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ON ENERGY AND MATERIAL TRANSITIONS: HEAVY INDUSTRY PATHWAYS IN A WELL-BELOW 2ºC WORLD

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SOBRE TRANSIÇÕES ENERGÉTICAS E MATERIAIS: TRAJETÓRIAS PARA A INDÚSTRIA PESADA EM UM MUNDO BEM ABAIXO DOS 2ºC

Marianne Zanon Zotin

Outubro/2024

Orientadores: Alexandre Salem Szklo
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Programa: Planejamento Energético

Esta tese examina o papel das indústrias pesadas em cenários alinhados às metas climáticas de aquecimento abaixo de 2°C, com foco nas interações entre materiais, energia e emissões de gases de efeito estufa nas transições energéticas. Combinando uma revisão histórica e modelagem prospectiva de cenários, aborda três questões-chave: (i) a interação histórica entre transições de materiais e energia, (ii) as contribuições do setor industrial para mitigar mudanças climáticas, e (iii) as limitações e oportunidades na substituição de matérias-primas químicas. Usando o modelo COmputable Framework For Energy and the Environment (COFFEE), um modelo de avaliação integrada de programação linear, as últimas duas questões exploram caminhos para a descarbonização de cimento, aço e produtos químicos primários em 18 regiões globais de 2010 a 2100. Os resultados mostram que, embora as indústrias pesadas sejam rotuladas como “hard-to-abate”, elas têm potencial significativo de mitigação em subsetores e regiões específicas. No subsetor químico, o potencial inclui tanto a remoção direta de carbono quanto a mitigação sistêmica indireta, reduzindo o uso de refinarias de petróleo. Contudo, esses resultados dependem da disponibilidade de biomassa primária e da rápida expansão de tecnologias de captura e armazenamento de carbono (CCS), o que pode levar à persistência de emissões residuais industriais, mesmo após a meta de emissões líquidas zero ser atingida globalmente.

Abstract of Thesis presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Doctor of Science (D.Sc.)

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This thesis examines the role of heavy industries in achieving global climate targets under well-below 2°C scenarios, focusing on the interactions of materials, energy, and greenhouse gas emissions in energy transitions. By combining a historical review approach with prospective scenario modelling, this thesis addresses three key research questions aiming to understand: (i) the historical interplay between material and energy transitions, (ii) the contributions of the industrial sector to climate change mitigation, and (iii) the limitations and opportunities associated with feedstock substitution of primary chemicals. Using the COmputable Framework For Energy and the Environment (COFFEE) model, a perfect-foresight linear programming integrated assessment model, the latter two research questions explore pathways for cement, steel, and primary chemicals decarbonization across 18 global regions from 2010 to 2100. Findings show that, while heavy industries are often labelled as "hard-to-abate", they present significant mitigation potential in specific subsectors and regions. For the chemicals subsector, this potential is found to have both direct carbon removal potential and indirect systemic mitigation through reduced petroleum refinery utilization factor, contributing to oil phase-out. However, these findings were highly dependent on primary biomass availability and the rapid scale-up of carbon capture and storage (CCS) technologies, leading to the persistence of industrial residual emissions after net-zero emissions is achieved globally.

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List of Acronyms

°C – degree Celsius

ACM – Alternative Cementitious Materials

AFOLU – Agriculture, Forestry, and Other Land Use

AR6 – Sixth Assessment Report

BAT – Best Available Technology

BCCS – Bio-based Industrial Carbon Capture and Storage

BECCS – Bioenergy with Carbon Capture and Storage

BDH - Bioethanol Dehydration

BGS - Biomass Gasification

BF – Blast Furnace

BOF – Blast Oxygen Furnace

BTX – Benzene, Toluene, and Xylenes

CAT - Catadiene®

CCS – Carbon Capture and Storage

CCU – Carbon Capture and Utilization

CCUS – Carbon Capture, Utilization and Storage

CDH - Carbon Dioxide Hydrogenation

CDR – Carbon Dioxide Removal

CGS - Coal Gasification

CR - Catalytic Reforming

COFFEE – COmputable Framework For Energy and the Environment model

COP28 – 2023 United Nations Climate Change Conference

COTC – Crude Oil-to-Chemicals

DAC – Direct Air Capture

DIM – Dimerization

DRI – Direct Reduced Iron

E/P – Ethylene/Propylene ratio

EAF – Electric Arc Furnace

EJ – Exajoule

EROI – Energy Return on Investment

ETB – Ethanol-to-Butadiene

EV – Electric Vehicle

FCC – Fluidized Catalytic Cracking

FCCS – Fossil Industrial Carbon Capture and Storage

FT-BtL – Fischer-Tropsch Biomass-to-Liquids

GDP – Gross Domestic Product

GHG – Greenhouse Gas

GST – Global Stocktake

HB – Haber Bosch synthesis

HDRI – Hydrogen Direct Reduced Iron

HHV – Higher Heating Value

HM – Hot Metal

HTH – High-Temperature Heat

IAM – Integrated Assessment Model

ICE – Internal Combustion Engine

ICT – Information and Communication Technology

IMO – International Maritime Organization

IMP – Illustrative Mitigation Pathways

IPCC – Intergovernmental Panel on Climate Change

ISBL – Inside Battery Limits

LCA – Life Cycle Assessment

LHV – Lower Heating Value

LPG – Liquified Petroleum Gas

MeOH – Methanol

MNET – Material Negative Emissions Technology

MTA – Methanol-to-Aromatics

MTO – Methanol-to-Olefins

MTT – Metathesis

NCC – Naphtha Catalytic Cracking

NG – Natural Gas

NPi – National Policies Implemented

OHF – Open Hearth Furnace

OSBL – Outside Battery Limits

PDH – Propane Dehydrogenation

PET – Polyethylene Terephthalate

PGM – Platinum Group Metals

POX – Partial Oil Oxidation

PV – Photovoltaic

REE – Rare Earth Elements

SAF – Sustainable Aviation Fuel

SMR – Steam Methane Reforming

SR – Smelting Reduction

SR1.5 – Special Report on Global Warming of 1.5 °C

SSP – Shared Socioeconomic Pathway

1 INTRODUCTION

Human-induced greenhouse gas (GHG) emissions have reached 59.1 GtCO2e.yr-1 in 2019, causing CO2 concentration levels to rise to 410 ppm and the global surface temperature to increase 1.1°C above pre-industrial levels [1]. To avoid irreversible and extreme climate impacts, limiting the global average temperature well-below 2°C climate threshold is considered unavoidable. Given the proportionality between cumulative GHG emissions and global mean temperature [2], it is imperative to peak cumulative emissions within the next few decades and reduce annual global emissions towards net-zero [3].

After being first mentioned in the Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report (AR5) [4] in 2013 and highlighted in the Paris Agreement by 2015, the concept of net-zero gained momentum with the IPCC Special Report on Global Warming of 1.5 °C (SR1.5) [5]. Since then, net-zero commitments have rapidly increased, with governments, companies, and organizations worldwide adopting, announcing, and considering net-zero pledges [6].

The concept of net-zero emissions refers to ʻa balance between anthropogenic emissions by sources and removals by sinks of greenhouse gases in the second half of this century ʻ [6], [7], and can refer to both net CO_2 emissions and GHG emissions, expected to be reached around 2050 and 2060, respectively[1]. This feeds an expectation that while some sectors have more straightforward decarbonization, others might be "hard-to-abate", leading to residual emissions after mid-century that need to be compensated by carbon dioxide removal technologies (CDR) [8]. Along with some non-CO_2, aviation, and shipping, the industry is one of the sectors that are expected to contribute to the residual emissions side of the balance rather than becoming mitigation or sinks, even with major transformations on the energy-side [9], [10].

1.1 Challenges of decarbonising heavy industries

The industrial sector is currently responsible for 24% and 34% of global direct and indirect emissions [11], respectively, and 37% of global energy use [12]. Non-metallic minerals, iron and steel, chemicals, paper and pulp, and non-ferrous metals are industrial subsectors, also referred to as heavy industries, are often mentioned as being hard-to-abate.

Various technical and economic challenges exist for decarbonising heavy industries. On the technical side, operating temperatures ranging between 900-1600°C are often required by industrial kilns, furnaces, and crackers. While heat requirements of up to 300°C can be met through electrification to reduce emissions, electrification of high-temperature heat is not technically nor economically feasible yet [13], although electrothermal heating could be a possibility in the future [14]. Moreover, many industrial processes generate GHG emissions as a result of chemical reactions other than combustion, such as those from CO_2 released in limestone calcination [15]. These so-called 'process emissions' are not mitigated with renewable energy sources as they are inherent to the production process chemistry. Furthermore, fossil hydrocarbons are also used as feedstock for the production of materials including plastics, fertilizers, and asphalt. The demand for such materials is thus deeply interdependent on fossil fuel production [16]. Our current energy system thus significantly locks-in the material basis of modern societies.

Energy-intensive industries also require significant upfront investments in machinery, infrastructure, and technology, with long payback periods. They often face a slow rate of capital stock turnover [17] due to the long lifespans of existing infrastructure, which poses financial barriers to adopting low-carbon alternatives, particularly in volatile or low-margin markets. This inertia further limits the deployment rate at which new, lower-emission technologies can be adopted. The costs associated with reducing emissions also tend to be higher compared to other sectors due to the energy-intensive nature of these processes [18]. These sectors operate within highly competitive international commodity markets, where cost considerations and trade dynamics often discourage unilateral decarbonization efforts [19]. Companies may be reluctant to invest in costly emission-reducing technologies if competitors do not face similar regulatory pressures.

Previous studies on scenario-based industrial decarbonization pathways conducted with Integrated Assessment Models (IAMs) have analysed the role of industrial sectors in achieving global climate change mitigation targets. IAMs are tools extensively used to support climate policy, designed to capture complex biophysical and systems interactions, synergies, and trade-offs of climate, energy, and land-use policies. When assessing pathways to net-zero in IAMs, anthropogenic emissions and removals are assessed in a single framework. In this context, model choices are typically based on cost optimization, which plays a critical role in determining technological pathways. This integration of cost considerations ensures that the selected pathways are economically viable and effective in achieving net-zero targets.

Significant improvements have taken place since the model intercomparison conducted by Edelenbosch et al. (2017) [20], who found limited resolution of industrial subsectors in global IAMs. IAMs have been used to assess the cement [21], [22], [23], steel [21], [23], [24], chemicals [25], including plastics [26] and other non-energy products [27]. There is a recent focus on exploring price feedback in industrial demand [28] and endogenous representation of material use in buildings, vehicles, appliances, and electricity generation [29], [30], [31], [32], [33], considering their stock-flow dynamics [32], [34], [35].

Yet, limitations remain to be addressed regarding the supply-side of materials in IAMs. For instance, linking refinery activity to petrochemical feedstock supply in the chemicals sector is critical to analyse fossil fuels phase out in detail, a consistency that none of the global IAMs has yet attained, as shown by [36]. Moreover, exploring the role of industrial pathways in different temperature ambitions has not been assessed considering key material-energy interlinkages.

1.2 Objectives of the thesis

Given the abovementioned literature gaps, the main research question of this thesis is: *How does the production of materials, specifically within the heavy industry, contributes to global decarbonization pathways to achieve net-zero targets?* Given the breadth and depth of the main research question's scope, it is divided into three research sub-questions:

RQ1: *How do material transitions influence and are influenced by energy transitions?*

To answer this question, a combination of historical review and interdisciplinary synthesis was used, aiming at understanding the intricate relationship between energy and materials transitions throughout history and their implications for the current transition to low-carbon technologies. Understanding these historical material-energy linkages is critical for planning emerging energy systems, particularly as we move towards a low-carbon economy. This study provided a framework to support the subsequent industry modelling work based on an integrated assessment approach, and it laid the foundations for defining a priority of materials to model and dynamics to represent.

Given our interest in the relationship between materials and climate change mitigation, priority was given to materials that:

1. Are produced on large-scale and relevant to global emissions, as these materials typically have more data available for representation on a global scale with regional detail. Additionally, as a global integrated assessment model (IAM), our focus is on understanding global mitigation pathways towards net-zero. Therefore, we prioritized adding detail to sectors already included in the model but lacking sufficient granularity to respond to simulated climate policy;

2. Generate process emissions during production, given it is a key challenge for reducing emissions towards zero and, therefore, a reason to justify residual emissions.

3. Use fossil fuels for non-energy purposes, as it allows addressing the multiple uses of fossil fuels beyond energy, highlighting a critical connection between energy and material systems currently lacking in IAMs.

Based on these criteria, the cement, iron and steel, and chemical sectors were chosen for detailed representation and further analyses, which are described in the next two RQs.

RQ2: *What is the contribution of the global industrial sector to climate change mitigation in well below 2°C scenarios?*

To address this question, the COmputable Framework For Energy and the Environment model (COFFEE), a linear programming optimization model based on the MESSAGE framework, was used. COFFEE is a global IAM and presents 18 regions with explicit representation of land and energy systems. With this work, the representation of the industrial sector in COFFEE was improved to understand how mitigation choices made in industrial subsectors vary in response to different carbon budgets representing different temperature ambitions. When addressing this RQ, we found an overlooked potential for the chemical sector to achieve not only net-zero targets but also reach net-negative emissions. This required a more targeted analysis, focusing on the chemicals sector, to be addressed by the next research question.

RQ3: W*hat are the impacts and limits of feedstock substitution in the chemicals sector to mitigate GHG emissions and phase-out fossil fuels?*

Transitioning from an (organic) fossil-based system to an electric (metal-based, inorganic) system requires scaling up low-carbon technologies and understanding the challenges of fossil fuels phase-out. This includes replacing carbon-based products derived from petroleum and coal beyond fuels, e,g., plastics, nitrogen fertilizers, and other organic chemicals. However, alternative carbon-based feedstocks such as biomass or captured CO_2 (i.e., Carbon Capture and Utilisation or CCU) are also extensively considered for other mitigation purposes. Failing to substitute carbon-based materials can lead refineries to remain operating, hence cheaply co-producing fuel products and undermining fossil fuels phase-out in energy systems. An integrated perspective is called for, given the complex interactions that take place in this problem, including: (i) the competition for resources (e.g., land-use for food, bioenergy, and biomaterials); (ii) the increasing long-term material demand and the need to reduce sectoral emissions; (iii) the reduction of long-term gasoline demand due to passenger vehicle electrification, which can generate a supply of fossil petrochemical naphtha; and (iv) the increasing petrochemical feedstock demand. Therefore, the COFFEE model was applied to run scenarios limiting alternative feedstock availability in the context of net-zero.

1.3 Thesis outline

The research sub-questions described above are explored individually in Chapters 2, 3, and 4, respectively. Chapter 2 is a book chapter published in the *Routledge Handbook of Energy Transitions* [37]. Chapter 3 is an article currently under review in the *Applied Energy Journal* under the manuscript number APEN-D-24-13067. Chapter 4 is an article published in *Nature Communications Journal* (DOI: 10.1038/s41467-024-52434-y). Chapter 5 presents a summary of the main findings and discusses the overarching conclusions of this thesis.

2 CRITICAL CONNECTIONS IN MATERIAL TRANSITIONS AND ENERGY TRANSITIONS

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Abstract

Energy transitions have always been associated with materials transitions, shaping and being shaped by the latter. Recent technological trends – renewable energy, vehicle electrification, digitalization – raise concerns about the scale and complexity of material use prospects. This chapter explores the connections between energy and materials transitions, focusing on three aspects. The first comprises fossil-based organic bulk materials, such as plastics and agrochemicals. Low-carbon energy transitions should address the substitution and/or lower use of such materials. The second refers to inorganic bulk materials, such as steel and cement, which provide the infrastructure to support low-carbon technologies. Primary metals will face declining ore grades by expanding production to lower quality mines, requiring ever-growing energy use. These materials extraction and processing have socioeconomic and environmental implications, including conflicts over the right to land, particularly in emerging economies. The third connection between energy and materials transitions refers to critical materials for the ongoing energy transition, which include: (i) minor metals, co- or by-products of a primary production; (ii) locally concentrated reserves and/or production/processing capacity; and/or (iii) specialty metals with low substitutability rate. Rare-earth metals, cobalt and indium, are examples of these materials for which the shortage of supply could slow down the deployment of clean energy technologies. This chapter shows that the ongoing energy transition needs to be accompanied by a simultaneous, sustainable materials transition on many levels.

2.1 Introduction

As non-linear, complex, far-reaching, and inherently uncertain processes, global energy transitions comprise a number of transformations inextricably linked to the diffusion of new prime movers – defined here as machines or devices that convert primary and/or secondary energy sources into energy services – and the structural change of global primary energy supply. Energy transitions in different scales may be driven by technoeconomic aspects, natural resources limitations and power relations in energy systems, among other influences. The implications of these processes echo in all other human systems [38].

Throughout history, energy transitions have been closely related to materials demand in quantitative and qualitative terms, determining the material foundations of societies. Likewise, advances in materials science and technology, as well as inexpensive availability of materials with desirable properties, have been necessary though not sufficient conditions for new energy systems to emerge, stabilize and expand. As a result, societal use has evolved from 13 elements known in the periodic table prior to 1750, to the material basis of the current global economy consisting of 80 stable chemical elements in a wide spectrum of natural and synthetic materials. Metal alloys, synthetic polymers, high-performance composites, fine chemicals, and ceramics have been invented, as well as their properties improved to meet material services demand.

While energy transition studies have substantially contributed to the understanding of how such processes unfold and shape (or are shaped by) economic development, technological innovation, and social change [39], [40], [41], socio-metabolic research has similarly provided a conceptual basis to understand society-nature interactions, offering valuable insights into how socioeconomic activity relates to biophysical flows and stocks use [42]. Furthermore, a fragmented literature on the role of biomaterials, materials efficiency strategies, circular economy, industry sector decarbonization, and critical materials in energy transitions has gained relevance in recent years [23], [35], [43], [44], [45], [46]. Nevertheless, how energy transitions shape materials transitions and vice-versa has not been well analysed in a systematic way.

Thus, the aim of this chapter is twofold: first, to present energy-materials interlinkages in past energy transitions (Section 2.2); and second, to discuss potential materials-related issues that may play a role in shaping the current energy transition and the material foundations of the 21st century (Section 2.3). Section 2.4 draws concluding remarks.

2.2 Materials-energy Linkages over Transitions

This section aims to highlight how the provision of material and energy services[1] have been intertwined through technical, socioeconomic, and environmental linkages throughout history. It is not our goal to fully cover materials use and technology history, nor the chronology of events that have led to profound shifts in energy production and consumption globally. Instead, the objective is to shed light on when and how energy and materials developments have been interdependent in such a way that when one shifted the other was also altered. While the historical trajectories of energy and materials consumption have been geographically and culturally diverse, we focus on how materials transitions shaped global energy transitions and vice-versa in the past. We aim to contribute to the debate on sustainability transitions by reviewing and analysing how materials can play the roles of constraints or opportunities in the ongoing energy transition to a low-carbon economy.

2.2.1 The Transition to Agrarian Societies

In the search for water, food, and firewood, hunter-gatherers were limited by the distances travelled, the productivity of the region, the inventiveness of the people and the efficiency of human metabolism to convert food into mechanical power [47]. Energy use (i.e., food intake and wood burning) in prehistoric times was therefore limited to physiological needs (energy and materials), movement, and human reproduction [48]. In turn, prehistoric innovations were driven by survival needs. Readily available natural materials, such as stones, bones, plant branches and vines, were used to tailor better tools

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[1] We build on the conceptualization adapted from Whiting et al. (2020) that defines material services as *those functions that materials contribute to personal or societal activity with the purpose of obtaining or facilitating desired end goals or states, regardless of whether or not a material flow or stock is supplied by the market*. The authors consider all energy flows (excl. non-material energy flows such as solar, wind and hydro) as materials; likewise, all energy services are also material services (e.g., illumination, transport). However, in our text, “materials” and “material services” will be used in reference to flows/stocks and their respective services only when they provide exclusively material functions (e.g., shelter, packaging) to emphasize how natural resources used for energy and non-energy purposes interacted in past transitions.

and weapons that ultimately delivered a necessary means for defence, for foraging and/or for hunting larger animals [49].

By the late palaeolithic, wooden vessels also facilitated transportation, expanding distance limits that constrained food access, and the deployment of animal hides was extensively used for resisting harsh winters and building tents. Small kilns or pits were also used in some regions to fire ceramics and shape them into tools for cooking and storage.

The increased availability of energy surpluses through the domestication of grains and animals around 10,000 B.C. in the Fertile Crescent region[2] provided the comparative advantages of sedentary societies over hunter-gatherers, raising population density on the order of a 100 times [50]. Establishing, maintaining and expanding towns required a significant quantity of energy to find and transport construction materials. From simple huts to sophisticated hydraulic systems, the supply of common natural materials, such as stones, wood, clay, limestone, and bamboo, required planning and basic empirical knowledge on materials properties. Thus, energy surpluses could be shifted to activities beyond the simple maintenance and reproduction of existing systems, increasing the complexity of human societies [51].

The use of metals depended on early energy developments. Leveraging mining and metallurgy fire-based techniques, such as fire-setting and smelting, was the necessary precondition to create access to metallic compounds and to shape them into useful objects [52]. In pre-modern agrarian societies, metals in limited availability were used when, as an alternative for or in combination with wood or stone, they presented a better cost-benefit ratio in materials services provision, such as shelter (nails), transport (horseshoes), production (tools in general) and security (weaponry) [53].

Even though the above events unfolded differently across the world, in Europe these advances had such a remarkable impact on materials culture that historical periods were named after materials. For some applications, stone could be replaced by copper (3200 – 2300 B.C.), whose malleability enabled humans to shape tools according to their needs.

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[2] This spans modern day Iraq, Syria, Lebanon, Jordan, Palestine, Israel, and parts of Turkey and Egypt.

Bronze, an alloy of copper and tin, replaced copper for the same reason (2300 – 700 B.C.): it had greater hardness, a lower melting point and greater resistance to corrosion. Iron, despite its higher melting point, was more abundant than copper and tin. Triggered mainly by tin production shortages, iron replaced bronze (1200 – 300 B.C.), although it would only be a better performing material when further processed to steel alloys, centuries later [54]. Naturally, previous knowledge of ceramic kilns and high-temperature heat was the pillar of early metallurgy, driving the former two materials transitions with performance opportunities. The latter materials transition, on the other hand, was driven by lack of materials availability due to trade disruptions.

Among the inorganic and more commonly used natural materials, stone use was generally oriented to durable infrastructure and ceramic bricks eventually came into use for construction where clay was easily found and fired. The Romans developed the *opus caementicium*, a concrete-like material resultant of mixing rock or ceramic tiles as aggregates with gypsium, quicklime or pozzolana as binders, rendering one of the most time-resistant construction materials.

2.2.2 Industrial Revolution and the Transition to Coal: Steel and Construction Materials

From ancient times to the XVIII century in Europe (and still today in several regions of the Global South), biomass was the main source for both materials and energy services provisioning. While metals have better mechanical and chemical properties (e.g., malleability, specific stiffness, corrosion resistance) than wood, their utilization was limited by mining productivity, smelting capacity, transportation distances and costs. Wood, on the other hand, was vastly used for buildings, vessels, furniture, and artisanal manufacturing, not to mention its energy uses for heating, lighting, and cooking. In other words, economic activities were constrained by energy resources (firewood and food), materials (timber, stone and clay for housing, transportation, and tools), energy converters (human and animal power), and innovation in traditional biomass energy systems [55].

In the slow transition to coal within Britain, a number of factors preceded Watt's engine in defining the turning point. The expansion of international trade for Great Britain with its colonies through the hegemony of the British merchant fleet, as well as the development of rural textiles manufacturing industries, gave rise to population growth and urbanization. London's population more than doubled from 1520 to 1550 [56]. The expanding trade also introduced news forms of knowledge. In addition, the price revolution (1560-1620) increased real wages, particularly high in Britain, leading to higher material well-being [57]. Taken together, the demand for energy and materials grew, pressing the renewability of the agrarian system.

If, on the one hand, deforestation meant more timber and wood production as well as more land available to feed the growing population, on the other, it implied the gradual reduction of forest stocks leading to wood transportation prohibiting costs [52]. Coal was considered of inferior quality due to the bad odour when combusted, but it offered greater availability and became cost competitive relative to depleting forest wood [40], given the lower costs of open pit mining and transportation via cabotage (sea coal). In addition, it had higher energy density and reduced the pressure on the land, as it was found underground [58]. The price advantage led to the early use of coal for thermal energy provision in glassworks, breweries, pottery, and ultimately metallurgy. As early as 1700, coal use was already over 48% of the total energy consumed in England and Wales [59].

The utilization of coke instead of charcoal in blast furnaces reduced the specific consumption of the reducing agent from around 20 m^3 of softwood/tonne of hot metal (t HM) in the XVIII century to around 1 m^3 of coking coal/t HM [60]. However, waterwheels remained operating blowers, hammers and rolling cylinders until James Watt's steam engine invention (1776) – which would be impossible without the use of iron cylinders.

Watt's steam engine was based on Newcomen's engine (1708) for water removal of the increasingly deeper coal mines. Therefore, coal mining provided not only a new source of energy but also set the stage for the development of the first prime mover to convert the chemical energy of coal into mechanical power; i.e., a device universally applicable in industry. The innovation initially driven by the repeated shortages of energy, materials and land not only relaxed the competition on wood for material and energy services but, mostly, led to unprecedented gains of productivity and cost reduction in transportation, metals and construction materials production [53].

Indirectly, coal use expansion also drove the reduction of wood demand in the construction sector by driving cost reductions of brick production since it provided cheaper high-temperature heat than charcoal. The use of coking coal enabled the construction of larger blast furnaces due to its greater mechanical strength compared to charcoal, reducing costs of iron products, machinery, and railroads. This reinforced the positive feedback on materials production and the further expansion of land and maritime transport prime movers and networks as well as urbanization. Later on, Portland cement (1824) and Bessemer steel (1856) processes were patented, enabling mass production of construction materials production to supply the rapidly growing demand in cities.

By removing the energy constraints set by the traditional organic system on one hand, and by creating demand to expand transportation and urban infrastructure on the other, the Industrial Revolution supported large scale and diversified delivery of materials services. The expansion of energy surpluses was the essence of the transition from organic to inorganic materials [61], including ferrous and non-ferrous metals, glass and bricks. These were, in turn, materials requirements for both producing and transporting raw materials and final products for a vast array of material and energy services.

2.2.3 The Transition to Oil: Automobiles, Polymers and Fertilizers

From its modern birth in the XIX century to the development of Henry Ford's model T by 1907, the emergent petroleum industry was mostly based on providing kerosene use as a cheap illuminating substitute to the whale oil and coal town gas, although a minor use also was evident as a lubricant to reduce friction in machinery parts, as asphalt and as other product [62]. As the coal-based energy system expanded to the rest of Europe and to North America, urbanization strengthened and cities widened, changing the urban transport regime [63]. The increased pressure on the horse-based transport system created favourable conditions to the diffusion of electric trams during the 1888-1914 period and, later, to the establishment of gasoline automobiles as a cheap and practical means of transportation.

The advent of petroleum-based liquid fuels overcame the shortcomings of steam engines to transform the land mobility landscape with internal combustion engines (ICE), smaller and with more power per volume or mass than the steam engine. Automobile's diffusion demanded increasing amounts of steel (used in the body structure and other parts) and concrete to expand roads and bridges networks. The emergent automobile industry both benefitted from and reinforced the existing oil-based infrastructure: not only gasoline, but also asphalt for road pavements and eventually synthetic rubber feedstock for tires production (in substitution for natural rubber) were inexpensively co-produced from oil refining and processing to fulfil the energy and materials requirements of the automobile industry.

The influence of warfare in energy technology innovation and in shaping energy and materials transitions cannot be overlooked. Though scientific and technological breakthroughs were achieved in the pre-World War I (WWI) period in the organic chemical industry, there was considerable uncertainty over the potential market for synthetic materials [64]. Major demand for such materials was created during the two world wars (mostly the WWII), which spurred further innovation and massive investments in the oil-based materials industry. Large-scale production of polyvinyl chloride (electrical insulation in wires), neoprene and other synthetic rubbers (tires, tubes, wear, and oil resistant applications), nylon (parachutes and hammocks), Teflon (proximity fuses and uranium isotopes separation) and polyethylene (insulator for radar cables) was driven not only by the opportunities to substitute metals whenever possible but also by their unique properties which yielded tremendous advantages in warfare (Ibid). After the war, organic chemical technology co-evolved with refining technologies, grasping opportunities for achieving economies of scope through diversification and verticalization.

Oil and gas also became central to fertilizer production in industrial scale, essential to feed the rapidly growing population in the XX century. The first ammonia plant in Oppau (Germany) in 1914, based on coal feedstock in the Haber-Bosch process, initially aimed at improving agricultural productivity until it was diverted to HNO_3 explosives and munitions production when the WWI broke out [65]. In general, the organic chemical industry back then – located mainly in Germany (IG Farben), France (Rhône-Poulenc), and the UK (ICI)

– was based on coal tars. After WWII, cheap availability of petroleum rapidly displaced coal as a chemical feedstock [66], and natural gas became the main source of hydrogen for ammonia synthesis. Hence, the improvement of average diets in growing populations after 1950 was enabled by large-scale ammonia production for fertilizer use, which in turn depended on the cheap feedstock co-production in refineries [47], [67].

Relative to the transition to coal, the transition to oil also represented an even more abundant energy surplus to support societal materials needs. The complexity achieved by modern industrial civilization is revealed in the material abundance and diversity that flooded global markets in the postwar period. New synthetic materials with a peerless combination of properties, such as chemical and thermal resistance, durability, strength, and low cost, underwent competition in several different markets providing a better combination of cost and performance than incumbent materials such as ivory, glass, tin, lead, steel, and many others. In the 1930s, global plastics production was around 50,000 t, reached 6 Mt in 1960 and 380 Mt in 2015, as a result of the expansion of oil production worldwide [53], [68]. The fast growth of plastics, fertilizers, lubricants, solvents, rubbers, fibres, dyes, waxes, surfactants, detergents, asphalt, and other organic fossil fuel-based materials production mainly after 1950 not only reveals the diversity of oil-based products and their pervasiveness in the global economy but also the extent to which the last energy transition radically transformed the materials culture worldwide.

The technology landscape of the post-war period also represented a shift from military to civil purposes. The reconstruction of the infrastructure destroyed by the war and supporting the growing middle class required intensive mining activity of widely known metals such as iron, aluminum, and copper. After the war, the demand for by-product (minor) metals – such as cobalt, titanium, vanadium, and many others –also increased as aviation, communications, rocketry, and nuclear power technologies were gradually introduced in modern civil society [69].

Thus, oil became a key feedstock in the XX century (so far, also in the XXI). The combining effects of expanding urban and agriculture frontiers and increasing the production of inorganic and organic materials led to human-made materials surpassing global living biomass in 2020 [70].

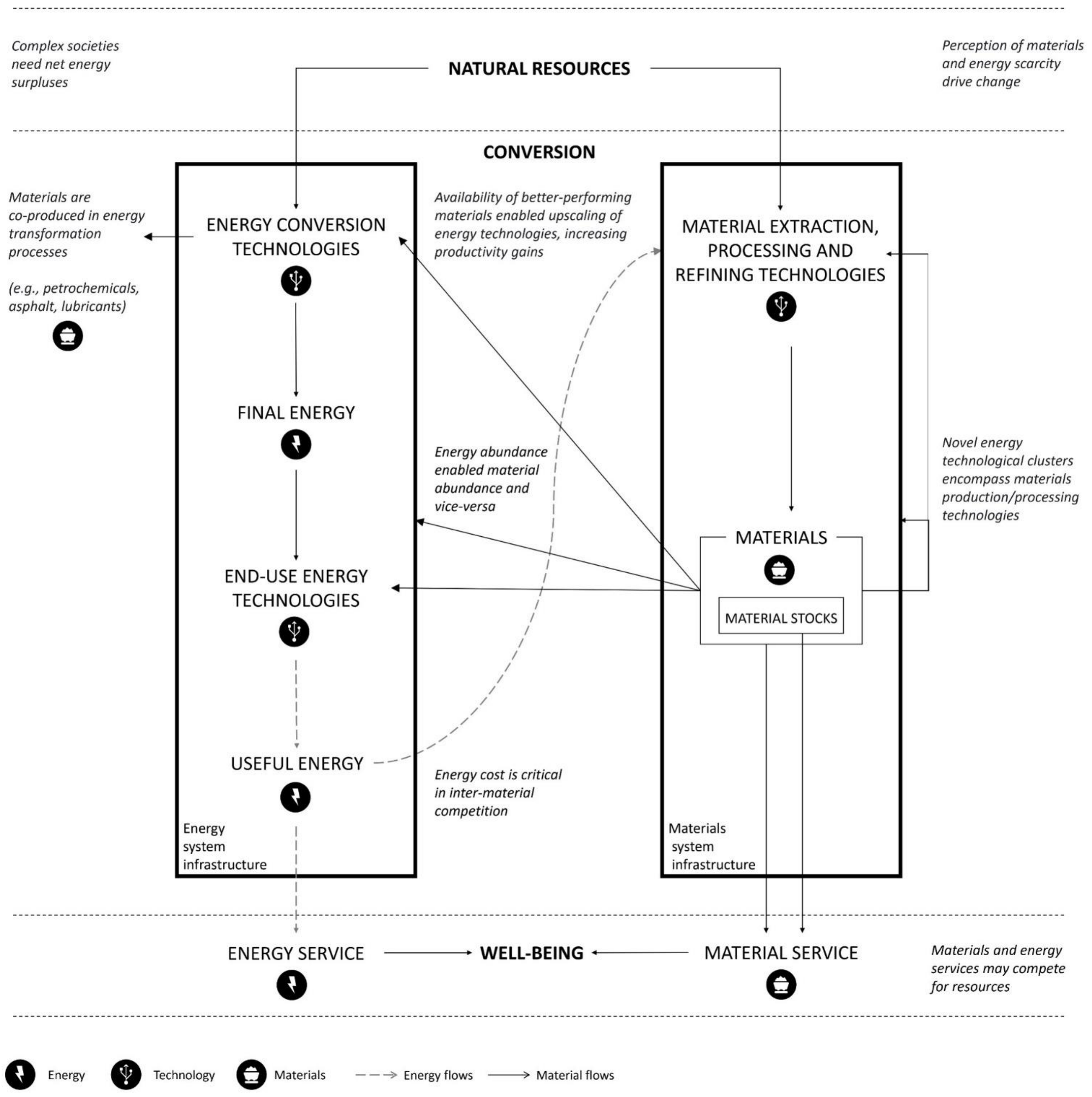

Figure 1. Main linkages between materials and energy sources/technologies.

2.3 Materials Opportunities and Constraints in the XXI Century Energy Transition

The conclusions drawn in the previous section add decisive questions for the unfolding energy transition. As greenhouse gas (GHG) emissions reduction targets become stricter every year due to insufficient climate action, an unprecedented and far-reaching global energy transition is urgently required so that all parties can meet their commitments under the Paris Agreement [5], [71]. In spite of the potential role of degrowth [72] or low energy demand scenarios [73], the required energy transition will entail expanding the diffusion of solar PV panels, wind turbines, and electric vehicles worldwide, as well as extensive transmission lines and industrial-scale carbon dioxide removal (CDR) strategies. This engineered energy transition [74], at unprecedented rates to deal with the climate emergency, has implications to materials use and production. Materials can act as constraints or opportunities to energy transition pathways. The following sub-sections summarize key issues underlying how different groups of materials may influence energy transition pathways.

2.3.1 Organic bulk materials

Organic bulk materials are those natural or synthetic materials (mostly made from petroleum, natural gas, and coal) containing covalently-bonded carbon and hydrogen – also oxygen, nitrogen, sulfur, chlorine, and other elements can be present – and produced in large quantities, usually associated with the coproduction of fuels. Fossil fuels can be used for combusted and non-combusted uses. In a typical refinery, some 75% of an oil barrel total volume is converted to gasoline, diesel, and jet fuel as its main products, and another 10% to other fuels. The remaining 15% is mostly petrochemical feedstock, non-combusted and cheaply co-produced with fuels, which feeds 90% of the modern chemical industry today [75]. They are subsequently transformed into primary chemicals, which are further processed into intermediates and, finally, converted to a vast array of final products among polymers, agrochemicals, and specialty chemicals in a complex supply chain.

Primary chemicals account for two-thirds of the energy demand in the chemical industry [75]. These are: ethylene, propylene, butadiene, and aromatics (benzene, toluene, and xylenes, or BTX) - also known as high-value chemicals (HVCs) -, methanol and ammonia. HVCs are the building blocks of plastics production. Ethylene and propylene are produced in larger volumes worldwide (around 165 Mt/yr and 120 Mt/yr, respectively) and are the key raw materials for thermoplastics production such as polyethylene and polypropylene, vastly used for a number of different applications from food packaging to electrical insulation [76]. Butadiene (around 10 Mt/yr) is critical to elastomers and synthetic rubbers production, essential in automotive tires. In turn, aromatics (~100 Mt/yr) are ring-structured molecules largely used for increasing fuel performance as a high-octane blend component but also as intermediates for polystyrene and polyethylene terephthalate (PET) production [77]. HVCs are conventionally produced in the steam cracking of (oil-based) naphtha or (natural gas-based) ethane, although there is a significant co-production of propylene and aromatics in the fluidized catalytic cracking and catalytic reforming units in refineries, respectively. Also, the last decade saw an increase in the dedicated development of propylene production capacity based on propane dehydrogenation in the Middle East and coal-to-olefins in China, as well as a green ethylene plant based on bioethanol dehydration in Brazil, although in a much smaller scale. This was distinct from traditional steam-cracking, multi-product facilities.

Ammonia (~170 Mt/yr) and methanol (~110 Mt/yr) production processes are based on the production of syngas, a mixture of hydrogen and carbon monoxide, through steam methane reforming, coal gasification (especially in China and South Africa) or partial oil oxidation [75]. Although ammonia is strictly an inorganic molecule, it requires large amounts of hydrocarbons to generate hydrogen, which further reacts with nitrogen. Around 80% of ammonia is consumed as nitrogen fertilizer (mostly in the form of urea and ammonium nitrate) [78], whereas methanol is used in a variety of energy (mostly as gasoline blending or substitute and in biodiesel production, but also in other forms) and non-energy (intermediate for formaldehyde, acetic acid, and silicone production, to name a few) applications. Although in ammonia-urea integrated facilities, CO_2 is captured and used within the process, in standalone ammonia facilities, process CO_2 emissions can increase from 2.1 to 4.6 tCO_2/t ammonia depending on the feedstock [79]. On the other hand, limited process emissions are generated in methanol production.

Hence, from high-performance engineering composites to grocery single-use plastic bags, these hydrocarbon-based raw materials constitute the core of synthetic materials production today. Therefore, the fates of the fossil fuel and fossil fuel-derived materials industries in the energy transition are thoroughly interdependent. An energy transition away from fossil fuels does not necessarily imply a materials transition that overthrows the non-energy use of petroleum, natural gas, and coal. Indeed, in the near- to medium-term, we shall expect an increasing refinery-petrochemical integration. As gasoline and diesel demands reduce due to passenger fleet electrification and carbon pricing, both refining capacity and cheap conventional feedstock free up for materials production. Intermediate streams from petroleum refineries are increasingly diverted towards petrochemicals production. For instance, [71] indicates that at a deep decarbonization scenario petroleum refinery throughput would reduce 85% in 2050 while its yield in petrochemicals would increase to 70%, almost leading to the survival of only refineries integrated to petrochemicals. Also, the increasing demand for low-carbon and energy-efficient technologies is already driving up the demand for lightweight, stiff, durable, fatigue resistant, and strong materials, such as polymer-based composites and carbon fibres [80]. The latter is at least four times lighter and its tensile strength three times higher than in steels [81]. This, coupled with the capital-intensive nature of chemical industries, make it very unlikely that a paradigm shift happens in the organic chemical technology and infrastructure anytime soon.

In the long-term, however, trends and uncertainties in the demand and supply sides may redefine the sector. From a demand side perspective, plastic marine pollution and microplastics contamination concerns are driving single-use plastics bans and changes in consumer profile towards circular economy, which might lead the industry to shift end-use markets [82]. At least 127 countries announced different laws and measures to limit single-use plastics use and manufacturing, though the COVID-19 pandemic delayed implementation [83]. Furthermore, the substitution of single-use non-degradable plastics for biodegradable alternatives has been considered but performance efficacy and potential for global scale substitution are yet to be proven.

In fact, large-scale plastic waste management methods must consider climate change mitigation, material efficiency, and circular economy principles. Mechanical recycling plays a role in reducing GHG emissions and the use of virgin raw materials by reconverting plastic waste back into valuable – though inevitably lower-grade - products. Chemical recycling, on the other hand, can be a game-changer in plastics demand if ever economically feasible, since it enables remanufacturing waste plastic to the original polymer with the same quality, other synthetic materials, or fuels, avoiding investment needs in new capacity. This material advantage comes with an energy penalty, however, due to heat requirements of pyrolysis and gasification processes as well as purification processes.

On the supply side, however, stringent climate targets can open opportunities to the chemical sector to develop and implement deep decarbonization measures Three general approaches arise to decarbonize the organic chemical industry. The first one consists of keeping up with oil, gas, and coal as raw materials but combining it with carbon capture and storage (CCS) to mitigate residual process and energy emissions. The second one counts on using CO_2 captured from other industrial processes or directly from air as the carbon (and oxygen) feedstock for chemical industrial processes (CCU). In the CCU case, cheap renewable electricity would play a central role in green hydrogen production and in promoting highly non-spontaneous reactions[3]. As renewable electricity costs decline, the conversion of electrolytic hydrogen (i.e., "Power-to-X") to both feedstock and energy carrier would become increasingly viable, enabling scaling up production. To date, green hydrogen technologies have not reached maturity. Policy coordination to expand hydrogen demand and develop the necessary infrastructure for large-scale transport and storage will be necessary. However, though a hydrogen-based strategy would deliver better climate and air pollution outcomes, concerns on safety and water requirements are still a challenge.

The third approach is to feed renewable biomass in direct chemical, biochemical and thermochemical processes. Though large-scale biomass harvesting may imply adverse side-effects, this approach could benefit from infrastructure, technological and logistics

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[3] In 2020, electrolysis-based hydrogen production reached 5% of the 8 Mt of global capacity (IEA 2021a).

synergies with similar bio-based strategies in other hard-to-abate sectors, such as aviation and shipping, which consider low-carbon fuels to comply with the International Maritime Organization (IMO) 50% reduction in carbon emissions goal by 2050 [44], [84]. Also, existing fossil fuel infrastructure can play a role in smoothing the transition in these sectors and reducing large-scale capital risks by co-processing bio-based feedstock in conventional refinery units aiming at producing biofuels and bio-derived chemicals.

Away from the chemical sector, organic bulk materials also play an essential role as reducing agents in the iron, steel, and ferroalloys industries, mainly coking coal in blast furnaces and natural gas in direct reduced iron (DRI) facilities to a lesser extent. Hydrogen and charcoal are potential substitute candidates, also scrap recycling in electric arc furnaces certainly plays a role by reducing mineral ore demand.

2.3.2 Inorganic bulk materials

Inorganic bulk materials are metallic (ferrous and non-ferrous) and non-metallic minerals produced in large volumes and whose production is energy- and/or emissions-intensive. The emphasis of this section lies on basic inorganic raw materials that are inextricably linked to the expansion of new electric and digital infrastructure for low-carbon technology deployment as well as to the intensification of potassium and phosphorous fertilizer use for bioenergy development. Thus, they influence energy transition pathways in: (i) the increment of energy inputs and direct and indirect GHG emissions; (ii) the material intensity of renewable energy technologies; and (iii) the potential reduction of the Energy Return on Investment (EROI) due to declining metal ore grade.

Today, some 4000 Mt of cement are produced every year, accounting for around 7% of both global direct GHG emissions and final energy consumption [85]. For iron and steelmaking processes these figures are 6% and 7%, respectively, and yearly global production reached around 1800 Mt of crude steel [86]. With very few cost-competitive substitutes, especially for structural applications, cement and steel demand have strong relationship with economies' GDP, industrialization and, in the future, probably with the new capital stock associated with renewable energy expansion as well – recognized as more material-intensive than traditional fossil fuel technologies. Actually, estimates show that global demand for steel in the power sector could grow by a factor of 2.6 in 2050 , driven by the deployment of renewable electricity technologies to limit global average temperature increase to 2 degrees Celsius [30].

Cement and steel are enablers of transitions, as traditional low-cost materials with the desired properties to be used in foundations for wind turbines, concentrated solar power towers, transmission lines, and CCS infrastructure. However, they are also constraints, as hard-to-abate and emissions-intensive sectors. Though energy efficiency played a central role in the past decades within these industrial sectors, replacing traditional with innovative technologies is unavoidable to limit emissions. Furthermore, shelter, transportation, and storage services demands will probably increase as populations grow, urbanize, and gain affluence worldwide. However, innovative low-carbon technologies are still on early stages of development and around 90% of the traditional existing capacity will reach the end of investment cycle only by 2040 [71].

Similar to the chemical industry, these are heavy, hard-to-abate, capital-intensive with long-lasting equipment industries. They demand high-temperature heat in metallurgical (i.e., reduction of hematite and magnetite ores in temperatures as high as 1400-1500ºC in blast furnaces and up to 1000ºC in direct reduction) and calcination (i.e., decomposition of limestone, releasing carbon at 850-900ºC) processes, which are energy services not easily electrified. It has been advocated that nuclear energy can be particularly useful in achieving these high temperatures or producing hydrogen as an energy carrier, thus playing a key role in hard-to-abate sectors as a mature, reliable, and low-carbon technology. But this comes with the acknowledged safety challenges faced by the nuclear energy itself and its toxic waste disposal, failing to meet circular economy principles [87], [88]. Nuclear plants are also high material consuming [89] with materials performance issues as well [90].

