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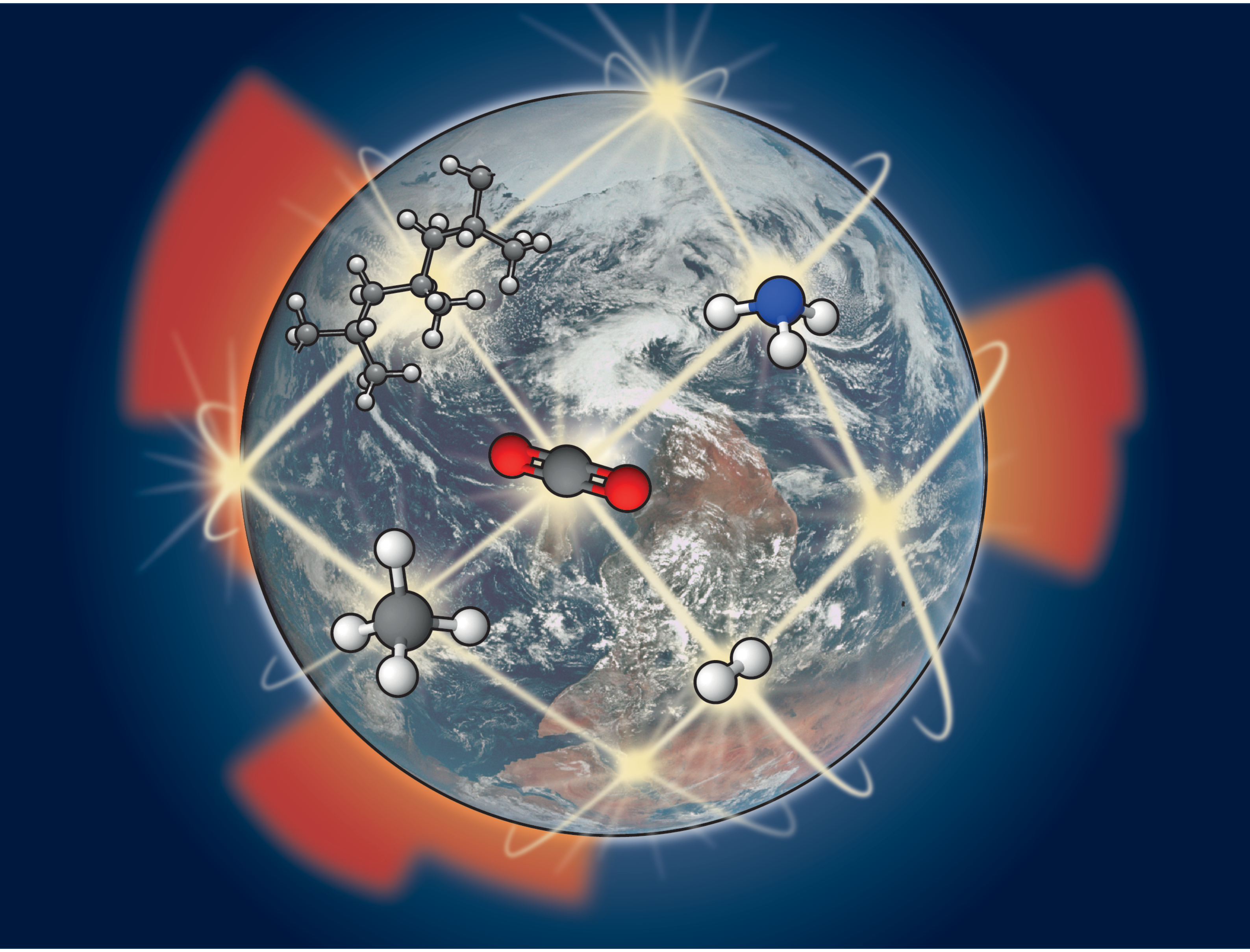

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An anthropocene-framed transdisciplinary dialog at the chemistry-energy nexus†

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At the energy-chemistry nexus, key molecules include carbon dioxide (CO_2), hydrogen (H_2), methane (CH_4), and ammonia (NH_3). The position of these four molecules and that of the more general family of synthetic macromolecular polymer blends (found in plastics) were cross-analyzed with the planetary boundary framework, and as part of five scientific policy roadmaps for the energy transition. According to the scenarios considered, the use of some of these molecular substances will be drastically modified in the coming years. Ammonia, which is currently almost exclusively synthesized as feedstock for the fertilizer industry, is envisioned as a future carbon-free energy vector. "Green hydrogen" is central to many projected decarbonized chemical processes. Carbon dioxide is forecast to shift from an unavoidable byproduct to a valuable feedstock for the production of carbon-based compounds. In this context, we believe that interdisciplinary elements from history, economics and anthropology are relevant to any attempted cross-analysis. Distinctive and crucial insights drawn from elements of humanities and social sciences have led us to formulate or re-raise open questions and possible blind-spots in main roadmaps, which were developed to guide, *inter alia*, chemical research toward the energy transition. We consider that these open questions are not sufficiently addressed in the academic arena around chemical research. Nevertheless, they are relevant to our understanding of the current planetary crisis, and to our capacity to properly assess the potential and limitations of chemical research addressing it. This academic perspective was written to share this understanding with the broader academic community. This work is intended not only as a call for a larger interdisciplinary method, to develop a sounder scientific approach to broader scenarios, but also – and perhaps mostly – as a call for the development of radically transdisciplinary routes of research. As scientists with different backgrounds, specialized in different disciplines and actively involved in

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contributing to shape solutions by means of our research, we bear ethical responsibility for the consequences of our acts, which often lead to consequences well beyond our discipline. Do our research and the knowledge it produces respond, perpetuate or even aggravate the problems encountered by society?

