2021	Production, fabrication, manufacturing, use, collection and sorting, processing and recycling, Post-consumer resin, industrial waste	US	Plastics (PE, PP, PET, PS, PVC, others)	2015	Considering an uncertainty of ±10% for all production stages until flow into use, and an uncertainty of ±25% for all end of life stages, it is possible to generate a matrix containing limit values for each of the plastic types at each of the relevant stages of the cycle
g	Jiang et al, 2020	2020	Production, Manufacturing, Use, Recycling	China	Plastics (PE, PP, ABS, PS, PVC)	1978-2017	Uncertainties in the dynamic-MFA mainly originated from the following six sources: the input of primary plastic in the production stage; the product split ratios in the manufacturing stage; the sector split ratios of the top-down method and the input of the bottom-up method in the use stage; the relevant coefficients and assumptions in the recycling and waste management stage; and the parameters of the lifetime distribution function. They calculate the variance in the final results in the cases of ± 10% change in each coefficient and data input. Sensitivity analysis of all variables is conducted.
h	Liang et al, 2021	2021	Waste trade and management	Asia	Plastics	2016, 2017,2018	Not found
i	Bureecam et al, 2018	2018	Production, use, collection and transportation, recycling	Thailand	Plastics	2013	Not found
j	Olatayo et al, 2021	2021	Production, use, trade, waste management	South Africa	Plastics	2017	A qualitative estimation of the uncertainty of the flow model

k	Liu Y., 2020	2020	Production, manufacturing, use, waste treatment	China	PVC	1980-2050	Not found
l	Van Eygen E, 2018	2018	use, end of life	Austria	Plastic packaging	2013	The estimated input uncertainties are subsequently propagated through the model using Gaussian error propagation (assuming normally distributed variables)
m	Kawecki D, 2018	2018	Production, manufacturing, use, waste treatment	Europe	plastic	2014	The distribution spread for a specific parameter is determined via a semi-quantitative approach
n	Singkran N., 2018	2018	Production, manufacturing	Bangkok Metropolis, Thailand	Plastic	2014	Not found
o	Ciacci L, 2017	2017	Production, Manufacturing, use, waste management	EU-27	PVC	1960-2012	Uncertainty range is set at ±15% for each end-use sector and the model was run 10,000 times
p	Van Eygen E, 2017	2017	Production, Manufacturing, use, waste management	Austria	Plastic	2010	There are two sources of uncertainty for a certain plas-tics flow: first, the mass flow itself, and second, the plastics content. Quantitative uncertainties expressed as coefficients of variation for the data quality indicators
q	Laner D, 2016	2016	use, waste management	Austria	Plastic	2010	Probability distributions (normal vs. log-normal) are examined
r	Nandy B, 2015	2015	Production, Manufacturing, use, waste management	India	Plastic waste	2012	Not found
s	Tukker A, 1997	1997		Sweden	PVC	1994	Guessed uncertainty
t	Duchin F., 1998	1998	use, waste management	US	Plastic	1987	Not found
u	Patel M K, 1998	1998	Production, manufacturing, use, waste treatment	Germany	Plastic	1994	Empirical analysis
v	Joosten L A J, 2000	2000	Production, manufacturing, use, waste treatment	Netherlands	Plastic	1990	Not found
w	Mutha N H, 2006	2006	Production, manufacturing, use, waste treatment	India	Plastic	2000/2001	Assumption of large uncertainty. Sensitivity analysis is carried out
x	Bogucka R, 2008	2008	Production, manufacturing, use, waste treatment	Austria and Poland	Plastic	1994/2004	Not found
y	Nakamura S, 2009	2009	Production, Manufacturing,	Japan	PVC	2000	Not found
z	Kuczenski B, 2010	2010		US	PET	1996-2007	Not found
aa	Zhou Y, 2013	2013	use	China	PVC	1957-2008	Not found
ab	Rochat D.,2013	2013	use and waste	Tunja, Colombia	PET	2003	Not found
ac	Lee J, 2014	2014	Production, Manufacturing, use, waste management and trade	EU-27+ Norway+ Switzerland	General plastics, DEHP, DBP and BBP	2012	Using lognormal distributions for phthalate concentrations in food and normal distributions for physiological parameters. The Monte Carlo model was set up to run 10,000 trial
ad	Lee J, 2014	2014	Production, Manufacturing, use, waste management and trade	EU-27+ Norway+ Switzerland	DEHP, DBP and BBP, Plastics	2012	Not found
ae	Lee S., 2015	2015	Production, Manufacturing, use, waste management	Korea	PBDEs	2011	Not found
af	Sevigné-Itoiz E, 2015	2015	Production, Manufacturing, use, waste management	Spain	General plastics	1999-2011	Not found
ag	Van Eygen E, 2015	2015	use, waste management	Austria		2010	Same as “A novel approach for characterizing data uncertainty in MFA and its application to plastics flows in Austria”

Table B-8: Peer-reviewed studies on petrochemical mass flows reviewed in this study

Appendix C

List of acronyms

Acronym	Definition
ACC	American Chemistry Council
BTX	Benzene, toluene and xylene
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilization
CDIAC	Carbon Dioxide Information Analysis Center
CEFIC	European Chemical Industry Council
CEH	Chemical Economics Handbook
CRF	Common Reporting Format
DOE	Department of Energy
ECHA	European Chemicals Agency
EDGAR	Emissions Database for Global Atmospheric Research
EEA	European Environment Agency
EIT	Economy in transition
ELCD	European Life Cycle Database
EOL	End of Life
EPD	Environmental Product Declaration
ESS	European Statistical System
EUROSTAT	Statistical Office of the European Communities
FAO	Food and Agriculture Association
GEIA	Global Emissions Inventories on NMVOC Compound Groups, Ammonia (NH_3)
GHG	Greenhouse Gas
HDPE	High-density polyethylene
HVC	High-value chemical
HYDE	History Database on the Global Environment
IEA	International Energy Agency
IFA	International Fertilisers Association
IOGP	International Association of Oil and Gas Producers
IPCC	Intergovernmental Panel on Climate Change
LCI	Life Cycle Inventory
LDC	Least-developed country
LDPE	Low-density polyethylene
LPG	Liquefied petroleum gas
MFA	Material flow analysis
NEAT model	Non-energy accounting tables model
OECD	Organisation for Economic Co-operation and Development
PBL	Netherlands Environmental Assessment Agency
PEP	Process Economics Program
PET	Polyethylene terephthalate
PP	Polypropylene
PS	Polystyrene
PUR	Polyurethane
PVC	Polyvinyl chloride
TRL	Technology Readiness Level
UNEP	United Nations Environment Programme
UNFCCC	United Nations Framework Convention on Climate Change
USEPA	United States Environmental Protection Agency
WHO	World Health Organisation
WRI	World Resources Initiative

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