Furthermore, these processes release not only energy- but also process-related emissions, thus requiring mitigation strategies such as clinker substitution, the substitution of coking coal as reducing agent in iron production, and Carbon Capture, Utilization and Storage (CCUS) in cement and steel production. Increasing the share of alternative materials into cement and the use of hydrogen as a reductant in the direct reduction of iron ore have been identified as key measures to achieve global net-zero emissions by 2050 [71]. However, permanently capturing CO_2 emissions and storing/using them is critical to address residual process emissions mitigation in these sectors. In this sense, while carbon capture as well as geological storage technologies are commercially available (though costly), using CO_2 as a feedstock could deliver additional economic revenues that would make the whole process economically viable [91].

The material-intensive aspect of energy transition also affects the supply and demand of other inorganic materials. Phosphate, potassium, and nitrogen fertilizers will be required to meet expanding needs for food and bioenergy. Aluminum is a light, malleable, corrosion-resistant, and ductile metal used for transportation, packaging, and transmission lines. Copper, as an essential metal in the electric and electronic industry, will be extensively used in electricity networks. Most of the nickel produced today is used to make stainless steel and other steel alloys, though increasingly demanded by the batteries industry. Zinc is widely used in steel galvanization and for anticorrosion protection in turbine types. Beyond their traditional uses and new energy applications, most of these metals are also part of the broader digital and electric technology cluster, which include mobile phones, ICTs, EVs, new lighting technologies, among others.

These metals' demands are expected to increase in unprecedented levels and most assessments assume an increase of around 215% for aluminium, 140% for copper, 140% for nickel, and 46% for zinc by 2050 [92]. Though abundant and produced in distributed regions, these materials usually present a cheaply available range of properties, making them hard to substitute. Hence, the more we delay large-scale deployment of low-carbon technology, much less densely packed than fossil fuel-based ones, the faster will be the ramp up of material extraction and production rates needed. Also, the stock of materials in use, thus prevented from being recycled, will also be higher, which can hamper the efficacy of material efficiency measures [93].

As a consequence, speculations over potential exhaustion of metal reserves emerge, in a way revisiting historical concerns over the scarcity of natural resources. While many researches point out evidence that mined ore grades have been declining over the years [94], others suggest that misconceptions over mining concepts and economics, as well as inappropriate analogies with petroleum reserves, have created a false idea of causality between observed declining mined ores and the depletion of higher grade deposits [95], [96]. The question though seems to be less about the physical limits of metal endowments and more about the implications of increasing energy intensity of metal extraction, how fast can metal extraction increase to respond to demand escalation, and the socio-environmental impacts that may arise from mining intensification.

Whether higher-quality deposits are indeed facing depletion or technological improvements enabled lower grade mining in high demand periods, it remains true that energy consumption and GHG emissions increased with decreasing ore grades [97]. This effect may be amplified with increasing depth of deposits and impurities concentration due to mining activity intensification. This underlies a key concern over the reduction of the net energy available to society if the energy return on investment (EROI) decreases, from which a vicious cycle would result: the energy transition to metal-intensive technologies would increase metal demand, gradually increasing the energy intensity of extraction, ultimately decreasing the EROI of the system and increasing the need for renewable technologies deployment [98]. Though only copper, zinc, lead and nickel have shown declining grade trends as of today, managing environmental impacts of mining and processing of all metals would add to the energy cost accountability.

Moreover, mining and metallurgical activities entail serious human health and environmental impacts. For instance, mining extraction provokes land-use change – affecting biodiversity and displacement of communities – as well as large water use and waste generation, which are increased with lower ore grades. For example, water use in brine lithium and copper production can be as high as around $1m^3/kg$ and $0.05m^3/kg$, respectively [99]. Depending on the ore, toxic pollutants may be emitted, such as SO_2 in copper chalcopyrite and HF in aluminum processing. Naturally, appropriate technology was developed for decades to minimize these impacts, not without affecting prices and leading to offshoring of mining activities to countries with less stringent environmental regulations. Thus, if social and environmental burden of mining, metallurgical and refining activities are not rigorously handled, energy transition pathways may result in extensive local impacts.

2.3.3 Critical Materials

Whilst inorganic and organic bulk materials directly relate to CO_2 emissions and energy transition pathways, critical materials neither have a rigorous physicochemical nature nor have its impacts on the basis of energy/CO_2 emissions accountability. The concept of critical materials has been evolving since its first use in the 1930s-40s to represent national security concerns over resource access: when the national security concept changed – from mainly military defence in war times to a vast array of economic securities – so did the critical materials concept to encompass material access concerns over energy transition strategies [100]. Since the late 2000's, this concept has been used in reference to materials that present a high risk of supply and are considered important in a given economy, corporation, or supply chain [101]. Criticality is, therefore, not an inherent feature of a material but a dynamic concept that changes depending on the perspective and historical time.

Naturally, the diversity of perspectives in criticality assessments often results in contrasting outcomes regarding which materials are and which are not critical [102]. For example, even bulk materials such as copper and phosphates are understood as critical in some assessments (e.g. [103], [104]). However, our focus here lies on the materials more frequently considered critical, which usually (but not always): (i) are used in small mass per product unit, for which its property is essential; (ii) are minor metals, mined in much smaller quantities compared to bulk or industrial metals (as a consequence, they usually cannot be considered mineral commodities); (iii) have increasing demand rates prospects; (iv) are co- or by-products of a major metal production; (v) have very low price elasticity of supply; (vi) require complicated (intensive in energy, chemicals and water use) extractive metallurgy; (vii) have low recycling rates; and/or (viii) have no substitutes with similar performance in the short/medium term. The fundamental issue is that some of these materials could delay or slow down energy technologies deployment on both supply (e.g., renewables) and demand (e.g., digitalization) sides as a consequence of geopolitical, economic, technological, or socioenvironmental aspects. Hence, if organic and inorganic bulk materials are the macronutrients of the socioeconomic metabolism, critical materials are the micronutrients [105].

Examples can be drawn. Lithium’s lowest standard reduction potential combined with the low electric and thermal conductivity of cobalt make them suitable for long-lasting and high energy density batteries. Rare earth elements (REE) such as dysprosium, neodymium, terbium, and praseodymium make up NdFeB magnets, which are capable of creating a powerful magnetic field without undergoing demagnetization in high temperatures, thus suitable for wind turbines and electric motors. Platinum Group Metals (PGMs) are extensively used in heterogeneous and electrochemical catalysis – also, potentially in biorefineries and hydrogen electrolysers – given its high chemical resistance, high catalytic activity, and stability properties.

The claim that the ongoing energy transition is one from an oil-based to a mineral-based economy finds evidence not only in the increasing dependence on material-intensive, digital, and low-carbon technologies, but also in the changing energy geopolitical landscape that emerges from it. The high geographical concentration of reserves, production, and/or processing capacity of some materials was what triggered off materials supply concerns and multiple criticality assessments in the last decade, after the 2010 rare earth crisis. China raised export taxes and decreased export quotas of rare earth elements in that year, which increased prices from 5 to 13 times [106]. By that time, 97% of REE production was in China and, despite the diversification and recycling measures taken by industry and governments, it reduced to 65% (90% of the processing capacity) in 2019 [99]. China also holds around 60% and 50% of the processing capacity of cobalt (whose global production is 70% in the Democratic Republic of the Congo) and lithium, respectively, and 40% of copper refining capacity [99]. China has been able to expand access to key resources of the energy transition so as to convert it to industrial advantage, fulfilling its own materials requirements for strategic emerging industries such as wind turbines, electronic equipment, and electric vehicles manufacturing [107].

Of particular importance is the limited capability of the mining industry to respond to such crises and general market fluctuations. New project development, from the discovery of a new deposit to the production, takes on average 17 years [99]. To further process the metal extracted, capital-intensive metallurgical and refining processes are required, and such investments can be hampered due to the characteristic price volatility of these materials. Price volatility is commonly observed for metals that are recovered as by- or co-products of a primary desired metal. They are not necessarily scarce in the earth's crust but sparsely distributed in specific orebodies and sometimes in such low grades that remain as waste products unless proven economical. Hence, co- and by-products pricing is highly dependent on the market dynamics of the main metal, which can make supply insensitive to high prices.

Besides geopolitical and economic factors, mining, recovering, and refining minor metals inflict major socioenvironmental impacts. As ore grades decrease, more waste is generated and more water, energy and chemicals are required to extract and purify the desired metals, frequently also exposing workers to toxic chemicals. It is estimated that over 50% of lithium and copper production today is carried out in high water stress regions [99]. Whilst steel production consumes around 23 MJ/kg, cobalt production ranges from 140 to 2100 MJ/kg and platinum group metals can reach up to 254,860 MJ/kg [108]. Child labour, unsafe work conditions in artisanal mining sites and political instability in the Democratic Republic of the Congo has been also documented as critical aspects of cobalt production in the country. Hence, measures to ensure material access to energy transition pathways must not overlook potential trade-offs between local and global impacts.

2.4 Concluding Remarks

All social and economic activities are mediated by the metabolic exchange of both matter and energy within nature, inextricably conditioned by the laws of thermodynamics [109]. Energy transition conceptualizations are diverse; they converge, though, in that materials aspects are often underrated as part of the transformations that go by with structural changes in energy production, transformation and consumption globally. As a result, energy transitions modelling that supports energy policy do not fully consider the materials-energy nexus as constraints or opportunities for deep decarbonization pathways.

From this perspective, an energy transition from fossil to renewable energy, not unusually envisioned as one from finite to infinite energy resources, may underestimate energy sources and/or prime movers substitutions triggered by unavailability of materials, much similar to that of the depletion of forests stocks in Europe. However, while back then material shortage revealed itself as a driver for harnessing the increasing availability of coal energy, as of today material shortage can hamper GHG emissions mitigation strategies to avoid irreversible climate change impacts. As the [99] recently ascertained, investment plans for expanding mineral supplies to the extent required by an accelerated transition are still insufficient, not to mention geopolitical and environmental risks that could disrupt the operating capacity.

Likewise, materials-related opportunities may be sidelined as well. Efforts to establish a fully circular economy can both strengthen energy security and reduce the pressure on local communities and the environment. Moreover, material efficiency strategies – such as material substitution, recycling, remanufacturing, design, repair, and lifetime expansion – can also become relevant to loosen the pressure over supplies and further reduce impacts and improve energy efficiency. Nevertheless, primary material supply is unavoidable to fulfil the increasing demand for materials in emerging countries where the build-up of new material stocks for infrastructure and buildings is required [110]. In addition, materials are part of the transition system and thus can affect energy technology choices (for example, facilities that co-produce materials and fuels from renewable sources may become systemically preferable compared to energy focused facilities). Therefore, energy transition strategies need a holistic and systemic approach so as to consider materials life cycles and industrial ecology in the cascading use of resources. Materials not only add up to energy and emissions accounting but can abruptly disrupt energy pathways as well as represent an underexplored potential to minimize socioenvironmental impacts of an inevitably fast transition on account of decades of global climate inaction. To make ends meet, a just global energy transition must be based on materials life cycle sustainability, taking stock of the materials-energy linkages revealed in past transitions.

3 INDUSTRIAL SECTOR PATHWAYS TO A WELL-BELOW 2ºC WORLD: A GLOBAL INTEGRATED ASSESSMENT PERSPECTIVE

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Abstract

The heavy industry is often regarded as *hard-to-abate* due to its importance to infrastructure build-up, capital stock, high-temperature heat requirements, and the critical role it plays in global supply chains and security. These complexities have often been invoked to justify the persistence of residual greenhouse gas (GHG) emissions from cement, steel, and chemicals production by 2050, which, in contrast, suggest the need for global-scale roll-out of carbon dioxide removal (CDR) technologies. In this study, we use the global integrated assessment model (IAM) COFFEE with a detailed representation of industrial processes to understand the role of the industrial sector in climate change mitigation scenarios with different temperature ambitions. Our findings reveal a nuanced picture. While the industrial sector presents residual emissions of 1300 - 7600 $MtCO_2yr^{-1}$ in well-below 2ºC scenarios by 2050, it also emerges as a key mitigation asset in some subsectors (e.g. chemicals and steel) and regions (e.g. AUS, BRA, CAN, CAM, SAM), depending on the level of climate ambition pursued and the availability of biomass and carbon capture scale-up. Thus, the sector's role in climate change mitigation is context-dependent, opening pathways for strategic planning and technological and regional targeted actions.

3.1 Introduction

The industrial sector has been regarded as hard-to-abate or difficult-to-decarbonize [8], [111], [112], [113], [114]. This is primarily due to: (1) the long-lasting and capital-intensive nature of industrial equipment; (2) the high-temperature and hard-to-electrify heat requirements; (3) the scale of production required to build and maintain urban infrastructures and services; (4) industrial process emissions, which result from chemical reactions other than combustion and are not mitigated through electrification or renewable energy; (5) the cross border competitiveness of industrial commodities and the challenge of attributing embodied greenhouse gas (GHG) emissions in traded products[115], and (6) the relationship between economic growth and industrial development, which affects the selection of sites for low-carbon industries [116]. Hence, there is an expectation that the industrial sector – along with the aviation, shipping, and part of the agriculture subsectors – will exhibit residual "recalcitrant emissions" by 2050, which will require offsetting by carbon dioxide removal (CDR) strategies [117] for global net-zero to be achieved [118]. Comparatively, “light-duty transportation, heating, cooling, and lighting may be relatively straightforward to decarbonize by electrifying” [8].

Approximately 25% and 35% of total direct and indirect global CO_2 emissions can be traced down to the industrial sector, respectively [119]. Therefore, the scale, location, and timeliness of industrial residual emissions remain a concern for effective policymaking and for sending clear signals about mitigation responsibilities and the necessity of CDR.

The main strategies considered as key to decarbonize the industrial sector are energy efficiency [120], [121], electrification, and fuel switching to low-carbon fuels (including feedstock substitution) [14], [122], [123], [124], [125], carbon capture and storage (CCS) [111], and reducing demand via material efficiency measures [126]. Scenario-based bottom-up sectoral assessments and the so-called roadmaps to net-zero have analysed the cement [127], steel [128], and chemicals [129] subsectors. However, studies with an integrated perspective that investigated the role of the industrial sector in global mitigation scenarios rarely find this sector to be carbon neutral by 2050, except in scenarios with very specific assumptions [21], [23], [25], [26], [130]. Sectoral studies typically focus on the question, "What does it take to reduce emissions in the industrial sector to zero by 2050?"; in contrast, Integrated Assessment Modelling (IAM) studies that focus on the industrial sector aim to understand its role within a broader decarbonization strategy, considering mitigation costs across all sectors under different carbon (shadow) price assumptions throughout the century. In other words, IAMs scenarios find global pathways by balancing residual emissions and carbon sinks across sectors towards net-zero emissions globally.

With this work, we aim to contribute to the literature about industrial residual and hard-to-abate emissions by running scenarios with different climate ambitions to understand the role of the industrial sector in "well-below 2ºC" scenarios. Our hypothesis is that, while presenting technical and market barriers for decarbonization, the global industrial sector will not necessarily present residual emissions in these scenarios, following different pathways depending on the subsector and region. In this study, we present the recently enhanced representation of the industrial sector in the COFFEE model, a global IAM, to test this hypothesis. COFFEE depicts an industrial sector that includes cement, steel, and chemical subsectors with the representation of conventional and innovative/low-carbon technologies. These technologies are used to produce clinker, cement, steel, high-value chemicals (HVCs), ammonia and methanol, meeting regional demands projected throughout the century. Capacity, costs, and lifetimes for industrial equipment were regionally assessed to represent industrial subsectors. Moreover, the link with the refining sector was also developed to ensure that the demand for petrochemicals was consistent with the activity of the oil refining sector and the production of primary fossil fuels, as required by other studies [36], [131].

The rest of this article is structured as follows. Section 3.2 describes the methodology behind this work, from technoeconomic assumptions to scenario design. Section 3.3 presents the results and Section 3.4 include the main discussion points and final remarks.

3.2 Methods

3.2.1 The COFFEE model

The COFFEE (COmputable Framework For Energy and the Environment) model is a linear programming model for intertemporal optimization (perfect foresight) of the global energy and land use systems. Its objective function is to minimize the cost of the energy and land use systems and simultaneously fulfil long-term demands for energy and food services, subject to restrictions. The sectors explicitly represented in COFFEE are energy, buildings (residential and commercial), passenger and freight transport, industry, and waste and residues. COFFEE is based on the MESSAGE platform developed by IIASA (International Institute for Applied System Analysis).

Further details of the COFFEE model can be found in refs. [132], [133], [134]. Material production and demand representation were improved in COFFEE to assess better potential synergies and trade-offs between materials-, energy- and land-use dynamics. Table 1 and Figure 2 provide the regional breakdown of the COFFEE model. The following sections provide details on module structure, data sources, assumptions, and scenario design used for this work.

Table 1. Region representation in the COFFEE model

Tag	Description
AFR	Africa (excl. South Africa)
AUS	Australia and New Zealand
BRA	Brazil
CAM	Central America
CAN	Canada
CAS	Caspian Region
CHN	China
EEU	European Union (28)
IND	India
JPN	Japan
KOR	South Korea
MEA	Middle East
RAS	Rest of Asia and Oceania
RUS	Russia
SAF	South Africa
SAM	South America (excl. Brazil)
USA	United States
XEU	Other Europe

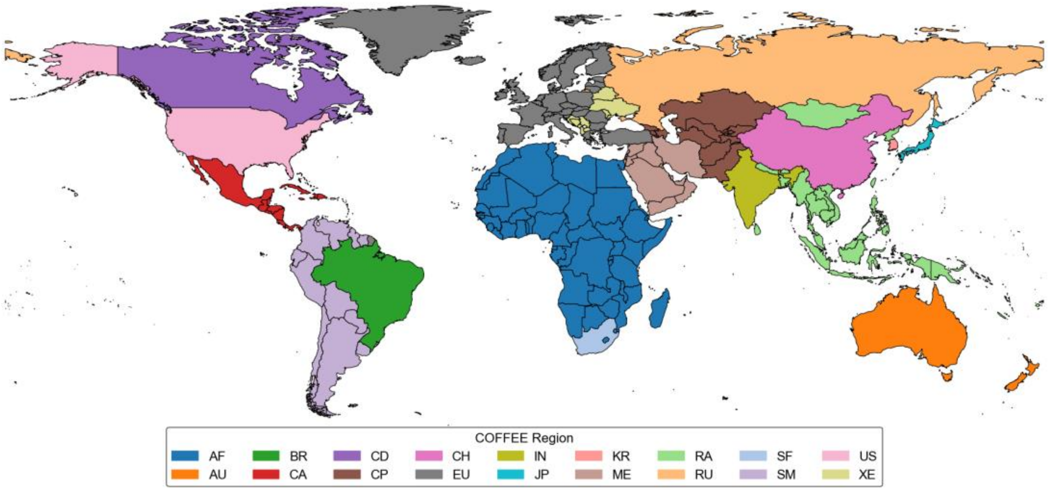


Figure 2. Regional breakdown of the COFFEE model

3.2.2 Demand assumptions

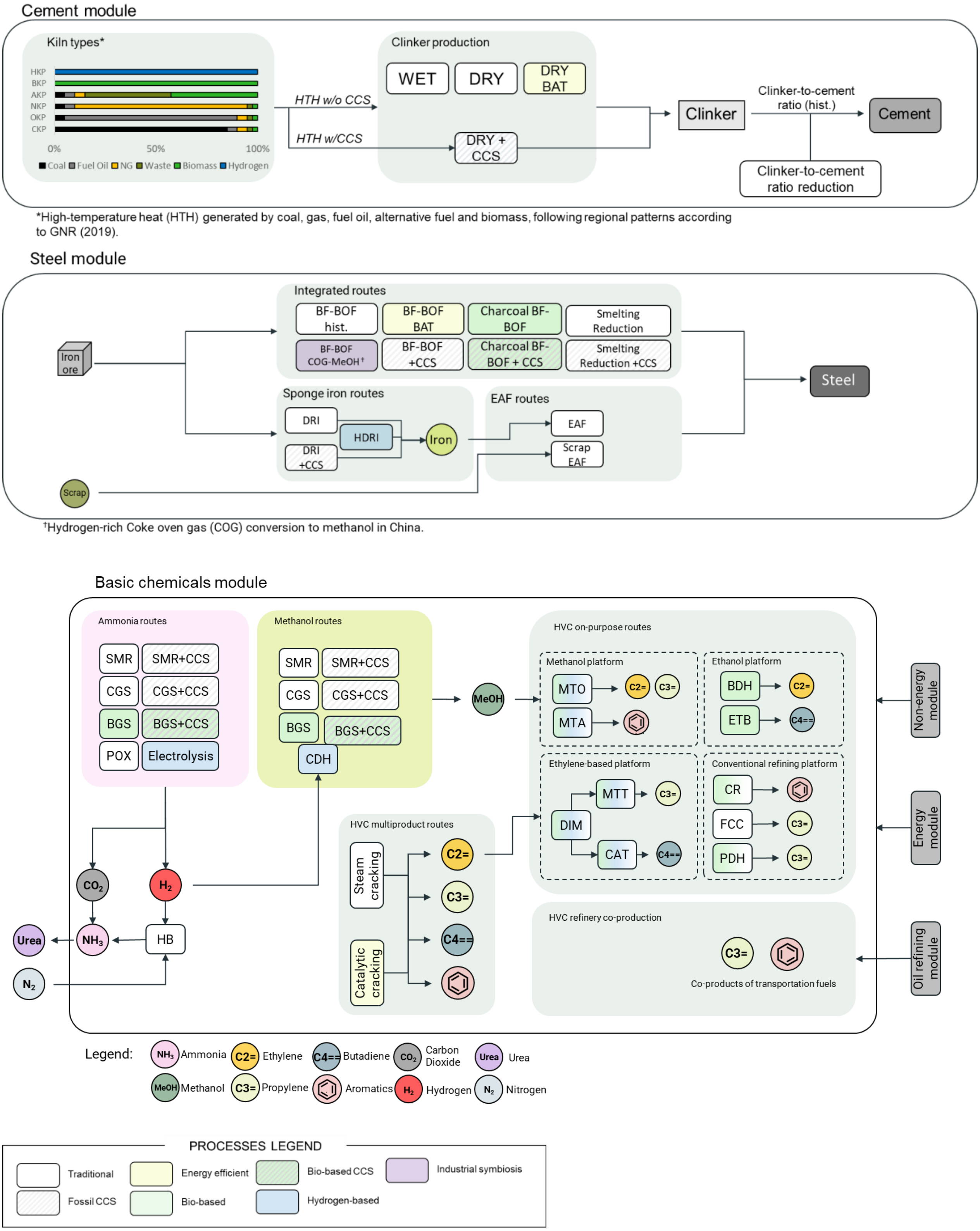
Exogenous demand pathways were developed based on the historical intensity of use between material demand (in physical, not service, terms) and socioeconomic variables – gross domestic product (GDP) and population [21], [135]. Historical apparent steel use and apparent steel use per capita data per country was derived from Worldsteel's Steel Statistical Yearbook (2000-2021) [136], and cement production by country from USGS's Minerals Yearbook: Cement (1999-2020) [137]. As for the chemicals sector, data on thermoplastics consumption per capita of 66 countries was used as a proxy for regional plastics demands [138]. Building on that, ethylene, propylene, butadiene, and BTX separate demands were calculated based on their share in thermoplastics production in 2013, based on the work of Levi and Cullen (2018), which were assumed to remain constant over time [139]. Ammonia demands were calculated based on USGS's Minerals Yearbook: Nitrogen (2003-2020) [140] and YARA (2018) [141]. Methanol used for biodiesel production and gasoline blending is an endogenous result of COFFEE. Hence, we only considered methanol demand for non-energy purposes, e.g., formaldehyde, acetic acid, and methylamine production. To that end, data on regional methanol demands were collected from EPE (2019) and Su et al. (2013), from which we calculated the difference of methanol use for energy purposes based on Chatterton (2018) and OECD & FAO (2021) [142], [143].

Material efficiency and circular economy measures that could reduce virgin material demand were out of the scope of this work and will be recommended as developments for further studies in the last section of this work.

3.2.3 Technology portfolio

To improve the industrial sector representation in COFFEE, we incorporated traditional and innovative production technologies represented by techno-economic parameters such as investment costs, fixed and variable operating and maintenance costs, energy inputs, process yields, and plant lifetime. These technologies fulfil exogenous demand projections of cement, steel, and primary chemicals (ethylene, propylene, butadiene, BTX, methanol, and ammonia) from 2010 to 2100 described above.

On the production side, innovative routes based on electrification/hydrogen, biomass, and CCUS were included in each sector as well as efficient alternatives for traditional technologies, so as to offer the model different technological and energy sources possibilities to fulfil regional long-term demands as cost-effectively as possible under carbon stringent scenarios. Moreover, a simplified approach to the trade of chemicals and steel was modelled by creating a global pool, which every region could export to and import from, and the age of existing plants was also accounted for whenever data was available. Figure 3 illustrates the explicitly represented industrial sector in the COFFEE model with its technologies, intermediate, and final products.



*High-temperature heat (HTH) generated by coal, gas, fuel oil, alternative fuel and biomass, following regional patterns according to GNR (2019).

†Hydrogen-rich Coke oven gas (COG) conversion to methanol in China.

Figure 3. Cement (upper), steel (middle) and primary chemicals (lower) modules representation in the COFFEE model

3.2.3.1 Cement

3.2.3.1.1 Production technologies

The cement module was divided into three sections: (1) HTH generation, which is generally responsible for 40% of global cement emissions via fossil fuels combustion; (2) clinker production via limestone calcination, which leads to CO_2 release and is responsible for roughly 50% of total cement emissions, and (3) cement production by adding alternative cementitious materials to the clinker mix.

Section (1) was developed to capture regional differences in final energy composition for thermal energy use in the clinker production stage. Different typologies of kilns were represented to account for current and alternative HTH technologies but also highlight the sector's characteristic flexibility in using multiple sources of energy, depending on a variety of regional factors such as local availability and cost. Thus, as represented in Figure 3, we included Kilns with coal, natural gas, and petroleum coke as being 85% of the total fuel feed (in the base year), with the other 15% being divided between fossil fuels, alternative fossil fuels (e.g., tires, solvents, refuse-derived fuel, waste oil), and bio-based fuels (e.g., charcoal, bio-waste). These kilns were also coupled with CCS, resulting in six fossil-based kilns. A kiln based on 42.5% of alternative fossil fuels and 42.5% in biomass (i.e., only 15% of conventional fossil fuels) and one based entirely on biomass were included, adding up to their respective CCS options. Finally, a hydrogen-based kiln was also included in the portfolio, summing up to eleven kiln typologies in total.

Kiln typologies split per region were calculated based on the energy use per country [85], which are described in Table 2.

Table 2. Fuel type profile in 2010 according to COFFEE regions based on ref. [85]. The model was calibrated until 2020 using values of the same database.

	Fossil fuel			Alternative fossil fuel	Biofuel
%	**Coal**	**Fuel Oil/ Pet coke**	**NG**	**Waste**	**Biomass**
AFR	30	48	20	1	1
AUS	81	10	2	2	5
BRA	2	79	0	7	12
CAM	8	80	2	9	1
CAN	45	21	21	11	2
CAS	48	1	50	1	0
CHN	94	0	0	5	1
EEU	28	41	1	24	6
IND	31	69	0	0	0
JPN	92	3	0	5	1
KOR	92	3	0	5	1
MEA	19	79	0	2	0
RAS	81	10	2	2	5
RUS	48	1	50	1	0
SAF	50	48	0	1	1
SAM	30	22	43	3	2
USA	45	21	21	11	2
XEU	48	1	50	1	0

The clinker production section receives HTH as an input from the previous section based on its requirements for limestone calcination in each of the technologies represented, including wet rotary (WET), dry with preheater (without pre-calciner) (DRY), efficient dry rotary (i.e., Dry with preheater and pre-calciner), and efficiency dry with on-site CCS technologies. This section also represents process emissions derived from the conversion of limestone (primarily composed by $CaCO_3$) to clinker (CaO). Country- or region-specific emissions factors based on the composition of limestone used in clinker production were used whenever available [144], [145], [146]; or else, we used the factor recommended by the IPCC guidelines [147].

As for the cement production part, we considered that clinker flows from the previous module and is mixed into a generic flow of *alternative cementitious materials* (ACM) to produce cement. We calibrated cement production according to historical data of clinker-to-cement ratio, which was derived from clinker and cement production at the country-level [85], [137]. To represent regional clinker-to-cement ratio reduction over time, we assumed that the costs of additives would grow exponentially, based on current costs of traditional (i.e., fly ash, blast furnace slag) and innovative (i.e., geopolymer cement) cementitious materials as references.

The technologies included in this module are represented in Figure 3, and the parametrization used in our modelling is described in Table 3.

Table 3. Techno-economic parameters for clinker production technologies

Technology	Main Input	Main Output	CO$_2$ capture	SEC[a]	Investment cost	O&M cost		Ref.
						FOM	VOM	
			%	GJ/GJ$_{MI}$	USD2010/t$_{MO}$py[b]	USD2010/t$_{MO}$		
WET	Heat	Clinker	-	5.75	180	4.9	4.9	[21], [85], [148]
DRY			-	3.72	190			[21], [85], [148]
DRY BAT			-	2.85	259			[21], [85], [148]
DRY+CCS[c]			60%	3.91	320			[21], [85], [148], [149]

FOM: Fixed operation and maintenance cost; VOM: Variable operation and maintenance cost; MO: Main Output.

[a]Includes heat, steam, and machine drive requirements. [b] Tonnes of main output per year. [c]Post-combustion CCS.

3.2.3.2 Iron and steel

The technologies included in the iron and steel module are categorized as: (1) integrated routes, (2) sponge iron routes, and (3) electric arc furnace routes (see Figure 3). Integrated routes include Blast furnace integrated to basic oxygen furnaces using both bituminous coal and charcoal (i.e., BFs in Brazil) as reducing agents, and smelting reduction and open-hearth furnaces. Consumption of coal in this sector also includes transforming coal in coke ovens. A variation of BF-BOF was also included to represent methanol production from hydrogen-rich coke oven gas in China as a co-product in integrated steel plants, which integrates with the chemical module. Sponge iron routes refer to the production of direct reduced iron (using both natural gas and hydrogen). Electric arc furnaces refer to the collection of steel scrap to feed electric arc furnaces where it is melted to steel. Whenever possible, alternatives combined with CCS were also included. The parametrization used in our modelling of the steel sector is described in Table 5.

Steel scrap baseline availability was limited over time based on the assumption that the relation consumption of scrap per demand, on a regional basis, would remain the same over time. This was defined as a simplification of steel scrap generation in the absence of a detailed stock flow model based on steel use in products and their lifetimes. A higher level of availability was created , with a higher cost to increase the baseline availability by 25% as a proxy to increasing recycling rates in the steel subsector.

Table 4. Scrap use as share of demand in 2010.

Scrap use as a share of demand in 2010 (in %)	
AFR	16
AUS	22
BRA	32
CAM	23
CAN	34
CAS	39
CHN	17
EEU	53
IND	33
JPN	43
KOR	50
MEA	2
RAS	32
RUS	39
SAF	44
SAM	13
USA	60
XEU	53

Table 5. Techno-economic parameters for iron and steel production technologies.

Technology	Main Input	Reductant	Main Output	Yield	CO_2 captured	SEC[a]	Investment cost	O&M cost		Ref.
								FOM	VOM	
				t_{MO}/t_{MI}	tCO_2/t_{MO}	GJ/t_{MO}	$USD2010/t_{MO}py^b$	$USD2010/t_{MO}$		
OHF	Iron ore	Coking Coal	Crude steel	1.6	-	29.5	300	44.5	44.5	[135]
BF-BOF	Iron ore	Coking Coal	Crude steel	1.6	-	23.0	471	44.5	44.5	[21], [148], [150], [151]
BF-BOF BAT	Iron ore	Coking Coal	Crude steel	1.6	-	18.0	563	44.5	44.5	[21], [148], [150], [151], [152]
Charcoal BF-BOF	Iron ore	Bio-Charcoal	Crude steel	1.6	-	24.8	471	44.5	44.5	[150], [151], [153]
SR	Iron ore	Non-coking coal	Crude steel	1.6	-	19.4	441	44.0	44.0	[21], [151], [154]
BF-BOF-MeOH	Iron ore	Coking Coal	Crude steel	1.6	-	24.6	518	44.5	44.5	[148], [155]
BF-BOF+CCS	Iron ore	Coking Coal	Crude steel	1.6	0.71	18.0	623	44.5	44.5	[21], [150]
Charcoal BF-BOF+CCS	Iron ore	Bio-Charcoal	Crude steel	1.6	1.69	24.8	623	44.5	44.5	[150], [151]
SR+CCS	Iron ore	Non-coking coal	Crude steel	1.6	1.69	19.4	491	44.0	44.0	[21], [150]
DRI	Iron ore	Methane	Sponge Iron	1.7	-	14.9	142	6.0	6.0	[21], [148], [150], [151], [153]
DRI+CCS	Iron ore	Methane	Sponge Iron	1.7	0.53	14.9	182	6.0	6.0	[21], [148], [150], [151], [153]
HDRI	Iron ore	Hydrogen	Sponge Iron	1.7	-	14.2	455	11.4	11.4	[124], [156], [157]
EAF	Sponge Iron	-	Crude steel	0.97	-	2.1	230	23	23	[21], [148], [150], [158]
Scrap EAF	Steel scrap	-	Crude steel	0.95	-	2.1	230	23	23	[21], [148], [150], [151], [153]

FOM: Fixed operation and maintenance cost; VOM: Variable operation and maintenance cost; MO: Main Output; MI: Main Input.

[a] Includes heat, steam, and machine drive requirements as well as energy carriers used as reductants.

[b] Tonnes of main output per year.

3.2.3.3 Chemicals

The chemicals subsector in COFFEE is divided in two segments: (1) a technology-rich and explicit representation of primary chemicals, i.e., High Value Chemicals (HVCs), methanol, and ammonia, which covers two-thirds of global energy use in the chemical sector [12]; and (2) an implicit representation of other chemicals. Total energy use was calibrated to the World Energy Balances per region. HVCs technologies are categorized as Refinery co-production, Multiproduct and On-purpose (i.e., facilities dedicated to producing a specific primary chemical, as opposed to multiproduct routes such as steam cracking). Refinery co-production technologies include propylene co-production in the fluidized catalytic cracking (FCC), and BTXs in the catalytic reforming (CR) units, which are integrated into five refinery typologies represented in the oil refining sector in COFFEE [131]. Multiproduct routes include steam cracking (ethane and naphtha-based) as well as naphtha catalytic cracking. On-purpose routes include propane dehydrogenation (PDH), methanol-to-olefins (MTO), bioethanol dehydration (BDH), ethanol to butadiene (ETB), metathesis (MTT), dimerization (DIM), Catadiene (CAT), and catalytic reforming (CR). Ammonia and methanol can be produced by steam methane reforming (SMR), coal gasification (CGS), biomass gasification (BGS), and partial oil oxidation (POX), with different considerations on process emissions as part of the carbon content of the feedstock remains in methanol but not in ammonia. For ammonia, electrolysis is also considered whereas carbon dioxide hydrogenation (CDH) is considered a CCU route for methanol. To fully represent the chemicals sector in COFFEE, data from the IEA's World Energy Balances was considered to account for the gap in energy use between primary chemicals production and the rest of the sector. Heat and machine drive provision technologies were included to fulfil this gap, allowing for fuel switching, electrification, and efficiency gains over time. Figure 3 depicts the primary chemical module structure in COFFEE and *Table 6*, *Table 7*, and Table 8 show the parametrization of HVCs, methanol, and ammonia production technologies, respectively.

Table 6. Techno-economic parameters of HVC production technologies.

Technology	Feedstock	Output yields						SEC[a]	Plant capacity	Investment cost	O&M cost		Ref.
		Ethylene	Propylene	Butadiene	BTX	C4 stream	H_2				FOM	VOM	
		t/t_F						GJ/GJ_F	kt_{MO}/yr	USD2010/ $t_{MO}py$[b]	USD2010/t_{MO}		
SC-Naphtha	Naphtha	**0.324**	0.168	0.050	0.104			10	500	2718	54	54	[75], [159], [160], [161], [162]
SC-Naphtha-b	Bionaphtha	***0.324***	*0.168*	*0.050*	*0.104*			10	500				
SC-NG	Ethane	**0.803**	0.016	0.023	0			15	500	1680	34	34	
NCC	Naphtha	**0.324**	0.324	0.050	0.130			9.3	400	3963	41	41	[75], [159], [163], [164]
NCC-b	Bionaphtha	***0.324***	*0.324*	*0.050*	*0.130*			9.3	400				
BDH	Ethanol	***0.575***						2.8	200	1190	84	84	
MTO	Methanol[c]	**0.190**	0.180					4.3	500	1340	34	34	[75], [159], [163], [164], [165], [166], [167], [168], [169]
MTO-b	Biomethanol	***0.190***	*0.180*					4.3	500				
PDH	Propane		**0.750**			0.19		9.1	500	855	23	23	[75], [159], [170], [171]
PDH-b	Biopropane		***0.750***			*0.19*		9.1	500				
MTT	Ethylene (+ C4s)[d]		**3.125**					3.6	300	750	44	44	[172], [173]
MTT-b	Bioethylene (+ bC4s) [d]		***3.125***					3.6	300				
ETB	Ethanol			***0.280***				21.5	50	800	67	23	[174]
MTA	Methanol[c]				**0.230**			3.8	500	1380	17	17	[75], [159], [166], [168]
MTA-b	Biomethanol				***0.230***			3.8	500				
CAT	C4 stream			**0.600**				11.4	500	855	23	23	[75], [159], [170], [171]
CAT-b	Bio C4 stream			***0.600***				11.4	500				
DIM	Ethylene					**0.800**		0.4	300	150	4	4	[172]
DIM-b	Bioethylene					***0.800***		0.4	300				
CR	Naphtha				**0.880**		3.6[e]	0.8	800	262	3	3	[175], [176]
CR	Bionaphtha				***0.880***		3.6[e]	0.8	800	262	3	3	[175], [176]

F: Feedstock (underlined); **MO: Main output (values in bold).** *Bioproducts in italic.* [a] Includes heat, steam, and machine drive requirements (thus excluding energy use as feedstock). [b] Tonnes per year. [c] Fossil-. or CCU-based. [d] Yields refer to 1t of ethylene and 3.03t of C4s. [e] Value in GJ/t_{MI}. SC: Steam cracking; NCC: Naphtha catalytic cracking; BDH: Bioethanol dehydration; MTO: Methanol-to-Olefins; PDH: Propane dehydrogenation; MTT: Metathesis; ETB: Ethanol-to-Butadiene; MTA: Methanol-to-Aromatics; CAT: Catadiene®; DIM: Dimerization; CR: Catalytic reforming; Suffix *-b*: bio-based feedstock and products.

Table 7. Techno-economic parameters for methanol production technologies

Technology	Feedstock	Yields		Machine drive requirement	Process Emissions	Investment cost	O&M cost		Ref.
		MO: Methanol	CO_2 *capture*/**use**				FOM	VOM	
		GJ_F [a] /t_{MO}	tCO_2/t_{MO}	GJ/t_{MO}	tCO_2 /t_{MO}	USD2010/t_{MO}py [b]	USD2010/t_{MO}		
SMR	Methane	33.9	-	0.3	0.8	340	4.5	4.5	[45], [57], [76]
SMR+CCS	Methane	33.9	*0.76*	0.3	0.04	540	6.7	6.7	[75], [78], [148]
CGS	Coal	46.3	-	3.7	3.3	820	10.3	10.3	[75], [78], [148]
CGS+CCS	Coal	55.3	*3.14*	3.9	0.17	1020	12.8	12.8	[75], [78], [148]
BGS	Solid biomass	47.9	-	5.0	0	5655	70.7	70.7	[75], [78], [148], [177]
BGS+CCS	Solid biomass	47.9	*3.25*	5.0	0	5855	73.3	73.3	[75], [78], [148], [177]
CDH	H_2 + CO_2	22.6	**1.38**	1.5	0	44	0.5	0.5	[75], [78], [148], [178]

F: Feedstock (underlined); MO: Main Output; FOM: Fixed operation and maintenance cost; VOM: Variable operation and maintenance cost. [a] Includes heat and feedstock requirements. [b] Tonnes of main output per year.

Table 8. Techno-economic assumptions for hydrogen and ammonia production technologies

Technology	Feedstock Inputs	Yields		Machine drive	Process Emissions	Investment cost	O&M cost		Ref.
		MO: H_2 or **NH_3**	CO_2 capture				FOM	VOM	
		GJ_{MO}^{a} /GJ_{MI} or **t_{MO}/GJ_{MI}**	tCO_2/t_{MO}	GJ/t_{MO}	tCO_2 /t_{MO}	USD2010/$kWyr_{MO}py^{b}$	USD2010/$kWyr_{MO}$		
SMR	Methane	0.74	-	-	8.90	545	12	12	[75], [78], [148], [179]
SMR+CCS	Methane	0.74	8.01	-	0.89	622	23	23	[75], [78], [148], [179], [180]
CGS	Coal	0.59	-	-	20.2	2086	20	20	[75], [78], [148], [179]
CGS+CCS	Coal	0.59	18.18	-	2.02	2255	22	22	[75], [78], [148], [179], [180]
POX	Fuel oil	0.70	-	-	13.6	800	10	10	[75], [78], [148], [179]
BGS	Solid biomass	0.67	-	-	-	2285	83	83	[75], [78], [148], [177], [179]
BGS+CCS	Solid biomass	0.67	16.4	-	-	2465	83	83	[75], [78], [148], [177], [179]
Electrolysis	Electricity + H_2O	0.64 (2010) 0.74 (2060)	**-**	-	-	896 (2010) 240 (2050)	12 (2010) 3 (2050)	12 (2010) 3 (2050) ^{c}	[75], [78], [148], [178], [179], [181]
Haber Bosch	H_2 + N_2	**0.04**	**-**	3.9	-	95	2.5	2.5	[75]

MI: Main Input (underlined); MO: Main Output; FOM: Fixed operation and maintenance cost; VOM: Variable operation and maintenance cost. ^{a} Includes heat and feedstock requirements. ^{b} tonnes per year. ^{c} Electrolysis VOM does not include potential revenues from oxygen sales.

3.2.3.4 Other industries

To ensure complete coverage, we introduced the “Other Industries” sector in COFFEE to represent the energy use and emissions of industrial sectors not explicitly modelled. The energy use for each sector and region was calibrated according to the IEA’s World Energy Balances [12]. The residual energy use in the industrial sector was then allocated to the “other industries” sector. For simplicity, we assumed that the residual industrial energy use would grow at a rate comparable to that of the cement sector.

While representing a significant share of total GHG emissions globally (approximately 35-40% of total industrial emissions in the base year), the Other industries comprises mostly of light industries, except for the paper and pulp, non-ferrous metals and other non-metallic minerals. Therefore, it was assumed that most of this sector’s energy services could transition to electrification, as most of the remaining sectors demand energy services that could be easily electrified, such as low and medium temperature heat [14]. A restriction on biomass use was also implemented to ensure that biomass consumption, reflecting the demand of the paper and pulp sector remained, at least, constant over the century.

3.2.4 Scenario development

Four scenarios representing distinct climate ambitions were designed to analyse the mitigation role of the industrial sector. All of the scenarios were built on the assumption of the Shared Socioeconomic Pathway 2 (SSP2), which extrapolates historical patterns of social, economic, and technological trends throughout the century [182], [183].

The National Policies Implemented (NPi) scenario reflects the energy and climate policies implemented until 2020 and their implications in GHG emissions over the century. It does not consider additional mitigation efforts. Building on the NPi scenario and based on the definitions of the remaining carbon budget from the IPCC Sixth Assessment Report (AR6) Working Group One (WGI) report [184], we created three scenarios compliant with the “well-below 2ºC” targets established under the Paris Agreement but reflecting distinct temperature ambitions: 2.0-Degree (2C), 1.7-Degree (1.7C), and 1.5-Degree (1.5C) Celsius Increase Limit. The budget relative to these scenarios is more than 66% consistent with the temperature target (Table 9).

Table 9. Scenario definition.

	$GtCO_2$		AR6 WGI	
Scenario \ Period	Budget COFFEE[a] (2018-2100)	Budget AR6 WGI[b] (2020-2100)	T_L (°C)	Likelihood
NPi	-	-	-	-
2C	1230	1150	2.0	67%
1.7C	780	700	1.7	
1.5C	480	400	1.5	

T_L: Temperature increase above pre-industrial levels limit. [a] The carbon budget variable in COFFEE starts in 2018. To account for the 2018-2020 gap, ~80 $GtCO_2$ was integrated into the COFFEE model's carbon budget based on [185]. [b] Source: based on ref. [184].

We performed a sensitivity analysis based on the assumptions of scenario 1.5C, which includes the following restrictions:

- Global biomass availability is restricted to the 100 EJ. yr^{-1} threshold, defined as the sustainable technical potential of primary biomass production [186];
- Global CCS deployment is limited to a linear growth to achieve 10 $GtCO_2.yr^{-1}$ by 2080.
- Carbon removal in non-incinerated and non-recycled biomaterials is not accounted for.