1. Introduction

1.1. Anthropocene: the overarching context

The term Anthropocene, popularized by Paul J. Crutzen (an atmospheric chemist) around 2000,[1] is becoming established both among scientists and the wider public. It reflects how Earth's biochemical processes have been profoundly altered by humanity's way of inhabiting the environment (housing, agriculture, industry, transportation, *etc.*). The effects extend to the composition of the Earth's crust and its atmosphere. Consequently, our activities have become an Earth-altering force of geological magnitude. The term was devised to refer to our current age, considering that the Earth had moved beyond the stable periods of the Holocene (the temperate period of the last 12 000 years, following the last Pleistocene glaciation) and the striving age of humanity (with the beginning of agriculture around 11 000 years ago). The Anthropocene age is characterized by fluctuations and uncertainty, which are further exacerbated by the "great acceleration" suggested by the analysis of several socio-economic and Earth Systems trends performed by scientists from the Stockholm Resilience Center.[2] With others, P. J. Crutzen and W. Steffen contributed to the definition of the "planetary boundaries"-framework aiming to assess the extent and consequences of our impact on nine Earth system processes.[3–14]

The challenges posed by the Anthropocene will need to be addressed, and science, including chemistry, is expected to be part of this process. Indeed, options for change, and their implementations to help either avoid or mitigate the multidimensional ecological crisis humanity faces will need to be scientifically informed. Among the pressing open questions, scientists must provide new knowledge to help the deployment of solutions to achieve an equilibrium between our energy and resource consumption and the planet's human habitability. Several sustainability-driven systemic frameworks have been proposed for chemistry, *e.g.*, the green and sustainable periodic table,[15] one-world-chemistry,[16] or "circular chemistry for circular economy".[17] Implementing sustainability has also been advocated for in chemistry education, through the teaching – among other principles – of systems thinking.[18–20]

In this paper, we particularly explore the importance of Anthropocene-spurred interdisciplinary connections between the social sciences, chemistry and the humanities as part of the search for the sustainability-driven balance at the chemistry-energy nexus.

1.2. About the authors

Chemistry's connections with ethical, social, economic, and political aspects have always been present, since chemistry both shapes and is being shaped by them. At the same time, these connections become more explicit in the Anthropocene, since the Anthropocene questions the roles of human societies in natural dynamics. The Anthropocene therefore explicitly calls for a dialog between, and even an interweaving of, the social and natural sciences in order to scientifically consider the state of the planet and its future course.

Since interweaving social and natural sciences is a defining stance of this manuscript, it seemed necessary to adopt aspects of the social sciences in our writing, even though they are rarely used in the natural sciences. We will therefore start by stating "from where we write". Indeed, social scientists have demonstrated that scientific discourse – including that in the natural science field – is rarely neutral. Despite all the methodological precautions, all scientific discourse is historically and culturally situated.[21,22] This contrasts with the idea of science as neutral and objective, which is a recurrent trope in the natural and physical sciences. Therefore, as a prelude to any attempt at interdisciplinarity of chemistry-centered academic research, it seemed necessary to make this teaching our own, and to specify aspects of our own situations and backgrounds (details in ESI, Section SI-1.1†). Briefly, we are a group of scholars with different profiles (age, career trajectory, nationality) and disciplinary backgrounds, including chemistry, economy, history, and ethics. We share a common viewpoint, that a narrow disciplinary approach cannot successfully guide chemistry-centered research in the context of the Anthropocene due to the complexity of the associated interdependencies. This shared viewpoint led us to formulate two questions: do we consider that the way chemists are called upon to work on the energy transition by some, if not most, leading research-shaping authorities satisfactorily aligns with Anthropocene-related challenges? Can interdisciplinarity help us to shape tools to answer this question?

1.3. Outline and scope of the paper

After the introduction, the paper is developed in three sections. In Section 2, elements of the planetary framework are presented through five representative molecular substances: carbon dioxide (CO_2), hydrogen (H_2), ammonia (NH_3), methane (CH_4), and (bio)polymers. For each of these substances, Section 3 presents an analysis of a selection of recently published scenarios produced by leading organizations guiding policy makers in Europe, where most of the authors are based (more details in the ESI, Section SI-1†), and at the global level. These include scenarios by the IPCC (Intergovernmental Panel on Climate Change),[25] the IEA (International Energy Agency),[24] Dechema,[25] Sunergy,[26] and Shell.[27] Section 4 builds upon a selection of insights provided by other disciplines, in particular drawing in the social sciences and humanities (history, economics, political science, ethics), to highlight some limitations that emerge when attempting to bring together the elements presented in the two previous sections. We then conclude and share our current perspectives on the topic.

Our focus on the chemistry-energy nexus, which is our main center of academic expertise, necessarily obscures other aspects for which chemistry is central. Indeed, we make no claims to exhaustivity nor to have selected the most important possible subfields. At the same time, this approach allowed us to define a perimeter, the energy transition, which attracts or even monopolizes a large segment of public and scientific discourse, thus justifying the scope, relevance, and timeliness of this manuscript. Our paper is intended to all scientists not familiar with transdisciplinary research: PhD students, early career researchers and more senior scholars, in chemical sciences or trained in other fields and working on the energy transition, who do not regularly have opportunities to experience what substantial integration of other disciplines can bring to their own research. Our aim is to share with our peers some of our thoughts and concerns about the transdisciplinary challenges associated with our research.

2. Five sample molecular substances at the energy/chemistry/planetary boundaries nexus

2.1. Why these five molecular substances?

The nine Earth system processes and their Planetary Boundaries (PB) scientific framework was developed in tight association with the Anthropocene concept in 2009 by authors from the Stockholm Resilience Centre and others. These PB correspond to quantitative limits associated with essential Earth system processes.[4] The framework attempts to define quantitative boundaries within which humanity can continue to evolve safely in the long-term with the stability that characterized the Holocene. PB have been quantified for many years for seven of these nine Earth system processes[3–11] – freshwater use, land-system change, biosphere integrity, climate change, stratospheric ozone depletion, ocean acidification, and

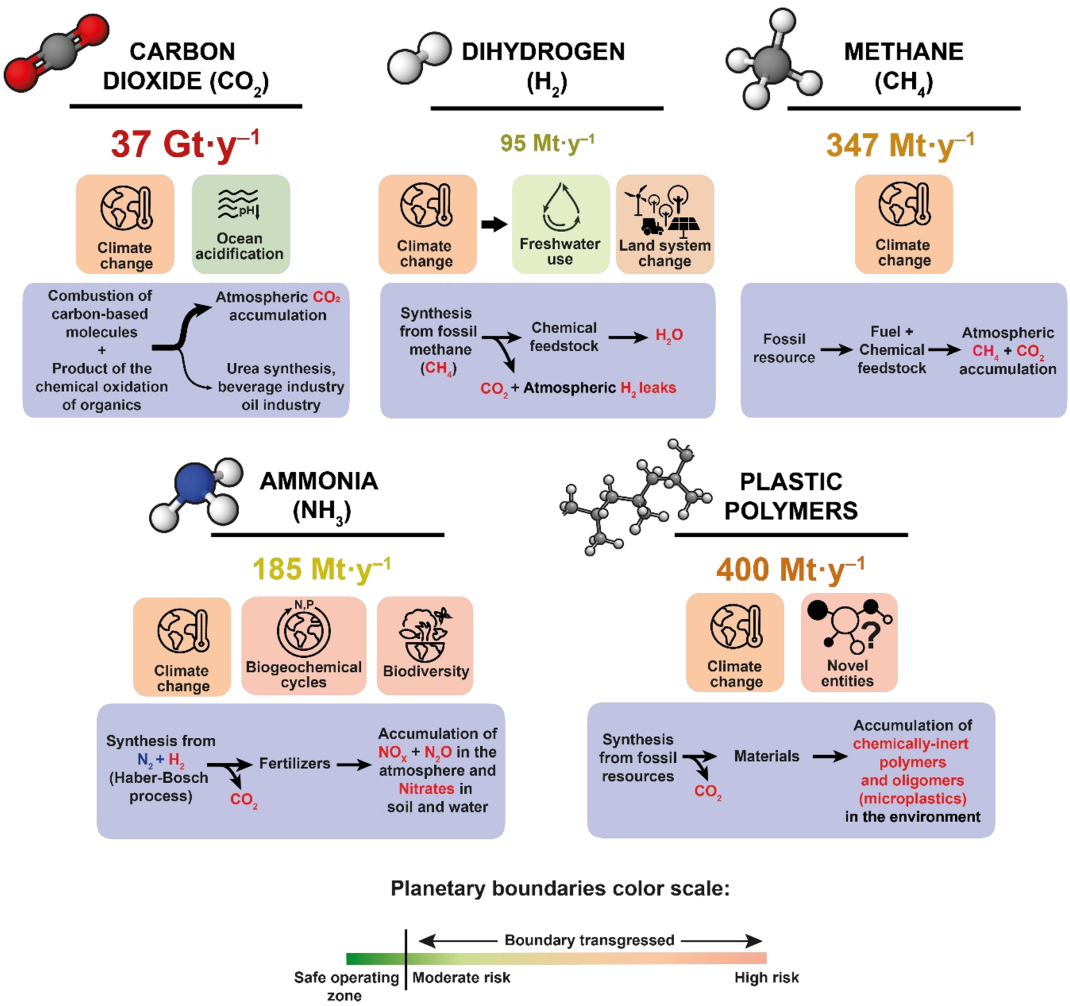


Fig. 1 The four molecules (CO_2, H_2, CH_4 and NH_3) and plastic polymers, chosen here as illustrative molecular substances sitting at the crux of the chemistry-energy nexus. For each of these substances, are reported: their current annual global production (in 2022), and the main Earth system processes with which they interact. In the case of dihydrogen, the shift in affected Earth system processes entailed by a shift towards production of "green hydrogen" (see Scheme 1 for definition) is materialized by an arrow. The current level of transgression of each planetary boundary estimated in literature is represented by its color, according to the caption at the bottom of the figure. Finally, current mode of production, main usage, and issues associated with end-of-life considerations are described in the blue boxes. More details in text and in ESI, Table SI-3.†

biogeochemical flows – and are updated regularly,[12,13] whereas estimation of the remaining two – atmospheric aerosol loading and novel entities – has only started recently.[12,14] All these Earth system processes have aspects which are at the heart of the chemical-energy nexus and are therefore closely related to the chemical sciences.

Here, we have chosen four molecules to focus on: carbon dioxide (CO_2), hydrogen (H_2), methane (CH_4), and ammonia (NH_3). We selected these molecules not only because their consumption and production are central to the fabric of modern society, but also because they have been repeatedly identified as key pieces of the global transition needed to wane from excessive fossil resources consumption. They are projected to fill crucial niches in alternative carbon-free or carbon-neutral processes. As such, they appear central to most energy-driven transition scenarios proposed by governments, scientific consortia, and companies in their roadmaps for the coming three decades, all of which emphasize the objective of "Net-Zero-Emissions by 2050", as called for by the COP2021 Paris agreement,[28] and the United Nations.[29] We have added to the four molecules listed above the broader family of synthetic macromolecules represented by polymer blends found in plastics. According to the IEA, "petrochemicals are rapidly becoming the largest driver of global oil demand",[30] and nowadays, 90% of these petrochemicals are used for the synthesis of polymers.[31] Plastics are thus currently tightly dependent on fossil resources: their inclusion in our scope aimed at introducing an indicator of fossil-based chemical production not directly embedded in energy-driven scenarios (Fig. 1).

Below, we present an overview of the space occupied by these five molecular substances in the current global chemical landscape, in particular in relation to energy, and how they can be linked to the Planetary Boundaries framework.

2.2. Carbon dioxide

Anthropic CO_2 overwhelmingly remains a waste product of oxidative fossil fuel use as a heat source, or for other energy generation. Four sectors were responsible for 94% of the 36.8 Gt of CO_2 released worldwide in 2022: power generation (14.65 Gt), industry (9.15 Gt), transportation (7.98 Gt), and building (2.97 Gt).[32] Among industrial processes, most emissions are linked to the production of cement, iron, and steel. In 2022, 4.16 Gt of cement were produced,[33] releasing 2.4 Gt of CO_2 into the atmosphere (0.58 t of CO_2 produced per ton of cement).[34] During the same year, 1.88 Gt of steel and iron were produced,[35] associated with 2.6 Gt of CO_2 (1.41 t of CO_2 per ton of steel).[36] Chemical and petrochemical production emitted 1.33 Gt of CO_2 in 2022.[37] This included the production of ammonia (419.80 Mt of CO_2 emitted), methanol (261.25 Mt of CO_2 emitted), and other high-value chemicals (*i.e.*, ethylene, propylene, benzene, toluene, xylenes, 255.29 Mt of CO_2 emitted in total).[38] Although the chemical sector ranks third in terms of direct CO_2 emissions (25% due to processes, 75% due to fuel combustion), it is the primary consumer of energy: 50% of primary petrochemicals are used as actual energy-source to fuel the processes, and 50% are used as feedstock – and are thus no longer available for energy generation.

The current main uses of CO_2 as a feedstock are for food and beverage purposes (230 Mt per year),[39] enhanced oil recovery (80 Mt per year),[39] and in the synthesis of key compounds: urea (130 Mt per year), methanol (2 Mt per year), salicylic acid (30 kt per year), and cyclic carbonate (40 kt per year).[26] Overall, these processes consume up to 422 Mt per year, which is only slightly more than 1% of the annual anthropogenic CO_2 emissions.