As heavily reliant on CCS and biomass, this sensitivity analysis aims to understand how the role of the industrial sector is affected when critical mitigation and feedstock substitution strategies are limited. In the results section, this scenario will be referred to as scenario 1.5C_r.

3.3 Results

3.3.1 Pathways for the industrial sector in increasing temperature ambitions

This section presents the results of the industrial sector from COFFEE 1.5. Section 473.3.1.1 covers global trends in emission and energy use by the industrial sector as a whole in the context of a global net-zero strategy, and Section 3.3.1.2 provides detailed results for cement, steel, and chemicals. Section 3.3.1.3 presents results for the sensitivity analysis.

3.3.1.1 Global industrial emissions and energy use

Figure 4 presents an overview of long-term industrial emissions and energy use across scenarios. Global net-zero industrial emissions are not achieved, with residual emissions reaching 7622, 3563, 1312 $MtCO_2yr^{-1}$ in scenarios 2C, 1.7C, and 1.5C by 2050, respectively (Figure 4a). The primary contributors of these residual emissions include CHN, MEA, and USA contributing to 595, 216, 122 MtCO$_2$yr^{-1}, respectively, in scenario 1.5C. On the other hand, annual emissions reach levels below 50 MtCO$_2$yr^{-1} in some regions (AFR, AUS, CAS, SAF) or even net negative emissions (BRA, CAM, CAN, XEU, SAM) by the same year.

Increased ambition in limiting temperature increases drives earlier deployment of mitigation strategies in the industrial sector (Figure 4a). Comparable levels of emissions are achieved by 2060 under scenario 2C (5742 MtCO$_2$yr^{-1}), by 2040 under scenario 1.7C (6270 MtCO$_2$yr^{-1}), and by 2030 under scenario 1.5C (6005 MtCO$_2$yr^{-1}). Post-mid-century pathways show a resurgence in emissions, suggesting that the 2025-2050 window is critical for reducing emissions. This resurgence is attributed to three main factors: 1) increased population and affluence driving demand in some regions after 2050; 2) decommissioning of a large fossil-based capacity of long-lived capital deployed in the 2000s-2010s (both within the industrial sector and in other sectors); 3) CCS and other mitigation measures reaching maturity and becoming more widely available, allowing for a higher level of industrial emissions that is compensated in sectors that are not “hard-to-abate”.

Total final energy use modestly increases by 10-14% from 2010 to 2070 in mitigation scenarios (Figure 4b). This is primarily explained by the enhanced efficiency from the electrification of low-temperature heat services within the ‘Other industries’ sector. However, total non-energy use more than doubles over the same period across all scenarios (Figure 4c). The increased substitution of fossil fuels with biomass, which has comparatively lower conversion yields, results in a 7-12% higher final energy use for non-energy purposes in mitigation scenarios compared to the NPi scenario.

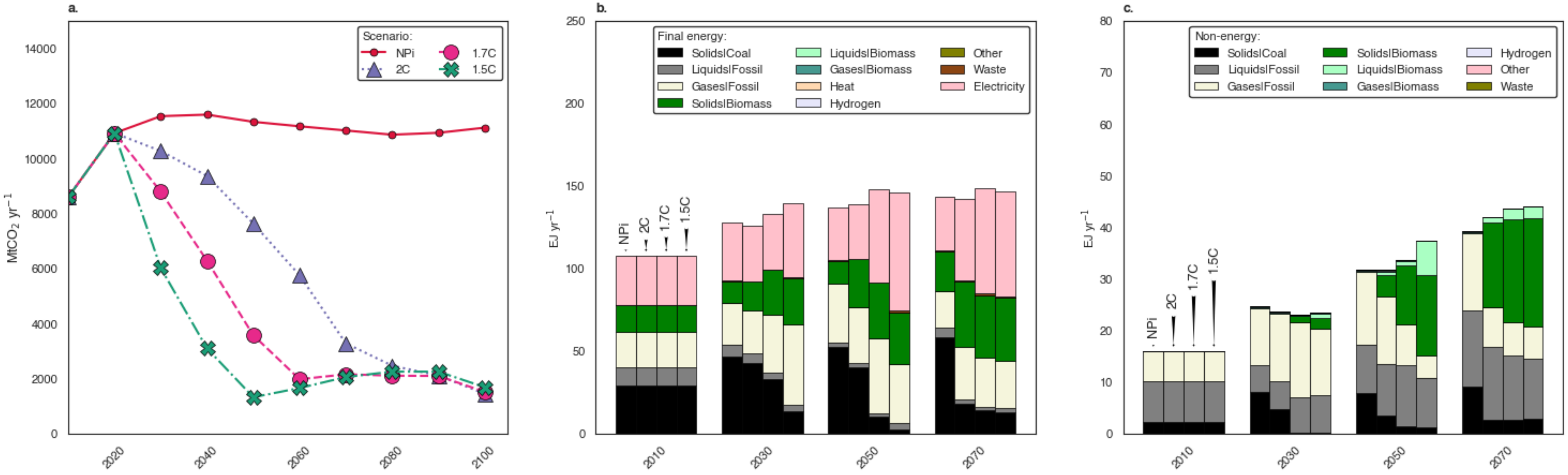


Figure 4. Global industrial energy and process net CO₂ emissions (a), final energy use per energy carrier (b), and non-energy use per energy carrier (c)

3.3.1.2 Sub-sectoral analysis

3.3.1.2.1 Cement

Figure 5 and Figure 6 provide an overview of the emissions trends, final energy use, technology split, and clinker-to-cement ratio for the cement sector.

Globally, cement demand and emissions stabilize around the 3600-4000 $Mt_{cement}yr^{-1}$ and 2000-2400 $MtCO_2yr^{-1}$ levels in the long run, respectively, after peaking in 2020 in the NPi scenario. In mitigation scenarios, CO_2 emissions reach 857-1581 $MtCO_2yr^{-1}$ by 2050 and stabilizes around ~1200 $MtCO_2yr^{-1}$ levels until the end-of-century. While regions such as AFR, AUS, CAS, IND, RAS, and SAF see their demand increase by 2-4.3 times between 2010 and 2050, regions like CHN, JPN, and KOR experience a sharp decline in domestic demand.

Climate ambition not only involves anticipating mitigation efforts but also changing strategies for the cement sector. The 1.7C and 2C scenarios have similar emissions pathways and strategy until 2050, i.e., increasing biomass use from ~3% in 2010 to 21-31% in 2050, while reducing coal use from 54% to 26-39%. Moreover, kiln capacity coupled with CCS reaches ~60% in the same year in both scenarios. Increasing climate ambition towards 1.5C targets involves not only anticipating and more aggressively deploying the same measures but also reducing the clinker-to-cement ratio. Coal use with and without CCS is virtually phased-out (i.e., <3% of total energy use) and biomass use share increases to 35% by 2050. Moreover, the increased use of ACM in cement lowers the clinker-to-cement ratio to 50% as early as 2030. These values are close to the 58% and 52% targets by 2030 and 2050, respectively, recommended by the GCCA [127].

After mid-century, clinker production capacity in all mitigation scenarios consists entirely of dry efficient kilns (i.e., with preheater and pre-calciner) equipped with CCS. There is a resurgence in coal use after mid-century, when CCS technologies are assumed to have reached maturity and scale-up gains momentum, allowing for a resurgence in sectoral CO_2 emissions while still achieving and sustaining global net-zero until 2100. While biomass has a role, especially until 2050, its share in cement final energy use reduces due to its critical importance and higher potential for net negative emissions in other sectors.

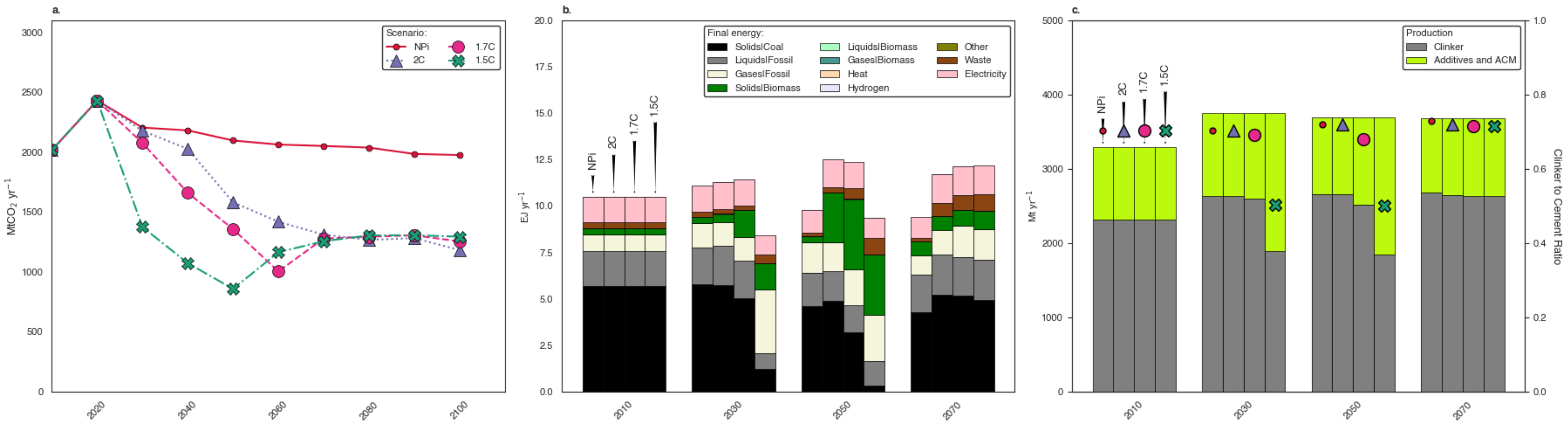


Figure 5. Global cement emissions (a), final energy use per energy carrier (b), clinker and additives production (c, left y-axis) as well as clinker-to-cement ratio (c, right y-axis).

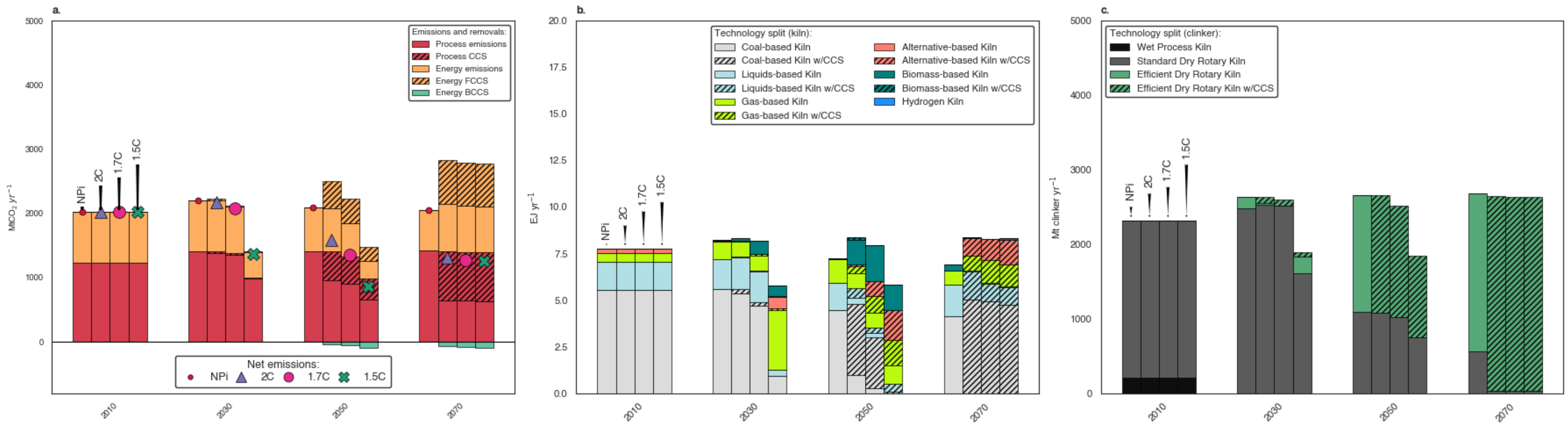


Figure 6. Global cement emissions and removals split (a), kiln technology split (b), and clinker technology split (c).

3.3.1.2.2 Iron and steel

Global direct CO_2 emissions from the iron and steel sector increased from 2700 $MtCO_2yr^{-1}$ in 2010, peaking at 2900 $MtCO_2yr^{-1}$ in 2030, and then presented a downward trend until reaching ~2300 $MtCO_2yr^{-1}$ by the end of the century under the scenario NPi (Figure 7a). Global production (incl. primary and secondary), on the other hand, increases from ~1400 Mt yr^{-1} in 2010 to ~2350 Mt yr^{-1} in 2050 (Figure 7c). Regional production trends are various: steel production AFR, CAS, IND, MEA, RAS, and SAM increase 2.9-7.2-fold between 2010 and 2050, while BRA, EEU, JPN, and KOR experience a decline.

Global direct emissions intensity, therefore, drops from ~1.70 tCO_2/t_{steel} in 2010 to 1.25 tCO_2/t_{steel} in 2050 and 0.98 tCO_2/t_{steel} in 2100 in the NPi. In mitigation scenarios, emissions intensity drops to 0.36-0.8 tCO_2/t_{steel} in 2050 and 0.28-0.31 tCO_2/t_{steel} by 2100. BRA is the only region that ever reaches net negative emissions, which happens in scenario 1.5C by 2045, due to increased recycling, expansion of Charcoal BOF w/CCS, and replacing Coal-based BOF to DRI-EAF.

As part of the global well-below 2-degrees strategy, the iron and steel sector reduces by 22%, 35%, and 59% its CO2 emissions by 2030 in scenarios 2C, 1.7C, and 1.5C, respectively, compared to scenario NPi in the same year. In 2050, these values are 36%, 68%, and 71%. Global emissions stabilize around 700-900 $MtCO_2yr^{-1}$ levels by 2040, 2050, 2070 in scenarios 1.5C, 1.7C and 2C, also indicating anticipated action in more stringent scenarios (Figure 7a).

Although global production increases, total final energy use stabilizes across all scenarios: 27-37 $EJyr^{-1}$ by 2030, 37-33 $EJyr^{-1}$ by 2050, and 32-33 EJ yr^{-1} by 2100 (Figure 7b). This is primarily due to efficiency gains, reductant switch from coal to gas, and increased recycling. Efficiency improvements are more relevant in the NPi and 2C scenarios, where efficient BOFs replace traditional BOFs (Figure 8b), whereas in scenarios 1.7C and 1.5C EAFs replace BOFs as the primary steelmaking technology, driving DRI production (Figure 8c). These shifts occur earlier and to a greater extent as mitigation ambition increases. After mid-century, BOF capacity is fully equipped w/ CCS in all mitigation scenarios, which allows for a resurgence in coal use. Interestingly, scenario 2C presents the earliest deployment of BOF w/ CCS, with 8% of total capacity in 2030. Scenarios 1.7C and 1.5C present this level only in 2040 and after 2050, respectively, as EAF (DRI-based) rapidly increases capacity to reach 49% and 54% by 2050, respectively.

This drives DRI production in these scenarios to reach 1154 Mt yr^{-1} and 1258 Mt yr^{-1} (32% w/CCS), respectively. This highlights a more important role of transitioning to gas than coupling CCS to BOFs in more ambitious scenarios, especially in the 2025-2050 period.

Additionally, the increased recycling across all scenarios (from 23% in 2010 to 31-40% over the century in all scenarios) contributes to lowering the total final energy use, as Scrap-EAF requires much less energy to remelt metal scrap back into crude steel. These figures are lower than in similar studies that assessed steel stocks and flows with higher detail, such as those conducted by Keramidas et al (2024) (57% by 2050) [130] and IEA's Net-zero Roadmap (48% by 2050) [187], which indicate an even higher potential of steel recycling in mitigation scenarios.

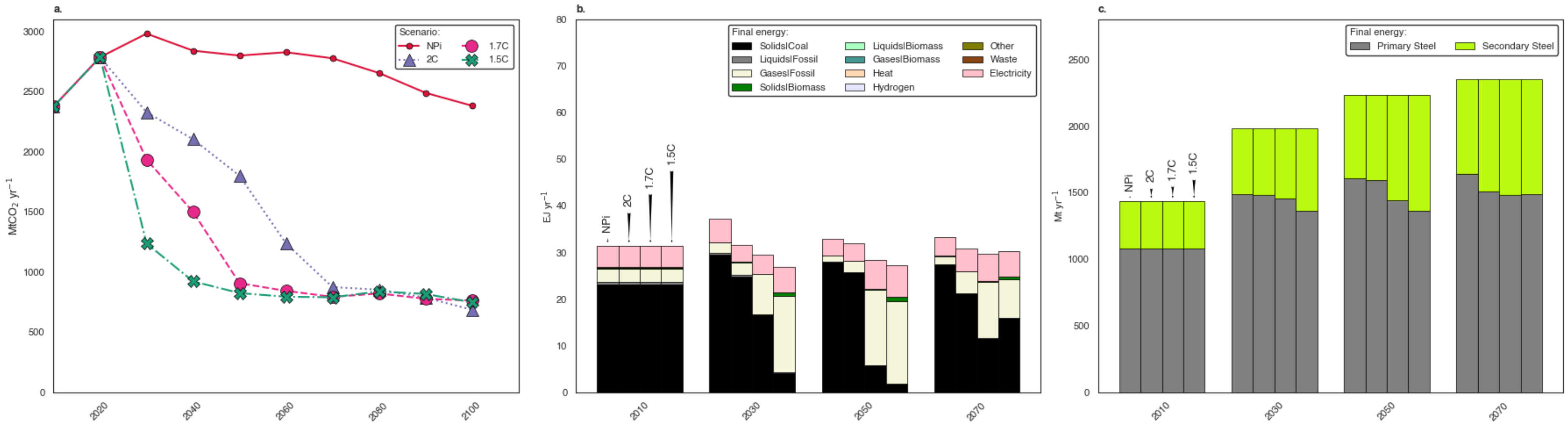


Figure 7. Global steel emissions (a), final energy use per energy carrier (b), primary and secondary steel production (c).

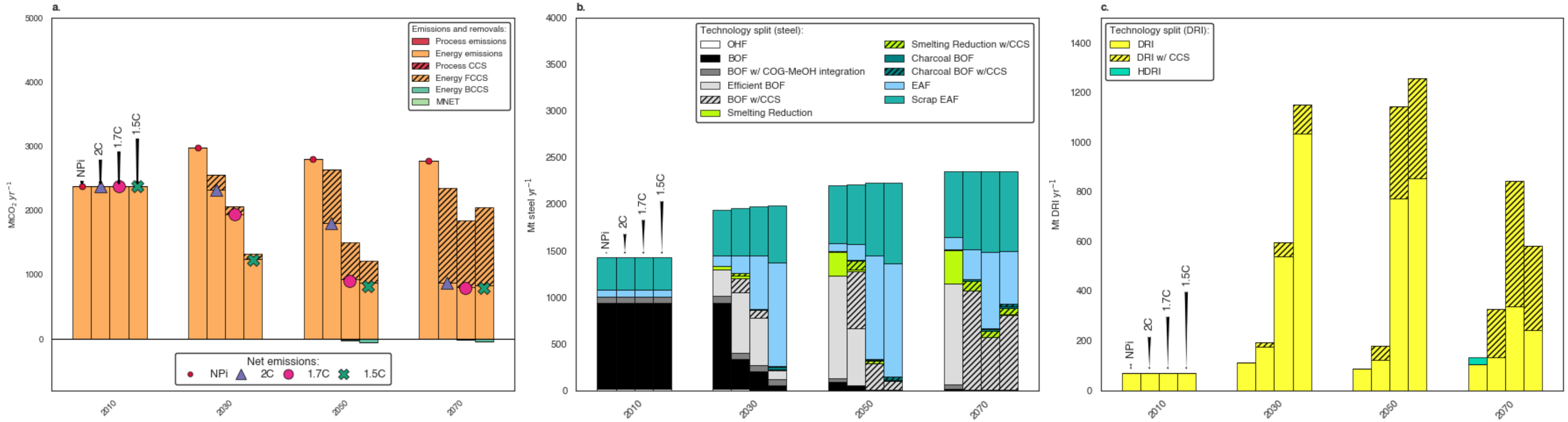


Figure 8. Global iron and steel emissions and removals split (a), steel production split (b), and DRI production split (c).

3.3.1.2.3 Chemicals

In contrast to the cement and steel sectors, results for the chemicals sector suggest the potential not only to achieve net-zero targets but also to contribute to net negative emissions, as depicted in Figure 9a. This happens in 2050 under the scenario 1.5C (-730 Mt CO_2 yr^{-1}) and 2060 under the scenario 1.7C (-452 Mt CO_2 yr^{-1}). Under scenario 2C, the chemicals sector reaches around net-zero by 2070 (3 MtCO_2 yr^{-1}). This result is largely associated with the increased use of biomass for non-energy purposes in mitigation scenarios, as illustrated in Figure 4c. Figure 10 a-c show that bio-based feedstock is predominantly used in ammonia production (Figure 10b), where biogenic carbon is captured via biomass gasification w/ CCS. Ammonia production with electrolysis-based H_2 increases its relevance in more stringent scenarios, as shown in Figure 10b.

Fossil fuels remain the most relevant feedstock for HVCs (Figure 10a), although the use of bio-based feedstock for non-recycled and non-incinerated plastics shows an opportunity for negative emissions, which is key for the chemicals sector to achieve negative emissions by 2050 (Figure 10a). Carbon storage in biomaterials become particularly relevant for AFR, BRA, CHN, and IND regions in mitigation scenarios, reaching 11-47, 20, 10-126, and 83 MtCO_2 yr^{-1} of removals by 2050 in mitigation scenarios, respectively. Since fuel switching to biomass and CCUS are strategies used for both feedstock substitution in the chemicals sector and mitigation measures across all sectors, there is competition for these resources. Because part of the carbon in fossil fuels used for non-energy purposes remains in products like long-lived plastics and asphalt, the model allocates biomass to sectors and applications where the fossil carbon would typically be released back into the atmosphere.

For methanol production, CO_2 hydrogenation (i.e., via CCU and hydrogen generation) becomes the key technology after mid-century (Figure 10c). The capacity for methanol-based processes (MTO/MTA) increases to 6% of total HVC production by 2050, 5-9% by 2070, and 9.6-9.9% by 2100. This expansion drives the demand for methanol for non-energy purposes, projected to rise by 1.3-4.5 times by 2050, 4.8-7 times by 2070, and 9.2-9.6 times by 2100, compared to 2010 levels. The increased role of methanol as a chemical intermediate to HVCs is supported by part of the chemistry and process engineering literature [188], focusing on the so-called “Methanol economy”, first introduced by Olah (2005) [189] and to some extent also the IAM literature [25].

Finally, low-temperature heat is electrified in the other chemicals sector, reducing total emissions from chemicals and increasing the electricity share in the total final energy use (Figure 9b).

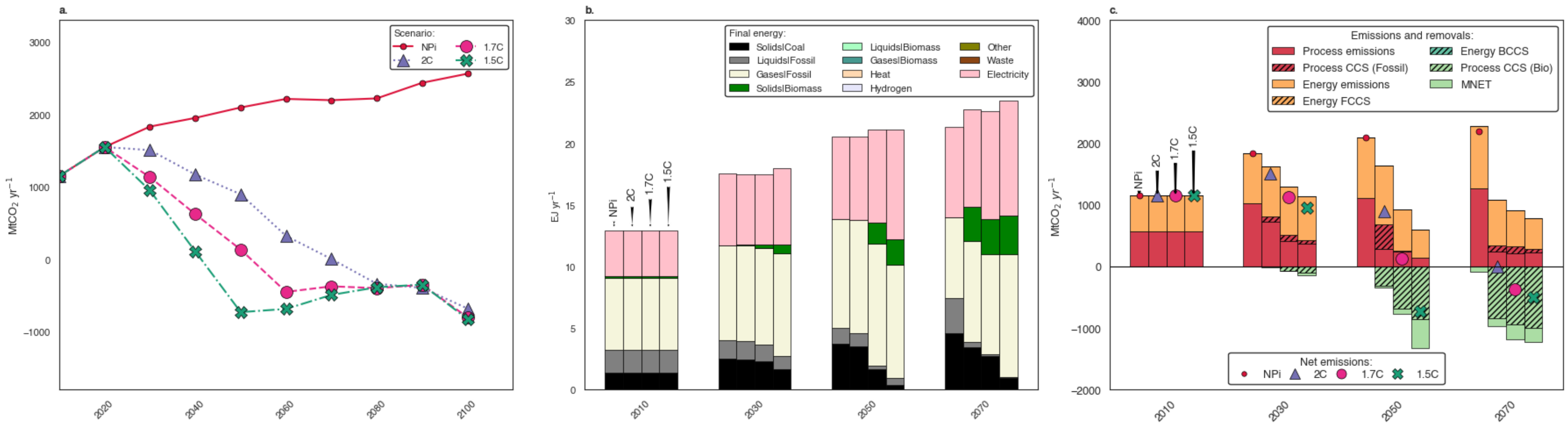


Figure 9. Global CO_2 emissions from the chemicals sector (a), final energy use per energy carrier (b), and CO_2 emissions and removals split (c)

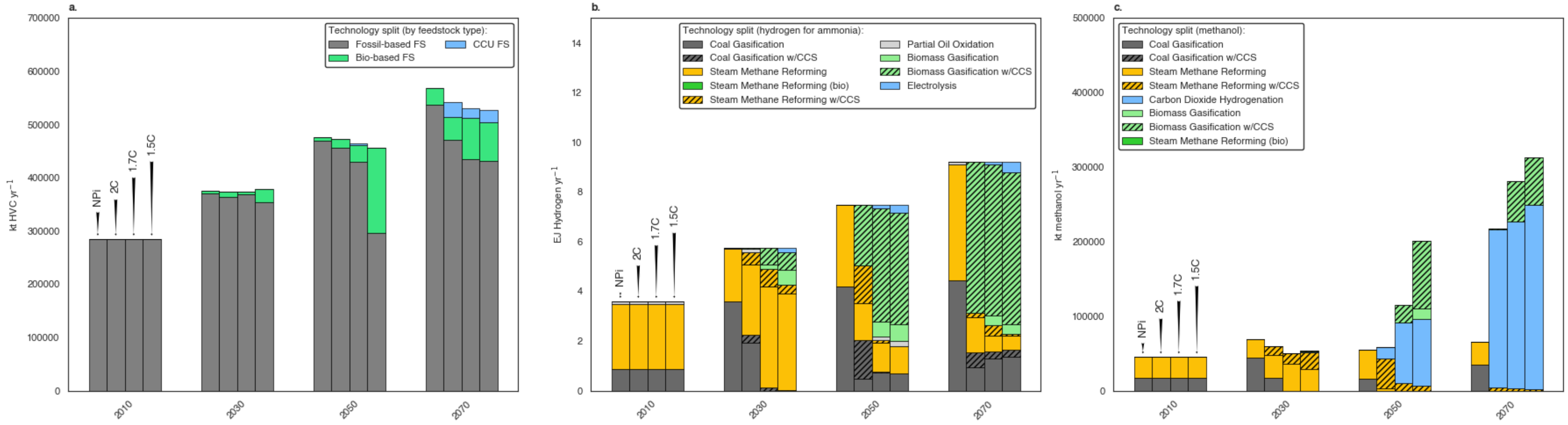


Figure 10. Technology split of HVC production by feedstock type (a), hydrogen production for ammonia (b), and methanol production (c).

3.3.1.2.4 Other industries

The Other industries sector encompasses all the other industries not explicitly represented in the model, i.e., paper and pulp, food and beverage, non-ferrous metals, and other manufacturing industries. In general, the strategy for the Other industries sector follows the total industry overview (Figure 4): the higher the climate ambition, the earlier the coal phase-out and the faster the electrification. This is particularly relevant for this sector, which can more easily electrify low-temperature energy services. From 28% in 2010, electricity use by 2050 reaches 46% under scenario 1.7C and 62% under scenario 1.5C.

3.3.1.3 Sensitivity Analysis

Results from the biomass and CCS restricted scenario (1.5C_r) indicate that industrial emissions do not reach the low levels observed in scenario 1.5C, with residual emissions summing up to 3171 $MtCO_2$ yr^{-1} by 2050. This is primarily due to the chemical sector failing to reach negative emissions because of reduced availability of alternative feedstock by 2050, although it still attains net-zero by 2070. After 2050, rather than experiencing emissions rebound, global industrial emissions continue to decline, reaching 2179 $MtCO_2$ yr^{-1} in 2070 and 1600 $MtCO_2$ yr^{-1} in 2100. This sustained reduction is largely driven by the cement and steel sectors, which maintain a similar emissions trajectory until 2050 as scenario 1.5C but continue to reduce emissions post-2050 by lowering the clinker-to-cement ratio and further reducing the use of coal w/ CCS, respectively.

This scenario demonstrates that while the chemical sector's ability to achieve net-negative emissions is compromised in the 1.5C_r scenario, the steel and cement sectors must perform more ambitiously to ensure the overall system achieves net-zero, compensating for the restricted emissions reductions in other "easier-to-abate" sectors (Figure 11 and Figure 12).

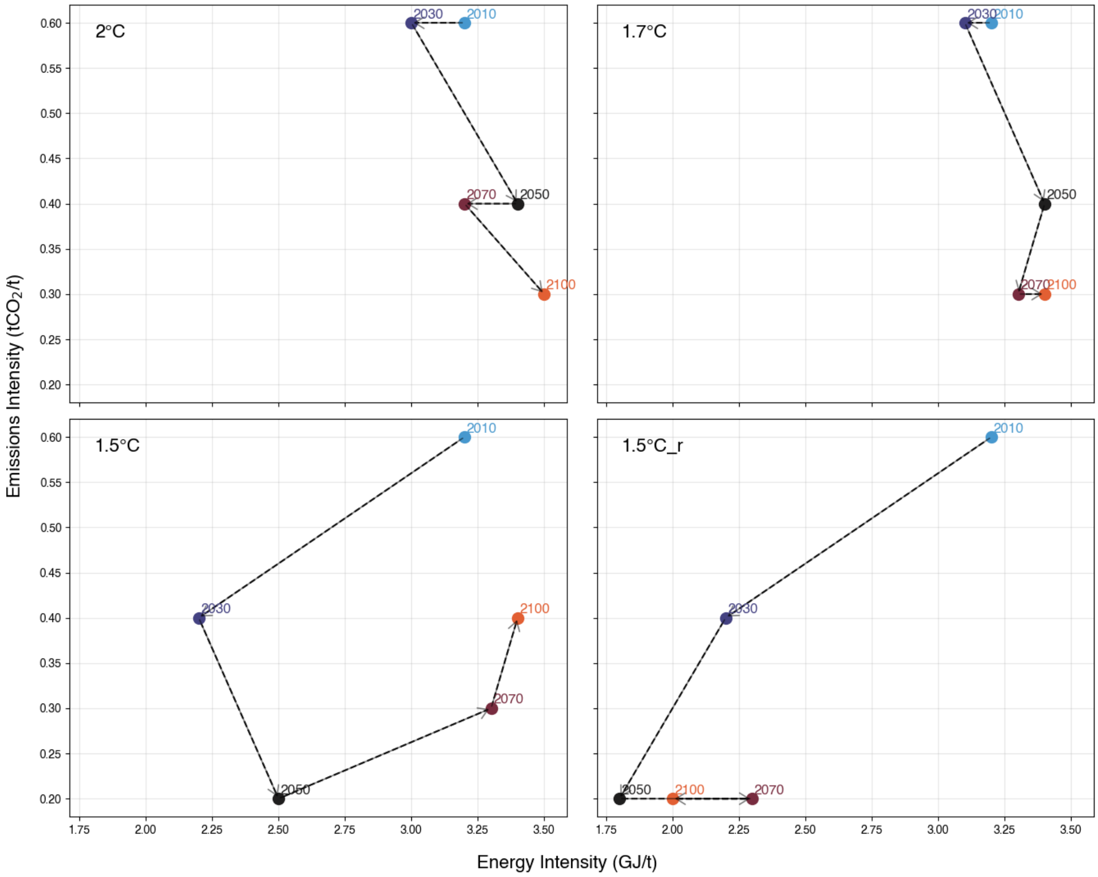


Figure 11. Energy and emissions intensity profile of the global cement industry

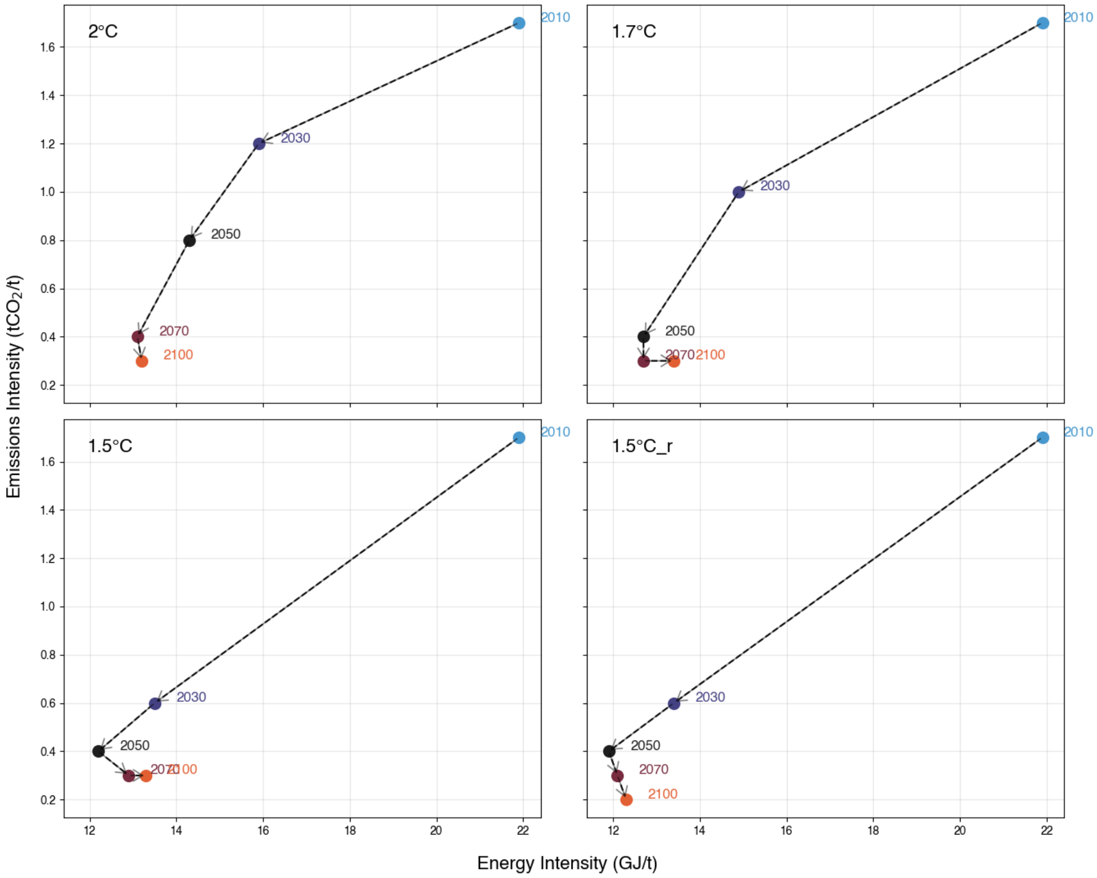


Figure 12. Energy and emissions intensity profile of the global steel industry

Figure 13 illustrates the scale and share of industrial CCS deployment compared to "Other CCS," which refers to carbon captured outside the industrial sector boundaries. As ambition increases, global CCS scale-up happens earlier and deployment in the 2025-2050 period becomes increasingly higher. However, increased ambition leads to total industrial CCS reduction in absolute and relative terms in the same period. In 2050, total industrial CCS amount to 2478 $MtCO_2yr^{-1}$ (72%), 2170 $MtCO_2yr^{-1}$ (30%), and 1868 $MtCO_2yr^{-1}$ (25%) under scenarios 2C, 1.7C, and 1.5C, respectively. Nevertheless, while fossil industrial CCS (FCCS) decreases, bio-based CCS increases, particularly in the chemical sector, due to its potential to deliver negative emissions. These are reduced in scenario 1.5_r as CCS and biomass are restricted.

Our least-cost pathway analysis indicates that, with increased ambition and if CCS in other sectors can offset residual industrial emissions, they will do so. However, when both CCS and biomass are limited, the model optimally allocates these restricted options across sectors. This means that some sectors may gain and others loose CCS capacity, while the whole system experiences an overall reduction in CCS availability. As a result, the industrial sector adopts alternative strategies to meet the 1.5-degree target. These results indicate that in scenarios with increased ambitions, fossil fuel assets have limited life expectancy, even if coupled with CCS. Particularly when CCS is restricted, a larger share of bio-based CCS is allocated to the industrial sector.

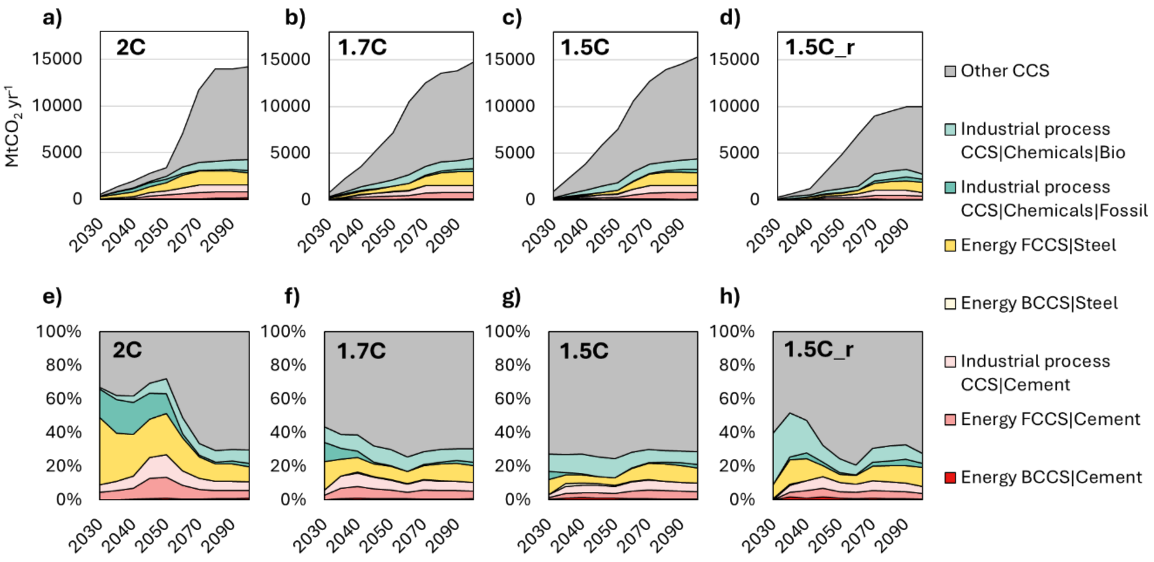


Figure 13. Carbon capture and storage (CCS) pathways for scenarios 2.C (a), 1.7C (b), 1.5C (c), and 1.5C_r (d), as well as their respective shares (e-h).

Industrial Process CCS refer to CCS of process emissions. Energy FCCS refer to CCS of fossil-based energy emissions within the industrial sector, and Energy BCCS refers to CCS bio-based energy emissions within the industrial sector

3.4 Discussion and final remarks

This study used a perfect foresight linear programming optimization model with an integrated view of the global energy-land-emissions system to explore the contribution of the industrial sector to climate change mitigation in well-below 2ºC scenarios. Residual emissions and their role as “hard-to-abate” were also analysed in each sub-sector. Below, we summarise its four main contributions.

Firstly, significant challenges hinder the industrial sector from achieving carbon-neutrality in all assessed scenarios, particularly due to the long lifespan of existing infrastructure such as kilns, BOFs, and crackers in the cement, steel, and chemicals sectors, respectively. Challenges include the difficulty of replacing fossil-based reductants and feedstocks in the steel and chemicals sectors and finding alternatives to clinker in cement production. Global industrial emissions reach 1300-7600 $MtCO_2yr^{-1}$ by 2050 in well-below 2ºC scenarios. However, several regions present net-zero industry by the 2040-2060 window (AUS, BRA, CAN CAM, SAM) in scenario 1.5C, indicating that there are sub-sectoral and regional opportunities to be leveraged and further explored. For instance, biomaterials used in long-lived applications coupled with biomass gasification coupled with CCS for ammonia production lead to negative chemicals sector across many regions, and the use of charcoal for steel production leads to BRA being the single region to achieve net-zero emissions in the sector in scenario 1.5 by 2045. Industrialization, population growth, and infrastructure development have a critical role in defining emissions and technology pathways across regions.

Secondly, regardless of the scenario assessed, the period up to 2030 is the most critical to the industrial transition; investments made now will significantly impact asset performance and emissions until at least 2070. This underscores the urgency of immediate action and investment in low-carbon technologies and infrastructure. Recent investments made in fossil-based petrochemical and steel capacity in China illustrate the increasing challenge of attaining high-levels levels of emissions reduction and feedstock switch as they lock in carbon-intensive infrastructure and long-lived equipment [190], [191].

Thirdly, an integrated perspective is critical to understand the role of the industrial sector considering the competition for low-carbon resources and investments to achieve global climate targets. Many studies that have a sectoral focus find ambitious results for the industrial sector, reaching net-zero and lack the integrated perspective. Therefore, they fail to capture the synergies and trade-offs of resource use within a broader system. For instance, the potential for negative emissions in the chemical sector is largely dependent on the availability of CCS and biomass, which is extensively used as a mitigation measure in other sectors as well and therefore require an integrated perspective. On the other hand, the integrated perspective may equally fail to capture the full potential of decarbonization of the so-called “hard-to-abate” sectors if other sectors can carry that burden of global mitigation with lower cost to the system. Our results show that, while industrial emissions stemming from high-temperature heat service provision and process emissions can be challenging to mitigate, the extent to which they still present residual emissions after global net-zero largely depends on how “easy” (i.e., less costly) it is to abate the emissions in other sectors. Therefore, we should be careful when interpreting sectors that present residual emissions as hard-to-abate when they could be simply compensated by “easier-to-abate” sectors. Therefore, “hard-to-abate” and “residual emissions” require consistent definitions and well-defined criteria. Understanding what makes a sector hard-to-abate—whether it is the technical feasibility, market dynamics, geopolitical context, or regulatory environment—is crucial for developing effective decarbonization strategies.

Fourth and lastly, our study highlights that the industrial sector demands solutions beyond supply-side energy-related solutions. These include demand-side (e.g., more intensive use of buildings, increased lifetimes and reuse of products) and supply-side (e.g., improving manufacturing yields, pre-consumer scrap recycling, product design changes, material substitution) material efficiency measures. These measures are hard-to-model and data-intensive in a global and integrated framework. However, the lack of consistent and comprehensive data further complicates industrial net-zero and reinforces the role of industrial sector as hard-to-abate. Therefore, if on one hand our results show the inflexibility of the industrial sector and support the difficulty to abate emissions in the industrial sector, on the other hand, it also indicates that a systemic transformation is required in materials production and use.

The potential for the industry to achieve net-zero emissions by 2050 is not fully accomplished in the COFFEE model due to several reasons. One key issue is the incomplete (i.e., in terms of limited coverage of materials explicitly represented) and inconsistent (i.e., between total material production and total material required in demand sectors) representation of material flows and stocks, which limit the ability of assessing material efficiency solutions in our model. While we account for recycling and clinker reduction, these measures are simplified and neither they capture the full spectrum of material efficiency strategies available, nor the material cycles. Understand the full mitigation potential of these measures is critical for designing policies that can harness of this potential and at the same time reduce the reliance in CDR.

Therefore, model development to support future studies should focus on three main topics: 1) representation of material stocks and flows, aiming to link material production to services and including circularity and material efficiency measures; 2) improving the representation of commodities trade to include the possibility of commercialization of intermediate of final products (i.e., low-carbon DRI or steel) as well as scrap metal; and 3) advance the representation of materials to the mineral extraction sector, in terms of energy use and related emissions, endogenous representation of resources and reserves along with regional cost supply curves, and linked to the technological development associated with the energy transition.

4 UNADDRESSED NON-ENERGY USE IN THE CHEMICAL INDUSTRY CAN UNDERMINE FOSSIL FUELS PHASE-OUT*

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Abstract

Around 13% of fossil fuels globally are used for non-combustion purposes. Fossil fuel processing plants, such as petroleum refineries, exhibit interdependent material and energy system dynamics, making the transition away from fossil fuels energy systems become more challenging without addressing the non-energy outputs. This study explores the future role of fossil fuels for non-energy purposes in climate-stringent scenarios with restrictions on alternative feedstock availability, focusing on the primary chemicals sector. Using a global integrated assessment model with detailed refining and primary chemicals sectors, findings across various scenarios reveal that up to 62% of total feedstock use in the chemical sector could be provided by alternative sources by 2050. This would require significant scale-up in biomass utilisation and carbon capture technologies. Annual CO_2 emissions from the chemical sector could be reduced to as low as -1Gt CO_2 by the same year if carbon storage in non-recycled and non-incinerated bioplastics is accounted for.

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* Supplementary Methods, Figures and Tables of this Chapter can be found in Appendix A.

4.1 INTRODUCTION

In the 2023 United Nations Climate Change Conference (COP28) Global Stocktake (GST), nearly 200 parties agreed on "transitioning away from fossil fuels in energy systems, (...), so as to achieve net zero by 2050 in keeping with the science". Around 30 Exajoules (EJ), or 13% of the world's total fossil fuel production, are used for non-energy purposes. Of this, two-thirds are used as feedstocks for primary chemicals production[12], [75], which contributes to approximately 1 $GtCO_2yr^{-1}$ of emissions. This earns the sector a dual role as hard-to-abate and hard-to-defossilize in mitigation pathways. Yet, there is no reference to the non-energy use of fossil fuels in the GST, revealing that key material-energy links remain unaddressed by global climate policy.