2.2.1 Link to Earth system processes and their planetary boundaries. The concentration of carbon dioxide in the atmosphere has increased from 277 ppm in 1750 to 417 ppm in 2022 (+51%).[40] This accumulation has led directly to an increase of the global mean surface temperature of more than 1 °C.[41] The PB associated with climate change is an atmospheric CO_2 concentration of 350 ppm, which has thus been crossed.[12] Any further increase in CO_2 emissions adds to the ocean acidification as well: the associated planetary boundary is set at a minimum level of aragonite saturation of 80% of the pre-industrial level, whereas the current value amounts to 81%.[12,42,43] Over the period 1980–2016, a decrease of pH from 8.11 to 8.06 was reported, which is 100 times faster than any change in acidity experienced during the previous 55 million years.[44] Crossing both of those PB has cascading consequences, such as rising sea levels or extreme weather events, and endangers many species. The rise in atmospheric CO_2

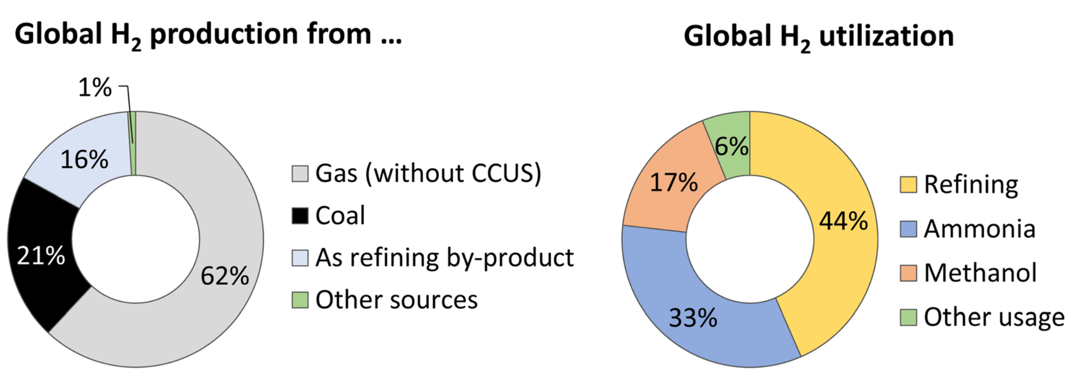


Fig. 2 Production (left) and utilization (right) of H_2 in 2022, according to IEA.[48] "Other sources" in the H_2 production panel include oil (0.5%), fossil fuels coupled to CCUS (0.6%), and water electrolysis (0.1%). "Other usage" in the H_2 utilization panel is mostly linked to the iron and steel industry (DRI, Direct Reduced Iron).

concentration results from CO_2-emissive anthropogenic activities: fossil fuel combustion and industrial activity were responsible for around 5 Gt of CO_2 in 1950, around 15 Gt in 1970, and more than 37 Gt in 2023.[32,41,45,46]

2.3. Hydrogen

Historically, large-scale hydrogen use was first developed in the 18th century with aerial transportation (Zeppelin airships). It expanded in the 20th century as part of massive industrial processes (mainly ammonia and methanol production and oil refining, Fig. 2, right), and also found niche applications in space propulsion or lubrication. Some consider the end of the 1990s as the period when the idea of a hydrogen-based society emerged, with applications expected in both transportation and energy.[47]

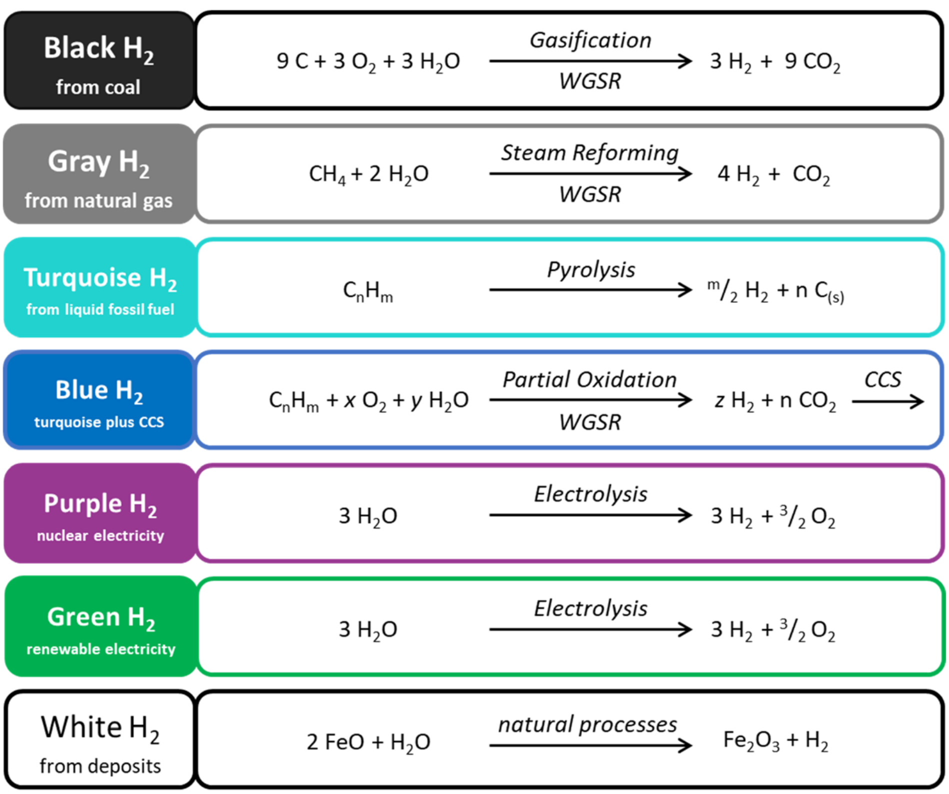
Global hydrogen production reached 95 Mt in 2022[49] of which less than 0.7% is low-emission hydrogen, *i.e.*, mostly from fossil fuel coupled to carbon capture, utilization and storage (CCUS) technologies (0.6%), or through water electrolysis (0.1%): in 2022, only 100 kt of H_2 was produced by electrolysis.[48] The remaining >99% was produced through fossil fuel-based industrial processes, primarily from natural gas through steam reforming (Fig. 2, left). The demand for hydrogen is mainly related to refining processes (*e.g.*, for the removal of sulfur from crude oil) and base chemical production, like key small molecules (*e.g.*, ammonia), chemical intermediates (*e.g.*, methanol), and fine chemicals (*e.g.*, for the food and pharmaceutical industries). These numerous applications reveal how hydrogen connects fossil resources to several global production processes.

2.3.1 Link to Earth system processes and their planetary boundaries. Since more than 99% of current hydrogen is produced using fossil fuels, its production bears a considerable planetary burden. In 2022, H_2 production was responsible for 1.144–1.291 Gt of $CO_{2eq.}$ emissions.[48,49] The well-to-gate greenhouse gas (GHG) emissions from natural gas-powered steam reforming were 9 $kgCO_{2eq.}$ per kgH_2.[48]

2.4. Methane

Most of the methane currently used in the industry and energy sector is of fossil origin, as it is a major component of natural and shale gas. Between 2010 and 2021, worldwide methane consumption rose by 28% to 4038 billion cubic meters (bcm) (132 EJ, 4.3×10^{13} kW h).[50] Methane is mainly used as an energy source through combustion. Compared to coal and oil, the combustion of methane is more carbon efficient: natural gas-powered plants emit about 50% less CO_2 than coal-powered plants[51] (see Scheme 1 for a relative comparison based on hydrogen production rather than fuel combustion).

About 15% of methane is used as a chemical feedstock.[52] Current upgrading routes of methane progress *via* steam methane reforming and the water-gas shift reaction (CO_2/CO/



Scheme 1 Simplified chemical reactions (only one possible representative reaction is shown) associated with current fossil-based and projected hydrogen syntheses, with CO_2 emissions decreasing top to bottom and the corresponding "color" scheme used in literature. WGSR: water–gas shift reaction. CCS: carbon capture and storage.[78–80]

H_2 mixtures). Direct routes for methane upgrading (either under oxidative or non-oxidative conditions) have been proposed as alternatives, yet limited advances have been made in converting methane into chemicals other than syngas. Given methane's important role in the current energy infrastructure, biomass methanization processes are being developed, and other biological, photo-, electro- or photoelectrochemical routes are explored (power-to-methane, either *via* direct electrolysis of captured CO_2 or *via* the intermediate production of green H_2, for example; see Scheme 1 for the definition of "green H_2").

2.4.1 Link to Earth system processes and their planetary boundaries. Methane is a potent GHG, with a Global Warming Potential over a 100 years period (GWP-100) estimated to be between 27 and 30 (*vs.* GWP-100 = 1 for CO_2). Methane emissions may arise from its production or transportation.

In 2021, 144 bcm (4.7 EJ, 1.5×10^{12} kW h) of natural gas were flared: besides being a waste of fuel, flaring also releases CO_2, soot, and other greenhouse gases in the atmosphere. In 2022, a 3% decrease in flaring was recorded.[53] More ambitiously, the World Bank's Zero Routine Flaring by 2030 initiative,[54] which is in line with the Net-Zero Emissions by 2050 scenario[24] calls for a complete stop to this practice.

Large distances often separate up- and downstream processing sites of methane, necessitating extensive and vulnerable infrastructures, particularly pipelines and tankers to transport liquefied natural gas (LNG). For instance, methane emissions from local distribution in the United States have been estimated at 0.69 Mt per year.[55] Methane leaks at various points in the natural gas supply chain can have detrimental environmental consequences.[56]

2.5. Ammonia

The Haber–Bosch process is at the root of industrial ammonia production. It converts atmospheric N_2 to NH_3, while consuming about 1.2% of the world's energy (about 39.3 GJ required per ton of ammonia produced). Current annual industrial ammonia production is 185 Mt.[57] This represents the amount of anthropogenic elemental nitrogen that enters the reactive nitrogen (Nr) pool every year: 75–80% in the form of fertilizers and 10% as explosives. Fertilizers include urea $(NH_2)_2CO$, ammonium sulfate (AS), diammonium phosphate (DAP), monoammonium phosphate (MAP), ammonium nitrate (AN), and calcium ammonium nitrate (CAN). The nitrates among these can be further combined with phosphates to generate NPK (nitrogen, phosphorus, potassium) fertilizers. When used, urea (~60% in N mass) will eventually release CO_2 back into the atmosphere.

15% in N mass of ammonia is converted to nitric acid (HNO_3) through the Ostwald process, *en route* to nitrates.[58,59] During the Ostwald process, 6–9 kg of N_2O, a potent GHG (298 $CO_{2eq.}$), are produced along each ton of nitric acid, although abatement measures may reduce this value down to 0.12 kg.[60] This main route to nitrates which starts with dinitrogen reduction *via* Haber–Bosch to ammonia followed by oxidative Ostwald process is a chemical detour and thus energy intensive.

Further down the "value chain" of ammonia utilization as fertilizer, the ammonia-to-eaten food arc has a deplorable nitrogen use efficiency.[61] Overall, between 86 and 96% of the nitrogen fixed as ammonia is not eaten, which represents a significant waste of energy and excess CO_2 emissions during NH_3 manufacturing, transformation, transport, and dispersal.[62] A significant fraction of losses occurs through denitrification of NH_3 to N_2: the non-denitrified "run-off" nitrogen excess contributes substantially to major pollution events such as eutrophication, marine anoxia, and fine particle emissions ($PM_{2.5}$, particulate matter <2.5 μm), leading to loss of biodiversity. Among these run-off nitrogen compounds, 3 to 5% of ammonia degraded through biological denitrification is released as the GHG N_2O.[63] In fact, if only 10% of annual ammonia production were biologically denitrified, the CO_2-equivalent footprint of N_2O byproducts would be comparable to that of the whole Haber–Bosch process, thus doubling the carbon footprint of ammonia synthesis.

2.5.1 Link to Earth system processes and their planetary boundaries. Because of this massive anthropogenic flux of Nr, the nitrogen geochemical cycle is among the most severely transgressed planetary boundaries. In the PB framework, the safe operating space has been estimated at 62 Mt per year of Nr:[8] the current anthropogenic Nr is 190 Mt per year, that is five-fold above the considered safe operating space limit (see Fig. 1 and Table SI-3†).[12] Current agricultural practices are reliant on the use of ammonia-based fertilizers and on other chemicals, which also require ammonia during their production: these include, but are not limited to, the herbicides metolachlor, glyphosate, or atrazine, and neonicotinoid insecticides like imidacloprid. These chemicals or their decomposition products are expected to negatively impact freshwater use and biosphere integrity.[64] Moreover, since – unlike ammonia – most of these synthetic chemicals do not belong to natural biochemical degradation manifolds, they contribute to current transgression of the planetary boundary associated with "Novel entities".[12] However, their impact remains to be quantified given no identification of a unique control variable for the Earth system process.

In summary, ammonia is produced, dispersed, and chemically transformed in quantities and ways that are difficult for Earth Systems to "metabolize" without entailing severe effects on Earth system processes, causing most planetary boundaries to be transgressed.