With the demand for fossil fuels in energy systems projected to decrease[192], the materials systems will also be affected primarily because fossil fuel plants simultaneously co-produce fuels and feedstock for materials production. Naphtha, the main feedstock used to produce high-value chemicals (HVCs) (i.e., ethylene, propylene, butadiene, and aromatics), is inexpensively co-produced with diesel, gasoline, and aviation fuels. Refinery units directly co-produce propylene[193] and aromatics[194] while producing fuels. Natural gas (for example, in North America and the Middle East) and coal (mainly in China and South Africa) are also key feedstocks for producing methanol[178] and ammonia[195].

Meanwhile, the last greenfield fuel-oriented petroleum refineries are expected to be those under construction[196] as new refining capacity presents increasingly higher petrochemical integration[197]. Nevertheless, fuel-oriented refineries are projected to remain operating after mid-century given the long-lived and capital-intensive nature of their assets.

Simultaneously, the demand for materials, as well as its feedstocks, are expected to grow [198]. These materials include but are not limited to synthetic polymers, chemicals, fertilisers, and other non-energy oil products such as lubricants, asphalt, and solvents [199]. This may be partly attributed to the energy transition itself in the form of the materials requirements for timely and at-scale deployment of renewable energy technologies such as lightweight car parts, solar panel components, wind turbine blades [200], and fertilisers for biomass production[201].

This shift in oil products' demand and supply patterns raises essential questions about the future of the symbiotic relationship between fossil fuels and primary chemicals in a world striving to achieve stringent climate targets. Many studies have addressed long-term strategies to reduce emissions of primary chemicals to reach climate targets based on fuels switch for process heat generation, feedstock substitution, carbon capture, utilization, and storage (CCUS), and circular (bio)economy. These strategies have been thoroughly analysed in the literature[23], [25], [26], [27], [129], [202] individually or in combination.

Despite the decreasing demand for fossil fuels in energy systems due to climate policies[192], [203], [204], the co-production of energy, feedstocks, and chemicals in petroleum refineries and implications to energy use and emissions pathways across sectors remain largely unexplored[205]. Aiming to fill this gap, this article investigates the role of the chemical sector in a global net-zero strategy. Our hypothesis is that the chemical sector, while being both hard-to-abate and hard-to-defossilize, can offer strategic contributions to deep decarbonisation, both sectoral and systemically. An integrated assessment perspective is essential to understand: 1) How the integration of a growing chemical sector with the oil refining sector affects fossil fuels phase-out and decarbonization of chemicals; and 2) The competition for CO_2 (i.e., CCUS), hydrogen, and biomass for feedstock substitution with other mitigation measures across sectors that also rely on these resources to reduce emissions. To address this, we use the Computable Framework For Energy and the Environment model (COFFEE), a global integrated assessment model (IAM) based on the MESSAGE framework that accounts for various types of oil qualities and refinery typologies, along with an explicit representation of primary chemicals [204], [206]. To our knowledge, none of the Intergovernmental Panel for Climate Change (IPCC) scenarios in the Sixth Assessment Report (AR6) assessed the role of fossil fuels as feedstocks for primary chemicals in detail while assessing refinery activity and co-production [132]. Questions that remain unaddressed, particularly from a global integrated assessment perspective, are the supply of materials co-produced in refineries with decreasing utilisation factors, the availability of alternative feedstocks in the required scale and speed, the final use of biomaterials and whether and for how long they store biogenic carbon. Beyond sector-specific net-zero targets, an integrated perspective is essential for understanding the nexus between energy, materials, emissions, land use, and carbon across different sectors, including primary chemicals.

With a focus on supply-side mitigation measures, we explore global technological pathways, carbon feedstocks, energy use and direct emissions scenarios for the primary chemicals industry in scenarios considering Implemented National Policies (NPi) and climate policies aiming at limiting global average temperature increase to below 1.5^{o}C above pre-industrial levels (1.5C) by 2100. We also test a set of restrictions to limit alternative feedstock availability throughout the century in different pathways aligning with a below 1.5^{o}C scenario, namely: (i) the assumption that biogenic carbon is stored in unrecycled/unrecovered biomaterials is turned off (MNEToff); (ii) limited scale-up of global carbon capture and storage (gCCS), which also affects the availability of CO_2 as carbon feedstock; (iii) limited global biomass availability (PBIO), which affects both energy and non-energy applications, and (iv) a combination of all restrictions above (all). We further discuss how these constraints impact and are influenced by the energy sector.

Our study demonstrates that the timely and scaled supply of alternative carbon feedstocks to the chemical sector is crucial for meeting climate goals and phasing out fossil fuels. Scenarios with limitations on biomass supply, carbon capture and storage (CCS) deployment, and carbon storage in biomaterials require earlier and more extensive climate action, and show an additional reduction of at least 6 $GtCO_2$ per year by 2030 compared to the 1.5C scenario. The competition between mitigation and feedstock substitution is evident, as restrictions on bio-based feedstocks and CCS lead to a higher reliance on fossil fuels for producing primary chemicals, prolonging oil use throughout the century. However, we also find that the chemical sector can adopt strategies to ease the burden on other sectors by reaching net removal levels as low as -1$GtCO_2yr^{-1}$ by 2050 if the right policies and conditions are established.

4.2 RESULTS

4.2.1 Global CO_2 emissions and fossil fuel use

Our results show that scenarios with stricter restrictions on global biomass availability, deployment of CCS, and biogenic carbon storage (or material net – MNET) require taking climate action faster, sooner, and on a larger scale, as demonstrated in Figure 14a. Global CO_2 emissions in the scenario with all restrictions must be reduced by at least 6 $GtCO_2$ per year more than in scenario 1.5C by 2030 to stay within the CO_2 budget. This illustrates that CCS and biomass availability are critical in mitigation across all sectors, including but not limited to the primary chemicals. These restrictions also explain the difference between achieving global net-zero CO_2 emissions around 2050 or 2060.

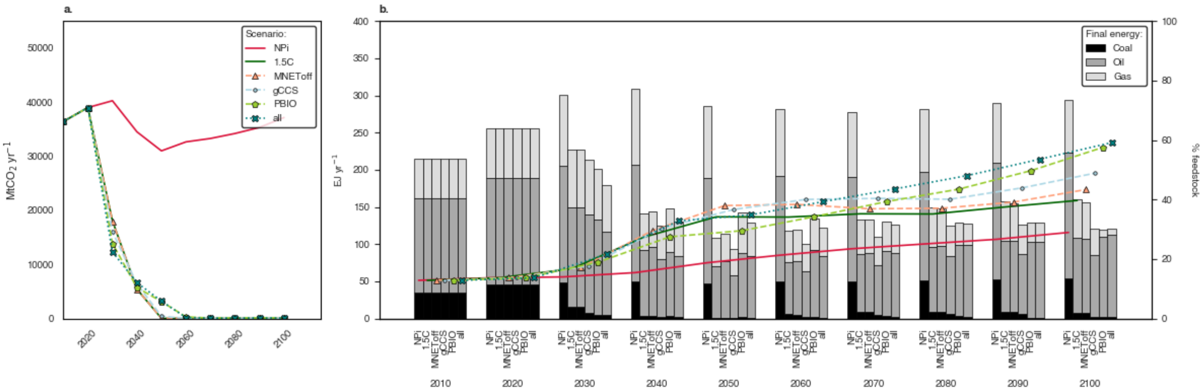


Figure 14. Long-term global CO_2 pathways, fossil fuel use and feedstock share across scenarios and sensitivities analysed.

a. Global CO_2 pathways (2010-2100). **b**. Global fossil fuels use (left axis, represented by the stacked bars) and its share used for feedstock purposes (right axis, represented by the lines with scenario markers) (2010-2100). EJ: Exajoules; NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. Source data are provided as a Source Data file.

While all mitigation scenarios present a similar trajectory to achieve 1.5°C below pre-industrial levels, we identify distinct fossil fuel use trends, especially after mid-century (Figure 14**Error! Reference source not found.**b). By 2050, we see that fossil fuels use is reduced from 2020 levels in all of the 1.5°C scenarios: coal use is reduced by 95-99%, gas by 19-47% and oil use by 40-60% (Figure 14b).

On the other hand, oil use shows less potential for reduction by 2100 (22-42%) when compared to gas (22-87%) and coal (82-97%). The resurgence in coal use observed after mid-century aligns with the IAM scenario literature and is attributed to the combining effects of: 1) A rising energy demand in regions projected to experience significant population and affluence growth post-2050 (i.e., Africa, Southeast Asia, and India), 2) Escalating costs of oil and gas, and 3) Coal use transitioning to include carbon capture[192].

At the same time, the output of fossil fuels transitions away from combustion to non-energy purposes in the NPi scenario, and this trend intensifies in mitigation scenarios. The share of fossil fuels use as non-energy increases from 14% in 2020 to 30-38% in mitigation scenarios by 2050; by 2100, these values further increase to 40-59%. In other words, as restrictions arise in the supply of bio-based feedstocks and the scale-up of CCS (i.e., feedstock based on Carbon Capture and Utilization - CCU), more fossil fuels – particularly oil – will be required to fulfil carbon-based feedstocks. This happens simultaneously with the electrification of passenger vehicles, leading to gasoline oversupply. As gasoline and naphtha share a similar carbon range, gasoline replaces naphtha as feedstock for HVCs. Therefore, oil use persists throughout the 21st century in our results through these two self-reinforcing mechanisms: (i) gasoline-naphtha substitution flexibility and (ii) insufficient expansion of alternative feedstocks to fulfil the growing primary chemicals demand. This combination leads oil refineries to remain operating in our model for longer, thereby producing fuels, chemicals and feedstocks.

4.2.2 Oil production and refineries' utilisation factors

Refineries are capital-intensive plants with limited flexibility concerning their product outputs[207], [208]. They are designed to optimise profit margins, which are influenced by the quality of crude oil and the product slate required by consumers. Typically, the complexity of refinery operations increases when the crude input shifts from sweet and light to sour and heavy grades, which requires advanced processing units such as Hydrocracking. The product slate is primarily focused on gasoline and diesel but may also extend the production of specialised products like aviation fuels, petrochemical naphtha, and lubricants, depending on market demands.

Our results highlight three trends in the refining sector in mitigation scenarios, which intensify in the more restrictive scenarios. Firstly, the refining sector shrinks in capacity throughout the century (see Supplementary Fig. 10); its utilisation factor also reduces until 2050. Total refining capacity in terms of oil input reduces from ~191

EJ.yr^{-1} in 2010 to 103 (1.5C) -132 (all) EJ.yr^{-1} in 2050 and 44 (gCCS) – 77 (all) EJ.yr^{-1} in 2070. The upper limits are set by the scenario all, not NPi, indicating that highly restricted scenarios foresee a greater demand for oil. Furthermore, the utilisation factors drop from ~70% in 2020 to 30-50% in mitigation scenarios by 2030 and then increase to 100% in 2070 once the new capacity is built. This follows the dynamics of capital optimization to maximize long-term value of newly built capacity considering energy and non-energy demands.

Secondly, greenfield refineries become more complex. While old and inefficient refinery capacity dies, new capacity is built based on the Hycon technology, the most complex refinery typology in the COFFEE model. It represents a refinery with hydrocracking and residue hydro desulphurisation units, thus allowing for different oil qualities while achieving higher conversion rates.

Thirdly, greenfield refineries have higher integration with petrochemicals. Although refinery-sourced chemicals are reduced by 49-77% in 2050 in mitigation scenarios (Supplementary Fig. 10), the refinery capacity that survives after mid-century is up to 15% more integrated to petrochemicals than current figures.

4.2.3 Carbon feedstock sources in a carbon-constrained world

Pathways for carbon feedstocks in primary chemical production are presented in energy (Figure 15a) and mass (Figure 15b) terms. By that, we aim to compare fossil and bio-based hydrocarbons, which can be used as either energy or feedstocks, and CO_2, which results from carbon capture in the model and is not an energy carrier. Results indicate that mitigation scenarios see an increase in liquid and solid biomass use in the chemical sector, reaching 6-25 EJ.yr^{-1} by 2050 and 12-25 EJ.yr^{-1} by 2070. To a lesser extent, CO_2 also becomes relevant as a feedstock, reaching up to 368 Mt.yr^{-1} by 2070. Interestingly, the most significant deployment of CCU is observed in scenarios where biogenic carbon storage is turned off (MNEToff and all), supporting studies that find that the climate advantages of biomass conversion to materials are somewhat contingent on this assumption [209], [210], [211]. Moreover, a comparative analysis of the two plots reveals that feedstock substitution requires more significant mass input to produce an equivalent basket of products. This highlights the variance in fossil and alternative feedstock conversion yields, which have implications for transportation logistics (Supplementary Fig. 7 presents the mass of carbon embedded in feedstocks).

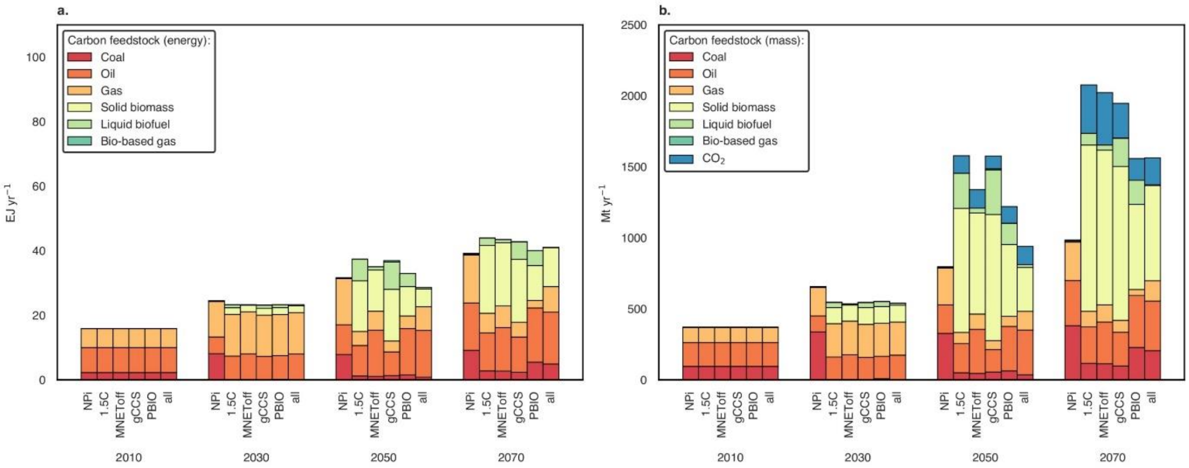


Figure 15. Carbon feedstock sources pathways for primary chemical production.

a. Carbon feedstock in energy terms. **b.** Carbon feedstock in mass terms. Supplementary Fig. 13 and 14 show the regional pathways for biogenic storage in biomaterials and primary biomass use across R5 regions, respectively. While Asia and the OECD90+EU have similar biomass use pathways, the Asian R5 region uses up to three times more for non-energy purposes based on the biogenic carbon storage results compared to the OECD90+EU by 2050. EJ: Exajoules; NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. Source data are provided as a Source Data file.

Fossil fuels used as feedstocks in mitigation scenarios achieve reductions of up to 62% by 2050, respective to NPi. This is quite ambitious considering challenges such as developing new supply chains and transportation logistics for alternative feedstocks. At least 500Mt of primary chemicals capacity is less than 20 years old, and massive investments in fossil-based capacity have been made in the past ten years, particularly in China and Southeast Asia [212], [213]. Significantly, scenarios that present reduced petroleum use as carbon feedstock are compatible with reduced oil production (Supplementary Fig. 9).

The upper bound of feedstock substitution (62%) refers to the gCCS scenario, indicating a higher opportunity for Bioenergy with Carbon Capture and Storage (BECCS) and materials use in long-term applications. The lower bound (28%) refers to the scenario all, reflecting the increased need for oil when alternative feedstock availability is constrained. However, as Supplementary Fig. 9 shows, reminiscent oil demand is met primarily with light and medium sweet oil. These qualities of crude oil have lower emissions and yield a higher output of products per input of raw material [131], [214], [215].

When only CCS is restricted, feedstock substitution is prioritised as a mitigation measure in the chemical sector. As Figure 16d and Figure 16e show, biomass gasification with CCS reaches its highest potential in ammonia and methanol production precisely when CCS is restricted globally. This indicates that, under constraints, BECCS is prioritised in the chemical sector.

4.2.4 Technology pathways and resource allocation

Our results show that Steam Cracking (SC) remains the leading technology for producing HVCs. Ethane SC increases from 9% to 25% of HVC production in all mitigation scenarios between 2010 and 2030, particularly in gas-rich regions such as the Middle East and the United States. Ethane SC has a higher selectivity towards ethylene over other HVCs, compared to Naphtha SC (Supplementary Fig. 2). As a result, switching from naphtha to ethane as a feedstock leads to propylene and aromatics gaps in demand/supply ratios.

Furthermore, as the passenger transport sector gradually electrifies, refineries reduce their utilisation factors and their HVC output (Figure 16**Error! Reference source not found.**b). This results in a gasoline surplus, which becomes cheaper and finds market in the primary chemical sector through Naphtha Catalytic Cracking (NCC) (32-52% of HVC market share by 2070). NCC has a more balanced ethylene/propylene ratio than conventional Naphtha SC[216] (Supplementary Fig. 2) – and catalytic reforming units. In scenario all, the share of electricity use in the transport sector reaches its highest level (37% on final energy use basis considering passenger and freight transport in 2070, see Supplementary Figs. 16 and 17) as biofuels reduce their importance for BECCS given CCS and biomass constraints.

Moreover, reduced HVC output from refineries makes the propylene and aromatics gap more pronounced. NCC deployment is not sufficient to bridge these gaps alone, and on-purpose routes such as Propane Dehydrogenation (PDH), Metathesis (MTT), and Methanol-to-Olefins (MTO) see substantial growth (Figure 16b).

Furthermore, bioethanol is also diverted from an internal combustion engine fuel to ethylene production. Interestingly, the highest level of ethylene from ethanol is achieved in the PBIO scenario, where biomass use is restricted but not CCS. This means that the model prioritises the limited availability of biomass in the ethanol industry, finding an opportunity to produce ethanol with CCS and later store biogenic carbon in biomaterials (Supplementary Fig. 8 presents detailed results on technology pathways for each HVC).

To put it concisely, HVC production remains dependent on fossil fuels throughout the century in mitigation scenarios and across all HVCs. However, scenarios 1.5C and gCCS show that 35% and 51% of HVCs are produced with bio-based feedstocks by 2050, respectively (Figure 16c). As restrictions increase, results for the all scenario seem more and more similar to the results for the NPi scenario, indicating that the lack of availability of alternative feedstocks for HVCs drives the persistent oil use in this sector.

Results on syngas products show that biomass gasification with CCS is favoured for ammonia production due to the potential for BECCS, whereas CCU is preferred for methanol production (Figure 16d, e). While in ammonia production carbon is largely converted into captured CO_2 with high purity, contingent on the efficiency of the capture process, in methanol production, some of the carbon remains in the final product. Therefore, scaling-up biomass use with carbon capture in ammonia production is identified by the model as a source of negative emissions. This can significantly reduce emissions across the overall system both in scale and pace required for reaching 1.5-degrees goals. Nevertheless, water electrolysis coupled with O_2 use in oxyfuel routes for capturing CO_2 could also be effective, although not assessed in this work. Overall, the use of fossil fuels for ammonia reduces over time but remains relevant, especially in more stringent scenarios.

Furthermore, in the gCCS scenario, we see is that the chemical sector is prioritized for capture across various sectors (see Supplementary Fig. 15). Although the global CCS roll-out declines in 2050 compared to other scenarios, the use of CCS in the chemical sector increases because the model chooses to reduce emissions in the sector with the lowest cost. Note that when biomass and CCS are constrained simultaneously (scenario all), this relative advantage disappears. Similarly, when only biomass is constrained, total CCS remains the same but “Energy CCS – Fossil fuels” increases in relative terms, leading to a greater relevance of Direct Air Capture – or ‘DAC’.

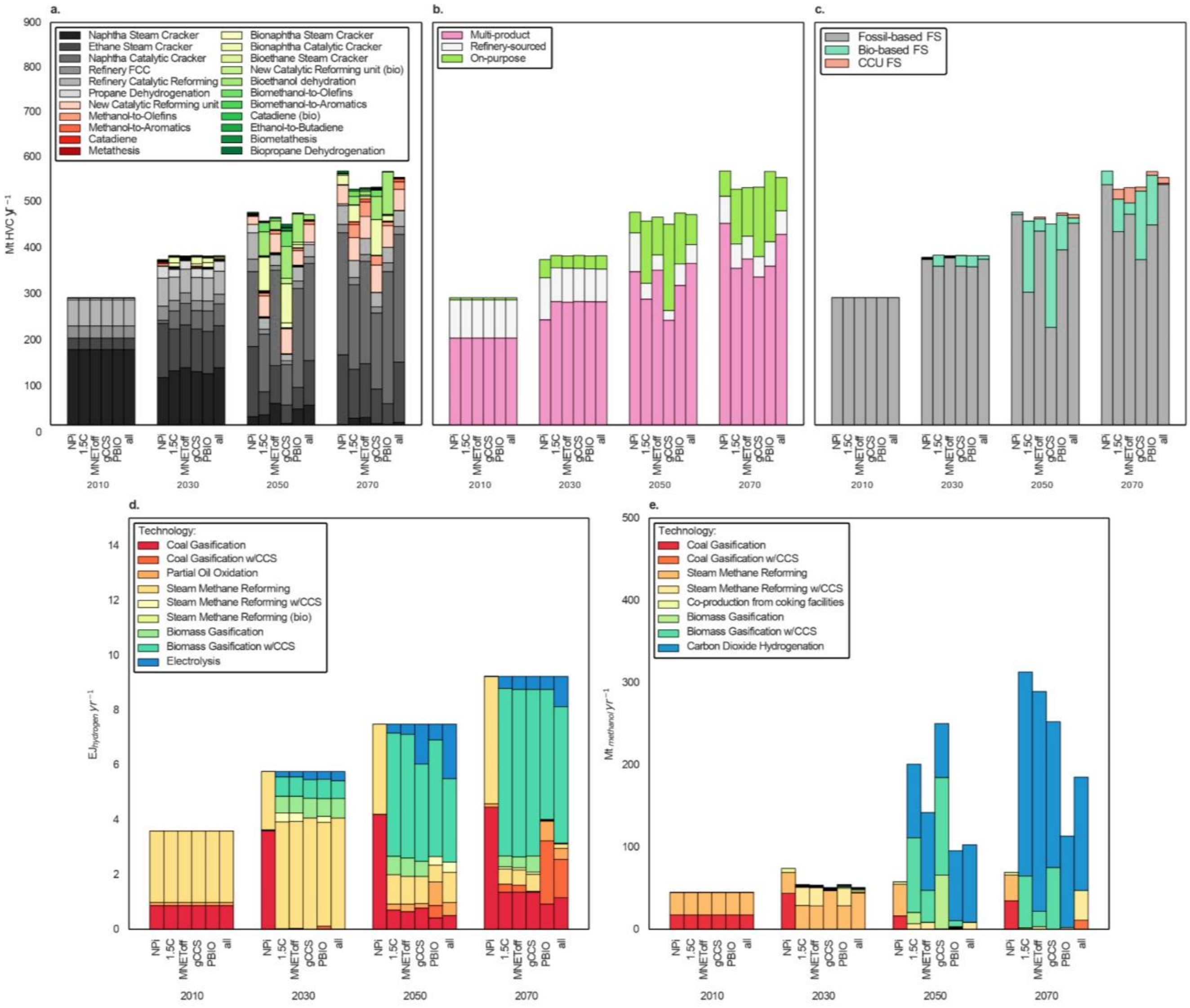


Figure 16.Technology pathways for High Value Chemicals (HVCs), ammonia and methanol.

HVC production is illustrated in three approaches, being **a.** technology split, **b.** technology typology, and **c.** carbon source. In the legend box for plot **a**, colours relate to the feedstocks used as inputs: grey: fossil-based; red: CCU (i.e., CO_2 captured from bio-based or process emissions sources as well as from Direct Air Capture) or fossil-based; green**:** bio-based. Demands for ethylene, propylene, butadiene, and Benzene, Toluene, and Xylenes (BTX) are static, but ethylene can be used as an intermediate for propylene and butadiene via Metathesis and Catadiene (Supplementary Method 2), thus explaining different production levels across scenarios. **d.** Technology split for hydrogen in ammonia. Ammonia demand is static. **e.** Methanol production (only non-energy). Methanol long-term demand is composed of both a static demand and an ancillary demand as an intermediate for ethylene, propylene, and BTX via MTO and MTA. This explains the increased demand after mid-century. EJ: Exajoules; NPi: Implemented National

Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNETоff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. FCC: Fluidized Catalytic Cracking. FS: Feedstock. CCU: Carbon Capture and Utilization. CCS: Carbon Capture and Storage. Source data are provided as a Source Data file.

4.2.5 Emission pathways for the global chemical sector

Figure 17 shows the role of the chemical sector in a 1.5ºC world subject to different restrictions. It achieves a net reduction of -0.73 $GtCO_2.yr^{-1}$ in scenario 1.5C and -1$GtCO_2.yr^{-1}$ in scenario gCCS by 2050. Direct emissions reduction stems mainly from BECCS in ammonia production and biogenic carbon storage, as well as increased efficiency in fossil fuels-based platforms. Not only does the chemical sector not always behave as hard-to-abate from an emissions standpoint, but it can also be a climate asset if bio-based resources are available and the potential of storing biogenic carbon in biomaterials is explored.

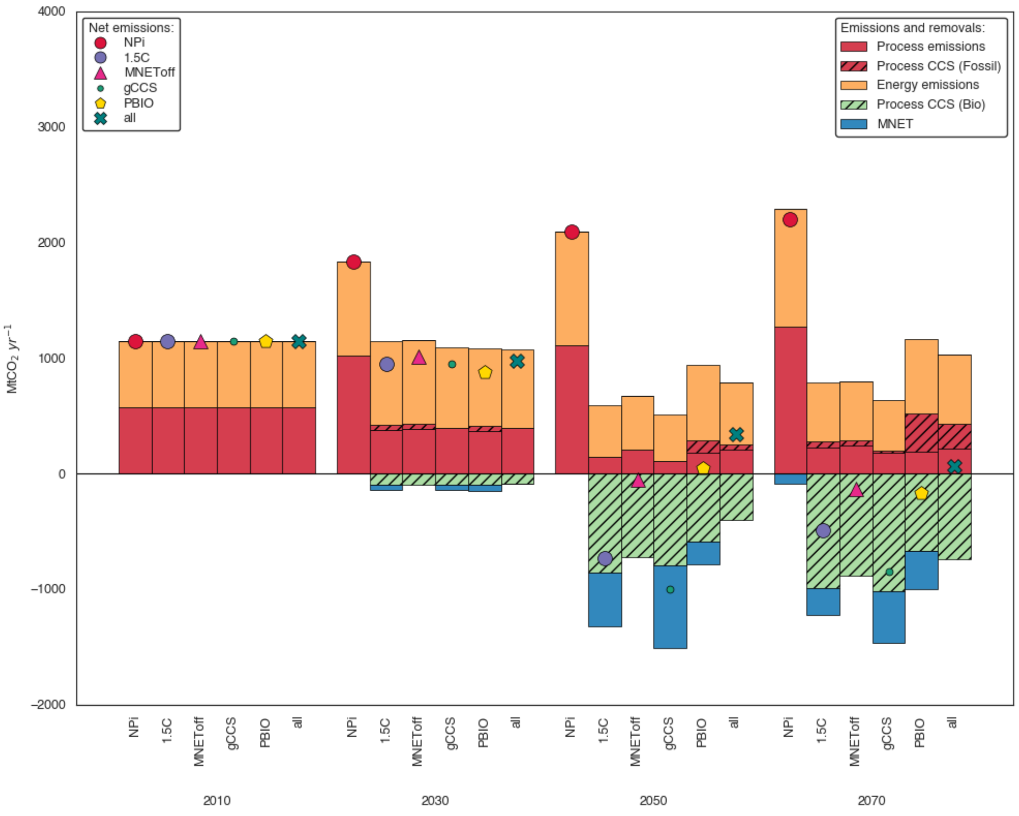


Figure 17. Global direct CO_2 emissions from the chemical sector. Includes direct (Scope 1) emissions from primary chemicals (explicitly modelled in the COFFEE model) and other chemicals (implicitly modelled in COFFEE).

Symbols represent net CO_2 emissions in each scenario. Energy and Process emissions refer to CO_2 emissions resulting from combustion and from chemical reactions not related to energy use, respectively. In this work, we consider emissions from hydrogen production for ammonia synthesis as process emissions. Emissions from incineration and mechanical recycling are also regarded as Process Emissions. ‘Process CCS (Fossil)’ reflects the reduction in emissions achieved through the CCS of fossil feedstock used to produce ammonia and methanol. ‘Process CCS (Bio)’ refers to the removal of CO2 emissions achieved through the CCS of bio-based feedstock used to produce ammonia and methanol. MNET refers to biogenic carbon storage in long-lived materials. Supplementary Fig. 12 presents regional pathways for CO2 emissions in the chemical sector across R5 regions. NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. CCS: Carbon Capture and Storage. Source data are provided as a Source Data file.

However, when all constraints are turned on in the model, the chemical sector remains with residual emissions in 2050, and reaches net-negative emissions only by 2070 (scenario all). This difference of ~1Gt $CO_2.yr^{-1}$ increases the burden on other sectors, which in turn have to extend and anticipate decarbonisation efforts. While accounting for biogenic carbon storage in bioplastics highlights the potential of carbon removal in long-lived applications as a mitigation strategy, it is essential to assess other sustainability dimensions to evaluate its effectiveness as a carbon mitigation strategy fully.

4.3 DISCUSSION

This work contributes to the research field of carbon emissions mitigation in the primary chemicals sector in four ways.

Firstly, we observe that primary chemicals are hard-to-abate but can have a role in promoting systemic decarbonisation. Although decarbonisation technologies are available and could reduce emissions to as low as -1 $GtCO_2yr^{-1}$ by 2050, these reductions heavily rely on the large-scale availability of alternative feedstocks and on accounting for bio-based carbon storage in bioplastics that are neither incinerated nor recycled. In scenarios where alternative feedstocks are limited and carbon storage in biomaterials is not assumed, achieving net-zero emissions in the chemicals sector by 2070 remains elusive.

Secondly, primary chemicals are hard-to-defossilize, leading to critical implications for decarbonisation of the chemicals sector and beyond. Our findings suggest that ambitious feedstock substitution could reduce fossil fuel dependence by approximately 60% by 2050 globally. However, if carbon capture and biomass use are constrained, the feedstock use profile remains essentially unchanged. This reflects both an opportunity and a challenge. On the one hand, substituting feedstock can significantly reduce refinery utilisation, bringing indirect decarbonisation across sectors. On the other hand, failing to transition away from fossil fuel use as feedstock could inadvertently sustain petroleum refining activities, prolonging fossil fuel reliance and delaying the broader transition away from fossil fuels. This scenario could lead to continued fossil fuel extraction and refining focused on feedstock production, potentially resulting in lower-cost fuel co-production, and assets becoming stranded before investments are amortised. These findings highlight critical implications for investments in fossil fuel assets and underscore the need for a more integrated approach to energy, climate, and resource regulation.

Thirdly, transitioning away from fossil fuels will require restructuring within the primary chemicals sector. Steam cracking remained the leading technology for HVC production over the century, largely influenced by the electrification of the transport sector and the resulting diversion of gasoline to the naphtha pool. However, refinery-sourced HVCs will decline due to the shrinking of the refining sector as a result of fossil fuels phase-out policies. On-purpose routes, particularly the ones based on methanol (via MTO, MTA) and ethanol (via BDH, and also influenced by oversupply due to transport electrification) as intermediates, will increase to accommodate feedstock substitutions. The restructuring will also affect methanol and ammonia production; biomass gasification with CCS becomes the preferred route for ammonia, while CCU plays a key role in methanol production. Demand for non-energy methanol in mitigation scenarios is expected to increase two to five times by 2050 compared to NPi. This is primarily due to its importance as an intermediate for HVC production. This shift indicates that solutions are product-specific and every carbon feedstock source will be relevant for achieving climate targets.

Importantly, our scenarios explore a limited set of technologies to understand the role of feedstock supply in achieving net-zero scenarios, assuming unchanged demand patterns for primary chemicals. Given the diverse products and services provided by primary chemicals, detailing and addressing their complexities is challenging. This work aimed to unravel the dynamics of petroleum production and refining within the emissions pathway of primary chemicals by developing drop-in substitution alternatives. Nevertheless, we acknowledge that more is needed to provide a comprehensive view of the potential futures lying ahead for the chemical sector. Historically, energy transitions have redefined systems and triggered material transitions and vice-versa[37]. Hence, transforming the complex network of feedstocks, products, and services developed under the petroleum-based economy and thermochemical foundations since the 1950s will require innovative solutions. Beyond phasing-out fossil fuels in energy systems, these include the development of biodegradable chemicals, material substitutions, and demand-side measures. While these aspects were not the focus of our assessment, they are crucial considerations for future policymaking.

Fourth and lastly, improving the representation of fossil fuels in IAMs to capture relevant material-energy links allows modellers to reach a higher degree of accuracy in depicting systems integration. Representing incumbent energy carriers set to be phased-out in detail enables modellers to provide realistic but ambitious recommendations to policymakers considering their pervasive use across sectors. In this sense, the scope and scale of the required transition in the chemical sector to respond to the climate challenges of the 21st century are diverse and in different stages of the supply chain.

A significant albeit deliberate limitation was not including the demand-side or final disposal insights. It is indisputable that these measures hold a highly relevant potential. Stegmann (2022), for instance, found that recycled plastics could make up to 60% of plastics produced yearly by 2050 [26]. Chemical recycling (e.g., via pyrolysis, gasification, solvolysis) is also highlighted as an alternative to drastically reduce the future demand for virgin plastics [217], [218]. However, we chose to exclude them from this work to analyse the supply-side dynamics in more detail while assuming demand and final disposal shares of plastics as unchanged throughout the century.

Nevertheless, we can draw meaningful conclusions on chemical demand, its final disposal, and its broader role in climate change mitigation. Reducing, Reusing, and Recycling/Recovering chemicals are critical circular economy strategies to minimise the investment needed in innovative technologies. Reducing material demand becomes more relevant to the chemical sector than others, given its reliance on fossil fuels as feedstock and the decarbonisation spillover across sectors. On the other hand, if demand reduces, the potential for negative emissions also reduces if feedstock transitions from fossil to bio-based, as was the case for ammonia production in our results.

Furthermore, introducing Crude-Oil-to-Chemicals (COTC) could significantly impact the chemical industry, potentially increasing yields to HVCs or other chemicals to eliminate the problem of material/energy co-production in refineries. However, we did not consider it in our module representation mainly due to a lack of reliable data, which should be covered in future studies. Moreover, we focus on the production of primary chemicals, assuming that the demand for those products remains similar to historical trends and that substitution follows a drop-in logic. In the long run, assuming increased use of biomass and the high weight of oxygen in bio-based feedstocks, oxidised and oxygenated materials such as polyesters or polycarbonates could become the leading platform for plastics. This is also something to be addressed in future work.

Despite these limitations, the significance of these results also lies in quantitatively assessing the climate burden of the carbon lock-in brought about by the increasing economies of scale and scope of fossil fuel resource abundance over decades. Beyond increasing ambition, a change in perspective is needed to embrace the complexity of systems to design climate and resource policy. Without targeting both energy and non-energy purposes in climate agreements such as the GST, the resilience of the fossil fuel industry will continue to be reinforced across decades. Hence, reimagining futures without oil requires targeted modelling and policymaking efforts beyond promoting renewable energy and green hydrogen scale-up. Therefore, policymakers must consider systems interdependencies to design policy frameworks that account for potential synergies and trade-offs between energy and materials systems as well as non-intended outcomes of climate and resource policy.

4.4 METHODS

4.4.1 The Computable Framework For Energy and the Environment (COFFEE) model

The Computable Framework For Energy and the Environment model (COFFEE) is a perfect foresight, linear programming, least-cost optimisation model built within the MESSAGE framework. The model depicts energy and land-use systems in a single framework for eighteen global regions. It is designed to support policymaking by evaluating potential trade-offs and synergies between climate, environmental and energy policies. GHG emissions are accounted for using the IPCC methodology, which includes emissions from fuels, industrial processes, waste, and Agriculture, Forestry, and Other Land Uses (AFOLU), covering greenhouse gases such as CO_2, N_2O, and CH_4. Emissions from biomass production (land-side) for subsequent conversion into energy carriers or materials are accounted for in the AFOLU sector. Additionally, the model incorporates options for carbon dioxide removal, such as land sinks, carbon storage associated with BECCS or DAC, and the use of materials in long-lived applications. Unlike life cycle assessments (LCA) studies that consider cradle-to-grave emissions, COFFEE focus solely on emissions directly associated with major energy, food, and industrial products. Therefore, energy renewable energy sources like solar and wind are considered to provide zero emissions electricity.

COFFEE was one of the five Illustrative Mitigation Pathways (IMPs) highlighted in the last IPCC 6th Assessment Report[132] and detailed information on its structure can be found in ref.[131].

4.4.2 Oil production and refining sector

COFFEE's resolution of the oil and gas sector is generally higher than that present in other IAMs, which includes the representation of oil qualities, crude trade, and fuel-oriented refinery typologies, thus allowing for a better understanding of supply dynamics under climate policy. Refinery typologies can be classified into Existing Topping, Cracking, and Hycon, as well as New Cracking and Hycon options. Each type of refinery has three activity modes, which focus on optimising diesel, gasoline, or kerosene (see ref.[131] for a detailed description of those typologies and technoeconomic assumptions).

With this work, we expand this representation to include the regional averages of propylene and BTX output from FCC and CR units, respectively, based on the OGJ Worldwide Refining Survey[219]. We also assumed that greenfield fuel-oriented refinery capacity could increase its HVC output up to 15% to assess potential opportunities for increased petrochemical integration under high-severity operation, based on ref.[220].

4.4.3 Process representation

Our research expands the scope of the industry sector in COFFEE by explicitly representing the production of HVCs, ammonia, and methanol in our model.

For HVC production, we included 12 technologies overall. The reasoning behind our approach was to provide the model with a variety of options for producing each HVC, using a diverse range of carbon feedstock (fossil fuels, biofuels, and CO_2 via CCU) and industry setups (multi-product or on-purpose routes). Only propylene and aromatics were considered options for refinery co-production, which aligns with prevailing practices and is completely integrated into the refining module's activity. Technologies for HVCs include (naphtha and ethane) Steam Cracking (SC), Naphtha Catalytic Cracking (NCC), Fluidized Catalytic Cracking (FCC) and Catalytic Reforming (CR) – both integrated and not integrated to refineries, Propane Dehydrogenation (PDH), Dimerization (DIM), Catadiene® (CAT), Metathesis (MTT), Ethanol to Butadiene (ETB), Methanol-to-Olefins (MTO), Methanol-to-Aromatics (MTA), and Bioethanol Dehydration (BDH).

For syngas products, the technologies are similar in the concept and feedstock but not in the emissions. The molecule of interest in ammonia production is hydrogen, which will then react with nitrogen. The remaining carbon is converted to CO_2, which can be used for urea production or is emitted into the atmosphere. In contrast, hydrogen and carbon monoxide are necessary for producing methanol. Detailed assumptions for emissions accounting can be found in Supplementary Method 1 Supplementary Method 3, and Supplementary Method 5 and Supplementary Method 6. The technologies considered for syngas products are Steam Methane Reforming (SMR), Coal Gasification (CGS), Biomass Gasification (BGS), Partial Oil Oxidation (POX) – only for ammonia, Electrolysis (ELE) – only for ammonia, and Carbon Dioxide Hydrogenation (CDH) – only for methanol. After hydrogen is produced from one of those routes, it is reacted with nitrogen to ammonia via the Haber-Bosch process (HB).

Supplementary Figure 1 illustrates the primary chemicals module and its technologies, and Supplementary Tables 1, 2 and 3 present all techno-economic assumptions. The method for calculating regional long-term demands for each primary chemical is described in Supplementary Method 4 .

4.4.4 Sources of carbon-based feedstock

Carbon-based feedstocks included in COFFEE are categorised as fossil-based, bio-based, and CCU-based, representing products derived from CO_2 conversion.

Fossil-based feedstocks include coal, natural gas, and products derived from crude oil processing in refineries, including Liquefied Petroleum Gas (LPG), naphtha, and heavy oil. Notably, gasoline can be converted to naphtha and vice-versa.

Bio-based feedstocks include bioethanol and co-products of Fischer-Tropsch Biomass-to-Liquids synthesis (FT-BtL), such as bio-naphtha and bio-LPG. These bio-based feedstocks are derived from processing raw agricultural materials, including sugary, starchy, lignocellulosic, and oily crops.

Currently, the only CCU-based feedstock represented is methanol, when produced via the hydrogenation of CO_2 captured from diluted (i.e. atmosphere via Direct Air Capture based on CO_2 absorption in sodium hydroxide solution) or concentrated sources. Concentrated sources include blast furnaces, power plants, cement kilns, and bio- or fossil-based hydrogen production processes, for example. CO_2 captured feeds into a regional "CO_2 pool" that can be either geologically stored or utilised as feedstock. Supplementary Method 1 presents a more detailed description of the abovementioned feedstocks.

4.4.5 Scenario development

All of the scenarios are built on the assumptions of the Shared Socioeconomic Pathway 2 – the "middle of the road" scenario, which extrapolates historical patterns of social, economic, and technological trends throughout the century [182], [183]. The assumptions for each scenario are described below and summarised in Supplementary Table 4. Plastics end-of-life and demand patterns were assumed to remain the same throughout the century to allow a more detailed analysis of the supply-side.

4.4.5.1 National Policies Implemented (NPi)

The National Policies Implemented (NPi) scenario accounts for the impact of national climate, energy, and land policies implemented until 2020, which have long-term implications on carbon dioxide emissions [114], [133]. This scenario does not consider additional efforts towards curbing temperature rise beyond what has already been enacted.

4.4.5.2 Scenario Compliant with 1.5-Degree Increase Limit (1.5C)

Building on the NPi scenario and based on the definitions of the remaining carbon budget from the IPCC Sixth Assessment Report (AR6) Working Group One (WGI) report[184], we create a scenario compliant with the climate targets established under the Paris Agreement: 1.5-Degree Celsius (1.5C) Increase Limit[184]**.** The budget relative to this scenario is more than 66% consistent with the temperature target (Supplementary Table 4).

We also performed four sensitivity analyses, which allow us to comprehend the model's behaviour when constraints are placed on factors such as CCS deployment (gCCS), biomass availability (PBIO), and assumptions regarding carbon storage in biomaterials (MNEToff), all of which affect either the availability of alternative carbon feedstock (CO_2 in gCCS and biomass in PBIO) and the sustainability of bio-based drop-in plastics (MNEToff). These are described below. Both gCCS and PBIO constraints were formulated in scenario protocols within the framework of model intercomparison initiatives. Specifically, these were undertaken as part of global IAM consortium projects such as the Exploring National and Global Actions to reduce Greenhouse gas Emissions (ENGAGE) and the Next generation of AdVanced InteGrated Assessment modelling to support climaTE policy making (NAVIGATE[221]).

4.4.5.3 Scenario with Restricted Deployment of CCS (gCCS)

Restricted Deployment of CCS scenario (gCCS) envisions a future world where the global deployment of Global Carbon Capture and Storage significantly falls short of expectations. By 2023, CCS facilities captured around 45 Mt.yr^{-1}, primarily for Enhanced Oil Recovery. Project announcements foresee a total capacity of 244 Mt.yr^{-1} in the next decade, a figure still below the capture requirement necessary to fulfil the objectives of the Paris Agreement [222]. According to 540 scenarios from IAMs – categories C1, C2 and C3 – in the AR6 IIASA Scenario Database, the maximum deployment of CCS projected for 2030, 2050, and 2100 was 21.0, 30.0, and 38.4 $GtCO_2$.yr^{-1}, respectively (Supplementary Fig. 5). This scenario assumes that global CCS achieves 10 Gt.yr^{-1} in 2080.

4.4.5.4 Scenario with Restricted Use of Biomass (PBIO)

Based on the AR6 scenario database, biomass use as primary energy ranges from 28.7 to 228.4 EJ.yr^{-1} in 2030, 33.5 to 310.1 EJ.yr^{-1} in 2050, and 41.1 to 530.4EJ.yr^{-1} in 2100 (Supplementary Fig. 6). The Restricted Use of Biomass scenario (PBIO) considers a world where the use of biomass is restricted to below 100 EJ.yr^{-1}, based on the high-confidence agreement in the literature found in ref.[186] for the sustainable technical potential of primary biomass production.

4.4.5.5 Scenario with Biogenic Carbon Storage Turned Off (MNEToff)

MNET – or material net – is a constraint specifically designed for this study. The Biogenic Carbon Storage Turned Off scenario (MNEToff) considers a world where biogenic carbon storage in materials is turned off. The baseline assumption considers that biomaterials act like a carbon sink provided they are not subjected to incineration or degradation [26], [210]. We turn that assumption off, thereby assuming that bioplastics can be produced but are not attributed any carbon credits for material storage.