2.6. Plastics

The definition of term "plastics" varies depending on the source.[65] The term generally refers to materials which contain as an essential ingredient synthetic polymers of high molecular mass. Plastics include some of the most widespread synthetic carbon-based materials. The roughly 400 Mt of plastics produced in 2022 are mainly constituted of the following polymers: polypropylene (PP) counts for 18.9% of the production, followed by low density and linear low-density polyethylene (PE-LD, PE-LLD) with 14.1%, polyvinyl chloride (PVC) at 12.7% and high density and medium density polyethylene (PE-HD, PE-MD)

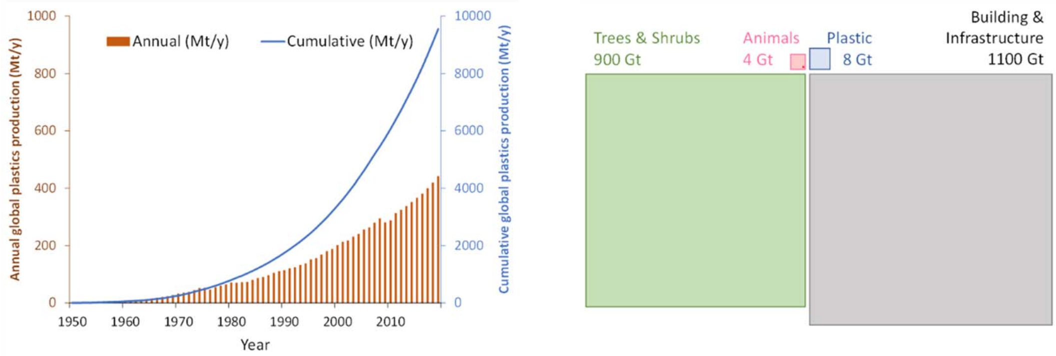


Fig. 3 Left: annual (brown bars) and cumulative (blue line) global plastic production between 1950 and 2019 (data by OurWorldinData, Licence CC-BY).[69] Right: comparison between the mass of animals (pink), trees & shrubs (green), plastic (blue), and building & infrastructure (gray). The areas of the squares are proportional to the total mass estimated for each group.[68] The red dot in the "Animals" square represents at scale the mass of all human beings (*ca.* 0.06 Gt of carbon).[70] Assumptions in mass accounting made in different studies explain the differences in absolute numbers between the left and right parts of the figure; the overall message remains the same in the two parts of the figure, with respect to the general trend discussed here.

at 12.2%.[66] The remainder share of production is mainly constituted by polyethylene terephthalate (PET), polyurethanes (PUR), and polystyrene (PS), together with the contribution of other less common polymers. More than 90% of the total amount of polymers is obtained from the polymerization of petrochemicals and are therefore fossil-based. "Circular" plastic (*i.e.* recycled or bio-based) is estimated to account for the remaining 10%.[66] The vast majority of plastics produced are used in the packaging industry (44%) followed by the building and construction industry (18%).[67]

Global plastics cumulative production has risen exponentially from 1950 to 2019 (Fig. 3, left), to the point where the total amount of plastics now accounts for twice as much as the total mass of animals on the planet,[68] contributing to 2020 being a landmark year: it is the date when the combined weight of man-made elements started exceeding that of all living biomass (Fig. 3, right).

2.6.1 Link to Earth system processes and their planetary boundaries. It was estimated that the global life-cycle GHG emissions of plastics were 1.8 Gt of $CO_{2eq.}$ worldwide in 2019, that is 3.4% of global GHG emissions, and 90% of these emissions are caused because plastics are manufactured from fossil resources.[71] These facts link plastics life-cycle to the "climate change" Earth system process.

Furthermore, synthetic polymers traditionally combine high chemical stability with the absence of any natural biogeological cycle, leading to long residence times in most environments. As such, their massive introduction at accelerating rates has recently been presented as the main evidence of transgression of the "Novel Entity" Earth system process.[14] Despite difficulties in accurately quantifying the PB related to this process, the claim that the boundary has been transgressed is linked to the fact that the rate of production and release of plastics is so rapid that it has outstripped our ability to assess safety and monitor adverse environmental effects. To support this, there is increasing evidence that plastic and microplastic ingestion and accumulation can lead to environmental and health damage,[72] affecting the biosphere integrity and the freshwater use Earth system processes.

3. Selected scenarios and projections through the prism of these molecular substances

3.1. Selected scenarios

The five molecular substances under discussion in this article are among key levers of the energy transition. Strategies for their production or management have been the subject of modelling efforts by a wide range of institutions ranging from intergovernmental, international, national, and private bodies to industry leaders.

These institutional and private stakeholders provide data and advice to policy makers, so that they can implement actions to meet the objectives and define regulations surrounding the production and use of chemicals on their territory and, by extension, globally. It is clear that many factors can influence the vision presented in these roadmaps, starting with the identity of the authors. Given our Europe-centered composition, using representative European examples, we will explore the visions most often presented to political leaders and policy makers, resulting in policy programs shaping the research objectives chemists are expected to meet.

Among the available scenarios, we selected five bodies that cover a part of this institutional diversity while largely maintaining a focus on United Nations-level, trans-Atlantic and Europe-centered institutions, organizations, and companies.

- The Intergovernmental Panel on Climate Change (IPCC):[23] the United Nations body assessing the science of climate change from a global perspective. IPCC reports are based on a diverse array of data and research from member countries and aim to provide policy makers with scientific assessments of climate change and to propose appropriate mitigation and adaptation approaches.

- The International Energy Agency (IEA):[24] this intergovernmental organization provides reports, data, and analyses of the global energy sector. In particular, it publishes policy recommendations to reach targets set by the political leadership of its members. It has 31 member-countries and 13 association countries, which overall represent 75% of the global energy demand. As an autonomous body under the umbrella of the Office of Community Economic Development (OECD), spurred from post-world war II Marshall plan, its membership reflects this trans-Atlantic barycenter. The current members, for example, do not include Africa, Russia, most of Asia and Middle East (Japan, South Korea, Turkey, and Israel are members).

- Dechema, the German Society for Chemical Engineering and Biotechnology:[25] a German non-profit organization representing over 5000 chemists, biotechnologists, and engineers, working at the interface between academic science, industry, economics, and the general public. Dechema has notably published several roadmaps for the use of chemicals in the European Union in the coming years.

- The Sunergy Initiative[26] powered by the EU-funded SUNER-C coordination and support action: this community groups together more than 300 academic and industrial stakeholders, with the aim of studying and promoting the development of breakthrough technologies to allow circular energy models at the European level.

- Private stakeholders, whose businesses involve the use or production of the substances of interest here, have regularly published data and perspectives on their activities. As a representative example, we selected the British–Dutch oil company Shell,[27] which is one of the largest multinationals. Shell regularly publishes reports on the future of fossil fuel and frequently lobbies policy makers regarding regulations on fossil fuel resource extraction, management, and use.

As summarized in Table 1, these scenarios are not synoptic. Their authors have vastly different roles in society, which results in a multitude of approaches and ultimately different individual goals. At the same time, we posit that a dominant picture for each of the five molecular substances described above can be proposed from a comparative analysis of these scenarios. While nuances or even differences exist between these scenarios, our goal is precisely to explore the possibility that a shared picture can be extracted, which surpasses the fragmented vision offered by focusing on the specificities of each scenario.

3.2. Dominant projected future for carbon dioxide

All scenarios consider anthropogenic CO_2 emissions to be the main cause of climate change, and share common views of future CO_2-related technologies. To reduce the concentration of CO_2 in the atmosphere it should be captured either from air (Direct Air Capture, DAC) or from point sources, where CO_2 is very concentrated (*e.g.*, industrial exhaust fumes). The captured CO_2 should then either be used as a starting material to produce fuels and primary chemicals (CCU, Carbon Capture and Utilization), or stored through geological storage or mineralization (CCS, Carbon Capture and Storage). All published scenarios share a demand for large-scale and low-cost "green energy" to power these processes, "green energy" ranging from energy from renewable sources (solar, wind, …) to energy production routes with lower carbon impact with respect to current dominant ones.

Potential solutions (carbon storage *vs.* carbon utilization) vary between the different authors involved – academia, policy makers or industry. As CO_2 is the key driver of climate change, the IPCC proposes a 2030 goal of a 45% reduction in CO_2 emissions. Shell sees CO_2 as an unavoidable byproduct of energy generation: to maintain the level of production of (petro-sourced) energy, Shell suggests that the emitted CO_2 should therefore be captured and kept in geological storage by the (petro)chemical industry itself. The required CCS (Carbon Capture and Storage) technologies should be powered by wind and solar energy, to decrease total CO_2 emissions by 50% in 2030.[27] The other scenarios analyzed here – Dechema and Sunergy – focus on either CO_2 captured from air or sequestered from point sources and its use as a key feedstock in the chemical value chain. To allow the maturation of the novel required processes, the significant emission-reduction goals in their scenarios are set only after 2030.[25,26]

Below we will discuss technologies directly related to CO_2, although some of them rely on other processes such as the production of "green" hydrogen (see Scheme 1) or the generation of decarbonized electricity. The level of detail available on the technologies to be promoted differs depending on the scenario.

3.2.1 Carbon capture. Carbon capture technologies are quite advanced, and proofs of concept have been established, with some facilities already running.[73] However, remaining difficulties are linked to, *inter alia*, high costs and energy consumption, which hamper scale-up and industrial applicability. Broader application will therefore depend on future efficiency gains.

Sunergy has reviewed various solutions for carbon capture. The most mature technology is amine-based CO_2 absorption: large plants are expected to capture from a point source up to 0.4 $MtCO_2$ per year at an energy cost of about 3.5–3.8 GJ/tCO_2, and an economic cost of less than 50 € per tCO_2. Higher modularity could be achieved by implementing membrane adsorption.[26] Direct air capture (DAC) is also possible, but poses the additional problem of separation and purification of the low-abundant CO_2 in air, if it is to be subsequently exploited. Today, each ton of CO_2 treated by DAC costs €300–600 and consumes 5–9 GJ of energy. Nevertheless, the IEA estimates that following scale-up and optimization, DAC costs could fall to less than 100 € per tCO_2.[24] Sunergy also proposes a long-term solution based on the direct capture of CO_2 from the air in small-scale, decentralized plants.[26] Dechema, in contrast, considers harnessing point sources to be the most appealing strategy as it would allow easier capture of highly concentrated CO_2 streams.[25]

The scenario proposed by the IEA involves large-scale facilities capable of capturing about 1200 $MtCO_2$ per year in 2050. In 2022, about 45 Mt of CO_2 were captured, and based on the TRL of future planned plants, the IEA estimates that about 390 Mt year could be captured in 2030, *i.e.*, less than a third of the Net Zero Emissions, NZE, goal.[74] Carbon dioxide removal technologies would only have a significant impact if emissions could be first reduced to ∼10–20% of their current levels.[75]

3.2.2 Carbon storage *vs.* carbon utilization. The different scenarios promote storage (CCS) and/or use (CCU) of the captured carbon to varying degrees. The IEA highlights the need

Table 1 Overview of the main applications and actions proposed by the energy scenarios considered here (IPCC, Dechema, Shell, IEA, Sunergy) for the five molecular substances under review (NH_3, H_2, CO_2, CH_4, plastics)[a]

	IPCC	Dechema	Shell	IEA	Sunergy
CO_2	- 1.5–2 °C warming is inevitable, measures should aim to manage this new reality	- Zero emissions 2050	- Net-zero 2050, 50% reduction by 2030	-3 scenarios: (1) STEPS: 32 $GtCO_2$ per year in 2050, +2.5 °C. (2) APS: 12 $GtCO_2$ per year in 2050, +1.7 °C. (3) NZE: 0 Gt per year in 2050, +1.4 °C	- CO_2 as a feedstock for localized on-demand production of chemicals
	- CCUS is a potential solution but with its own negative environmental impact	- Point sources (*via* CCUS) and biomass as dual feedstocks for industry	- Switch to renewables, geological storage and reforestation	- Need to decouple CO_2 emissions from chemical value chains, requires massive, immediate investments	- Sourced from DAC
		-4 scenarios described	-0.4 Mt CO_2 in CCS in 2021, up to 25 Mt in 2035	- Notes huge discrepancy between required and realized CCS capacity	- DAC currently not at CCUS level, low TRL
H_2	- Low-carbon hydrogen required (*e.g.*, electrolysis of water)	- Hydrogen from different types of electrolyzers	- Investment in increased H_2 production	- H_2 mostly produced by electrolysis of water, but also from fossil resources, coupled with CCUS	- Solar to hydrogen technologies, photo(electro)chemical technologies
	- Low-carbon hydrogen as an energy carrier when electrification not possible	- Poor electrolyzer scaling makes direct large-scale industrial use difficult due to land occupancy	- Maritime and terrestrial transportation - Development of refueling stations	- Low carbon H_2: 90 Mt in 2030, and 450 Mt in 2050	- Water electrolysis
CH_4	- CH_4 fugitive emissions from transportation of fossil fuels could be avoided to reduce the GHG emissions linked to CH_4	- Potential use as H_2 vector if methane is green, but CH_4 pyrolysis is low TRL	- Reduction of methane emissions and methane flaring	- All non-emergency flaring must cease by 2030	- CH_4 as a solar fuel
		- SNG as potential energy storage for renewables (CO_2 hydrogenation)		- Biomethane production to double by 2025, either by biogas upgrading or gasification of biomass	- DAC and subsequent upgrading of CO_2 to CH_4 using solar energy
		- SNG synthesis has to deal with H_2O byproduct and energy costs		- Beneficial to US and Europe with well-established gas grids	
NH_3	- Reduction of fertilizer consumption through innovation and best practice - NPK recovery from wastewater	- Production in current infrastructure but with green H_2 - Most important lever is cost of "green" (as in CO_2-neutral) energy	- Use as maritime fuel	- Emissions from NH_3 synthesis need to drop despite growth in demand - Envisions NH_3 as low-emission H_2 fuel	- Precision farming to reduce Nr pollution - Multiple "green" pathways toward NH_3, but all low TRL
				- Will consume 25% of "greener" H_2 in 2050	- Requires significant improvements to Haber–Bosch to become viable
				- NH_3 and H_2 make up 45% of energy use in shipping 2050 - H_2/NH_3 for seasonal storage of renewables, NH_3 to transport H_2 by sea	- Emphasis on decentralized NH_3

Table 1 (Contd.)