The assumption on biogenic carbon storage currently corresponds to biomaterials in landfills since we consider current regional rates of recycling, landfill and incineration.

4.4.5.6 Scenario with all restrictions implemented (all)

The All Restrictions Combined scenario (all) implements all the abovementioned constraints. Not only does the global deployment of CCS develop significantly below expectations, but the use of biomass is also heavily restricted, and carbon credits are not attributed for material storage in biomaterials. This scenario paints a picture of an especially stringent set of restrictions, which helps us to understand the role of the chemical industry in responding to CO_2 emissions reduction targets.

4.5 Data availability

Source data are provided with this paper. The data used generated by this study are available in the Figshare repository [223].

4.6 Code availability

Although it is not an open-source model, COFFEE is documented on the common integrated assessment model documentation website (https://www.iamcdocumentation.eu/index.php/IAMC_wiki). The code used to generate the figures of this study are available from the corresponding author upon request.

5 CONCLUSIONS

Driven by concerns over the impacts of climate change and rising global temperatures, the ongoing energy transition requires an equivalent shift in material production and use paradigms [224]. Cement, steel, and chemicals are bulk materials considered to be essential for modern life. Together, they are responsible for 19-24% of global direct CO_2 emissions, often regarded as hard-to-abate due to market, technical, and policy constraints.

This work explored the intricate relationship between materials, energy, and GHG emissions in energy transitions. Furthermore, it aimed to evaluate the contribution of the heavy industry to global climate change mitigation pathways under various scenarios combining different assumptions on temperature ambitions and alternative feedstock availability. It combined a historical review and prospective scenario modelling to address research questions related to two key issues: the relevance of materials in energy transitions and the challenges of reducing emissions in materials systems to meet temperature goals compatible with human life as we currently know.

Based on the energy-material linkages identified in past energy transitions in Chapter 2, an integrated assessment approach was chosen to represent key energy-material linkages and analyse industrial emissions pathways in climate change mitigation scenarios, which is presented in Chapter 3. This chapter analyses the role of industrial subsectors in decarbonization pathways within an integrated framework by running well-below 2ºC scenarios with different temperature ambitions. Steel, cement, and chemicals sectors remain contributing to residual emissions globally in the year of reaching net-zero CO_2 emissions, but not in every region and scenario. The discussion focuses on the concept of the industrial sector as “hard-to-abate” and responsible for “residual emissions” in the context of integrated assessment modelling. It highlights how current materials modelling practices in IAMs might reinforce the expectation that these sectors will continue to produce residual emissions in net-zero pathways by suggesting that most of the mitigation effort is concentrated in other areas such as transportation and energy.

Chapter 4 further explored the conditions under which industrial subsectors – specifically the chemicals sector (the major consumer of non-energy petroleum products) – not only achieve net-zero goals but also contribute to the sink side in the balance with residual emissions. This result is highly dependent on: 1) the global availability of biomass and CCUS technologies to replace fossil-based feedstock, and 2) the assumption of carbon storage in long-lived biomaterials. Therefore, the role of fossil fuels as both energy and feedstock for materials was investigated. Moreover, in light of the outcomes of COP28 concerning the commitments made by parties to transition away from fossil fuels in energy systems, we analyse how this is affected by feedstock substitution. To that end, the representation of the ability (or inflexibility) of petroleum refineries to co-produce material feedstock for petrochemical plants was improved in COFFEE.

By examining past transitions and exploring future pathways, we derive the conclusions from these chapters in the sections below. Section 5.1 summarizes the main findings of each chapter responding to their respective RQ. Section 5.3 reflects on overarching conclusions of this study that are relevant for policymaking, accounting for the limitations in modelling capabilities and analytical boundaries. Section 5.2 lists the main limitations to be addressed and suggests recommendations for future studies.

5.1 Main findings

RQ1*: How do material transitions influence and are influenced by energy transitions?*

Energy and material transitions are deeply interconnected. To understand the intricate relationship between energy and materials transitions throughout history, a combination of historical review and interdisciplinary synthesis was used, aiming also to shed light into the implications for the current transition to low-carbon technologies. Table 10 presents a summary of the main mechanisms through which materials and energy systems interacted in the past and are expected to interact in the future.

Table 10. Mechanisms through which energy and materials transitions affect each other.

Mechanism	Transition to Agrarian Societies	Transition to Coal	Transition to Oil	Transition to Renewables
1. **Material and energy resource constraints influencing change**	♦ Limited availability of fertile land and water within nomadic distances ♦ Increasing pressure for agricultural land use ♦ Bronze substitution for iron due to scarcity of tin	♦ Deforestation to supply high demand for timber (for fuel, construction, shipbuilding, etc.) → pressure over forests and land in the UK ♦ Local scarcity of traditional biomass fuel	♦ Overhunting of whale and shortages of whale oil as fuel for lamps and lubricants.	♦ 1973 and 1979 oil shocks ♦ Peak oil concerns (2000s) ♦ Environmental degradation and crossing planetary boundaries ♦ Critical materials, mostly minor metals co-produced in small volumes and very few substitutes ♦ Geographical concentration of metal reserves
2. **Energy surpluses enabling material abundance and complexity**	♦ Surpluses from cereal cultivation and animal domestication enabled permanent settlements ♦ Increased demand for construction materials (stone, wood, clay)	♦ Higher energy density of coal → mass production of cement and steel to support industrial expansion and urban growth	♦ Easier to transport, cleaner combustion, and higher energy density than coal → allows high-efficiency energy systems ♦ Natural gas DRI (steel) and petroleum coke (clinker) ♦ Metal co-products production scale-up to meet military and civil needs	♦ Lower cost of solar PV and wind turbines → enabling the deployment of new technologies and infrastructures (smart grids, EVs, storage systems). ♦ Potential for massive electrification of transport and heating

3. Co-production of materials in energy transformation processes	♦ Wood being used for timber (material) and firewood (energy) ♦ Agricultural products (grains, fibres, hides) serve dual purposes	♦ Coal tar, coke, and other by-products used in metallurgy and the chemical industries.	♦ Petroleum refineries co-produce feedstock for plastics, fertilizers and textiles, as well as asphalt, lubricants and a myriad of chemicals	♦ H_2 production for energy and feedstock (methanol, ammonia) purposes
4. Co-evolution of energy and materials technology innovation	♦ Smelting, fire-setting (access to copper, bronze, iron) leading to better-performing ploughs, increasing agricultural productivity. ♦ Biomechanical technological cluster	♦ Coal mining and steam engine co-evolution enables deeper extraction and broader industrial applications (locomotives, textile/paper mills, steamships, foundries, etc) ♦ Steam engines reduce transport costs, further driving coal demand ♦ Thermomechanical and metallurgical technological cluster	♦ Development of internal combustion engines revolutionized land and sea transport ♦ Oil refining enabled the mass production of synthetic materials (plastics, rubber) ♦ Thermochemical and catalytic technological cluster	♦ Innovations in battery storage, wind turbines, and solar PV technologies linked to material developments based on minor metals and high-technology applications ♦ Electrical and digital technological cluster
5. Energy costs driving inter-material competition	♦ Construction: Stone, clay bricks, wood ♦ Transport and Mobility: Animal-drawn carts (wood, leather)	♦ Construction: Coal-fired cement (replacing wood) ♦ Transport and Mobility: Steam locomotives	♦ Construction: Modern cement, plastics (replacing glass) ♦ Transport and Mobility:	♦ Construction: Low-carbon concrete, recycled materials (replacing cement, steel) ♦ Transport and Mobility: Electric vehicles

	♦ Warfare: Copper, bronze (replacing bones, wood) ♦ Clothing: Animal hides, plant fibres ♦ Packaging: Clay pots, woven baskets	(iron, steel replacing wood) ♦ Warfare: Steel, iron (replacing bronze, copper) ♦ Clothing: Early synthetics (replacing natural fibres) ♦ Packaging: Glass containers (replacing clay)	Automobiles, airplanes (aluminium, plastics, rubber replacing steel) ♦ Warfare: Synthetics, lighter metals ♦ Clothing: Nylon, polyester (replacing wool) ♦ Packaging: Plastic (replacing glass, metal)	(aluminium, lightweighting synthetics replacing steel) ♦ Warfare: Composites, recycled metals (replacing heavy metals) ♦ Clothing: Organic, recycled fibres (replacing synthetics) ♦ Packaging: Biodegradable plastics, paper packaging
6. **Positive feedback loops between material and energy systems (systemic shift)**	♦ Intensification of access to food (energy) → increased population → permanent settlements → demand for construction materials → expansion of agriculture to support population growth	♦ Expansion of coal use → development of steam engine → locomotives and rail networks → scale-up of steel production → higher coal demand	♦ Growth in automobile use → gasoline demand → expansion of petroleum infrastructure and associated products (asphalt, rubber, etc)	♦ Expansion of renewable energy → increased demand for rare metals and high-tech materials → increased energy intensity for metal extraction/separation → decreasing EROI ♦ Uncertain future of plastics, cement, and steel with low-density variable renewable energy deployment
7. **Environmental impacts and resource depletion**	♦ Overuse of local natural resources leading to local	♦ Urban smog and air pollution crises in cities (e.g., London's Great Smog of 1952) →	♦ Automobile emissions and industrial activity → Severe air pollution	♦ Climate change, dependence in energy and emissions intensive materials

	shifts in material and energy use ♦ Soil degradation and deforestation	cleaner alternatives to coal ♦ Habitat destruction and soil erosion from mining and deforestation	and smog in cities (e.g., Los Angeles, Beijing) → cleaner fuels and pollution control ♦ Oil spills and ecological disasters → environmental regulation	♦ Deep sea mining ♦ Renewable energy policy to end local air pollution → global GHG mitigation co-benefit

Table 10 demonstrates key mechanisms linking energy and material transitions with examples for each transition. These links are critical for climate modeling because they highlight the deep interdependence between transitioning to low-carbon energy systems and the material demands this transition entails. This interdependence means that any effective strategy for reducing greenhouse gas emissions must consider both energy and material dynamics. For instance, renewable energy infrastructure—like solar panels and wind turbines—requires substantial amounts of materials, many of which are geographically concentrated or have limited availability, posing geopolitical risks and supply chain vulnerabilities. Moreover, the projected demand for carbon-based feedstock while fossil fuels for energy systems is projected to decrease also raises questions about the scalability of alternative feedstocks. By capturing these energy-material interlinkages, integrated assessment models (IAMs) can more accurately project the mitigation pathways, considering resource requirements, and potential material constraints and opportunities introduced into the energy transition.

RQ2*: What is the contribution of the global industrial sector to climate change mitigation in well below 2°C scenarios?*

The global industrial sector – especially heavy industries such as cement, steel, and chemicals – faces significant challenges to reaching net-zero emissions goals in well-below 2°C scenarios. Results from the COFFEE IAM show that industrial emissions could reach 1300-7600 $MtCO_2yr^{-1}$ by 2050 (compared to emissions in 2020 of 10900 $MtCO_2yr^{-1}$) in scenarios that only consider supply-side mitigation measures. Overall, immediate action is critical to reach more ambitious temperature targets, particularly within the next decade, as investments made until 2030 in low-carbon technologies and infrastructure will shape emissions and technology pathways up to 2070 and beyond.

While some strategies vary across subsectors, others remain uniform. For example, model results show increased use of alternative renewable fuels and drastically reducing clinker-to-cement ratio in the cement sector. For the steel sector, on the other hand, transitioning from conventional BOF to EAF and Scrap-EAF contributes to dramatic decrease coal consumption until 2050. For the chemicals sector, feedstock substitution (biomass in ammonia and HVCs, and CCU for methanol) drove the emissions reduction. CCS deployment was observed as critical in all subsectors, particularly after mid-century. The timing and extent of CCS deployment and shifts from coal to gas and biomass are crucial, particularly under scenarios with more stringent climate ambitions. Finally, while in global analysis residual industrial emissions remain, analysis of different subsectors and regions reveal opportunities for net-zero or even negative emissions in scenarios with increased temperature ambition. These opportunities were found to be relevant in the chemicals and steel sector, particularly in Australia, South and Central America, Canada, which was explored in more detail in Chapter 4.

Industrialization, urbanization, and infrastructure development play a critical role in shaping emissions and technology pathways across regions. By modelling material demand based on the macroeconomic correlation between material intensity and GDP per capita, we implicitly assume that patterns of material use and service provision will remain unchanged throughout the century. Therefore, limitations on reaching net-zero targets also highlight the need for systemic transformation in materials production. To fully assess the sector's potential to reach net-zero emissions, it is essential to improve material demand modeling by explicitly representing flows, stocks, and their relation to the demand for services as well as potential substitutes.

Given these limitations, it becomes clear that not only “residual emissions” require a clear and consistent definition, as recently argued by the literature [10], [118], [225], but so does the term “hard-to-abate”. What exactly makes certain sectors easier or harder to decarbonize, and which aspects of mitigation can be effectively captured through quantitative modelling of mitigation pathways? While an integrated assessment perspective is essential to understanding synergies and trade-offs in decarbonizing various sectors simultaneously, assumptions about the challenges of decarbonization should be grounded on specific criteria and compared across sectors. Without a consistent and robust material modelling approach in IAMs that allows for the representation of material efficiency measures, the residual industrial emissions reported in IAMs assessments should not be taken as definitive indicator of being hard-to-abate.

RQ3: *What are the impacts and limits of feedstock substitution in the chemicals sector for fossil fuels phase-out and climate change mitigation?*

Feedstock substitution was found to be highly dependent on two factors: 1) availability of alternative carbon-based feedstock – biomass and captured CO_2, and 2) dynamics of the refining sector under stringent carbon budgets. While the effect of the former is more direct, i.e., higher availability leads to higher levels of substitution in mitigation scenarios, the latter is not so straightforward given the diverging trends of fuels and feedstock demands in the long run. We observe that the petroleum refining sector impacts the chemical sector by providing cheap naphtha feedstock as a result of gasoline oversupply driven by increasing vehicle fleet electrification. Simultaneously, the shrinking of refining capacity reduces the direct production of propylene and aromatics in FCC and CR units. These two effects lead the chemical industry to restructure in terms of technology typologies (i.e., increasing on-purpose routes) but remain largely fossil-based, even in scenarios with unconstrained feedstock availability. At first glance, focusing only on the chemicals sector might suggest that the petroleum sector as a whole is unchanged; however, a closer look reveals the opposite: non-energy demands are increasingly the primary factor keeping petroleum refineries operating, therefore undermining the full transition away from fossil fuels in energy systems due to fuel co-production. The timing of phasing out different oil products therefore remain key to climate policy and the indirect effect they have in each other′s decarbonization pathways.

Therefore, climate policy should target primary chemicals not only due to their direct contribution to global emissions, but also because targeting these chemicals can indirectly reduce refinery activity, thereby supporting a full phase-out of oil use beyond just the energy sector. The petroleum sector will probably increase the share of feedstock in the overall products but without addressing co-production, fuels and their emissions will also be produced. We did not assess the effect of COTC here, which is expected to have an important impact on the supply-side by separating energy and materials processing, thus allowing for non-energy fossil-based production without energy co-production. Moreover, the effect of recycling and demand reduction was also not in the scope, but should be a key aspect not only to climate change mitigation but also to plastic pollution control, as concluded in many other studies.

Concerning the effect of feedstock availability, we found the chemical sector to be a key to deploy CDR (BECCS through ammonia production and biogenic carbon storage in long-lived applications), which is frequently overlooked. Even in biomass stringent scenarios, biomass use in ammonia production coupled with CCS remains relevant. This indicates a cost-efficient carbon removal, primarily because ammonia requires only hydrogen, and therefore all of the carbon is captured. Naturally, this effect directly depends on the demand for ammonia, which was assumed to grow in line with historical trends. Transitioning to regenerative agriculture systems and shifting diet patterns would, therefore, reduce this effect but also reduce emissions from ammonia in general. This potential should be, therefore, further assessed considering changes in land-use and food systems.

Finally, the terminology used to describe the chemicals sector is critical. While primary chemicals are called "hard-to-abate", our results indicate that they could act as a sink. The core challenge is not merely the difficulty of mitigation – shared across other sectors labelled as hard-to-abate – but the lack of sufficient (i.e., scalable) alternative feedstock to replace fossil fuels for non-energy purposes. Thus, the issue extends beyond being *hard-to-abate* to being *hard-to-defossilize,* with implications beyond the boundaries of primary chemicals production. Given the complex interactions between energy and materials, resource competition, and the impact of climate policy, using an IAM to address this problem proved highly effective.

5.2 Limitations and research recommendations

Given that the main value of integrated assessment models is, most of all, in the evaluation of interactions between the endogenously represented systems, conclusions must be analysed carefully, considering the system boundaries, the feedback loops considered, and the solution method applied. These three main points will be discussed below before future recommendations are suggested.

5.2.1 On model development and sectorial resolution

Model improvements in the COFFEE model included in the scope of this thesis were limited to the supply-side and for a few sectors only.

The main limitation of this work is the reliance on static material demand projections, which are unresponsive to carbon prices and calculated based on macroeconomic and demographic drivers. Long-term material use is assumed to follow historical patterns in quantity and quality. Therefore, several measures were excluded from the analysis due to limitations of the model framework, most of which related to the inability of representing material flows and service provisioning through stock dynamics. Whenever representing materials flows per time step was strictly necessary – e.g., when determining steel scrap or plastic waste availability for regional steel and plastic recycling potentials, respectively – a stylized approach was adopted based on current regional shares and assumptions for long-term development. These assumptions were conservative, leading to a lower than expected mitigation potential to ensure the model would not over rely on them while still allowing for identifying potentials on the demand-side. Hence, a more comprehensive understanding of the effects of materials production and use in mitigation pathways requires an equally comprehensive representation of both materials supply and demand, beyond the representation of industries as energy demand sectors.

To start exploring demand-side solutions, an approach for future studies would be to run various demand (all materials), and final disposal (steel and plastics) scenarios defined exogenously. This would contribute to understanding the mitigation potential of reducing material demand. However, these exogenous material demand scenarios would not be consistent with the demand for materials in sectors such as buildings and transportation, which are endogenously represented in the model. A lightweight measure to reduce the steel demand, for instance, would not impact fuel or electricity consumption in passenger vehicles. Likewise, modal changes in the transport sector do not affect the material demands used as inputs in COFFEE.

To fully capture these feedbacks, future studies should focus on improving the demand-side while increasing consistency between the industry sector activity and the material demand from sectors endogenously represented. Creating a dynamic stock-flow model with the same sectoral and regional split would help to address this issue. A few examples of similar soft-link approaches can be found in the recent literature [32], [34] via soft- and hard-link of stock-flow models with IAMs. Ultimately, building a link between materials, material use in sectors, and material services ensures a consistency between supply and demand as rigorous as we find in energy system modules in process-based IAMs.

Therefore, enhancing the representation of materials and their links with energy and land-use systems includes expanding the bottom-up supply-side approach and representing material demand consistent with the existing sectors in COFFEE. As such, here lies a non-exhaustive list of recommendations for future model development in COFFEE and related analyses to address the abovementioned limitations:

- Expanding technology representation of sectors currently represented:
    - Representation of oxy-combustion processes for clinker production using oxygen co-produced with electrolysis-based hydrogen. This solution has the potential to promote CO_2 enrichment, thus facilitating the capture of flue gas stream, and reduce O_2 costs compared to conventional air separation units [226].
    - Expand the representation of steel production routes. This includes electrolysis-based ironmaking technologies such as molten oxide electrolysis and alkaline iron electrolysis, which would allow using electricity as a reducing agent and energy, as well as a top gas recycling blast furnace (TGR-BF).
    - Explicit representation of biodegradable plastics and chemical recycling in the chemicals sector. Adding alternative products and recycling technologies would enable performing analyses about the final disposal and demand patterns of HVCs.
- Expanding the industrial subsectors beyond the ones currently modelled:
    - Explicit representation of the chlor-alkali sector, including its connection to DAC technologies through the consumption of KOH/NaOH. This link would directly associate DAC expansion with the demand for these chemicals and account for the co-production of chlorine.
    - Explicit representation of the aluminium sector. This could include also lightweight measures in the transportation sector and studies assessing the increase of electricity use due to increased aluminium demand.
    - Add a detailed representation of the paper and pulp sector, focusing on opportunities for biogenic carbon capture and storage.

        - Representation of the extractive mineral industry, considering metal resources and cost-supply curves for extraction.

    - Improve material demand representation by linking COFFEE with the Total Economy Assessment (TEA) model, a computable generable equilibrium (CGE) with a regional and sectoral split similar to COFFEE`s.

    - Improve material demand representation by creating a dynamic stock-flow model with a similar sectoral and regional split as COFFEE, including age cohorts and lifetime distributions of buildings, transportation, and energy technologies.

5.2.2 On scenario development, modelling approach, and solution method

For this work, we only assessed two types of peak budget scenarios (i.e., implementation of a CO_2 budget from the base year until the year of net-zero, following Rogelj et al., 2019 [227]) based on the assumptions of SSP2. One set of scenarios represents distinct temperature ambitions while staying below 2°C above preindustrial levels; the other set represents limited availability of alternative feedstock for the chemicals sector, which also constrained mitigation measures and CDR relying on biomass and CCS. The choice of peak budget scenarios over the full century with or without overshoot, for example, was made to prevent a delayed action from the industry sector and to avoid overreliance on high levels of CDR after mid-century.

A natural step forward would be to explore these dynamics in SSPs beyond SSP2 to understand how these different socioeconomic narratives affect industrial mitigation pathways. Moreover, conducting uncertainty analyses on the carbon budget and future technology costs, for instance, could help assess the findings' robustness. New scenarios based on changes in material demand patterns and intersectoral integration could also be explored in future studies.

From a modelling perspective, it is relevant to recognize that cost-optimal pathways do not capture the full complexity of biophysical and economic systems nor economic and market barriers. Future studies should address non-linearities (e.g., technology learning and cost feedbacks, damages from extreme climate events that affect productivity) and justice considerations for carbon budget allocation, for instance.

5.3 Overarching conclusions

This thesis seeks to address the question "How does the production of materials, specifically within the heavy industry, integrates global decarbonization pathways to achieve net-zero targets?". Addressing the sub-research questions in Chapters 2, 3, and 4 allows further reflection on the main research question. The four main conclusions are outlined below.

1. Limited decarbonisation capacity of heavy industries from supply-side solutions

Supply-side solutions to mitigate climate change as conventionally modelled in IAMs – such as fuel switch, energy efficiency, and technological innovation of material production – have limited capacity to drive the heavy industry towards net-zero emissions by 2050. While regional and sectoral specificities may challenge this general outcome, as found in Chapter 3, the reliance on cost-optimal approaches in these models tends to allocate low-carbon resources to sectors representing the highest mitigation benefits. Within an integrated and cost-optimal framework that assumes energy, food, and material service demands to grow according to historical patterns, these resources are allocated to sectors or technologies that capture and store CO_2 more efficiently than others.

Conversely, these "less-efficient" sectors contribute to reducing emissions as much as possible with the remaining resources. Therefore, residual emissions are, in this case, not a measure of *difficulty*, but evidence of less-efficient allocation of low-carbon resources. Since this work analysed in detail only supply-side solutions, residual industrial emissions represent the scale of the remaining effort required from solutions that could not be explicitly modelled due to scope and/or data limitations, which include strategies such as material efficiency, substitution, and sufficiency.

Therefore, while there is reasoning behind heavy industries being hard-to-abate – whether based on technical feasibility, market dynamics, geopolitical context, or regulatory environment – residual industrial emissions found in cost optimization IAMs results cannot always be directly linked to these dimensions precisely because a framework based on the relationships between sectors will naturally tend to overestimate the mitigation/carbon removal potential of solutions expected to be cost-optimal within their availability constraints (e.g., BECCS) while underestimating in others sectors. Therefore, as key tools to understand synergies and trade-offs of climate policies globally, IAMs need to broaden their scope of material modelling to remain crucial to understand optimal resource allocation in climate and resource-constrained scenarios.

2. Addressing energy-materials links in climate policy

Energy transitions involve creating the conditions for new systems to emerge and destabilizing existing ones; therefore, scaling-up renewable, regenerative systems and phasing-out fossil fuels are related but distinct processes. Climate policy should address both.

Phasing out fossil fuels involves addressing all applications and services today provided. While energy-related uses such as power generation, transportation, heating, and cooking are more commonly addressed, the heavy industry concentrates many applications beyond their use as combustion agents. These include 1) metallurgical uses as a carbon-based reducing agent for steel production, 2) carbon-based feedstock for a myriad of light to heavy organic chemicals production (asphalt, lubricants, synthetic rubbers, textiles), 3) hydrogen-rich feedstock for nitrogen fertilizers, 4) high-density energy source for high-temperature heat provision in cement, steel, chemicals, glass, and ceramics production. However, because oil refineries are multiproduct petroleum processing plants – as explored in Chapter 4 – not phasing out fossil fuels in these applications could lead to the continued co-production of easily substitutable, low-temperature, clean combustion energy sources for which alternatives already exist. In this context, some bulk materials should be understood as carrying not only embodied emissions, but also embodied fossil fuels, for which substitutes are critical to promote phase-out.

3. Questioning hard-to-abate narratives based on material necessity

As part of broadening the material modelling scope in IAMs, reaching ambitious climate mitigation targets requires challenging the perception of cement, steel, and chemicals as indispensable, unavoidable, easily accessible, and economically optimal materials with unique properties. These industrial subsectors expanded as integral parts of the fossil fuel transition, largely due to extraordinary net energy surpluses. Transitioning away from these materials – i.e., exploring local and low-carbon material alternatives – is a critical yet underexplored aspect of climate policy.

Exploring material substitution could help heavy industries to reach net-zero sooner and reduce the reliance in CDR deployment to offset their residual industrial emissions. Integrating inter-material substitution into IAMs similarly to how energy is currently modelled concerning extraction, processing, and service delivery, can be rather complex and data-intensive. However, simplified approaches to model material substitution could bring attention and drive data collection and standardization efforts for future developments.

Another factor that contributes to hard-to-abate narrative in IAMs is the macro-scale and global focus, which can be partly attributed to data availability. To reduce emissions from material systems rooted in fossil-based technologies, institutions, and networks, it is essential to reimagine material services provision through locally-led climate solutions. There is a growing body of literature on alternative building materials – such as bio-concrete [228], timber [229], rammed earth [230], bamboo [231] – that could be integrated into IAMs, for example. Although systemic changes in material systems are even more challenging to model than energy systems, this complexity should not be ignored by models assessing climate change mitigation pathways. To fully understand and implement effective global scale decarbonization strategies targeting materials, data, and metrics surrounding material extraction, production, (re)use, recycling, and substitution should be improved. New, locally adapted solutions should also be explored.

Away from the modelling realm, assuming certain materials or material services as harder-to-abate based on necessity within the current material paradigm also contributes to limiting the solution space. Not representing or acknowledging that global material use patterns could change and that demand for those materials can be reduced is failing to recognize the dynamics of winners and losers in energy transitions. While power structures can be challenging to dismantle (let alone to model), social revolutions have historically been central in these processes [232] and acknowledging it is critical for triggering change.

4. The role of terminology in shaping expectations and actions

Terminology shapes expectations and actions. Terms such as *hard-to-abate* sectors and the expectation of producing *residual emissions* during *energy transitions*, among others, can affect or even prescribe the potential, necessity, and limits of change and therefore assign responsibilities and roles. Referring to sectors as hard-to-abate highlights the difficulties of decarbonization, but it also implies that other sectors are expected to meet net-zero targets or even become net-negative. This assumption is not universally applicable across regions, nor does it hold true for every service currently provided by fossil fuels. Failing to recognize that the challenges of decarbonization are geographic- and sector-specific might reinforce a view that limits innovative and local solutions. This perspective should not undermine the development of policies that promote broader systemic changes.

REFERENCES

[1] K. Calvin *et al.*, 'IPCC, 2023: Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, H. Lee and J. Romero (eds.)]. IPCC, Geneva, Switzerland.', Intergovernmental Panel on Climate Change (IPCC), Jul. 2023. doi: 10.59327/IPCC/AR6-9789291691647.

[2] H. D. Matthews, N. P. Gillett, P. A. Stott, and K. Zickfeld, 'The proportionality of global warming to cumulative carbon emissions', *Nature*, vol. 459, no. 7248, pp. 829–832, Jun. 2009, doi: 10.1038/nature08047.

[3] H. D. Matthews and K. Caldeira, 'Stabilizing climate requires near-zero emissions', *Geophysical Research Letters*, vol. 35, no. 4, p. 2007GL032388, Feb. 2008, doi: 10.1029/2007GL032388.

[4] R. K. Pachauri *et al.*, *Climate change 2014: synthesis report. Contribution of Working Groups I, II and III to the fifth assessment report of the Intergovernmental Panel on Climate Change*. Ipcc, 2014.

[5] IPCC, *Summary for Policymakers. Global Warming of 1.5°C. An IPCC Special Report on the impacts of global warming of 1.5 °C above pre-industrial levels.* 2018. doi: 10.1017/CBO9781107415324.

[6] M. R. Allen *et al.*, 'Net Zero: Science, Origins, and Implications', *Annual Review of Environment and Resources*, vol. 47, no. Volume 47, 2022, pp. 849–887, Oct. 2022, doi: 10.1146/annurev-environ-112320-105050.

[7] P. Agreement, 'Adoption of the Paris agreement proposal by the president, united nations framework convention on climate change', FCCC/CP/2015/L. 9 https://unfccc. int/resource/docs/2015/cop21/eng/l09. pdf …, 2015.

[8] S. J. Davis *et al.*, 'Net-zero emissions energy systems', *Science*, vol. 360, no. 6396, p. eaas9793, Jun. 2018, doi: 10.1126/science.aas9793.

[9] G. Luderer *et al.*, 'Residual fossil CO2 emissions in 1.5–2 °C pathways', *Nature Clim Change*, vol. 8, no. 7, pp. 626–633, Jul. 2018, doi: 10.1038/s41558-018-0198-6.

[10] W. F. Lamb, 'The size and composition of residual emissions in integrated assessment scenarios at net-zero CO2', *Environ. Res. Lett.*, vol. 19, no. 4, p. 044029, Mar. 2024, doi: 10.1088/1748-9326/ad31db.

[11] Intergovernmental Panel On Climate Change (Ipcc), Ed., 'Emissions Trends and Drivers', in *Climate Change 2022 - Mitigation of Climate Change*, 1st ed., Cambridge University Press, 2023, pp. 215–294. doi: 10.1017/9781009157926.004.

[12] IEA, 'Extended world energy balances, IEA World Energy Statistics and Balances (database)', 2022.

[13] G. P. Thiel and A. K. Stark, 'To decarbonize industry, we must decarbonize heat', *Joule*, vol. 5, no. 3, pp. 531–550, Mar. 2021, doi: 10.1016/j.joule.2020.12.007.

[14] S. Madeddu *et al.*, 'The CO $_2$ reduction potential for the European industry via direct electrification of heat supply (power-to-heat)', *Environ. Res. Lett.*, vol. 15, no. 12, p. 124004, Dec. 2020, doi: 10.1088/1748-9326/abbd02.

[15] M. Schneider, 'The cement industry on the way to a low-carbon future', *Cement and Concrete Research*, vol. 124, p. 105792, Oct. 2019, doi: 10.1016/j.cemconres.2019.105792.

[16] C. Forsberg, 'What is the long-term demand for liquid hydrocarbon fuels and feedstocks?', *Applied Energy*, vol. 341, p. 121104, Jul. 2023, doi: 10.1016/j.apenergy.2023.121104.

[17] E. Worrell and G. Biermans, 'Move over! Stock turnover, retrofit and industrial energy efficiency', *Energy Policy*, vol. 33, no. 7, pp. 949–962, May 2005, doi: 10.1016/j.enpol.2003.10.017.

[18] D. J. C. MacKay, 'Could energy-intensive industries be powered by carbon-free electricity?', *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 371, no. 1986, 2013, doi: 10.1098/rsta.2011.0560.

[19] C. Bataille *et al.*, 'A review of technology and policy deep decarbonization pathway options for making energy-intensive industry production consistent with the Paris Agreement', *Journal of Cleaner Production*, vol. 187, pp. 960–973, 2018, doi: 10.1016/j.jclepro.2018.03.107.

[20] O. Y. Edelenbosch *et al.*, ‘Comparing projections of industrial energy demand and greenhouse gas emissions in long-term energy models’, *Energy*, vol. 122, pp. 701–710, 2017, doi: 10.1016/j.energy.2017.01.017.

[21] B. J. Van Ruijven, D. P. Van Vuuren, W. Boskaljon, M. L. Neelis, D. Saygin, and M. K. Patel, ‘Long-term model-based projections of energy use and CO2 emissions from the global steel and cement industries’, *Resources, Conservation and Recycling*, vol. 112, pp. 15–36, 2016, doi: 10.1016/j.resconrec.2016.04.016.

[22] A. Müller *et al.*, ‘Decarbonizing the cement industry: Findings from coupling prospective life cycle assessment of clinker with integrated assessment model scenarios’, *Journal of Cleaner Production*, vol. 450, p. 141884, Apr. 2024, doi: 10.1016/j.jclepro.2024.141884.

[23] M. A. E. van Sluisveld, H. S. de Boer, V. Daioglou, A. F. Hof, and D. P. van Vuuren, ‘A race to zero - Assessing the position of heavy industry in a global net-zero CO2 emissions context’, *Energy and Climate Change*, vol. 2, no. July, p. 100051, 2021, doi: 10.1016/j.egycc.2021.100051.

[24] X. Wang, B. Yu, R. An, F. Sun, and S. Xu, ‘An integrated analysis of China’s iron and steel industry towards carbon neutrality’, *Applied Energy*, vol. 322, p. 119453, Sep. 2022, doi: 10.1016/j.apenergy.2022.119453.

[25] W. E. Fritzeen *et al.*, ‘Integrated Assessment of the Leading Paths to Mitigate CO2 Emissions from the Organic Chemical and Plastics Industry’, *Environ. Sci. Technol.*, Nov. 2023, doi: 10.1021/acs.est.3c05202.

[26] P. Stegmann, V. Daioglou, M. Londo, D. P. van Vuuren, and M. Junginger, ‘Plastic futures and their CO2 emissions’, *Nature*, vol. 612, no. 7939, pp. 272–276, Dec. 2022, doi: 10.1038/s41586-022-05422-5.

[27] V. Daioglou, A. P. C. Faaij, D. Saygin, M. K. Patel, B. Wicke, and D. P. Van Vuuren, ‘Energy demand and emissions of the non-energy sector’, *Energy and Environmental Science*, vol. 7, no. 2, pp. 482–498, 2014, doi: 10.1039/c3ee42667j.

[28] M. Pehl, F. Schreyer, and G. Luderer, ‘Modelling long-term industry energy demand and CO_2 emissions in the system context using REMIND (version 3.1.0)’, *Geoscientific Model Development*, vol. 17, no. 5, pp. 2015–2038, Mar. 2024, doi: 10.5194/gmd-17-2015-2024.

[29] S. Deetman, S. Pauliuk, D. P. Van Vuuren, E. Van Der Voet, and A. Tukker, ‘Scenarios for Demand Growth of Metals in Electricity Generation Technologies, Cars, and Electronic Appliances’, *Environmental Science and Technology*, vol. 52, no. 8, pp. 4950–4959, 2018, doi: 10.1021/acs.est.7b05549.

[30] S. Deetman, H. S. de Boer, M. Van Engelenburg, E. van der Voet, and D. P. van Vuuren, ‘Projected material requirements for the global electricity infrastructure – generation, transmission and storage’, *Resources, Conservation and Recycling*, vol. 164, no. October 2020, 2021, doi: 10.1016/j.resconrec.2020.105200.

[31] S. Deetman, S. Marinova, E. van der Voet, D. P. van Vuuren, O. Edelenbosch, and R. Heijungs, ‘Modelling global material stocks and flows for residential and service sector buildings towards 2050’, *Journal of Cleaner Production*, vol. 245, 2020, doi: 10.1016/j.jclepro.2019.118658.

[32] G. Ünlü *et al.*, ‘MESSAGEix-Materials v1.0.0: Representation of Material Flows and Stocks in an Integrated Assessment Model’, Mar. 20, 2024. doi: 10.5194/egusphere-2023-3035.

[33] A. Mastrucci and B. van Ruijven, ‘Global residential scenarios towards low energy and material demands’, *IOP Conf. Ser.: Earth Environ. Sci.*, vol. 1196, no. 1, p. 012008, Jun. 2023, doi: 10.1088/1755-1315/1196/1/012008.

[34] IRP, ‘Global Resources Outlook 2024: Bend the Trend – Pathways to a liveable planet as resource use spikes’, International Resource Panel. United Nations Environment Programme, Nairobi, 2024. [Online]. Available: https://wedocs.unep.org/20.500.11822/44901

[35] K. Kermeli, O. Y. Edelenbosch, W. Crijns-Graus, B. J. van Ruijven, D. P. van Vuuren, and E. Worrell, ‘Improving material projections in Integrated Assessment Models: The use of a stock-based versus a flow-based approach for the iron and steel industry’, *Energy*, p. 122434, 2021, doi: 10.1016/j.energy.2021.122434.

[36] G. Cardoso, A. Szklo, J. Portugal-Pereira, P. R. R. Rochedo, and R. Schaeffer, ‘Fossil materials demand within deep decarbonization scenarios: A feasibility assessment’, *Energy Strategy Reviews*, vol. 54, p. 101479, Jul. 2024, doi: 10.1016/j.esr.2024.101479.

[37] M. Zotin, P. Rochedo, J. Portugal-Pereira, A. Szklo, and R. Schaeffer, ‘Critical Connections in Material Transitions and Energy Transitions’, in *Routledge Handbook of Energy Transitions,* 1st ed., in Araújo, K. (Ed.). , London: Routledge, 2022. [Online]. Available: https://doi.org/10.4324/9781003183020

[38] C. Wilson, A. Grubler, and C. Zimm, ‘Energy Services-led Transformation’, in *Energy Transitions Handbook*, 2022.

[39] F. W. Geels, B. K. Sovacool, T. Schwanen, and S. Sorrell, ‘The Socio-Technical Dynamics of Low-Carbon Transitions’, *Joule*, vol. 1, no. 3, pp. 463–479, 2017, doi: 10.1016/j.joule.2017.09.018.

[40] K. Araujo, *Low carbon energy transitions: Turning Points in National Policy and Innovation*. OUP: New York, 2017.

[41] A. Grubler and C. Wilson, *Energy technology innovation: Learning from historical successes and failures*. 2014. doi: 10.1017/CBO9781139150880.

[42] H. Haberl, D. Wiedenhofer, S. Pauliuk, F. Krausmann, D. B. Müller, and M. Fischer-Kowalski, ‘Contributions of sociometabolic research to sustainability science’, *Nature Sustainability*, vol. 2, no. 3, pp. 173–184, 2019, doi: 10.1038/s41893-019-0225-2.

[43] J. M. Allwood, M. F. Ashby, T. G. Gutowski, and E. Worrell, ‘Material efficiency: A white paper’, *Resources, Conservation and Recycling*, vol. 55, no. 3, pp. 362–381, 2011, doi: 10.1016/j.resconrec.2010.11.002.

[44] C. C. N. Oliveira, G. Angelkorte, P. R. R. Rochedo, and A. Szklo, ‘The role of biomaterials for the energy transition from the lens of a national integrated assessment model’, *Climatic Change*, vol. 167, no. 3–4, 2021, doi: 10.1007/s10584-021-03201-1.

[45] E. Hertwich *et al.*, *RESOURCE EFFICIENCY AND CLIMATE CHANGE*. 2020. doi: 10.5281/zenodo.3542680.

[46] IEA, ‘The challenge of reaching zero emissions in heavy industry: Heavy industries both facilitate and complicate the transition to a net-zero emissions energy system’.

[47] B. S. L. Cunha, J. Portugal-Pereira, A. Szklo, and R. Schaeffer, ‘The Role of Food Systems in Energy Transitions’, in *Energy Transitions Handbook*, 2022.

[48] I. G. Simmons, ‘Environmental Change and Energy’, in *Encyclopedia of Energy*, 2004.

[49] J. Diamond, *Guns, Germs, and Steel: The Fates of Human Societies*. New York: Norton, 2005.

[50] J. R. Burger, V. P. Weinberger, and P. A. Marquet, ‘Extra-metabolic energy use and the rise in human hyper-density’, *Scientific Reports*, vol. 7, pp. 1–5, 2017, doi: 10.1038/srep43869.

[51] C. A. S. Hall and K. A. Klitgaard, *Energy and the Wealth of Nations: Understanding the Biophysical Economy*. 2012.

[52] J. Perlin, *A Forest Journey: the story of wood and civilization*. 2005.

[53] V. Smil, *Making the Modern World - Materials & Dematerialization*. 2014.

[54] J.-C. Debeir, J.-P. Deléage, and D. Hémery, *Les servitudes de la puissance. Une histoire de l’energie*. Flammarion, 1992. doi: 10.2307/3768761.

[55] V. Smil, ‘Energy Transitions: History, Requirements, Prospects’, 2010.

[56] P. Rutter and J. Keirstead, ‘A brief history and the possible future of urban energy systems’, *Energy Policy*, vol. 50, pp. 72–80, 2012, doi: 10.1016/j.enpol.2012.03.072.

[57] R. C. Allen, ‘Backward into the future: The shift to coal and implications for the next energy transition’, *Energy Policy*, vol. 50, pp. 17–23, 2012, doi: 10.1016/j.enpol.2012.03.020.

[58] R. P. Sieferle, *The Subterranean Forest The Subterranean Forest Energy Systems and the Industrial Revolution*. 2001.

[59] P. Warde, *Energy Consumption in England & Wales 1560-2000*. 2007.

[60] A. Babich and D. Senk, *Coke in the iron and steel industry*. Elsevier, 2018. doi: 10.1016/B978-0-08-102201-6.00013-3.

[61] E. . A. . Wrigley, ‘The Supply of Raw Materials in the Industrial Revolution’, *The Economic History Review, New Series*, vol. 15, no. 1, pp. 1–16, 1962.

[62] D. Yergin, *The Prize: the epic quest for oil, money and power*. 1991.

[63] F. Geels, ‘The dynamics of transitions in socio-technical systems: A multi-level analysis of the transition pathway from horse-drawn carriages to automobiles’, *Technology Analysis & Strategic Management*, vol. 17, no. 4, pp. 445–476, 2005.

[64] J. K. Smith, ‘World War II and the Transformation of the American Chemical Industry’, *Science, Technology and the Military*, vol. XII, pp. 307–322, 1988, doi: 10.1007/978-94-017-2958-1_2.

[65] V. Smil, *Enriching the earth - Fritz Haber, Carl Bosch, and the Transformation of World Food Production*, vol. 79, no. 34. 2001.

[66] S. J. Bennett and P. J. G. Pearson, ‘From petrochemical complexes to biorefineries? The past and prospective co-evolution of liquid fuels and chemicals production in the UK’, *Chemical Engineering Research and Design*, vol. 87, no. 9, pp. 1120–1139, 2009, doi: 10.1016/j.cherd.2009.02.008.

[67] V. Smil, *Enriching the earth. Fritz Haber, Carl Bosch, an the Transformation of World Food Production*. 2001.

[68] R. Geyer, J. R. Jambeck, and K. L. Law, ‘Supplementary Materials for Production, use, and fate of all plastics ever made’, *Science Advances*, vol. 3, no. 7, pp. 19–24, 2017, doi: 10.1126/sciadv.1700782.

[69] R. Kleijn, *Materials and energy: a story of linkages*, vol. PhD. 2012.

[70] E. Elhacham, L. Ben-Uri, J. Grozovski, Y. M. Bar-On, and R. Milo, ‘Global human-made mass exceeds all living biomass’, *Nature*, vol. 588, no. 7838, pp. 442–444, 2020, doi: 10.1038/s41586-020-3010-5.

[71] IEA, ‘Net Zero by 2050: A Roadmap for the Global Energy Sector’, 2021.

[72] L. T. Keyßer and M. Lenzen, ‘1.5 °C degrowth scenarios suggest the need for new mitigation pathways’, *Nature Communications*, vol. 12, no. 1, pp. 1–16, 2021, doi: 10.1038/s41467-021-22884-9.

[73] A. Grubler *et al.*, ‘A low energy demand scenario for meeting the 1.5 °c target and sustainable development goals without negative emission technologies’, *Nature Energy*, vol. 3, no. 6, pp. 515–527, 2018, doi: 10.1038/s41560-018-0172-6.

[74] B. K. Sovacool and F. W. Geels, ‘Further reflections on the temporality of energy transitions: A response to critics’, *Energy Research and Social Science*, vol. 22, pp. 232–237, 2016, doi: 10.1016/j.erss.2016.08.013.

[75] IEA, ‘The Future of Petrochemicals, Towards more sustainable plastics and fertilisers’, 2018, doi: 10.1016/B978-0-12-394381-1.00002-7.

[76] Oil&Gas Journal, ‘International Survey of Ethylene From Steam Crackers — 2015’, pp. 85–91, 2015.

[77] M. Bender, ‘An Overview of Industrial Processes for the Production of Olefins – C4 Hydrocarbons’, *ChemBioEng Reviews*, vol. 1, no. 4, pp. 136–147, 2014, doi: 10.1002/cben.201400016.

[78] IEA, ‘The Future of Hydrogen’, 2019. doi: 10.1787/1e0514c4-en.

[79] IPCC, ‘Chemical Industry Emissions’, *2006 IPCC Guidelines for National Greenhouse Gas Inventories. Volume 3: Industrial Process and Product Use*, p. 110, 2006.

[80] L. Mishnaevsky, K. Branner, H. N. Petersen, J. Beauson, M. McGugan, and B. F. Sørensen, ‘Materials for wind turbine blades: An overview’, *Materials*, vol. 10, no. 11, pp. 1–24, 2017, doi: 10.3390/ma10111285.

[81] Y. Liu, B. Zwingmann, and M. Schlaich, ‘Carbon fiber reinforced polymer for cable structures-a review’, *Polymers*, vol. 7, no. 10, pp. 2078–2099, 2015, doi: 10.3390/polym7101501.

[82] J. R. Jambeck, Q. Ji, Y.-G. Zhang, D. Liu, D. M. Grossnickle, and Z.-X. Luo, ‘Plastic waste inputs from land into the ocean’, *Science*, vol. 347, no. 6223, pp. 764–768, 2015, doi: 10.1126/science.1260879.

[83] C. Excell, C. Salcedo-La Viña, J. Worker, and E. Moses, ‘Legal Limits on Single-Use Plastics and Microplastics: A Global Review of National Laws and Regulation.’, *United Nations Environment Programme, Nairobi, Kenya*, pp. 1–118, 2018.

[84] F. Carvalho *et al.*, ‘Prospects for carbon-neutral maritime fuels production in Brazil’, *Journal of Cleaner Production*, vol. 326, no. October, p. 129385, 2021, doi: 10.1016/j.jclepro.2021.129385.

[85] GCCA, ‘GNR database - Getting the Numbers Right’, 2019.

[86] IEA, ‘Iron and Steel Technology Roadmap’, *Iron and Steel Technology Roadmap*, 2020, doi: 10.1787/3dcc2a1b-en.

[87] R. Costanza, C. Cleveland, B. Cooperstein, and I. Kubiszewski, ‘Can Nuclear Power Be Part of the Solution?’, *Solutions Journal*, vol. 2, pp. 29–31, 2011.

[88] S. Thomas, ‘Competitive energy markets and nuclear power: Can we have both, do we want either?’, *Energy Policy*, vol. 38, no. 9, pp. 4903–4908, 2010, doi: 10.1016/j.enpol.2010.04.051.

[89] P. F. Peterson, H. Zhao, and R. Petroski, ‘Metal And Concrete Inputs For Several Nuclear Power Plants Per F. Peterson, Haihua Zhao, and Robert Petroski’, pp. 1–20, 2005.

[90] S. J. Zinkle and G. S. Was, ‘Materials challenges in nuclear energy’, *Acta Materialia*, vol. 61, no. 3, pp. 735–758, 2013, doi: 10.1016/j.actamat.2012.11.004.

[91] IEA, ‘Transforming Industry through CCUS’, 2019, doi: 10.1787/09689323-en.

[92] T. Watari, K. Nansai, and K. Nakajima, ‘Major metals demand, supply, and environmental impacts to 2100: A critical review’, *Resources, Conservation and Recycling*, vol. 164, no. August 2020, p. 105107, 2021, doi: 10.1016/j.resconrec.2020.105107.

[93] O. Vidal, B. Goffé, and N. Arndt, ‘Metals for a low-carbon society’, *Nature Geoscience*, vol. 6, no. 11, pp. 894–896, 2013, doi: 10.1038/ngeo1993.

[94] G. Calvo, G. Mudd, A. Valero, and A. Valero, ‘Decreasing ore grades in global metallic mining: A theoretical issue or a global reality?’, *Resources*, vol. 5, no. 4, pp. 1–14, 2016, doi: 10.3390/resources5040036.

[95] J. West, ‘Decreasing Metal Ore Grades: Are They Really Being Driven by the Depletion of High-Grade Deposits?’, *Journal of Industrial Ecology*, vol. 15, no. 2, pp. 165–168, 2011, doi: 10.1111/j.1530-9290.2011.00334.x.

[96] S. A. Northey, G. M. Mudd, and T. T. Werner, ‘Unresolved Complexity in Assessments of Mineral Resource Depletion and Availability’, *Natural Resources Research*, vol. 27, no. 2, pp. 241–255, 2018, doi: 10.1007/s11053-017-9352-5.

[97] M. Azadi, S. A. Northey, S. H. Ali, and M. Edraki, ‘Transparency on greenhouse gas emissions from mining to enable climate change mitigation’, *Nature Geoscience*, vol. 13, no. 2, pp. 100–104, 2020, doi: 10.1038/s41561-020-0531-3.

[98] F. Fizaine and V. Court, ‘Renewable electricity producing technologies and metal depletion: A sensitivity analysis using the EROI’, *Ecological Economics*, vol. 110, pp. 106–118, 2015, doi: 10.1016/j.ecolecon.2014.12.001.

[99] IEA, ‘The Role of Critical Minerals in Clean Energy Transitions’, *IEA Publications*, p. 283, 2021.

[100] D. G. Haglund, ‘The new geopolitics of minerals. An inquiry into the changing international significance of strategic minerals’;, *Political Geography Quarterly*, vol. 5, no. 3, pp. 221–240, 1986, doi: 10.1016/0260-9827(86)90035-2.

[101] H. F. Leslie, M. Nordvig, and S. Brink, ‘Critical Materials Strategy 2010’, no. December, pp. 1–166, 2010.

[102] D. Schrijvers *et al.*, ‘A review of methods and data to determine raw material criticality’, *Resources, Conservation and Recycling*, vol. 155, no. June 2019, p. 104617, 2020, doi: 10.1016/j.resconrec.2019.104617.

[103] G. Sokhna, E. Hache, C. Bonnet, M. Simoën, and S. Carcanague, ‘Copper at the crossroads : Assessment of the interactions between low- carbon energy transition and supply limitations’, *Resources, Conservation & Recycling*, vol. 163, no. July, p. 105072, 2020, doi: 10.1016/j.resconrec.2020.105072.

[104] D. Cordell, J. O. Drangert, and S. White, ‘The story of phosphorus: Global food security and food for thought’, *Global Environmental Change*, vol. 19, no. 2, pp. 292–305, 2009, doi: 10.1016/j.gloenvcha.2008.10.009.

[105] S. Pauliuk and E. G. Hertwich, ‘Socioeconomic metabolism as paradigm for studying the biophysical basis of human societies’, *Ecological Economics*, vol. 119, pp. 83–93, 2015, doi: 10.1016/j.ecolecon.2015.08.012.

[106] R. D. Kiggins, *The Political Economy of Rare Earth Elements: Rising Powers and Technological Change*. 2015. doi: 10.1057/9781137364241.

[107] T. Kenderdine, ‘China’s Industrial Policy, Strategic Emerging Industries and Space Law’, *Asia and the Pacific Policy Studies*, vol. 4, no. 2, pp. 325–342, 2017, doi: 10.1002/app5.177.

[108] EU Commission, ‘Report on Critical Raw Materials and the Circular Economy’, 2018.

[109] N. Georgescu-Roegen, ‘The Entropy Law and the Economic Process in Retrospect’, *Eastern Economic Journal*, vol. XII, no. 1, pp. 3–25, 1986.

[110] F. Krausmann *et al.*, ‘Global socioeconomic material stocks rise 23-fold over the 20th century and require half of annual resource use’, *Proceedings of the National Academy of Sciences of the United States of America*, vol. 114, no. 8, pp. 1880–1885, 2017, doi: 10.1073/pnas.1613773114.

[111] S. Paltsev, J. Morris, H. Kheshgi, and H. Herzog, ‘Hard-to-Abate Sectors: The role of industrial carbon capture and storage (CCS) in emission mitigation’, *Applied Energy*, vol. 300, p. 117322, Oct. 2021, doi: 10.1016/j.apenergy.2021.117322.

[112] X. Yang, C. P. Nielsen, S. Song, and M. B. McElroy, ‘Breaking the hard-to-abate bottleneck in China’s path to carbon neutrality with clean hydrogen’, *Nat Energy*, vol. 7, no. 10, pp. 955–965, Oct. 2022, doi: 10.1038/s41560-022-01114-6.

[113] O. Y. Edelenbosch *et al.*, ‘Reducing sectoral hard-to-abate emissions to limit reliance on carbon dioxide removal’, *Nat. Clim. Chang.*, vol. 14, no. 7, pp. 715–722, Jul. 2024, doi: 10.1038/s41558-024-02025-y.

[114] I. Dafnomilis, M. den Elzen, and D. P. van Vuuren, ‘Achieving net-zero emissions targets: An analysis of long-term scenarios using an integrated assessment model’, *Annals of the New York Academy of Sciences*, vol. 1522, no. 1, pp. 98–108, 2023, doi: 10.1111/nyas.14970.

[115] C. G. F. Bataille, ‘Physical and policy pathways to net-zero emissions industry’, *Wiley Interdisciplinary Reviews: Climate Change*, vol. 11, no. 2, pp. 1–20, 2020, doi: 10.1002/wcc.633.

[116] M. Kniivilä, ‘Industrial development and economic growth: Implications for poverty reduction and income inequality’, *Industrial development for the 21st century: Sustainable development perspectives*, vol. 1, no. 3, pp. 295–333, 2007.

[117] W. F. Lamb *et al.*, ‘The carbon dioxide removal gap’, *Nat. Clim. Chang.*, pp. 1–8, May 2024, doi: 10.1038/s41558-024-01984-6.

[118] H. J. Buck, W. Carton, J. F. Lund, and N. Markusson, ‘Why residual emissions matter right now’, *Nat. Clim. Chang.*, vol. 13, no. 4, pp. 351–358, Apr. 2023, doi: 10.1038/s41558-022-01592-2.

[119] W. F. Lamb *et al.*, ‘A review of trends and drivers of greenhouse gas emissions by sector from 1990 to 2018’, *Environmental Research Letters*, vol. 2, no. 1, pp. 0–31, 2020.

[120] A. Boulamanti and J. A. Moya, *Energy efficiency and GHG emissions: Prospective scenarios for the Chemical and Petrochemical Industry*. 2017. doi: 10.2760/20486.

[121] E. Worrell, L. Bernstein, J. Roy, L. Price, and J. Harnisch, ‘Industrial energy efficiency and climate change mitigation’, *Energy Efficiency*, vol. 2, no. 2, pp. 109–123, 2009, doi: 10.1007/s12053-008-9032-8.

[122] A. Babich and D. Senk, ‘Biomass use in the steel industry: back to the future’, *Stahl und Eisen*, vol. 133, no. 5, p. 2013, 2013.

[123] R. T. Kusuma, R. B. Hiremath, P. Rajesh, B. Kumar, and S. Renukappa, ‘Sustainable transition towards biomass-based cement industry: A review’, *RENEWABLE & SUSTAINABLE ENERGY REVIEWS*, vol. 163, 2022, doi: 10.1016/j.rser.2022.112503 WE - Science Citation Index Expanded (SCI-EXPANDED).

[124] V. Vogl, M. Åhman, and L. J. Nilsson, ‘Assessment of hydrogen direct reduction for fossil-free steelmaking’, *Journal of Cleaner Production*, vol. 203, pp. 736–745, 2018, doi: 10.1016/j.jclepro.2018.08.279.

[125] D. S. Mallapragada *et al.*, ‘Decarbonization of the chemical industry through electrification: Barriers and opportunities’, *Joule*, vol. 7, no. 1, pp. 23–41, Jan. 2023, doi: 10.1016/j.joule.2022.12.008.

[126] J. M. Allwood, M. F. Ashby, T. G. Gutowski, and E. Worrell, ‘Material efficiency: Providing material services with less material production’, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 371, no. 1986, 2013, doi: 10.1098/rsta.2012.0496.

[127] GCCA, ‘Concrete Future Roadmap: The GCCA 2050 Cement and Concrete Industry Roadmap for Net Zero Concrete’, 2022. Accessed: Jul. 04, 2024. [Online]. Available: https://gccassociation.org/concretefuture/wp-

content/uploads/2022/10/GCCA-Concrete-Future-Roadmap-Document-AW-2022.pdf

[128] MPP, ‘Making Net Zero Steel possible: An industry-backed, 1.5°C-aligned transition strategy’. Accessed: Dec. 19, 2023. [Online]. Available: https://missionpossiblepartnership.org/wp-content/uploads/2022/09/Making-Net-Zero-Steel-possible.pdf

[129] F. Meng *et al.*, ‘Planet-compatible pathways for transitioning the chemical industry’, *Proceedings of the National Academy of Sciences*, vol. 120, no. 8, p. e2218294120, Feb. 2023, doi: 10.1073/pnas.2218294120.

[130] K. Keramidas, S. Mima, and A. Bidaud, ‘Opportunities and roadblocks in the decarbonisation of the global steel sector: A demand and production modelling approach’, *Energy and Climate Change*, vol. 5, p. 100121, Dec. 2024, doi: 10.1016/j.egycc.2023.100121.

[131] R. Draeger, B. S. L. Cunha, E. Müller-Casseres, P. R. R. Rochedo, A. Szklo, and R. Schaeffer, ‘Stranded crude oil resources and just transition: Why do crude oil quality, climate ambitions and land-use emissions matter’, *Energy*, p. 124451, Jun. 2022, doi: 10.1016/J.ENERGY.2022.124451.

[132] IPCC, ‘AR6 Climate Change 2022: Mitigation of Climate Change — IPCC’. Accessed: Jul. 29, 2022. [Online]. Available: https://www.ipcc.ch/report/sixth-assessment-report-working-group-3/

[133] M. Roelfsema *et al.*, ‘Taking stock of national climate policies to evaluate implementation of the Paris Agreement’, *Nature Communications*, vol. 11, no. 1, pp. 1–12, 2020, doi: 10.1038/s41467-020-15414-6.

[134] P. Rochedo, ‘Development of a global integrated energy model to evaluate the Brazilian role in climate change mitigation scenarios’, COPPE/UFRJ, 2016.

[135] M. Neelis and M. Patel, *Long-term production, energy consumption and CO2 emission scenarios for the worldwide iron and steel industry*. 2006.

[136] Worldsteel, ‘Steel statistical yearbook 2020 Extended Version’, p. 46, 2020.

[137] USGS, ‘Mineral Commodity Summaries: Cement’, *U.S. Geological Survey, MIneral Commodity Summaries*, vol. 2022, no. 703, pp. 44–45, 2022.

[138] EUROMAP, ‘Plastics Resin Production and Consumption in 63 Countries Worldwide 2009-2020’, no. October 2016, p. 80, 2016.

[139] P. G. Levi and J. M. Cullen, ‘Mapping Global Flows of Chemicals: From Fossil Fuel Feedstocks to Chemical Products’, *Environmental Science and Technology*, vol. 52, no. 4, pp. 1725–1734, 2018, doi: 10.1021/acs.est.7b04573.

[140] USGS, ‘Nitrogen Statistics and Information | U.S. Geological Survey (2003 - 2020)’. Accessed: Jul. 16, 2024. [Online]. Available: https://www.usgs.gov/centers/national-minerals-information-center/nitrogen-statistics-and-information

[141] YARA, ‘Yara Fertilizer Industry Handbook’, *Yara*, p. 90, 2018.

[142] C. Chatterton, ‘METHANOL AS AN ALTERNATIVE FUEL’, Methanol Institute, 2018.

[143] OECD and FAO, ‘OECD-FAO Agricultural Outlook 2021-2030’, 2021.

[144] R. M. Andrew, ‘Global CO 2 emissions from cement production , 1928 – 2018’, no. September, pp. 1–67, 2019.

[145] *SUMÁRIO EXECUTIVO: MODELAGENS SETORIAIS E OPÇÕES TRANSVERSAIS PARA MITIGAÇÃO DE EMISSÕES DE GASES DE EFEITO ESTUFA*. [Online]. Available: www.mcti.gov.br

[146] IEA and CSI, ‘Technology roadmap for cement’, *International Energy Agency*, p. 66, 2018.

[147] K. Paustian, N. Ravindranath, and A. van Amstel, ‘2006 IPCC guidelines for national greenhouse gas inventories’, 2006.

[148] D. Lerede, C. Bustreo, F. Gracceva, M. Saccone, and L. Savoldi, ‘Techno-economic and environmental characterization of industrial technologies for transparent bottom-up energy modeling’, *Renewable and Sustainable Energy Reviews*, vol. 140, no. January, p. 110742, 2021, doi: 10.1016/j.rser.2021.110742.

[149] T. Hills, D. Leeson, N. Florin, and P. Fennell, ‘Carbon Capture in the Cement Industry: Technologies, Progress, and Retrofitting’, *Environmental Science & Technology*, vol. 50, pp. 368–377, 2016, doi: 10.1021/acs.est.5b03508.

[150] Z. Fan and S. J. Friedmann, ‘Low-carbon production of iron and steel: Technology options, economic assessment, and policy’, *Joule*, vol. 5, no. 4, pp. 829–862, 2021, doi: 10.1016/j.joule.2021.02.018.

[151] R. G. D. Pinto, A. S. Szklo, and R. Rathmann, ‘CO2 emissions mitigation strategy in the Brazilian iron and steel sector–From structural to intensity effects’, *Energy Policy*, vol. 114, pp. 380–393, Mar. 2018, doi: 10.1016/J.ENPOL.2017.11.040.

[152] E. Worrell, L. Price, M. Neelis, C. Galitsky, and Z. Nan, ‘World Best Practice Energy Intensity Values for Selected Industrial Sectors’, vol. LBNL-62806, no. June, pp. 1–45, 2007.

[153] Empresa de Pesquisa Energética, ‘Análise da Eficiência Energética em Seguimentos Industriais Selecionados - Segmento Cadeia Siderúrgica’, p. 187, 2018.

[154] S. VAI, ‘SIMETAL Corex technology Industrially and commercially proven iron making’, pp. 1–15, 2011.

[155] L. Deng and T. A. Adams, ‘Techno-economic analysis of coke oven gas and blast furnace gas to methanol process with carbon dioxide capture and utilization’, *Energy Conversion and Management*, vol. 204, no. November, p. 112315, 2020, doi: 10.1016/j.enconman.2019.112315.

[156] A. Otto, M. Robinius, T. Grube, S. Schiebahn, A. Praktiknjo, and D. Stolten, ‘Power-to-steel: Reducing CO2 through the integration of renewable energy and hydrogen into the German steel industry’, *Energies*, vol. 10, no. 4, 2017, doi: 10.3390/en10040451.

[157] M. Pei, M. Petäjäniemi, A. Regnell, and O. Wijk, ‘Toward a Fossil Free Future with HYBRIT: Development of Iron and Steelmaking Technology in Sweden and Finland’, *metals*, vol. 10, no. 972, pp. 1–11, 2020, doi: 10.3390/met10070972.

[158] X. Li, W. Sun, L. Zhao, and J. Cai, ‘Material Metabolism and Environmental Emissions of BF-BOF and EAF Steel Production Routes’, *Mineral Processing and Extractive Metallurgy Review*, vol. 39, no. 1, pp. 50–58, 2018, doi: 10.1080/08827508.2017.1324440.

[159] A. M. Bazzanella, F. Ausfelder, and DECHEMA, ‘Low carbon energy and feedstock for the European chemical industry’, *The European Chemical Industry Council*, p. 168, 2017.

[160] T. Ren, M. Patel, and K. Blok, ‘Olefins from conventional and heavy feedstocks: Energy use in steam cracking and alternative processes’, *Energy*, vol. 31, no. 4, pp. 425–451, 2006, doi: 10.1016/j.energy.2005.04.001.

[161] T. Ren and M. K. Patel, ‘Basic petrochemicals from natural gas, coal and biomass: Energy use and CO2 emissions’, *Resources, Conservation and Recycling*, vol. 53, no. 9, pp. 513–528, 2009, doi: 10.1016/j.resconrec.2009.04.005.

[162] TechnipFMC, ‘Ethylene Production’, vol. 225, pp. 1019–1022, 2017.

[163] G. Chem *et al.*, ‘Catalytic Cracking of Naphtha into Light Olefins’, vol. 240, no. 1981, p. 2006, 2006.

[164] C. N. Eng, S. C. Kang, S. Choi, S. H. Oh, and Y. K. Park, ‘A Catalytic Cracking Process for Ethylene and Propylene From Paraffin Streams: The Advanced Catalytic Olefins (ACO) Process’, 2007.

[165] Flowserve Corporation, ‘Coal to Olefins (CTO) / Methanol to Olefins (MTO) API Production’, no. December, 2019.

[166] N. Nesterenko, J. Aguilhon, P. Bodart, D. Minoux, and J. P. Dath, *Methanol to Olefins: An Insight Into Reaction Pathways and Products Formation*. 2016. doi: 10.1016/B978-0-444-63506-8.00006-9.

[167] D. Xiang, S. Yang, X. Liu, Z. Mai, and Y. Qian, ‘Techno-economic performance of the coal-to-olefins process with CCS’, *Chemical Engineering Journal*, vol. 240, pp. 45–54, 2014, doi: 10.1016/j.cej.2013.11.051.

[168] X. Xu, Y. Liu, F. Zhang, W. Di, and Y. Zhang, ‘Clean coal technologies in China based on methanol platform’, *Catalysis Today*, vol. 298, no. December, pp. 61–68, 2017, doi: 10.1016/j.cattod.2017.05.070.

[169] Z. Xu, Y. Zhang, C. Fang, Y. Yu, and T. Ma, ‘Analysis of China’s olefin industry with a system optimization model – With different scenarios of dynamic oil and coal prices’, *Energy Policy*, vol. 135, no. June, p. 111004, 2019, doi: 10.1016/j.enpol.2019.111004.

[170] H. A. Maddah, ‘A Comparative Study between Propane Dehydrogenation (PDH) Technologies and Plants in Saudi Arabia’, *American Scientific Research Journal for Engineering, Technology, and Sciences (ASRJETS)*, vol. 45, no. 1, pp. 49–63, 2018.

[171] R. A. Meyers, *CHAPTER 3.3: LIGHT OLEFINS/DIOLEFINS PRODUCTION VIA LUMMUS’S CATOFIN®/CATADIENE® PROCESSES*. McGraw-Hill Education, 2019. Accessed: Jun. 10, 2022. [Online]. Available: https://www.accessengineeringlibrary.com/content/book/9781259643132/chapter/chapter27

[172] Intratec, *Propylene Production via Metathesis - Cost Analysis*. 2012.

[173] R. M. Venner and S. I. Kantorowicz, ‘Metathesis: Refinery and ethylene plant applications’, *Petroleum Technology Quarterly*, vol. 6, no. 2, pp. 141-142,144, 2001.

[174] S. Farzad, M. A. Mandegari, and J. F. Görgens, ‘Integrated techno-economic and environmental analysis of butadiene production from biomass’, *Bioresource Technology*, vol. 239, pp. 37–48, 2017, doi: 10.1016/j.biortech.2017.04.130.

[175] F. Guedes, ‘A MULTI-REGIONAL OPTIMIZATION MODEL FOR THE BRAZILIAN OIL REFINING INDUSTRY’, Universidade Federal do Rio de Janeiro, 2019.

[176] F. Lantz, V. Saint-Antonin, J.-F. Gruson, W. Suwala Editor, and B. Saveyn, ‘The OURSE model: Simulating the World Refining Sector to 2030’, doi: 10.2791/73210.

[177] Y. K. Salkuyeh, B. A. Saville, and H. L. MacLean, ‘Techno-economic analysis and life cycle assessment of hydrogen production from different biomass gasification processes’, *International Journal of Hydrogen Energy*, vol. 43, no. 20, pp. 9514–9528, 2018, doi: 10.1016/j.ijhydene.2018.04.024.

[178] International Renewable Energy Agency (IRENA), *Renewable Methanol*. 2021. [Online]. Available: http://www.irena.org/

[179] E. Müller-Casseres *et al.*, ‘Are there synergies in the decarbonization of aviation and shipping? An integrated perspective for the case of Brazil’, *iScience*, vol. 25, no. 10, p. 105248, Oct. 2022, doi: 10.1016/j.isci.2022.105248.

[180] W. Summers, ‘Baseline Analysis of Crude Methanol Production from Coal and Natural Gas’, *National Energy Technology Laboratory*, p. DOE/NETL-341/101514. 1-83, 2014.

[181] M. Carmo, D. L. Fritz, J. Mergel, and D. Stolten, ‘A comprehensive review on PEM water electrolysis’, *International Journal of Hydrogen Energy*, vol. 38, no. 12, pp. 4901–4934, Apr. 2013, doi: 10.1016/J.IJHYDENE.2013.01.151.

[182] B. C. O’Neill *et al.*, ‘The roads ahead: Narratives for shared socioeconomic pathways describing world futures in the 21st century’, *Global Environmental Change*, vol. 42, pp. 169–180, Jan. 2017, doi: 10.1016/j.gloenvcha.2015.01.004.

[183] K. Riahi *et al.*, ‘The Shared Socioeconomic Pathways and their energy, land use, and greenhouse gas emissions implications: An overview’, *Global Environmental Change*, vol. 42, pp. 153–168, 2017, doi: 10.1016/j.gloenvcha.2016.05.009.

[184] Intergovernmental Panel On Climate Change, *Climate Change 2021 – The Physical Science Basis: Working Group I Contribution to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*, 1st ed. Cambridge University Press, 2021. doi: 10.1017/9781009157896.

[185] European Commission. Joint Research Centre., *CO2 emissions of all world countries :JRC/IEA/PBL 2022 report.* LU: Publications Office, 2022. Accessed: Jul. 28, 2023. [Online]. Available: https://data.europa.eu/doi/10.2760/730164

[186] F. Creutzig *et al.*, ‘Bioenergy and climate change mitigation: An assessment’, *GCB Bioenergy*, vol. 7, no. 5, pp. 916–944, Sep. 2015, doi: 10.1111/GCBB.12205.

[187] IEA, ‘Net Zero Roadmap: A Global Pathway to Keep the 1.5 °C Goal in Reach’, Paris, 2023. [Online]. Available: https://www.iea.org/reports/net-zero-roadmap-a-global-pathway-to-keep-the-15-0c-goal-in-reach

[188] S. Sollai, A. Porcu, V. Tola, F. Ferrara, and A. Pettinau, ‘Renewable methanol production from green hydrogen and captured CO2: A techno-economic assessment’, *Journal of CO2 Utilization*, vol. 68, p. 102345, Feb. 2023, doi: 10.1016/j.jcou.2022.102345.

[189] G. A. Olah, ‘Beyond Oil and Gas: The Methanol Economy’, *Angewandte Chemie International Edition*, vol. 44, no. 18, pp. 2636–2639, 2005, doi: 10.1002/anie.200462121.

[190] IEA, ‘China’s petrochemical surge is driving global oil demand growth – Analysis’, IEA. Accessed: Aug. 12, 2024. [Online]. Available: https://www.iea.org/commentaries/china-s-petrochemical-surge-is-driving-global-oil-demand-growth

[191] IEA, ‘Average age and typical lifetime of assets in the iron and steel and cement industries, China – Charts – Data & Statistics’, IEA. Accessed: Aug. 12, 2024. [Online]. Available: https://www.iea.org/data-and-statistics/charts/average-age-and-typical-lifetime-of-assets-in-the-iron-and-steel-and-cement-industries-china

[192] P. Achakulwisut, P. Erickson, C. Guivarch, R. Schaeffer, E. Brutschin, and S. Pye, ‘Global fossil fuel reduction pathways under different climate mitigation strategies and ambitions’, *Nat Commun*, vol. 14, no. 1, Art. no. 1, Sep. 2023, doi: 10.1038/s41467-023-41105-z.

[193] A. Farshi, F. Shaiyegh, S. H. Burogerdi, and A. Dehgan, ‘FCC Process Role in Propylene Demands’, *http://dx.doi.org/10.1080/10916460903451985*, vol. 29, no. 9, pp. 875–885, Jan. 2011, doi: 10.1080/10916460903451985.

[194] M. Bender, ‘Global Aromatics Supply - Today and Tomorrow’, in *New Technologies and Alternative Feedstocks in Petrochemistry and Refining*, 2013, pp. 59–64.

[195] International Energy Agency, *Ammonia Technology Roadmap: Towards more sustainable nitrogen fertiliser production*. OECD, 2021. doi: 10.1787/f6daa4a0-en.

[196] IEF and S&P Global, ‘Oil Refining Industry Insights: Stretched Sector Fuels Market Volatility’. Accessed: Jan. 23, 2024. [Online]. Available: https://www.ief.org/_resources/files/news/stretched-sector-fuels-market-volatility/ief-sp-global-downstream-investment-outlook---vf.pdf?v=2

[197] E. Turner and P. Hickin, ‘Oil refining landscape to resume transformation in 2023 after hiatus’. Accessed: Jan. 23, 2024. [Online]. Available: https://www.spglobal.com/commodityinsights/en/market-insights/latest-news/chemicals/121922-oil-refining-landscape-to-resume-transformation-in-2023-after-hiatus

[198] R. Geyer, J. R. Jambeck, and K. L. Law, ‘Production, use, and fate of all plastics ever made’, *Science Advances*, vol. 3, no. 7, pp. 25–29, 2017, doi: 10.1126/sciadv.1700782.

[199] IEA, ‘Oil 2021’, *International Energy Agency*, p. 167, 2021.

[200] ICCA, ‘Plastics Are Essential to Meeting Climate and Sustainability Goals’. Accessed: Dec. 18, 2023. [Online]. Available: https://icca-chem.org/wp-content/uploads/2022/01/Plastics-Are-Essential-to-Meeting-Climate-and-Sustainability-Goals.pdf

[201] FAO, ‘World fertilizer trends and outlook to 2020: Summary Report’, 2017.

[202] J. Zheng and S. Suh, ‘Strategies to reduce the global carbon footprint of plastics’, *Nature Climate Change 2019 9:5*, vol. 9, no. 5, pp. 374–378, Apr. 2019, doi: 10.1038/s41558-019-0459-z.

[203] H. L. van Soest *et al.*, ‘Global roll-out of comprehensive policy measures may aid in bridging emissions gap’, *Nature Communications 2021 12:1*, vol. 12, no. 1, pp. 1–10, Nov. 2021, doi: 10.1038/s41467-021-26595-z.

[204] K. Riahi *et al.*, ‘Cost and attainability of meeting stringent climate targets without overshoot’, *Nat. Clim. Chang.*, vol. 11, no. 12, Art. no. 12, Dec. 2021, doi: 10.1038/s41558-021-01215-2.

[205] I. Bashmakov *et al.*, ‘Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change, Chapter 11’, 2022.

[206] P. R. R. Rochedo *et al.*, ‘Is Green Recovery Enough? Analysing the Impacts of Post-COVID-19 Economic Packages’, *Energies*, vol. 14, no. 17, Art. no. 17, Jan. 2021, doi: 10.3390/en14175567.

[207] M. M. de Barros and A. Szklo, ‘Petroleum refining flexibility and cost to address the risk of ethanol supply disruptions: The case of Brazil’, *Renewable Energy*, vol. 77, pp. 20–31, May 2015, doi: 10.1016/j.renene.2014.11.081.

[208] J. Bengtsson, D. Bredström, P. Flisberg, and M. Rönnqvist, ‘Robust planning of blending activities at refineries’, *Journal of the Operational Research Society*, vol. 64, no. 6, pp. 848–863, Jun. 2013, doi: 10.1057/jors.2012.86.

[209] M. Zanon-Zotin *et al.*, ‘Unpacking bio-based alternatives to ethylene production in Brazil, Europe, and the United States: A comparative life cycle assessment’, *Journal of Cleaner Production*, vol. 428, p. 139376, Nov. 2023, doi: 10.1016/j.jclepro.2023.139376.

[210] C. C. N. de Oliveira, M. Z. Zotin, P. R. R. Rochedo, and A. Szklo, ‘Achieving negative emissions in plastics life cycles through the conversion of biomass feedstock’, *Biofuels, Bioproducts and Biorefining*, vol. 15, no. 2, 2021, doi: 10.1002/bbb.2165.

[211] S. M. Hafezi, H. Zarea-Hosseinabadi, M. A. J. Huijbregts, and Z. J. N. Steinmann, ‘The importance of biogenic carbon storage in the greenhouse gas footprint of medium density fiberboard from poplar wood and bagasse’, *CLEANER ENVIRONMENTAL SYSTEMS*, vol. 3, 2021, doi: 10.1016/j.cesys.2021.100066.

[212] IEA, ‘Age profile of global production capacity for the chemicals sector (ammonia, methanol and HVC production) – Charts – Data & Statistics’, IEA. Accessed: Apr. 10, 2024. [Online]. Available: https://www.iea.org/data-and-statistics/charts/age-profile-of-global-production-capacity-for-the-chemicals-sector-ammonia-methanol-and-hvc-production

[213] IEA, ‘Investment in petrochemical plants by region, 2014-2019’. Accessed: Apr. 10, 2024. [Online]. Available: https://www.iea.org/data-and-statistics/charts/investment-in-petrochemical-plants-by-region-2014-2019

[214] G. Karras, ‘Combustion Emissions from Refining Lower Quality Oil: What Is the Global Warming Potential?’, *Environ. Sci. Technol.*, vol. 44, no. 24, pp. 9584–9589, Dec. 2010, doi: 10.1021/es1019965.

[215] ICCT, ‘Carbon Intensity of Crude Oil in Europe’. Accessed: Dec. 22, 2023. [Online]. Available: https://theicct.org/sites/default/files/ICCT_crudeoil_Eur_Dec2010_sum.pdf

[216] C. Dean, ‘Naphtha Catalytic Cracking in FCC Units Past & Present ?’, 2015.

[217] G. W. Coates and Y. D. Y. L. Getzler, ‘Chemical recycling to monomer for an ideal, circular polymer economy’, *Nat Rev Mater*, vol. 5, no. 7, pp. 501–516, Jul. 2020, doi: 10.1038/s41578-020-0190-4.

[218] S. Thiyagarajan, E. Maaskant-Reilink, T. A. Ewing, M. K. Julsing, and J. van Haveren, ‘Back-to-monomer recycling of polycondensation polymers: opportunities for chemicals and enzymes’, *RSC Advances*, vol. 12, no. 2, pp. 947–970, 2022, doi: 10.1039/D1RA08217E.

[219] OGJ, ‘Worldwide Refining Survey’, Oil & Gas Journal.

[220] A. Akah and M. Al-Ghrami, ‘Maximizing propylene production via FCC technology’, *Applied Petrochemical Research*, vol. 5, no. 4, pp. 377–392, 2015, doi: 10.1007/s13203-015-0104-3.

[221] ‘Next generation of AdVanced InteGrated Assessment modelling to support climaTE policy making | NAVIGATE Project | Fact Sheet | H2020’, CORDIS | European Commission. Accessed: Dec. 16, 2023. [Online]. Available: https://cordis.europa.eu/project/id/821124

[222] GCCSI, ‘Global Status of CCS 2022’. Accessed: Jul. 27, 2023. [Online]. Available: https://status22.globalccsinstitute.com/wp-content/uploads/2023/03/GCCSI_Global-Report-2022_PDF_FINAL-01-03-23.pdf

[223] M. Zanon-Zotin, L. B. Baptista, R. Draeger, P. Rochedo, A. Szklo, and Schaeffer, ‘Unaddressed non-energy use in the chemical industry can undermine fossil fuels phase-out’. figshare. doi: https://doi.org/10.6084/m9.figshare.25867120.

[224] F. Creutzig *et al.*, ‘Demand-side strategies key for mitigating material impacts of energy transitions’, *Nat. Clim. Chang.*, vol. 14, no. 6, pp. 561–572, Jun. 2024, doi: 10.1038/s41558-024-02016-z.

[225] J. F. Lund, N. Markusson, W. Carton, and H. J. Buck, ‘Net zero and the unexplored politics of residual emissions’, *Energy Research & Social Science*, vol. 98, p. 103035, Apr. 2023, doi: 10.1016/j.erss.2023.103035.

[226] D. R. Nhuchhen, S. P. Sit, and D. B. Layzell, ‘Decarbonization of cement production in a hydrogen economy’, *Applied Energy*, vol. 317, p. 119180, Jul. 2022, doi: 10.1016/j.apenergy.2022.119180.

[227] J. Rogelj *et al.*, ‘A new scenario logic for the Paris Agreement long-term temperature goal’, *Nature*, vol. 573, no. 7774, pp. 357–363, Sep. 2019, doi: 10.1038/s41586-019-1541-4.

[228] L. Rosse Caldas, A. Bernstad Saraiva, V. M. Andreola, and R. Dias Toledo Filho, ‘Bamboo bio-concrete as an alternative for buildings’ climate change mitigation and adaptation’, *Construction and Building Materials*, vol. 263, p. 120652, Dec. 2020, doi: 10.1016/j.conbuildmat.2020.120652.

[229] A. Mishra *et al.*, ‘Land use change and carbon emissions of a transformation to timber cities’, *Nat Commun*, vol. 13, no. 1, p. 4889, Aug. 2022, doi: 10.1038/s41467-022-32244-w.

[230] J.-C. Morel, R. Charef, E. Hamard, A. Fabbri, C. Beckett, and Q.-B. Bui, ‘Earth as construction material in the circular economy context: Practitioner perspectives on barriers to overcome’, *Philosophical Transactions of the Royal Society B: Biological Sciences*, vol. 376, no. 1834, 2021, doi: 10.1098/rstb.2020.0182.

[231] C. Maraveas, ‘Production of Sustainable Construction Materials Using Agro-Wastes’, *Materials*, vol. 13, no. 2, Art. no. 2, Jan. 2020, doi: 10.3390/ma13020262.

[232] M. Fischer-Kowalski, F. Krausmann, P. P. Pichler, R. K. Schaeffer, and S. Stadler, ‘Great transformations: Social revolutions erupted during energy transitions around the world, 1500–2013’, *Energy Research & Social Science*, vol. 105, p. 103280, Nov. 2023, doi: 10.1016/j.erss.2023.103280.

[233] R. Baciocchi, G. Storti, and M. Mazzotti, ‘Process design and energy requirements for the capture of carbon dioxide from air’, *Chemical Engineering and Processing: Process Intensification*, vol. 45, no. 12, pp. 1047–1058, Dec. 2006, doi: 10.1016/j.cep.2006.03.015.

[234] R. H. Socolow *et al.*, ‘Direct Air Capture of CO2 with Chemicals: A Technology Assessment for the APS Panel on Public Affairs’, 2011. [Online]. Available: https://api.semanticscholar.org/CorpusID:107482441

[235] IHS Markit, ‘Global Propylene Market: Motivated to Change’. Accessed: Jul. 25, 2023. [Online]. Available: http://cdn.ihs.com/www/pdf/asia-chem-conf/Carr.pdf

[236] W. C. White, ‘Butadiene production process overview’, *Chemico-Biological Interactions*, vol. 166, no. 1–3, pp. 10–14, 2007, doi: 10.1016/j.cbi.2007.01.009.

[237] K. A. Couch, J. P. Glavin, D. A. Wegerer, and J. A. Qafisheh, ‘FCC propylene production’, *Petroleum Technology Quarterly*, vol. 12, no. 4, pp. 33–43, 2007.

[238] IHS Markit, ‘Crude oil-to-chemicals (COTC): An industry gamechanger?’

[239] T. Ren, B. Daniëls, M. K. Patel, and K. Blok, ‘Petrochemicals from oil, natural gas, coal and biomass: Production costs in 2030-2050’, *Resources, Conservation and Recycling*, vol. 53, no. 12, pp. 653–663, 2009, doi: 10.1016/j.resconrec.2009.04.016.

[240] T. Ren, M. K. Patel, and K. Blok, ‘Steam cracking and methane to olefins: Energy use, CO2 emissions and production costs’, *Energy*, vol. 33, no. 5, pp. 817–833, 2008, doi: 10.1016/j.energy.2008.01.002.

[241] OGJ, ‘INTERNATIONAL SURVEY OF ETHYLENE FROM STEAM CRACKERS — 2015’, 2015.

[242] M. L. Neelis, M. Patel, and K. Blok, ‘CO2 emissions and carbon storage resulting from the non-energy use of fossil fuels in the Netherlands, NEAT results for 1993-1999’, *Resources, Conservation and Recycling*, vol. 45, no. 3, pp. 251–274, 2005, doi: 10.1016/j.resconrec.2005.05.004.

[243] Y. P. Chul, W. Lee, N. Young, and D. S. Park, ‘Catalytic Cracking of Lower-Valued Hydrocarbons for Producing Light Olefins’, pp. 75–84, 2010, doi: 10.1007/s10563-010-9089-1.

[244] M. Monai and B. M. Weckhuysen, ‘Propane to olefins tandem catalysis: a selective route towards light olefins production’, *Chemical Society Reviews*, no. January, 2021, doi: 10.1039/D1CS00357G.

[245] K. Van Geem, ‘Production of bioethylene: Alternatives for green chemicals and polymers’, *AIChE Ethylene Producers Conference Proceedings*, pp. 303–313, 2012.

[246] P. Tian, Y. Wei, M. Ye, and Z. Liu, ‘Methanol to Olefins (MTO): From Fundamentals to Commercialization’, *ACS Catal.*, vol. 5, no. 3, pp. 1922–1938, Mar. 2015, doi: 10.1021/acscatal.5b00007.

[247] M. R. Gogate, ‘Methanol-to-olefins process technology: current status and future prospects’, *Petroleum Science and Technology*, vol. 37, no. 5, pp. 559–565, 2019, doi: 10.1080/10916466.2018.1555589.

[248] G. Pomalaza, P. Arango Ponton, M. Capron, and F. Dumeignil, ‘Ethanol-to-butadiene: the reaction and its catalysts’, *Catalysis Science & Technology*, vol. 10, no. 15, pp. 4860–4911, Aug. 2020, doi: 10.1039/D0CY00784F.

[249] American Chemical Society, ‘A National Historic Chemical Landmark - The Houdry Process for Catalytic Cracking’, 1996.

[250] ‘Ullmann’s Encyclopedia of Industrial Chemistry’, *Ullmann’s Encyclopedia of Industrial Chemistry*, Jun. 2000, doi: 10.1002/14356007.

[251] Y. Bicer, I. Dincer, C. Zamfirescu, G. Vezina, and F. Raso, ‘Comparative life cycle assessment of various ammonia production methods’, *Journal of Cleaner Production*, vol. 135, pp. 1379–1395, 2016, doi: 10.1016/j.jclepro.2016.07.023.

[252] I. Dincer and Y. Bicer, *Ammonia Production*, vol. 3–5. 2018. doi: 10.1016/B978-0-12-809597-3.00305-9.

[253] C. Smith, A. K. Hill, and L. Torrente-Murciano, ‘Current and future role of Haber-Bosch ammonia in a carbon-free energy landscape’, *Energy and Environmental Science*, vol. 13, no. 2, pp. 331–344, 2020, doi: 10.1039/c9ee02873k.

[254] FAO, ‘Food and Agriculture Organization of the United Nations - FAOSTAT Statistical Database’, 2021, [Online]. Available: https://www.fao.org/faostat/en/#search/wheat production

[255] GPCA and Integer Research, ‘China Fertilizer Industry Outlook to 2017 summary’, 2017.

[256] F. Dalena, A. Senatore, A. Marino, A. Gordano, M. Basile, and A. Basile, *Methanol Production and Applications: An Overview*. Elsevier B.V., 2018. doi: 10.1016/B978-0-444-63903-5.00001-7.

[257] L. W. Su, X. R. Li, and Z. Y. Sun, ‘The consumption, production and transportation of methanol in china: A review’, *Energy Policy*, vol. 63, pp. 130–138, 2013, doi: 10.1016/j.enpol.2013.08.031.

[258] Zhiyan Consulting, ‘**我国焦炉煤气制甲醇**项目发展概况_**智研咨**询 (“The Development Situation of Coke Oven Gas to Methanol Project in China”)’. Accessed: Jul. 26, 2020. [Online]. Available: https://www.chyxx.com/industry/201312/225545.html

[259] D. Xiang, S. Yang, Z. Mai, and Y. Qian, ‘Comparative study of coal, natural gas, and coke-oven gas based methanol to olefins processes in China’, *Computers and*

Chemical Engineering, vol. 83, pp. 176–185, 2015, doi: 10.1016/j.compchemeng.2015.03.007.

[260] SASOL b, ‘Ammonia Information’, pp. 1–2, 2021.

[261] Methanex, ‘Methanex Annual Reports’, 2021 2010. Accessed: Jul. 28, 2023. [Online]. Available: https://www.annualreports.com/HostedData/AnnualReports/PDF/NASDAQ_MEOH_2022.pdf

[262] IIP, *Ammonia*, 2015. Accessed: Sep. 25, 2020. [Online]. Available: http://www.iipinetwork.org/wp-content/Ietd/content/ammonia.html#key-data

[263] ‘Ministry of Energy and Energy Industries | Methanol’. Accessed: Jul. 28, 2023. [Online]. Available: https://www.energy.gov.tt/our-business/lng-petrochemicals/petrochemicals/methanol/

[264] EPE, ‘Competitividade do Gás Natural: Estudo de Caso na Indústria de Metanol’, *Informe técnico*, p. 16, 2019.

[265] ‘Ammonia | Climate Technology Centre & Network | 1181779’. Accessed: Jul. 29, 2023. [Online]. Available: https://www.ctc-n.org/technology-library/chemicals-management/ammonia

[266] S. Shiva Kumar and H. Lim, ‘An overview of water electrolysis technologies for green hydrogen production’, *Energy Reports*, vol. 8, pp. 13793–13813, Nov. 2022, doi: 10.1016/j.egyr.2022.10.127.

[267] W. M. Vatavuk and others, ‘Updating the CE plant cost index’, *Chemical Engineering*, vol. 109, no. 1, pp. 62–70, 2002.

[268] P. G. Levi and J. M. Cullen, ‘Mapping Global Flows of Chemicals: Supporting Information’, *Environmental Science & Technology*, 2018.

[269] R. Garaffa, B. S. L. Cunha, T. Cruz, P. Bezerra, A. F. P. Lucena, and A. C. Gurgel, ‘Distributional effects of carbon pricing in Brazil under the Paris Agreement’, *Energy Economics*, vol. 101, p. 105396, Sep. 2021, doi: 10.1016/j.eneco.2021.105396.

[270] B. S. L. Cunha, R. Garaffa, and Â. C. Gurgel, ‘TEA Model Documentation’, Jan. 2020, Accessed: Jan. 22, 2024. [Online]. Available: https://hdl.handle.net/10438/28756

[271] World Bank Group, *WHAT A WASTE 2.0 - A Global Snapshot of Solid Waste Management to 2050*. Washington, 2018.

[272] A. C. Köberle *et al.*, *Can global models provide insights into regional mitigation strategies? A diagnostic model comparison study of bioenergy in Brazil*, vol. 170, no. 1–2. Springer Netherlands, 2022. doi: 10.1007/s10584-021-03236-4.

[273] T. Hasegawa *et al.*, ‘Land-based implications of early climate actions without global net-negative emissions’, *Nat Sustain*, vol. 4, no. 12, pp. 1052–1059, Dec. 2021, doi: 10.1038/s41893-021-00772-w.

[274] IAMC, ‘IAMC Model Documentation’.

[275] O. Cavalett, S. Norem Slettmo, and F. Cherubini, ‘Energy and Environmental Aspects of Using Eucalyptus from Brazil for Energy and Transportation Services in Europe’, *Sustainability*, vol. 10, no. 11, Art. no. 11, Nov. 2018, doi: 10.3390/su10114068.

Appendix A

Supplementary Method 1. Sources of carbon feedstock

COFFEE represents fossil-, bio- and CCU-based feedstocks as options for producing primary chemicals.

Fossil-based feedstock: Primarily includes natural gas (i.e., methane and ethane), oil (i.e., LPG, naphtha and heavy oil), and coal. Natural gas can be produced in fields associated with oil or in dedicated fields. Ethane and methane can be recovered from natural gas and used for steam cracking and steam methane reforming units, respectively. LPG, naphtha and heavy oil are outputs of the petroleum refining sector, which is described in ref.[131]. LPG is an input to propane dehydrogenation process, naphtha can be used in steam cracking and catalytic reforming units whereas heavy oil is used for hydrogen to ammonia production via partial oil oxidation. Coal is produced in different qualities in the resource module (bituminous, subbituminous, and lignite) but only bituminous coal is allowed in coal gasification processes.

Bio-based feedstock: Primarily includes solid and liquid biofuel produced from planted forests and energy crops. Solid biofuel is obtained from woody (eucalyptus) and grassy sources as well as agriculture residues, including sugarcane bagasse. Eucalyptus can be used for biomass gasification processes to produce hydrogen (for energy or ammonia production), methanol, or can be used in Fischer-Tropsch Biomass-to-Liquids (FT-BtL) to produce advanced liquid biofuels. Sugarcane bagasse can be used for 2G bioethanol production.

Liquid biofuels included as feedstocks for the chemical sector are bioethanol (via fermentation/distillation from sugarcane, maize, wheat, sugar beet, and agricultural residues), and bio-naphtha, and bio-LPG as co-products of hydrotreated vegetable oils (HVO) or hydroprocessed esters and fatty acids (HEFA) production from soybean oil, maize oil, or animal fat. HVO and HEFA are advanced biofuels alternatives to be used in diesel engines as green diesel or jet fuel (or sustainable aviation fuel – SAF), and might co-produce bio-naphtha and bio-LPG to be used in other sectors, including as feedstocks.

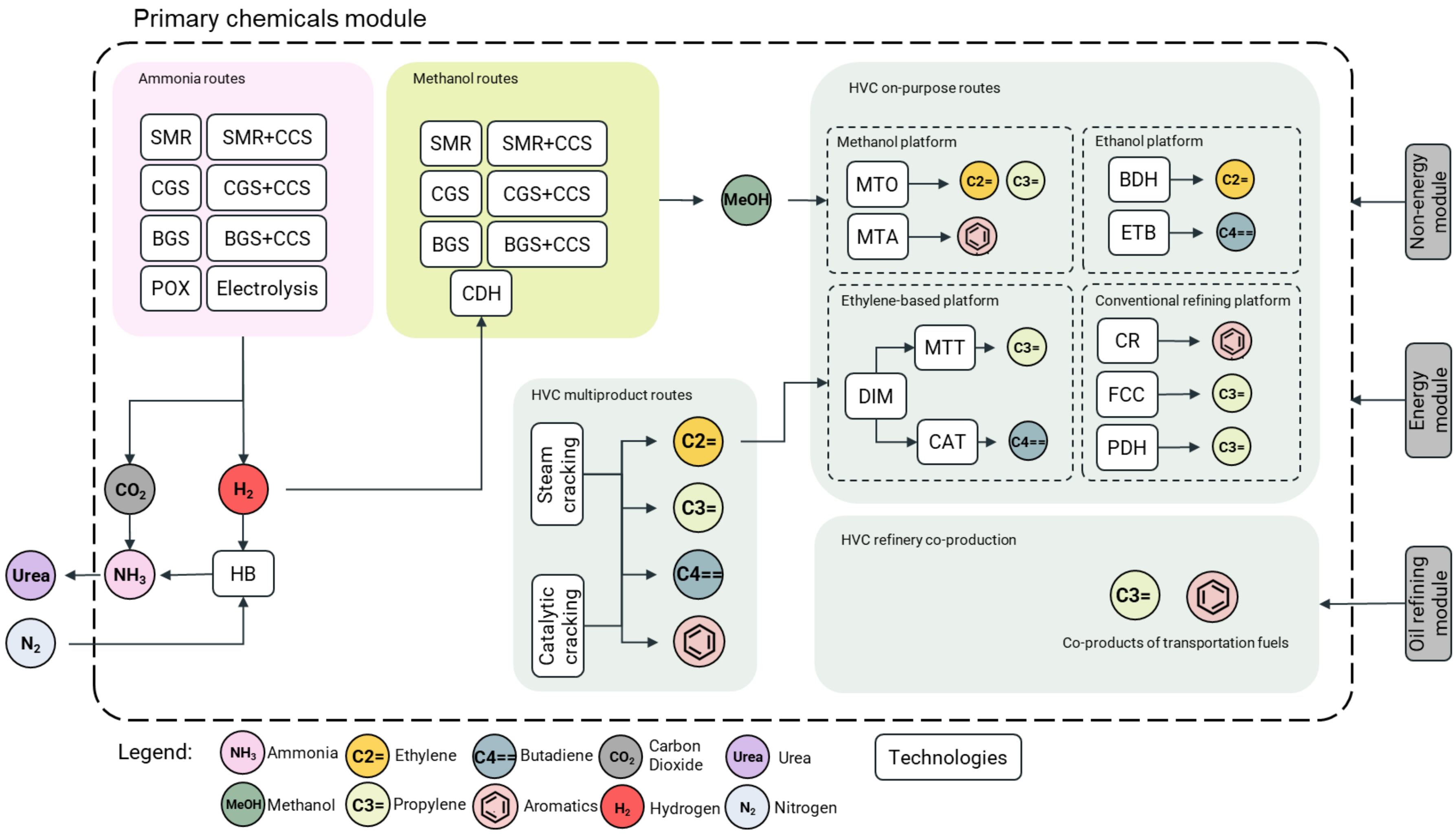
Biomethane could be a promising alternative feedstock. However, its supply chain is not yet developed in COFFEE and it remains as a topic to be further explored in future work.

CCU-based feedstock: CO_2 as a feedstock is sourced from a "CO_2 pool", which is composed by CO_2 captured from: 1) fossil- or bio-based concentrated sources such as power plants, cement kilns, blast furnaces, and methanol/ammonia plants (via gasification/partial oxidation, but not electrolysis). Both energy and process emissions can be captured from concentrated sources, and costs for CO_2 transportation are considered; 2) diluted CO_2 in the atmosphere via Direct Air Capture (DAC) based on absorption in sodium hydroxide solution, based on refs,[233], [234]. Captured CO_2 feeds into a regional "CO_2 pool" in the model, where the model decides whether it is geologically stored or used for CCU.

Supplementary Method 2. Technology representation

In this study, we categorize ammonia, methanol and high-value chemicals (i.e., ethylene, propylene, butadiene and BTX) as primary chemicals. They are the building blocks in multiple downstream processes that convert them into more complex chemicals for a multitude of material services. While capturing the use of primary and final energy sources for combustion in IAMs is critical to evaluate the climate-related challenges associated with replacing the primary energy source in the current global economy, it is equally important to understand their non-energy uses. This detailed perspective helps us to identify the broader implications of replacing fossil fuels, given their ubiquitous role in society as sources of both energy and materials.

The following sections provide details on technoeconomic parameters and other relevant data of the primary chemicals technologies included in the COFFEE model. Supplementary Figure 1 presents the technologies included in the primary chemicals module and their respective products, as well as the interaction with the oil refining module. Supplementary Table 1, Supplementary Table *2*, and Supplementary Table 3 summarize the techno-economic parameters used in this study.



Supplementary Figure 1. Primary chemicals module represented in the COFFEE model. SMR: Steam Methane Reforming; CGS: Coal Gasification; BGS: Biomass Gasification; POX: Partial Oxidation of Oil; HB: Haber Bosch synthesis; CDH: Carbon Dioxide Hydrogenation; DIM: Dimerization; CAT: Catadiene®; MTT: Metathesis; CR: Catalytic Reforming; FCC: Fluidized Catalytic Cracking; PDH: Propane Dehydrogenation; BDH: Bioethanol Dehydration; ETB: Ethanol to Butadiene; MTO: Methanol-to-Olefins; MTA: Methanol-to-Aromatics

<u>High-value Chemicals</u>

High Value Chemicals (HVCs) are basic chemicals widely used as building blocks for numerous chemical products. **Ethylene** (C_2H_4) is the primary raw material for the downstream petrochemical industry, and its main derivatives include (high-density, low-density, and linear low-density) polyethylene, polyethylene terephthalate (PET), ethylene oxide (intermediate for ethylene glycol), ethylene dichloride (precursor of PVC), and ethylbenzene (intermediate of polystyrene - PS), among others. Global ethylene production – approximately 190 $Mt.yr^{-1}$ – has been steadily growing over the past decades.

Propylene (C_3H_6) is the second basic chemical in importance, being the building block for several polymers and synthetic fibres such as polypropylene, propylene oxide, acrylonitrile, and others. Global propylene production reached around 85 Mt in 2015 [235].

Butadiene (C_4H_6) is a linear diolefin produced as a by-product of ethylene with a global production capacity around 11 $Mt.yr^{-1}$ [77], [236]. It is mostly used for rubbers such as styrene-butadiene rubber (SBR) and polybutadiene (PB), which are essential for tires production, but also acrylonitrile-butadiene-styrene resins (ABS) and other rubbers.

BTX stands for **Benzene** (C_6H_6), **Toluene** (C_7H_8) and **Xylenes** (C_8H_{10}, which includes ortho, meta and para isomers) and global production is approximately of 95 $Mt.yr^{-1}$ [194]. While p-xylene is mostly used for terephthalic acid production (i.e., PET precursor), benzene applications are more diverse such as for ethylbenzene (for PS production), cumene and cyclohexane, chemicals widely used as solvents, paints, and intermediates. In this study, the terms *aromatics* and *BTX* are used interchangeably.

Thus, by including these products in an IAM, we aim to capture the role of downstream chemicals produced in large scale such as plastics, synthetic fibres and rubbers in future energy and carbon feedstock demand as well as carbon emissions. HVCs technologies are categorized as <u>Refinery co-production</u>, <u>Multiproduct</u> and <u>On-purpose</u> (i.e., facilities dedicated to produce a specific primary chemical, as opposed to steam cracking) to account for potential structural changes that the petrochemical sector may experience due to feedstock transition and climate stringent targets. Below, we describe each technology and present the modelling strategy to represent this sector as well as data sources for regional installed capacity in the base year. Techno-economic assumptions for all technologies are also summarized in Supplementary Table 1.

Refinery co-production technologies (FCC-o and CR-o)

A significant share of the global propylene and BTX production is recovered from oil refineries, mainly in gasoline-producing refineries Fluidized Catalytic Cracking (FCC) and Catalytic Reforming (CR) units, respectively. While propylene is recovered diluted in the propane stream in the FCC unit, BTX is produced in Catalytic Reforming unit primarily as an octane rating booster for gasoline but also as a building block for polymers production.

Regional propylene and BTX recovery from FCC and RC were assumed based on country-specific data from the OGJ Worldwide Refining Survey [219]. While aromatics production is explicitly informed in the referred reference, propylene recovery yield in FCC units was assumed to be 5.0 wt% on fresh feed [237].

In the COFFEE model, three refinery schemes (Cracking and Coking, Topping and Hydroskimming, and Hycon), seven oil qualities (Light, Medium Sweet, Medium Sour, Heavy, Extra Heavy, Bitumen, and Kerogen) and three operating modes (Kerosene, Diesel and Naphtha runs) are combined to represent current and future oil resources and reserves, oil derivatives production and refining capacity [131]. To harmonize this with petrochemical co-production, we assume that regional historical rates of propylene and BTX recovery per total atmospheric distillation (ADU) capacity remains constant over time (FCC-o and RC-o, respectively). New refinery capacity with propylene and BTX yields 15% higher than historical were also made available in the model as a simplified and conservative approach to represent the potential increase in refinery-petrochemical integration over time, which could be achieved with e.g. high-severity FCC units and assuming that BTX availability for petrochemical use increases as its demand as a high-octane blend component in the gasoline pool decreases over time [194], [220].

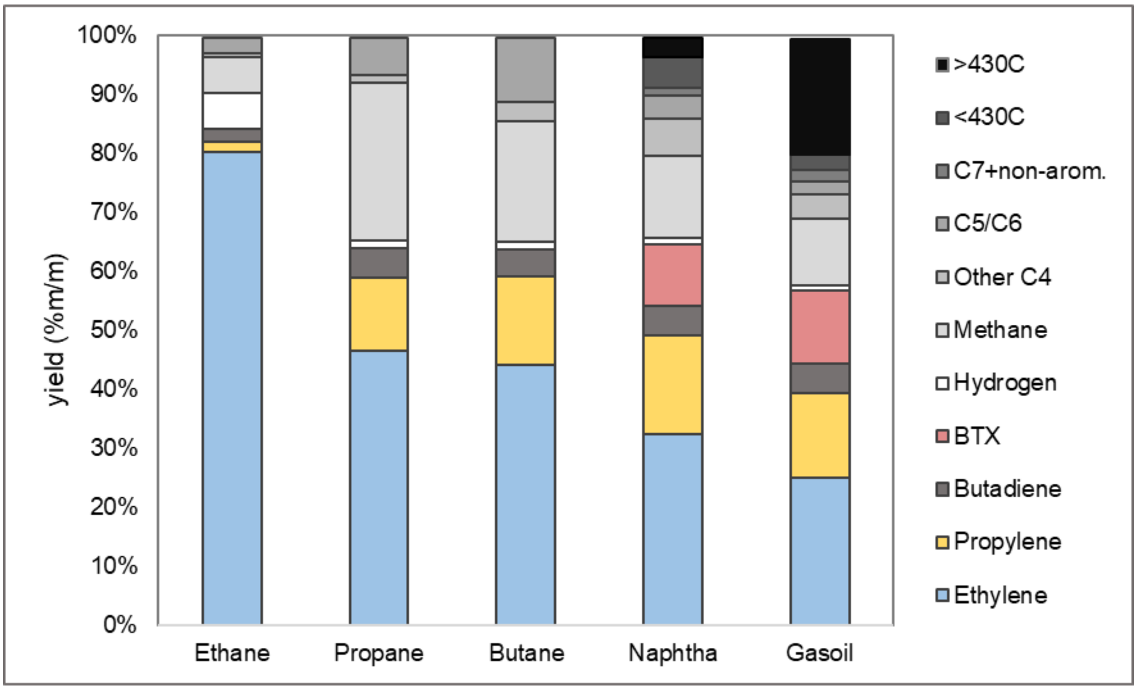
Several Crude-Oil-to-Chemicals (COTC) projects that primarily convert light crude into chemicals are already in stage of development or trial operation – mostly in China (Hengli Petrochemical, Zhejiang Petrochemical, Hengyi Shenghong) and Saudi Arabia (Aramco/SABIC) – with an estimated chemical conversion rate of more than 40% [238]. While an important trend in the petrochemical sector, representing COTC technologies was not possible given the lack of reliable and publicly available data. For now, we are aware that our results on future oil use for non-energy purposes may be underestimated (especially in less carbon constrained scenarios) and that refinery-petrochemical integration is a critical topic in the future role of oil and gas that should be addressed in future studies.

Multiproduct technologies

Steam cracking (SC-Naphtha and SC-Ethane)

Steam crackers are at the heart of the petrochemical industry. They break down saturated hydrocarbon streams (ethane, propane, butane, naphtha, and gasoil) into unsaturated compounds such as ethylene, propylene, butadiene, and BTX.

The steam cracking process is a non-catalytic pyrolysis of hydrocarbons, performed under temperatures that go up to 900°C, low pressure (around 1.5 bar) and short residence time (<1s). Under those conditions, carbon-carbon and carbon-hydrogen bonds are broken to make olefins and aromatics. Steam cracking of lighter streams (i.e., ethane) result in higher relative yields for ethylene whereas heavier streams (i.e., gasoil) yield a more balanced basket of products and fuel-grade by-products (e.g., hydrogen, methane, and butanes) (Supplementary Figure 3).



Supplementary Figure 2. Steam cracking yields according to feedstock. Source: own elaboration based on [239], [240].

Naphtha steam cracking has traditionally been pivotal in the production of HVCs. Compared to other feedstocks, naphtha use has been more advantageous given its higher flexibility to HVCs demand and pricing fluctuations. However, over the past two decades, there has been a transition in feedstock use towards ethane, especially in gas-rich regions. The Ethylene/Propylene ratio (E/P) resulting from ethane steam cracking is much higher than those of other feeds (Supplementary Figure 3). This has resulted in a significant deficit in propylene supply worldwide, notably in Asia. To bridge this propylene gap, several on-purpose technologies were deployed worldwide (e.g, Methanol-to-Olefins in China, and Propane Dehydrogenation in the Middle East and in the US).

Historical capacity data was sourced from the International Survey Of Ethylene From Steam Crackers [241]. Our model only included ethane and naphtha steam crackers in the model; for simplicity, we treated the capacity of propane, butane, and gasoil steam crackers as though it were from naphtha steam crackers.

Furthermore, we deem bionaphtha (e.g., co-product of HVO or SAF production via Fischer–Tropsch synthesis or oligomerization) to be chemically indistinguishable from fossil naphtha, and therefore, it can also be used in SC-Naphtha units. Also, we considered that the part of the process energy demand is met by fuel-grade by-products such as hydrogen and methane [160], [242].

Naphtha catalytic cracking (NCC)

Naphtha Catalytic Cracking (NCC) is an alternative steam cracking solution to make up for propylene gap while still using naphtha as feed. While P/E ratio in traditional naphtha steam cracking is around 0.5, NCC can deliver P/E ratios up to 1 with an increase in yield for aromatics as well [75], [164], [243]. Employing zeolite catalysts enhances the overall process, boosting both the selectivity for olefins and aromatics and the efficiency of the operation. To date, a singular commercial plant utilizing the New Catalytic Cracking (NCC) process has been established in Korea. This plant mirrors a standard Fluid Catalytic Cracking (FCC) unit in design, but is specifically configured for petrochemical production [164].

On-purpose technologies

Propane dehydrogenation (PDH)

Propane dehydrogenation (PDH) is one of the main technologies used so far to bridge the propylene supply gap, mainly in the United States, Middle East, and China. PDH has been available for decades as an alternative to produce polymer-grade propylene with a high selectivity from propane-rich streams and is usually carried out in the presence of a Platinum or Chromium catalyst under low pressure and high temperatures [170]. Bio-propane from bio-LPG streams was also considered as a feedstock. PDH regional historical capacity data was collected from [244].

Bioethanol dehydration (BDH)

Bioethanol, the most produced biofuel globally, primarily originates from maize in the United States, sugarcane in Brazil, and sugar beet in Europe. Unlike biodiesel, bioethanol is chemically identical to its fossil fuel-based counterpart and is utilized in internal combustion engine. As the long-term demand for gasoline and ethanol for passenger transportation declines, the dehydration of bioethanol (BDH) to ethylene emerges as a promising technology to decarbonize ethylene production. In 2010, Braskem deployed a bioethanol dehydration plant with annual ethylene capacity of 200kt [245]. Furthermore, ethylene can undergo oligomerization to form bio-jet fuel, green diesel, and bio-naphtha, aligning with decarbonization strategies in traditionally challenging sectors such as aviation and shipping.

Methanol-to-olefins (MTO)

Methanol-to-olefins (MTO) is an autocatalytic reaction that converts methanol from any feedstock to ethylene and propylene, often over a zeolite catalyst. It assumed significant strategic importance in China as a viable alternative source of olefins, particularly during periods of elevated oil prices [246].

In our modelling, methanol is identified as a critical pathway through which every HVC can be sourced via Carbon Capture and Utilization (CCU) methods. Initially, CO_2 is hydrogenated to methanol (see Carbon Dioxide Hydrogenation below), which can subsequently be converted to ethylene and propylene via MTO. The resulting ethylene can undergo a sequence of dimerization and Catadiene processes to form butadiene. Finally, aromatics can be generated through the Methanol-to-Aromatics (MTA) pathway, further detailed below.

Regional historical capacity data was collected from numerous references, with a particular relevance for China. This focus is due to the significant implementation of this technology in the country, where methanol production, primarily sourced from coal, is prevalent [165], [167], [168], [247].

Dimerization (DIM)

The dimerization (DIM) of ethylene is a chemical process that combines two ethylene molecules to produce butenes, commonly referred to as a C4 stream, which includes a mixture of both 1-butene and 2-butene isomers. In our modelling approach, we accommodate the use of alternative bio-/CCU-based feedstock, while also allowing the use of ethylene into olefin conversion technologies. Dimerization thus enables the conversion of ethylene to propylene via dimerization followed by metathesis [172].

Metathesis (MTT)

Metathesis (MTT) is a chemical process that transforms ethylene and either 2-butene or 1-butene (referred to as a C4 stream) into propylene. In the COFFEE model, this C4 stream is primarily generated from the dimerization of ethylene, but also as a co-product of the PDH process. Metathesis reactions entails the formation and cleavage of carbon-carbon double bonds, facilitated by catalysts that typically employ ruthenium, molybdenum, or tungsten. 1-butene molecules undergo isomerization to become 2-butene, which subsequently react with ethylene in the presence of a tungsten oxide catalyst [172]. On a stoichiometric basis, this reaction yields two moles of propylene for every mole of ethylene.

Ethanol-to-Butadiene (ETB)

Ethanol-to-Butadiene (ETB) is being considered as a bio-based alternative to butadiene production based on the renewable ethanol platform. Although the reaction mechanism is still under debate, the process generally consists of ethanol dehydrogenation to acetaldehyde, which then reacts with ethanol to form butadiene [174], [248].

Methanol-to-aromatics (MTA)

The methanol-to-aromatics (MTA) process is a catalytic conversion process that transforms methanol into BTX. Much similar to the MTO technology, the process involves several steps, including dehydration, dehydrogenation, and aromatization, but requires higher temperatures (500-700°C) and lower pressures (0.01-0.1 MPa). Furthermore, specialized zeolite catalysts are used to increase the selectivity to aromatics [75], [247].

Catadiene© (CAT)

Catadiene© (CAT) is based on the Houdry process – a catalytic cracking process developed in the early 1940s to convert heavy oil fractions to gasoline – and consists of a catalytic dehydrogenation of n-butanes and n-butenes (C4s stream) into butadiene [171], [236], [249], [250].

Catalytic Reforming unit (CR-n)

Conventional catalytic reforming is a process that converts low octane straight run naphtha into high-octane gasoline. This is performed by converting paraffinic and naphthenic compounds into aromatics, which increases the octane value of the gasoline.

An alternative option was also created to produce aromatics in the model, but outside the oil refining module. However, for this study, aromatics in this unit are produced exclusively for petrochemical production, being fed either by fossil fuel-based or bio-based naphtha. Cost assumptions were based on Guedes (2019). These costs include not only the expenses for the process unit (inside battery limits or ISBL) but also the direct and indirect costs associated with supporting infrastructure. This includes utilities, piping, storage, and electrical installations, among others (outside battery limits or OSBL).

Methanol and ammonia

Processes for ammonia, methanol and hydrogen production are quite similar in that they all have syngas (a mixture of carbon monoxide and hydrogen) as intermediates. In the COFFEE model, syngas can be produced via steam methane reforming (SMR), coal gasification (CGS), biomass gasification (BGS), partial oil oxidation (POX). Water electrolysis and carbon dioxide hydrogenation (CDH) are alternative routes to hydrogen (as input to ammonia production) and to methanol production, respectively.

Ammonia (NH_3) is the primary chemical of all nitrogen fertilizer and one of the top 3 chemicals transported globally [251], [252]. Agriculture uses cover around 70% of its global demand, and other applications span across several industrial sectors, including the production of nitric acid, an essential precursor for explosives, plastics, and polyurethanes [195]. Its conventional production method is the Haber-Bosch process, in which N_2 and H_2 react in a 1:3 ratio under high pressure and temperature. N_2 is separated from air mixture in a conventional air separation unit (cryogenic distillation/ pressure swing adsorption) and H_2 is usually sourced by steam methane reforming (SMR) followed by a water-gas shift reaction [253]. Ammonia supplied from H_2 produced by coal gasification (CGS) is particularly relevant in China and South Africa, whereas partial oxidation (POX) of heavy oil is still produced in Europe and India. Global production reached around 150 million tonnes in 2015 [201].

In ammonia production, carbon monoxide in syngas is converted to CO_2 and then either emitted or captured to be used in urea production. Therefore, given that CO_2 capture and utilisation is a common practice in ammonia-urea integrated facilities, ammonia’s process emissions have been adjusted according to regional urea production available in FAOSTAT [254], [255]. We assumed that the stoichiometric CO_2 demand for urea production is fulfilled by ammonia captured emissions, assuming that regional Urea/Ammonia production ratio remained constant over the century. The residual CO_2 (i.e., that which is not utilized by urea production facilities) is assumed to be released into the atmosphere as process emissions. Alternatively, if CO_2 from ammonia production is not available, urea can be synthesized using CO_2 sourced from other methods (e.g., carbon capture).

Methanol (CH_3OH), a simple alcohol with the formula CH_3OH, is a key chemical with a wide array of applications – mostly as feedstock, solvent, or fuel. It serves as a crucial feedstock for the production of formaldehyde, acetic acid, and several other chemicals, as well as an alternative fuel in internal combustion engines [256].

Methanol is primarily produced through steam methane reforming as well, given that the production of methanol often takes place in a fertilizer plant, where the same synthesis gas is utilized to manufacture ammonia and urea. Coal gasification processes are also relevant, particularly in China and South Africa. While ammonia synthesis requires a highly pure hydrogen stream, methanol production utilizes syngas in a 2:1 H_2/CO ratio, which leads to considerably lower process emissions in the latter.

Global methanol production increased from 50 million tonnes in 2010 to 100 million tonnes in 2019, approximately [178]. The primary drivers of demand growth have been the expansion of Methanol-to-Olefins (MTO) facilities and the introduction of standards for blending methanol into gasoline (ranging from M5 to M100), predominantly occurring in China. Methanol is also quite relevantly sourced from coke oven gas facilities integrated to steel production in China [257]. This information was incorporated into the steel module in COFFEE. We added a technology that simultaneously generates methanol and steel, taking into account technoeconomic data cited in references [148], [258], [259].

Data regarding historical regional production capacity and the technology split for methanol and ammonia were gathered from a variety of sources, including company reports [260], [261], scientific articles [251], [257] and associations and government reports [178], [195], [254], [262], [263], [264], [265].

Below, we describe the technologies incorporated into the COFFEE model to improve the representation of methanol and ammonia production. We present steam methane reforming, coal gasification, partial oil oxidation, and biomass gasification as syngas-based technologies, as well as carbon dioxide hydrogenation (for methanol) and electrolysis (for ammonia) as hydrogen/electricity-based technologies. Lastly, the respective methanol and ammonia synthesis are described.

Synthesis gas production routes

Steam methane reforming (SMR) is well-established process that converts methane into syngas through a catalytic reaction with steam under temperature and pressure at approximately 700-1000°C and 25 bar, respectively. The heat required for this endothermic reaction is provided by an external source [256]. As opposed to using light sulphur-free hydrocarbons such as methane, the conversion of heavier hydrocarbons such as coal into syngas requires higher temperatures (i.e., up to 1800°C) that make the catalytic pathway unfeasible. As a result, **coal gasification (CGS)** has been prioritized in countries with vast coal reserves and where the transportation of natural gas is not economical, such as China and South Africa. It is a process in which pulverized coal is mixed with a gasifying agent such as steam, air, or oxygen to produce syngas. The high temperature syngas follows steps of cooling, which sometimes happens with heat recovery to achieve better energy efficiency, and clean up to remove sulphur, ammonia, mercury and other contaminants as well as particulate matter. Furthermore, gasification is usually the process to handle solid hydrocarbons, which makes **Biomass gasification (BGS)** a similar but renewable alternative to produce syngas. Lastly, **partial oxidation (POX)** aims to react heavy liquid hydrocarbon feedstocks – such as fuel oil and petroleum residues – with sub-stoichiometric oxygen. Its H_2 to CO ratio is lower than SMR (which is around 3-4) but higher than coal/biomass gasification (around 0.3-0.7).

Given the similar initial steps in producing syngas, methanol and ammonia production share are often integrated to benefit from synergies like shared infrastructure and energy efficiency, for example.

Carbon Capture and Storage (CCS) technologies

We use CGS, SMR and BGS technologies integrated with carbon capture and storage (CCS) based on the amine-based chemical absorption. This is a well-established method currently used to capture CO_2 to produce urea in integrated facilities.

Electrolysis/Carbon dioxide Hydrogenation

Electrolysis and Carbon Dioxide Hydrogenation (CDH) are alternatives to syngas-based technologies to produce hydrogen for ammonia production and methanol, respectively.

Electrolysis refers to the splitting of the water molecule into H_2 and O_2 with electricity. In COFFEE, electricity is supplied to this technology directly from the electricity generation module of each region, thus it can include both renewable and non-renewable electricity. Furthermore, we assume that O_2 is vented for simplification purposes, thus incomes from potential revenues or use in oxy-fuel or oxidation processes are not accounted for.

Current electrolysis technologies considered for large-scale deployment are: i) Alkaline electrolysis, which is well-established and cost-effective but requires high-quality water and is less efficient (50-78%); ii) anion-exchange membrane (AEM), which can utilize various water types but is still under development and is more expensive; iii) proton-exchange membrane (PEM) electrolysis, an alternative highly efficient and adaptable to changing power inputs, but it requires pure water and is costly; and iv) solid oxide electrolysis, which present high efficiency (>85%) and has high operating temperatures but also presents low TRL [181], [266]. In COFFEE, we use technoeconomic data available for the PEM electrolysis to represent this technology.

Carbon dioxide hydrogenation converts CO_2 into methanol via hydrogenation followed by reversed WGS reactions. In the COFFEE model, CDH is the key CCU pathway to produce carbon-bearing primary chemicals. In COFFEE, hydrogen inputs to CDH can be sourced by any of the technologies above (SMR, CGS, POX, their CCS counterparts or Electrolysis) and CO_2 is likewise supplied by any carbon capture technology across the model.

Haber-Bosch synthesis and methanol synthesis

The syngas produced via SMR, CGS, POX, or BGS is followed by the water gas shift (WGS) reaction, during which CO and H_2O are converted to CO_2 and H_2.

For the methanol synthesis, this step has the role of adjusting the syngas composition to the optimal CO/H_2 ratio for methanol synthesis through catalytic hydrogenation using a copper-based catalyst under approximately 300°C and 2000-3000MPa.

In contrast, for ammonia production, WGS is designed to maximize the output of hydrogen. The excesses of CO_2 and CO are removed via chemical absorption and methanation, respectively, preventing the poisoning of the Haber-Bosch synthesis catalyst. After purification, H_2 is mixed with nitrogen in a high pressure synthesis over an iron catalyst to produce ammonia (Haber-Bosch synthesis). This step is the same followed by hydrogen production via water electrolysis.

Other chemicals

To achieve a comprehensive representation of the chemical sector (encompassing energy use and CO_2 emissions from both organic and inorganic chemicals) in the COFFEE model, we used data from the International Energy Agency's World Energy Balances[12]. By doing this, we accounted for the regional energy use gap between the production of primary chemicals and the remainder of the chemicals sector. We integrated heat and machine drive production technologies into the model to bridge this gap, thereby facilitating fuel switching, electrification, and efficiency improvements over time.

Supplementary Method 3. Technoeconomic parametrization of chemical processes

Supplementary Table 1, Supplementary Table 2, and Supplementary Table 3 detail the technoeconomic parameters for the production of HVCs, methanol, and ammonia, respectively. Primary references were used for refinery[175], [176] and chemical processing[75], [78], [148] units data, which were validated and complemented drawing on multiple sources.

To ensure consistency and comparability across processes, we standardized all values to the same units and currency. This process included the conversion of economic and physical units. For economic conversions, the Chemical Engineering Plant Cost Index (CEPCI)[267] was used to adjust the investment costs of chemical plants to 2010 US dollars. This accounts for inflation and variations in the costs of equipment, materials, and labour over time. Moreover, due to the diversity in original data – often presented in various currencies and/or from different years – we performed extensive conversions and validations.

For physical conversions, we used densities, heat of combustion, and basic unit conversion for handling material and energy efficiencies. When using heat of combustion, we applied the Higher Heating Value (HHV) when steam was explicitly included in the exhaust gases, capturing the total energy released, including the latent heat of vaporization of water. Conversely, we used the Lower Heating Value (LHV) when steam was not explicitly represented, which omits the energy associated with water vapor condensation. This differentiation ensures accuracy in energy conversion calculations depending on the presence of steam in the combustion exhaust.

In our analysis, we treated units that process bio-based, CCU-based, and fossil-based feedstocks as equivalent. For example, we assumed that catalytic reforming units convert both naphtha and bio-naphtha with identical efficiency. Similarly, whether derived from fossil, CCU or bio-based processes, methanol is chemically identical. Therefore, we maintained consistent costs and yields across all these units regardless of the feedstock origin.

Supplementary Table 1. Techno-economic parameters of HVC production technologies.

Technology	Feedstock	Output yields						SEC^a	Plant capacity	Investment cost	O&M cost		Ref.
		Ethylene	Propylene	Butadiene	BTX	C4 stream	H_2				FOM	VOM	
		t/t_F						GJ/GJ$_F$	kt_{MO}/yr	USD2010/ $t_{MO}py^b$	USD2010/t_{MO}		
SC-Naphtha	Naphtha	**0.324**	0.168	0.050	0.104			10	500	2718	54	54	[75], [159], [160], [161], [162]
SC-Naphtha-b	Bionaphtha	***0.324***	*0.168*	*0.050*	*0.104*			10	500				
SC-NG	Ethane	**0.803**	0.016	0.023	0			15	500	1680	34	34	
NCC	Naphtha	**0.324**	0.324	0.050	0.130			9.3	400	3963	41	41	[75], [159], [163], [164]
NCC-b	Bionaphtha	***0.324***	*0.324*	*0.050*	*0.130*			9.3	400				
BDH	Ethanol	***0.575***						2.8	200	1190	84	84	
MTO	Methanol^c	**0.190**	0.180					4.3	500	1340	34	34	[75], [159], [163], [164], [165], [166], [167], [168], [169]
MTO-b	Biomethanol	***0.190***	*0.180*					4.3	500				
PDH	Propane		**0.750**			0.19		9.1	500	855	23	23	[75], [159], [170], [171]
PDH-b	Biopropane		***0.750***			*0.19*		9.1	500				
MTT	Ethylene (+ C4s)^d		**3.125**					3.6	300	750	44	44	[172], [173]
MTT-b	Bioethylene (+ bC4s)^d		***3.125***					3.6	300				

ETB	Ethanol			***0.280***				21.5	50	800	67	23	[174]
MTA	Methanol[c]				**0.230**			3.8	500	1380	17	17	[75], [159], [166], [168]
MTA-b	Biomethanol				***0.230***			3.8	500				
CAT	C4 stream			**0.600**				11.4	500	855	23	23	[75], [159], [170], [171]
CAT-b	Bio C4 stream			***0.600***				11.4	500				
DIM	Ethylene					**0.800**		0.4	300	150	4	4	[172]
DIM-b	Bioethylene					***0.800***		0.4	300				
CR	Naphtha				**0.880**		3.6[e]	0.8	800	262	3	3	[175], [176]
CR	Bionaphtha				***0.880***		3.6[e]	0.8	800	262	3	3	[175], [176]

F: Feedstock (underlined); **MO: Main output (values in bold).** *Bioproducts in italic.* [a] Includes heat, steam, and machine drive requirements (thus excluding energy use as feedstock). [b] Tonnes per year. [c] Fossil-. or CCU-based. [d] Yields refer to 1t of ethylene and 3.03t of C4s. [e] Value in GJ/t_{MI}. SC: Steam cracking; NCC: Naphtha catalytic cracking; BDH: Bioethanol dehydration; MTO: Methanol-to-Olefins; PDH: Propane dehydrogenation; MTT: Metathesis; ETB: Ethanol-to-Butadiene; MTA: Methanol-to-Aromatics; CAT: Catadiene®; DIM: Dimerization; CR: Catalytic reforming; Suffix *-b*: bio-based feedstock and products.

Supplementary Table 2. Techno-economic parameters for methanol production technologies.

Technology	Feedstock	Yields		Machine drive	Process Emissions	Investment cost	O&M cost		Ref.
		MO: Methanol	CO_2 *capture*/**use**				FOM	VOM	
		GJ$_F$ [a] /t$_{MO}$	tCO_2/t$_{MO}$	GJ/t$_{MO}$	tCO_2 /t$_{MO}$	USD2010/t$_{MO}$py [b]	USD2010/t$_{MO}$		
SMR	Methane	33.9	-	0.3	0.8	340	4.5	4.5	[75], [78], [148]
SMR+CCS	Methane	33.9	*0.76*	0.3	0.04	540	6.7	6.7	[75], [78], [148]
CGS	Coal	46.3	-	3.7	3.3	820	10.3	10.3	[75], [78], [148]
CGS+CCS	Coal	55.3	*3.14*	3.9	0.17	1020	12.8	12.8	[75], [78], [148]
BGS	Solid biomass	47.9	-	5.0	0	5655	70.7	70.7	[75], [78], [148], [177]
BGS+CCS	Solid biomass	47.9	*3.25*	5.0	0	5855	73.3	73.3	[75], [78], [148], [177]
CDH	H_2 + CO_2	22.6	**1.38**	1.5	0	44	0.5	0.5	[75], [78], [148], [178]

F: Feedstock (underlined); MO: Main Output; FOM: Fixed operation and maintenance cost; VOM: Variable operation and maintenance cost. [a] Includes heat and feedstock requirements. [b] Tonnes of main output per year.

Supplementary Table 3. Techno-economic assumptions for hydrogen and ammonia production technologies. SMR, SMR+CCS, CGS, CGS+CCS, POX, BGS, BGS+CCS, and Electrolysis are hydrogen production technologies, which can be used for energy and non-energy purposes (i.e., in ammonia production via Haber-Bosch reaction).

Technology	Feedstock Inputs	Yields		Machine drive	Process Emissions	Investment cost	O&M cost		Ref.
		MO: H_2 or **NH_3**	CO_2 capture				FOM	VOM	
		GJ$_{MO}$[a] /GJ$_{MI}$ or **t$_{MO}$/GJ$_{MI}$**	tCO_2/t$_{MO}$	GJ/t$_{MO}$	tCO_2 /t$_{MO}$	USD2010/kWyr$_{MO}$py [b]	USD2010/kWyr$_{MO}$		
SMR	Methane	0.74	-	-	8.90	545	12	12	[75], [78], [148], [179]
SMR+CCS	Methane	0.74	8.01	-	0.89	622	23	23	[75], [78], [148], [179], [180]
CGS	Coal	0.59	-	-	20.2	2086	20	20	[75], [78], [148], [179]
CGS+CCS	Coal	0.59	18.18	-	2.02	2255	22	22	[75], [78], [148], [179], [180]
POX	Fuel oil	0.70	-	-	13.6	800	10	10	[75], [78], [148], [179]
BGS	Solid biomass	0.67	-	-	-	2285	83	83	[75], [78], [148], [177], [179]
BGS+CCS	Solid biomass	0.67	16.4	-	-	2465	83	83	[75], [78], [148], [177], [179]
Electrolysis	Electricity + H_2O	0.64 (2010) 0.74 (2060)	**-**	-	-	896 (2010) 240 (2050)	12 (2010) 3 (2050)	12 (2010) 3 (2050) [c]	[75], [78], [148], [178], [179], [181]
Haber Bosch	H_2 + N_2	**0.04**	**-**	3.9	-	95	2.5	2.5	[75]

MI: Main Input (underlined); MO: Main Output; FOM: Fixed operation and maintenance cost; VOM: Variable operation and maintenance cost. [a] Includes heat and feedstock requirements. [b] tonnes per year. [c] Electrolysis VOM does not include potential revenues from oxygen sales.

Supplementary Method 4. Regional demand scenarios

This section delves into the methodology used to model demand scenarios across regions, taking an econometric approach to provide a general understanding of scale and rate of future petrochemicals demand. We discuss these methodologies in detail in the following subsections.

High-value chemicals

The production of resin and fibres are key factors that drive the demand for high-value chemicals (HVC). Thus, to calculate the long term demands for each HVC, we initially relied on per capita plastics consumption data specific to 63 countries [138]. This data was used as a proxy to estimate total plastic demands from 2010 to 2100 for the 18 regions in COFFEE. The historical data used in this study is illustrated in Supplementary Figure 4.

Subsequently, we conducted a regression analysis to project future demand. We incorporated data on GDP and population data according to the second shared socioeconomic pathway (SSP2) [182]. We use a simple modified form of exponential growth model (Supplementary Equation 1) based on macroeconomic assumptions to project long-term demands:

$$Cpc_t = Cpc_{t-1} \, . \left(\frac{GDPpc_t}{GDPpc_{t-1}}\right)^{\frac{ln\left(\frac{Cpc_{2015}}{Cpc_{2010}}\right)}{ln\left(\frac{GDPpc_{2015}}{GDPpc_{2010}}\right)}} \qquad (1)$$

where:

Cpc_t: Plastics Consumption per capita at timestep t

Cpc_{t-1}: Plastics Consumption per capita at the previous timestep $t\ -1$

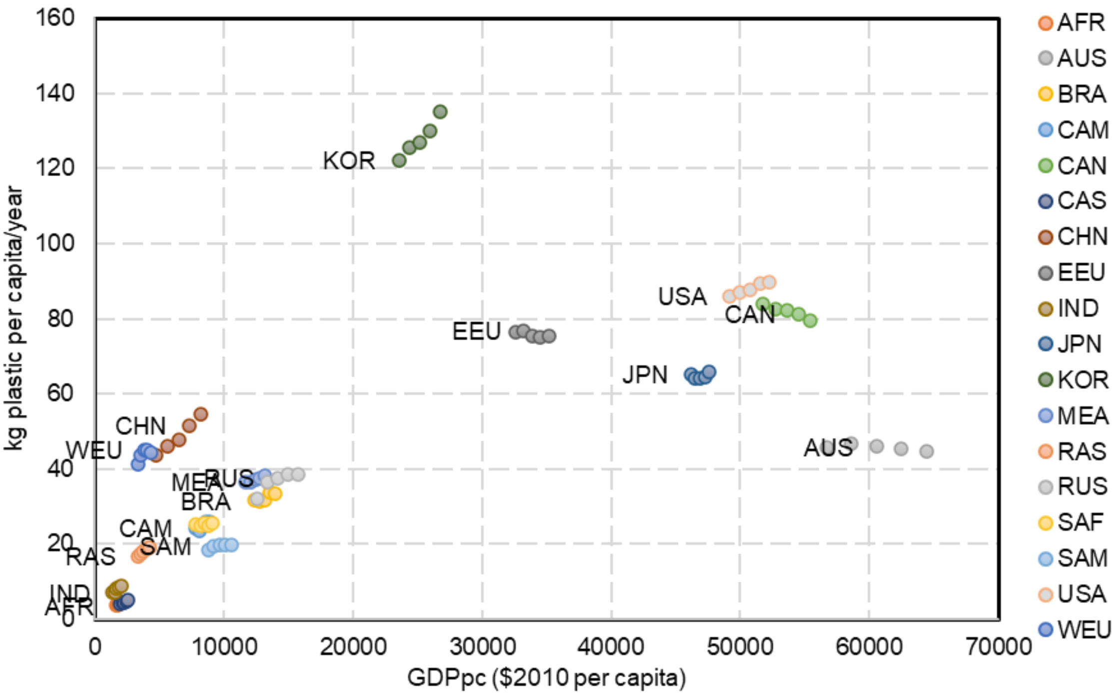
$GDPpc_t$: Gross Domestic Product per capita at timestep t

$GDPpc_{t-1}$: Gross Domestic Product per capita at the previous timestep t-1.

Cpc_{2010}, Cpc_{2015}, $GDPpc_{2010}$, and $GDPpc_{2010}$: The respective Plastics Consumption per capita and Gross Domestic Product per capita in the timesteps 2010 and 2015.

The model uses the ratio of growth rates between the current year and the previous year to adjust the rate of growth changes over time. Additionally, the logarithmic term normalizes the projection based on historical trends by comparing the ratio of plastic consumption per capita in a base year (i.e., 2015) to a prior year (i.e., 2010) with the ratio of growth rates over the same period. Due to low availability data, we decided to undertake this conservative approach to estimate future consumption per capita (i.e., it assumes that plastic consumption will continue to grow at a rate proportional to its current level, and that the rate of growth will be constant over time).

We compared the first estimates with other studies[26], [139], [198] and reached the conclusion that: 1) the primary data for plastics per capita consumption had a reduced scope compared to the assessment made by [75], [198], and 2) HVCs are also used in other applications such as solvents, surfactants and detergents. Thus, to account for this “other” component of HVC demand, we normalized global demands based in the figures provided by Geyer et al. (2017). We then calculated the content of ethylene, propylene, butadiene, and BTX in 1 kg of plastic, based on figures from a material flow analysis work of 2013 [139], [268]. These shares were assumed to remain constant over time.



Supplementary Figure 3. Development of per capita consumption of plastics per region.

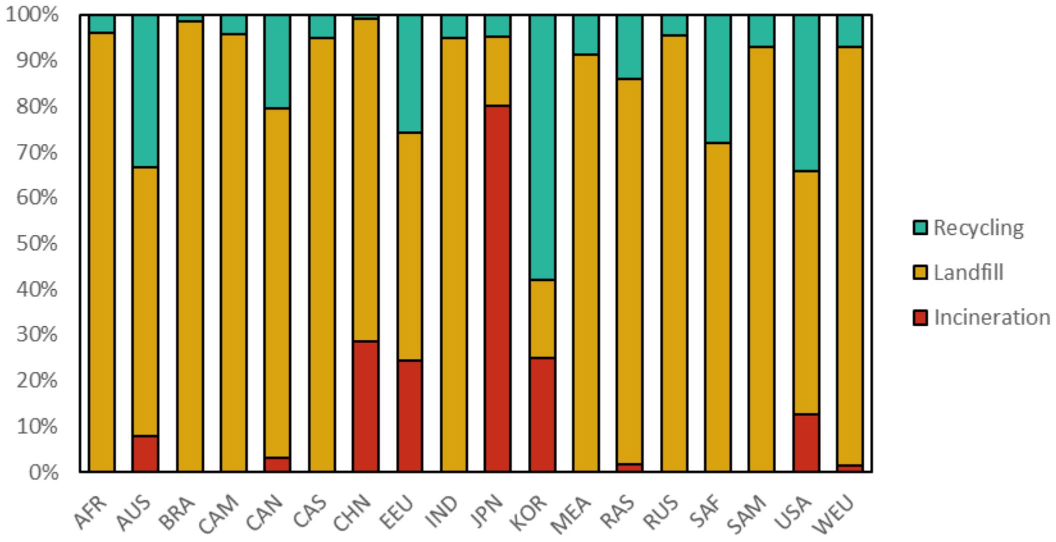
Methanol and Ammonia

A similar approach was followed to project methanol long-term regional demands. Given that methanol use in biodiesel production and gasoline blending was already endogenously represented in COFFEE, we model methanol demand for non-energy purposes separately, e.g., formaldehyde, acetic acid, and methylamine production. To that end, data on regional methanol demands were collected from EPE (2019) and Su et al. (2013) [257], [264], from which it was reduced the energy-related demands based on Chatterton (2018) and OECD & FAO (2021) [142], [143].

In the case of ammonia, we used long-term regional demands for food outputs the TEA (Total-Economy Assessment) model, which is a multi-regional and multi-sectorial Computable General Equilibrium (CGE) model used in soft-link with COFFEE[269], [270]. Future studies aim to make ammonia demand endogenous with the land-use module in COFFEE.

Supplementary Method 5. Final disposal assumptions

Solid waste management data from World Bank's *What a Waste 2.0* database was used as a baseline to estimate regional shares for incineration, landfilling (i.e., controlled landfilling plus mismanagement) and mechanical recycling (see Supplementary Figure 4). Incineration and recycling emissions were calculated based on ref.[210]. For plastics incineration, it was assumed that the carbon content of each HVC was emitted as CO_2. Therefore, 3.14 tCO_2/t ethylene, 3.14 tCO_2/t propylene, 3.25 tCO_2/t butadiene, and 3.38 tCO_2/t aromatics (using benzene as a proxy) were assumed when accounting for those emissions. Mechanical recycling considers 10% of material loss at every cycle and emissions account for electricity use from shredding, extrusion, and agglomeration.



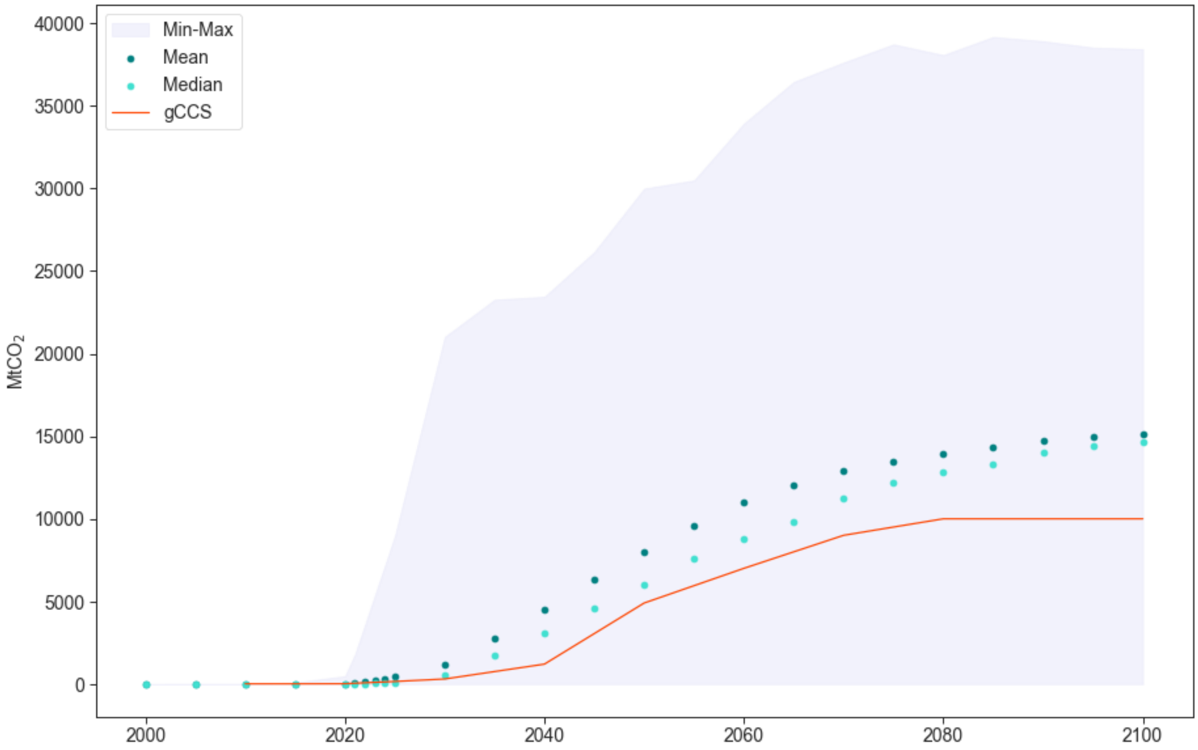
Supplementary Figure 4. Final disposal shares assumed in the base year for COFFEE regions. Source: own elaboration based on ref.[271].

Supplementary Method 6. Land-use emissions considerations

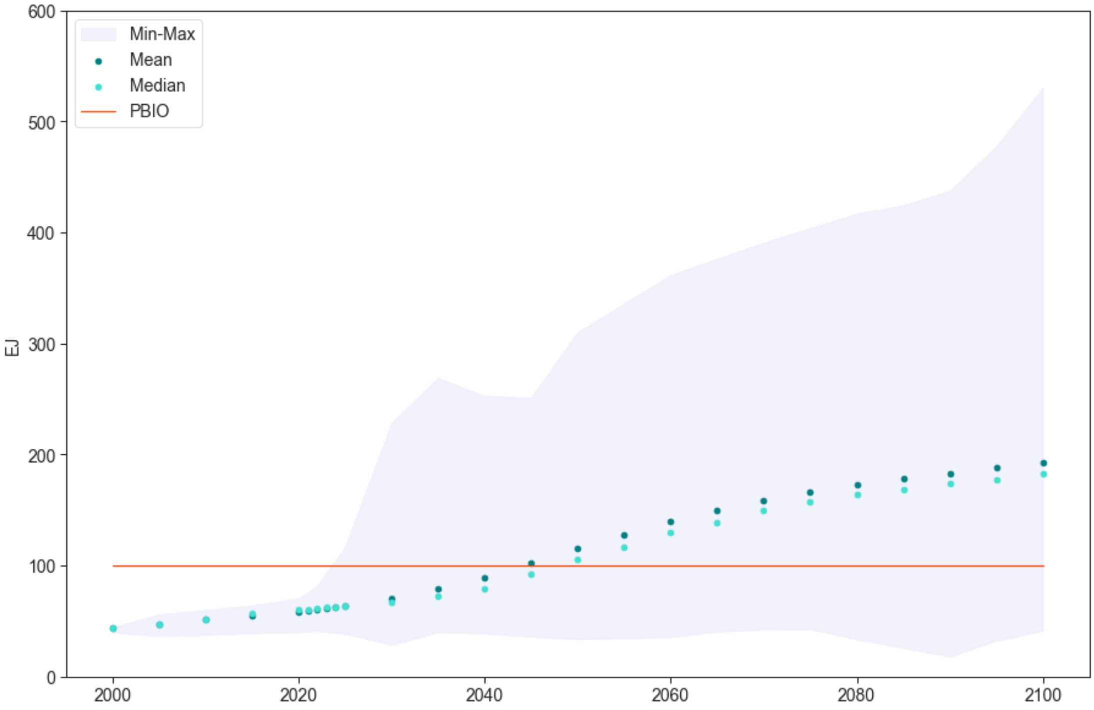
COFFEE assumes carbon neutrality for biomass based on specific conditions. Firstly, the model includes emissions from land-use changes, energy use during agricultural practices and logistics, agricultural residues, fertilizer use, and other relevant sources. It also considers carbon sequestration during biomass growth and the final storage of carbon, either geologically or in materials. Within the balance between carbon emissions and sinks, the model identifies and favours options and agriculture practices that guarantee net negative carbon emissions.

COFFEE represents Sugarcane, Corn, Wheat, Woody biomass, Grassy biomass, Beet, Bagasse, Residues. It considers the growth rates and carbon uptake capacities of different species to ensure that the biomass used has a high potential for carbon neutrality. Harvest methods are not explicitly represented, but are indirectly assumed via crop yields, energy inputs, capital investment and operating costs (incl. labour). The model does not account for soil carbon changes due to biomass harvesting. Soil carbon is affected only through land-use change.

More information on the land-use sector in COFFEE can be found in refs.[134], [272], [273], [274].



Supplementary Figure 5. Assumptions concerning the global deployment of CCS in 1p5C_gCCS scenario compared with outcomes derived from 540 scenarios across categories C1, C2, and C3 from the IPCC AR6 scenario database.

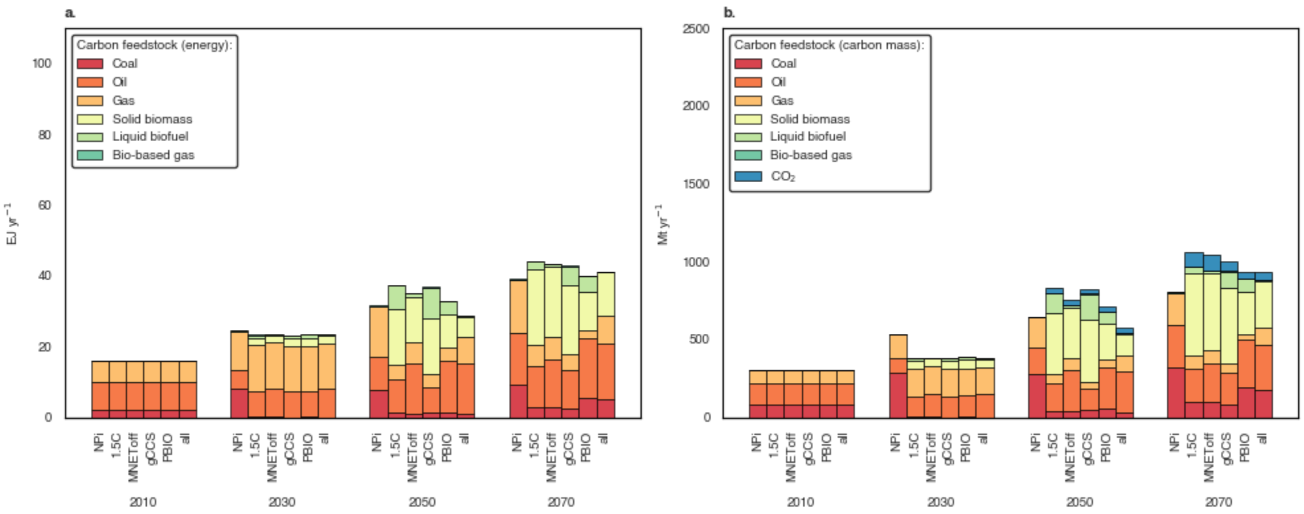


Supplementary Figure 6. Assumptions concerning the utilization of global biomass as a primary energy source in 1p5C_PBIO scenario compared with outcomes derived from 540 scenarios across categories C1, C2, and C3 from the IPCC AR6 scenario database.

Supplementary Table 4. Scenario definition and constraints assumptions.

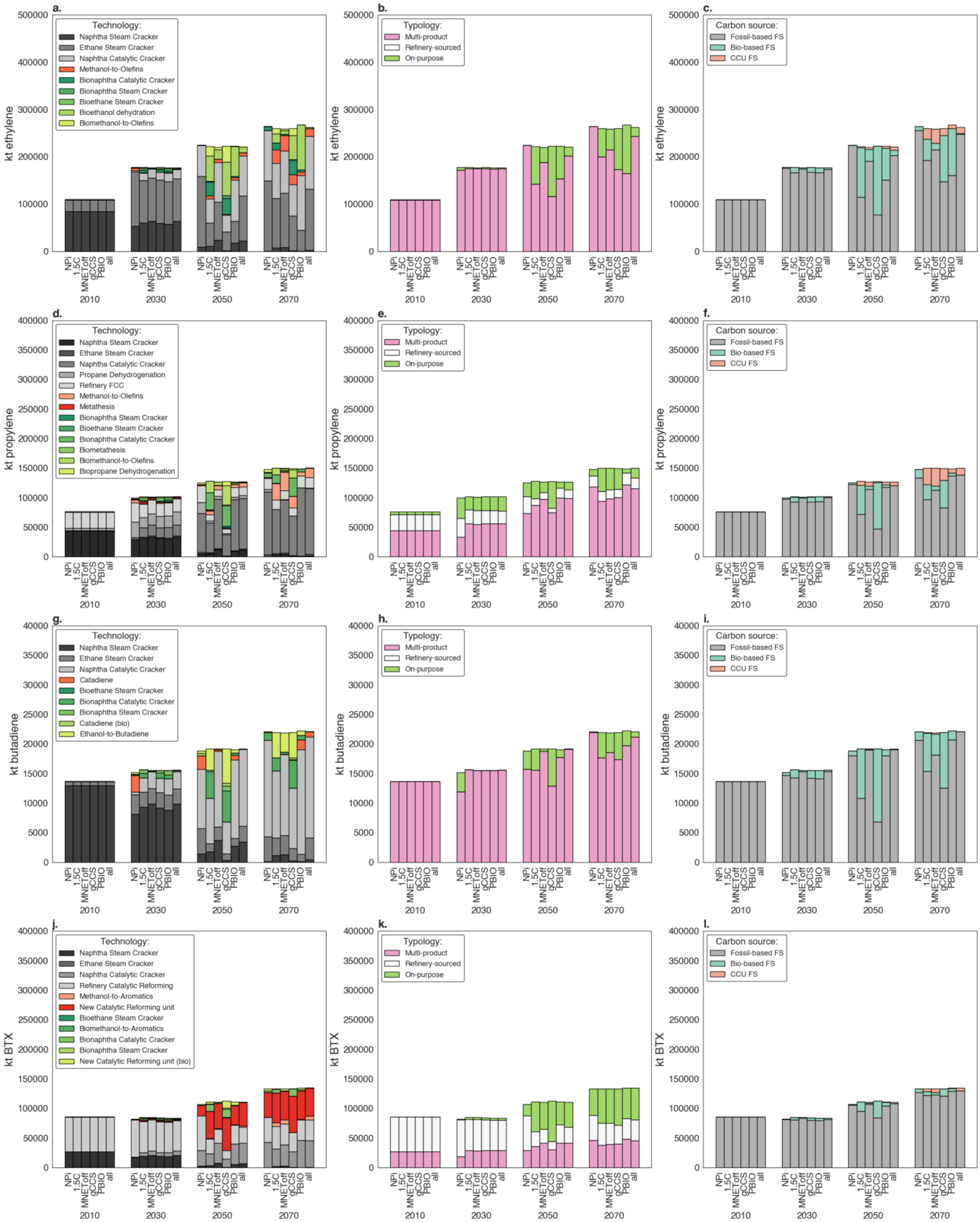
					Global CCS restriction, reaches 10 Gt/yr in 2080	Biogenic carbon storage in biomaterials	Restricts biomass use below 100 EJ/yr globally after 2040
	$GtCO_2$		AR6 WGI		COFFEE constraints		
Scenario / Period	Budget COFFEE[a] (2018-2100)	Budget AR6 WGI[b] (2020-2100)	T_L (◦C)	Likelihood	gCCS	MNET	PBIO
NPi	-	-	-	-	off	on	off
1p5C	480	400	1.5	67%	off	on	off
sensitivity analysis							
1p5C_gCCS	480	400	1.5	67%	on	on	off
1p5C_MNEToff					off	off	off
1p5C_PBIO					off	on	on
1p5C_all					on	off	on

T_L: Temperature increase above pre-industrial levels limit. [a] The carbon budget variable in COFFEE starts in 2018. To account for the 2018-2020 gap, ~80 $GtCO_2$ was integrated into the COFFEE model's carbon budget based on ref. [185]. [b] Source: [184].



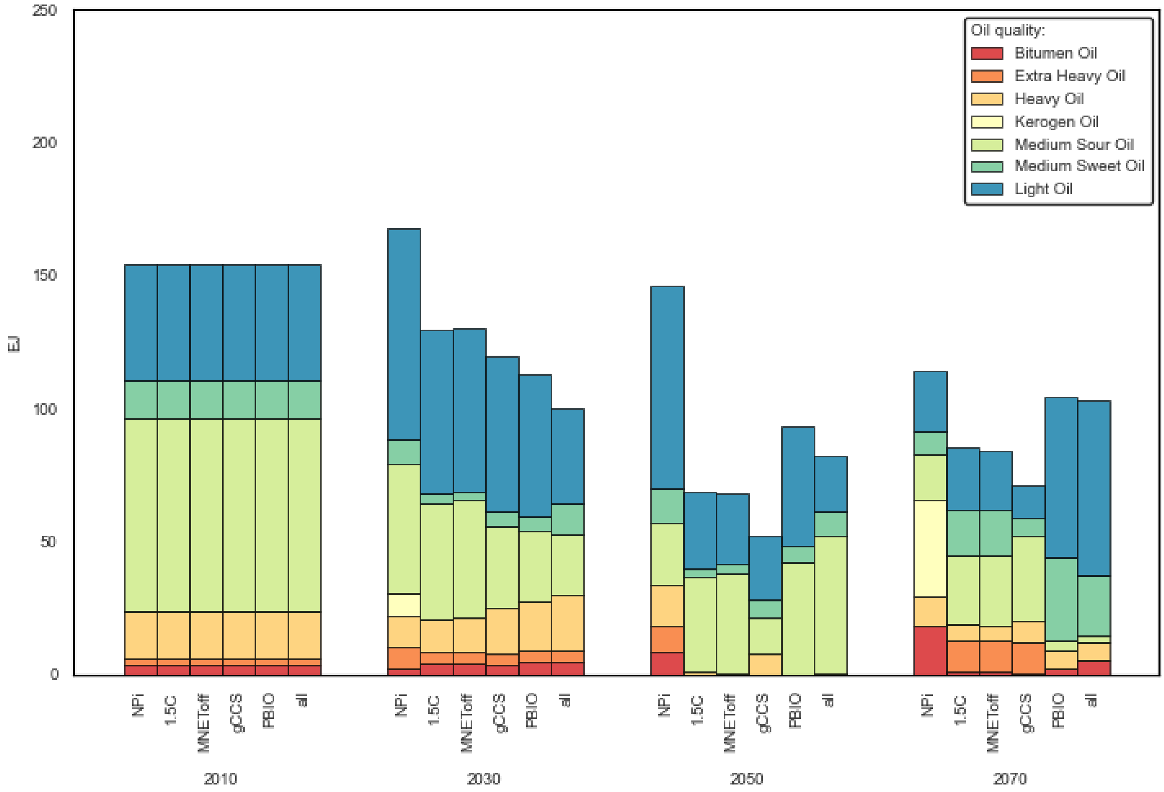
Supplementary Figure 7. Carbon feedstock in energy (a) and carbon mass (b) terms.

We considered the following carbon contents of each feedtock source: Coal: 85% (on average, considering bituminous coal with high carbon content); Oil: 84.2%, based on naphtha (C_8H_{18} as a proxy); Gas: 75.0%, based on methane (CH_4) Solid Biomass: 44.7%, based on eucalyptus (see ref.[275]) Liquid Biomass: 52.2% based on bio-ethanol (C_2H_5OH); Bio-based gas: 75%, based on biomethane (CH_4); and CO_2: 27.3%. NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



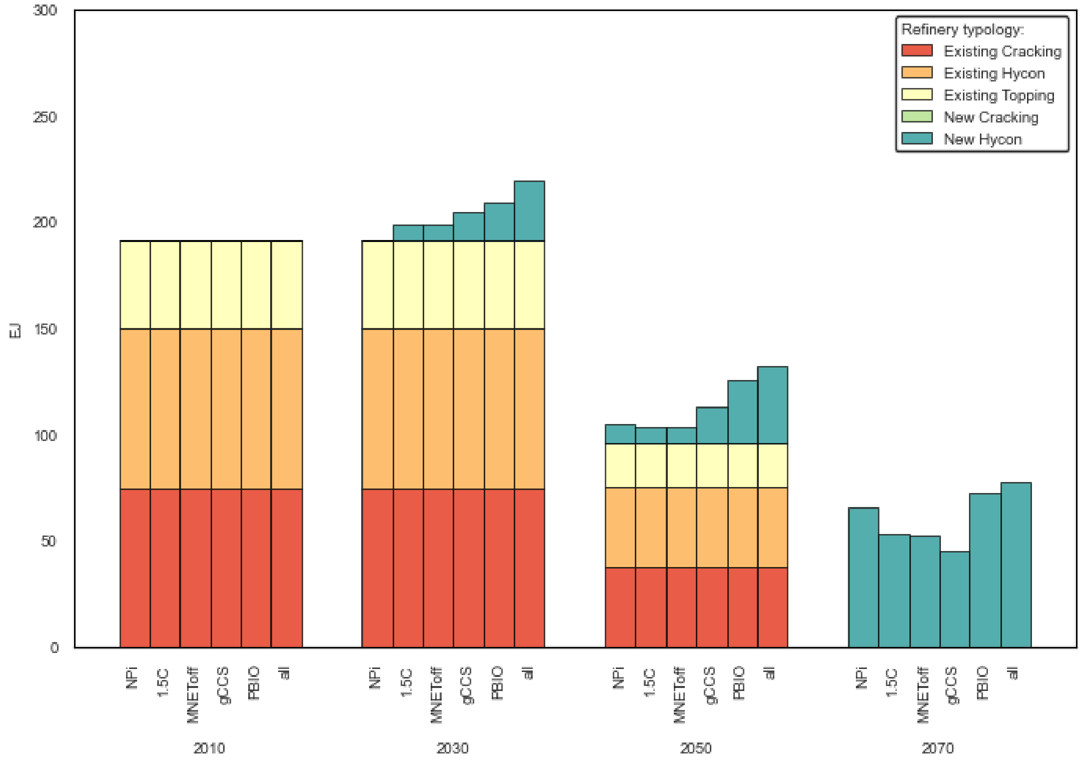
Supplementary Figure 8. Technology split, typology and carbon source for ethylene (a-c), propylene (d-f), butadiene (g-i), and Benzene, Toluene and Xylenes (BTX) (j-l) production.

NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



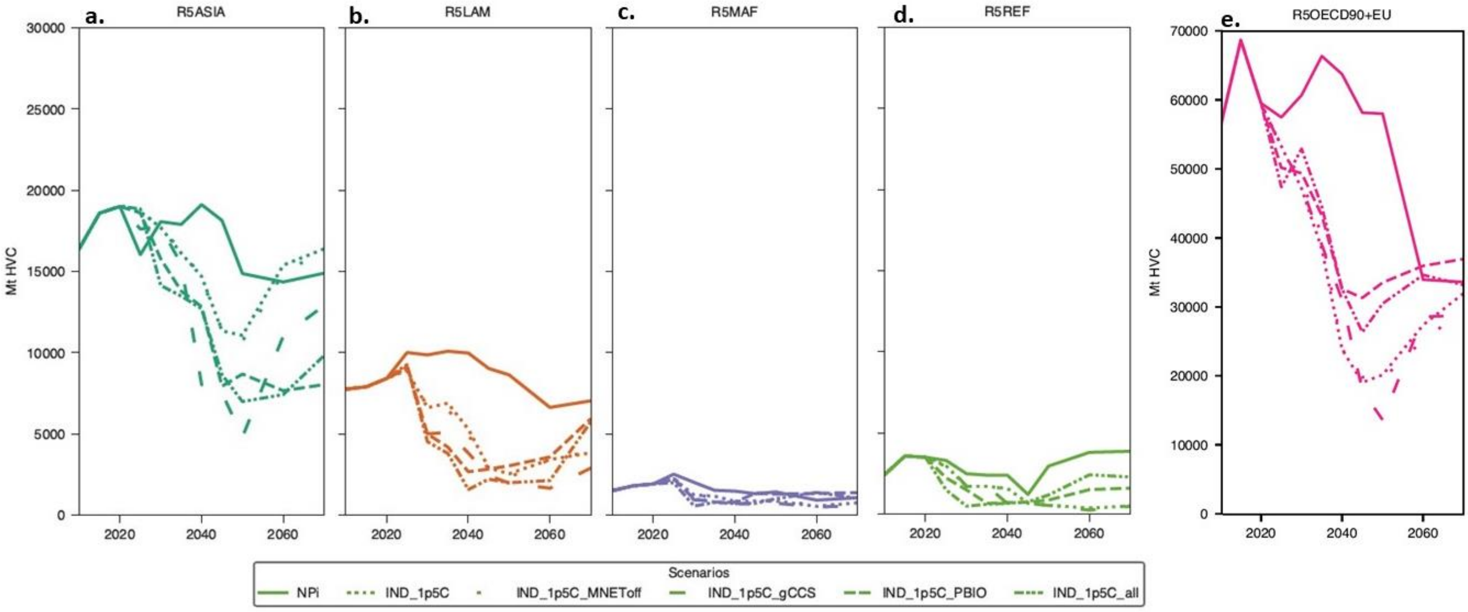
Supplementary Figure 9. Global oil production disaggregated according to oil quality.

NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



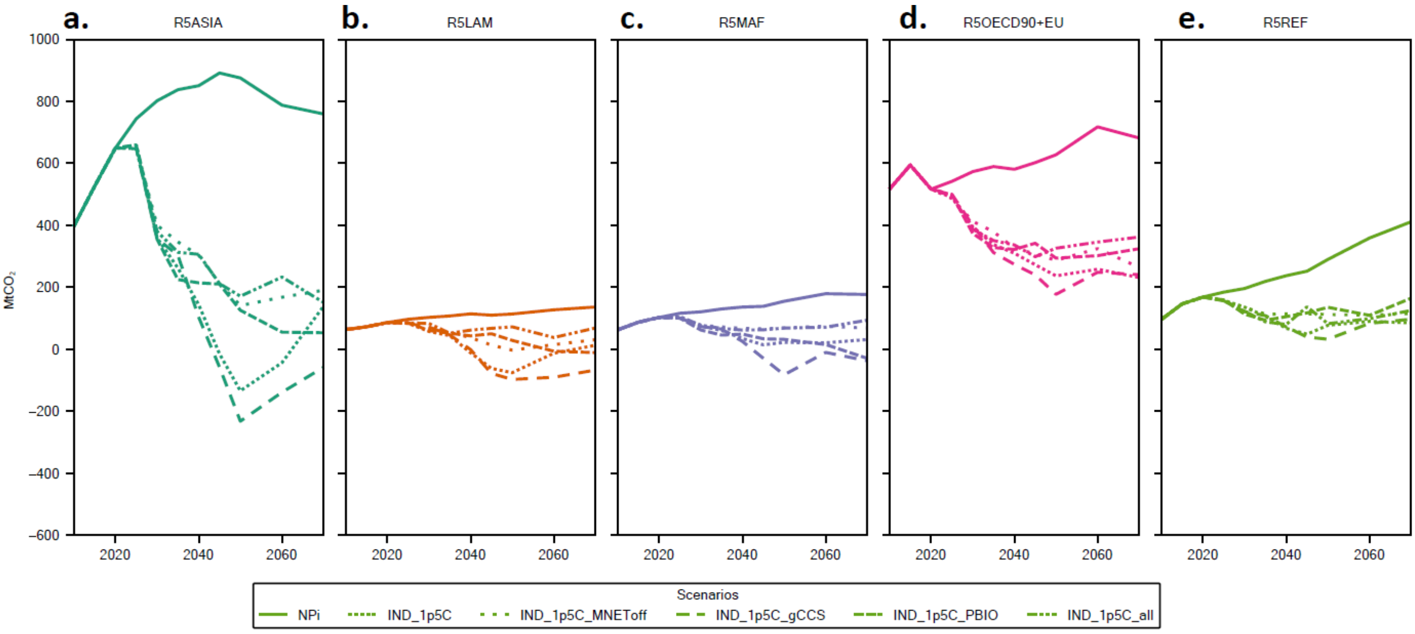
Supplementary Figure 10. Global refinery capacity per refinery typology.

NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



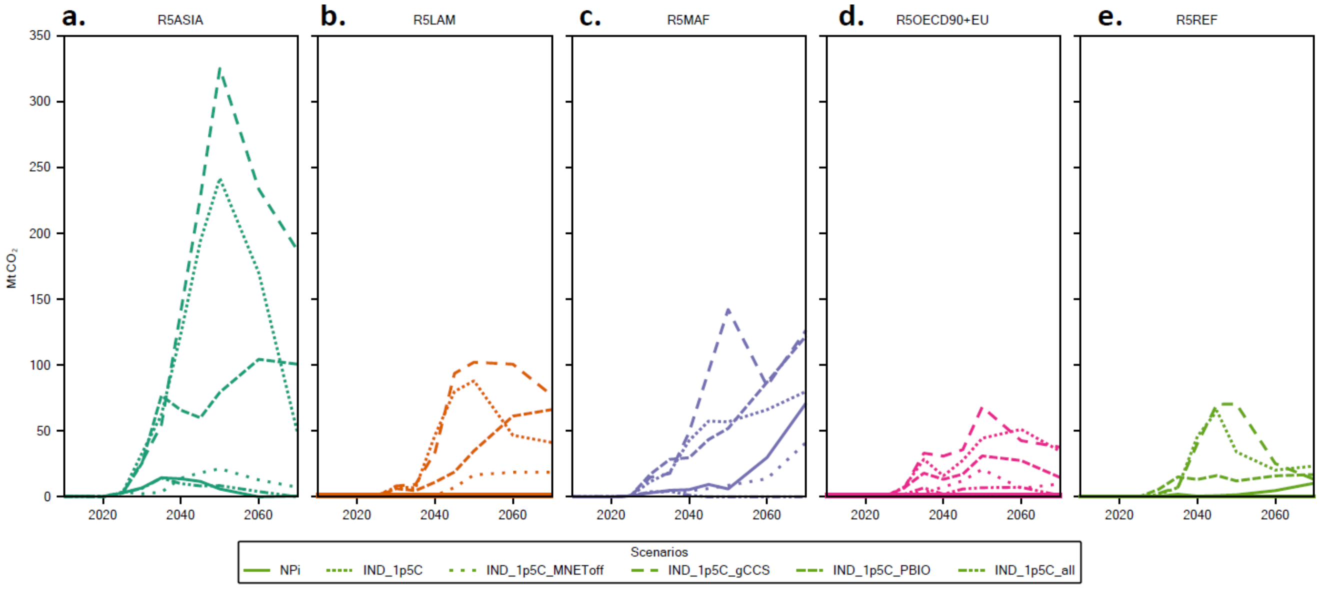
Supplementary Figure 11. Regional refinery-sourced HVCs per R5 region.

R5ASIA: Asia (excluding Middle East); R5LAM: Latin America; R5MAF: Middle East and Africa; R5OECD90+EU: OECD countries; R5REF: Reforming Economies (Eastern Europe, former Soviet Union). NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



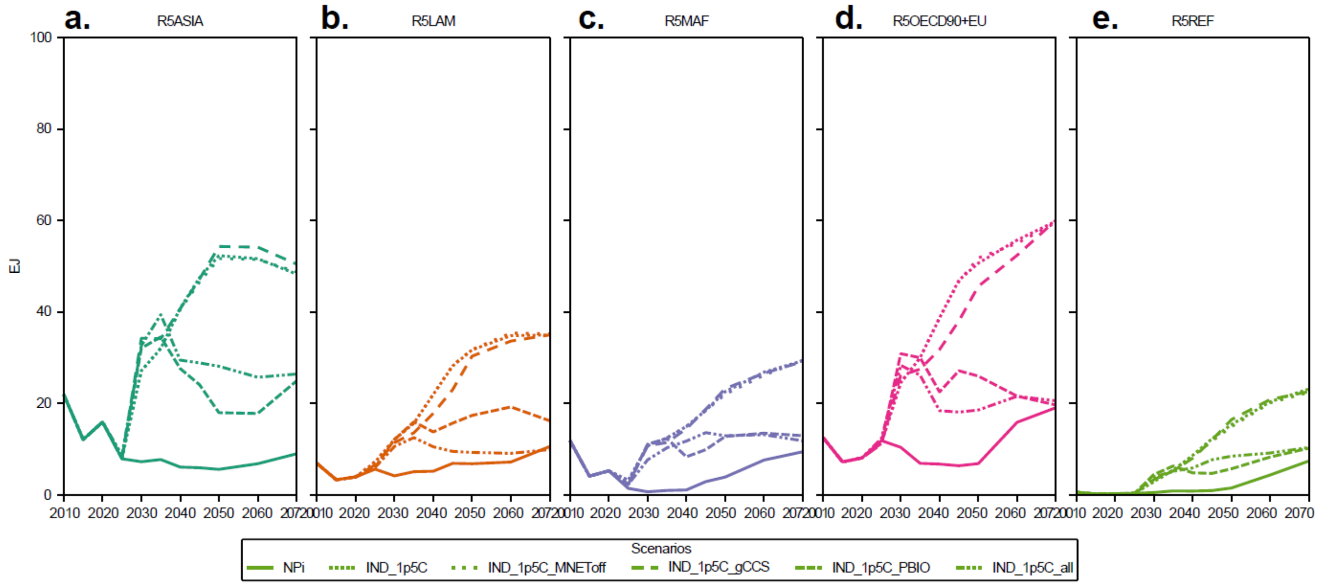
Supplementary Figure 12. Regional CO_2 emissions pathways for the chemical sector per R5 region.

R5ASIA: Asia (excluding Middle East); R5LAM: Latin America; R5MAF: Middle East and Africa; R5OECD90+EU: OECD countries; R5REF: Reforming Economies (Eastern Europe, former Soviet Union). NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



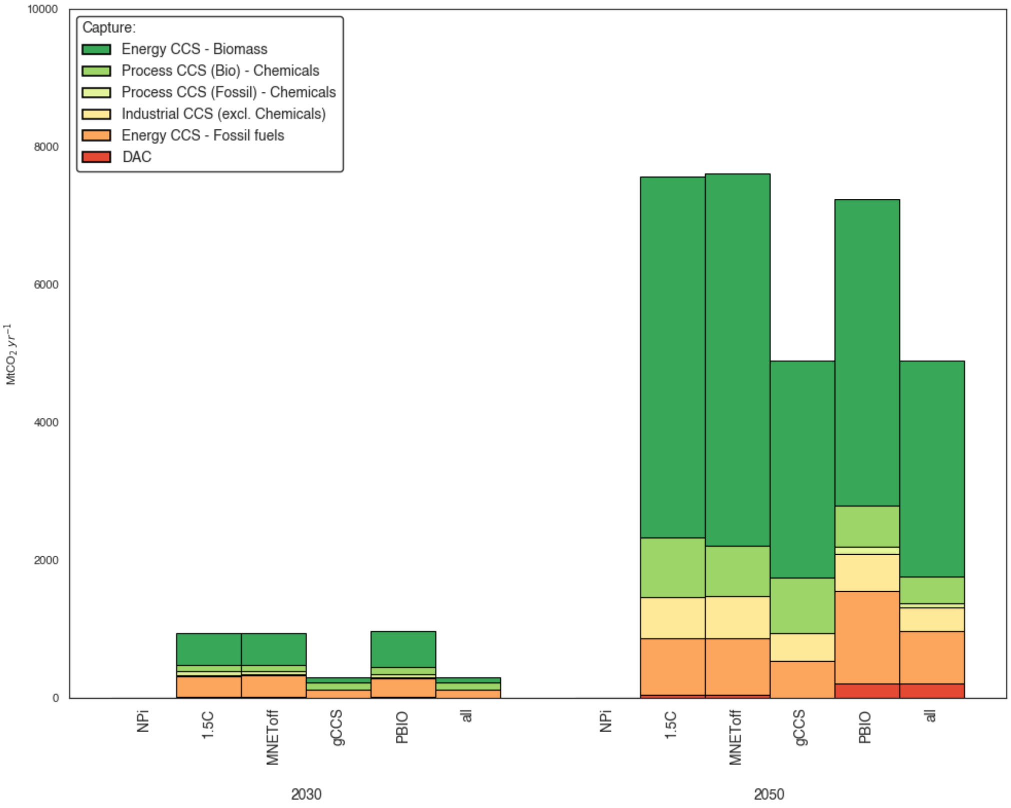
Supplementary Figure 13. Regional biogenic storage of carbon in biomaterials per R5 region.

R5ASIA: Asia (excluding Middle East); R5LAM: Latin America; R5MAF: Middle East and Africa; R5OECD90+EU: OECD countries; R5REF: Reforming Economies (Eastern Europe, former Soviet Union). NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNETOff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions.



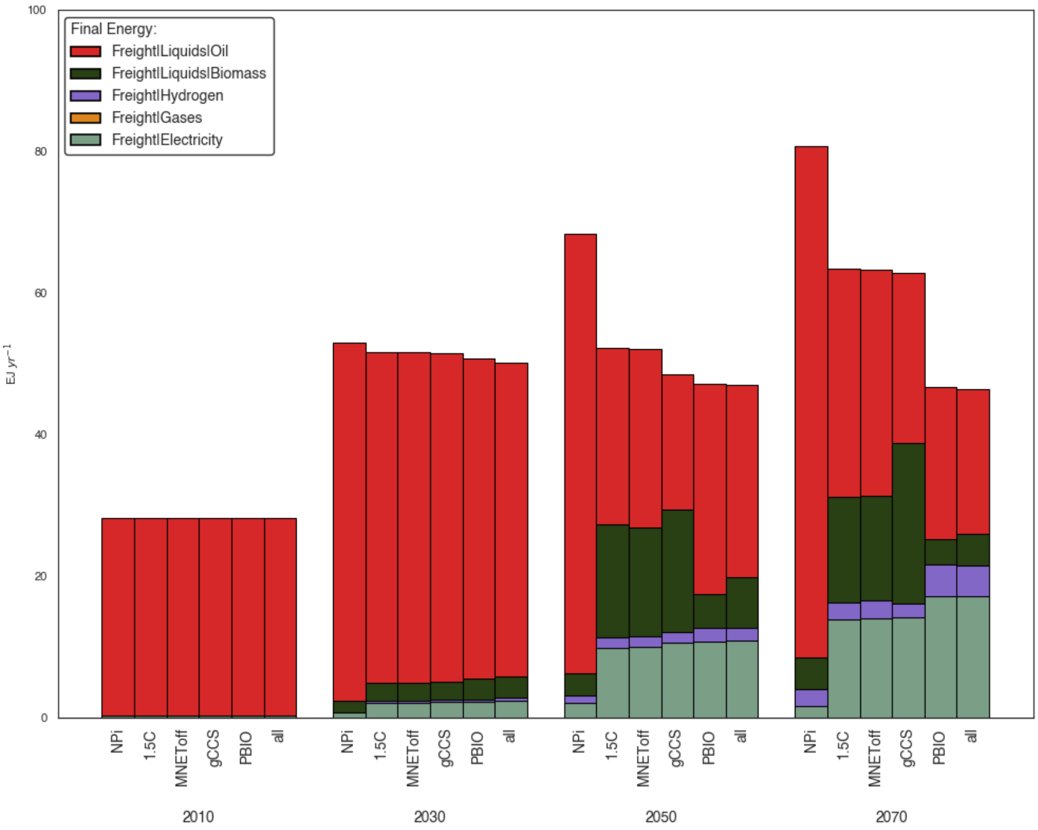
Supplementary Figure 14. Biomass use as primary energy in R5 regions.

R5ASIA: Asia (excluding Middle East); R5LAM: Latin America; R5MAF: Middle East and Africa; R5OECD90+EU: OECD countries; R5REF: Reforming Economies (Eastern Europe, former Soviet Union). NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. EJ: Exajoules.



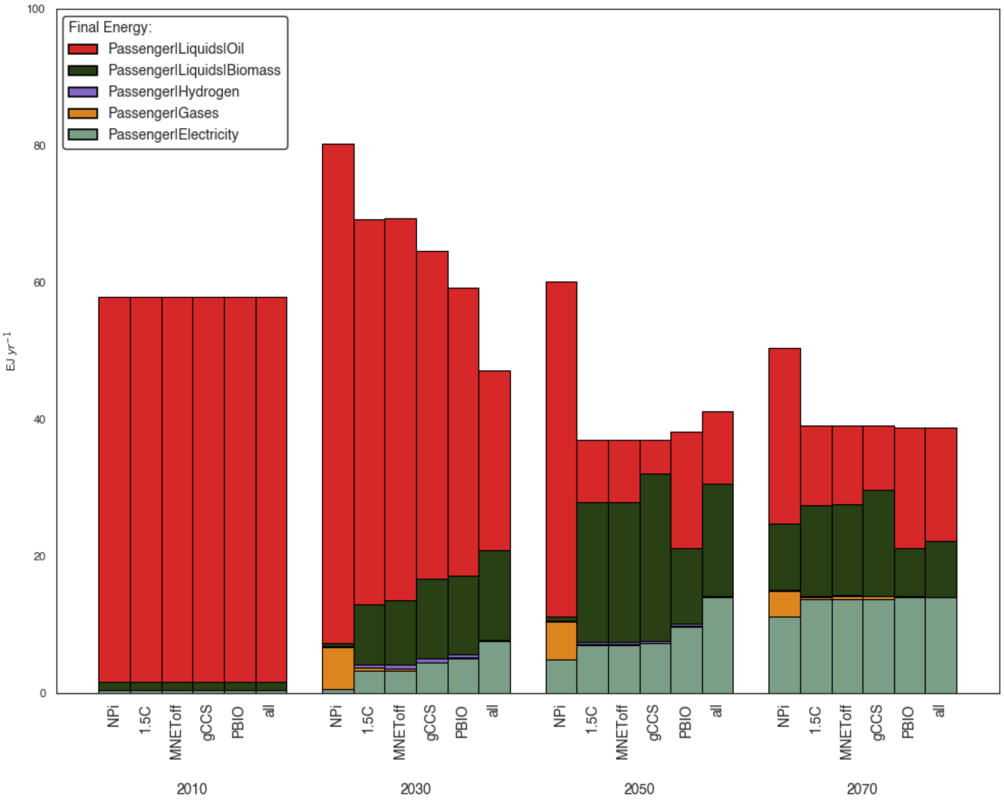
Supplementary Figure 15. Sources of carbon capture across scenarios in 2030 and 2050.

NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNETOff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. DAC: Direct Air Capture. CCS: Carbon Capture and Storage.



Supplementary Figure 16. Final energy use in the freight transportation sector across scenarios.

NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. EJ: Exajoules.



Supplementary Figure 17. Final energy use in the passenger transportation sector across scenarios.

NPi: Implemented National Policies; 1.5C: carbon budget consistent with limiting global warming to 1.5°C; gCCS: a 1.5C scenario with restrictions on global CCS deployment; PBIO: a 1.5C scenario with constraints on global primary biomass use; MNEToff: a 1.5C scenario that turns off the assumption of biogenic carbon storage in materials; and all: a comprehensive 1.5C sensitivity scenario incorporating all the abovementioned restrictions. EJ: Exajoules.