	IPCC	Dechema	Shell	IEA	Sunergy
Plastics	- Switch from fossil to biomass as carbon source	-4 scenarios for more sustainability: 1) CO_2 to MeOH. 2) from biomass. 3) circular economy. 4) CO_2 copolymers - In addition: Improvements in recycling	—	- Switch toward biopolymers to improve footprint - Main emphasis on recycling of existing polymer	- Incorporation of bio-based feedstocks into chemical industry - CO_2 as building block for polymers - Highly durable biopolymers act as a carbon-negative technology

[a] NPK: nitrogen, phosphorus, potassium fertilizer; Nr: reactive nitrogen; TRL: technology readiness level; CCUS: carbon capture, utilization, and storage; STEPS: stated policies scenario; APS: announced pledges scenario; NZE: net-zero-emissions; DAC: direct air capture; SNG: synthetic natural gas. See Scheme 1 and Fig. 4 for definitions of "green H_2" and "green NH_3".

for negative emissions, and thus the decisive role of long-term carbon storage: 95% of the carbon captured should be geologically stored by 2030, and only 5% should be used.[24] In the Shell scenario, the use of "nature-based" CCS is promoted, mostly *via* reforestation in addition to geological undersea storage.[27] Conversely, Sunergy discards the option of CCS, estimating that sequestration would be too energy intensive, and that geological pits would be too scarce.[26] Rather, they set a goal of finding innovative ways to use CO_2, as a feedstock, an option that is also promoted by Dechema.[25] For Dechema, the use of H_2 generated by green water electrolysis (see Scheme 1) constitutes a sustainable pathway toward conversion of CO_2 to methanol, which is a major platform chemical in the production of value-added products such as ethylene, propylene, or benzene/toluene/xylene (BTX), as well as for fuel production.[25]

While Dechema sees CCU as a technology to be integrated into existing large-scale industrial infrastructure, Sunergy aims to decentralize the entire value chain, thanks to small-scale DAC setups with subsequent valorization *via* microplants producing chemicals for local needs. Sunergy also presents various strategies to exploit CO_2, starting with biohybrid systems, involving biocatalytic conversion (*e.g.*, by bacteria or enzymes), and extending to electrochemical CO_2 reduction, powered by green electrons from solar energy, or, ideally, artificial photosynthesis and photoelectrochemical conversion of CO_2. Once again, the TRLs of the solutions proposed by Sunergy range from low to medium, which means that they may not be ready to implement in time to address the most urgent challenges.[26] This concern is shared by the IEA scenario,[24] for which more than 60 of the required technologies are at the prototype or demonstration stage. In the long-term, Sunergy aims to harness processes encompassing both CO_2 capture and its conversion. Direct air capture and conversion (DACC) would selectively yield valuable chemicals – such as syngas, hydrocarbons, or methanol – through the formation of carbonate or carbamate intermediates. Thermally-powered DACC to syngas is envisioned by 2030, with a photoelectrochemical process projected by 2040. The ideal processes would be insensitive to oxygen and nitrogen present in captured air, to allow immediate conversion of CO_2 without the need for its purification from the air stream – which would have advantages in energy terms.[26]

3.2.3 Conclusion on CO_2-related scenarios. Carbon dioxide has been, is and is expected to remain at the crux of the energy-chemistry nexus. CO_2 has been released into the atmosphere mostly because the energy we have used and are still using stems from carbon-intensive chemical processes (burning fossil resources). Today, the paradigm accepted for the future of chemistry focuses on using CO_2 as a feedstock and/or on finding processes that can reduce its release. Although CO_2 is widely accepted as the main GHG responsible for global warming and ocean acidification, its capture, storage and/or use are currently not affordable enough for a wide application. Profitable dissemination of CCS and/or CCU technologies, as well as a CO_2-based economy, is not yet on the cards.

Notwithstanding its possible limitations,[76] the concept of the carbon footprint – the analysis of the positive or negative emissions caused by chemical processes – has become one of the major criteria by which the sustainability of chemical processes is assessed. This choice affects the four other molecular substances considered here (H_2, CH_4, NH_3, plastics), and drives research in academia and industry into modifying processes accordingly.

3.3. Dominant projected future for hydrogen

Hydrogen is presented as one of the most promising short-term fossil-free and carbon-free energy carriers in all the scenarios studied. With a stored energy per weight of 120 MJ kg^{-1}, it surpasses all other chemicals (*e.g.*, 50 MJ kg^{-1} for methane). This has led to massive policy incentives for production of so-called green H_2 at individual country and international levels.

The next section will help clarify the chemical definition of the color associated with hydrogen. More broadly, the term "green" will be used hereafter with the same ambiguity found in common literature: while it can, in some context, be associated with the idea of sustainability and absence of detrimental environmental impact, the term green can also more prosaically mean less impactful than current routes (mostly in terms of overall CO_2 emissions, ideally tending toward CO_2-neutrality). Water electrolysis powered by renewable electricity is the current technology of choice for green H_2 production. Thus, the European Strategic Roadmap envisions a rapid increase in green H_2 production, from 6 GW to 40 GW of available electrolyzer power in the 2024–2030 period.[77] Some further details on green H_2 production infrastructure technologies are reported in ESI, Section SI-4.† Importantly, beyond its potential role as an energy vector, H_2 remains a central reducing chemical involved in a multitude of large-scale chemical processes (see Fig. 2), for which a switch to green H_2 could directly reduce CO_2 emissions.

3.3.1 The hydrogen production color chart – going for green. While green hydrogen generated by renewable power with no CO_2 emission is the stated target for all scenarios, the path toward large-scale production can take various routes, including a gradual transition or branching through different production methods, often distinguished by color-coding (Scheme 1).[78–80] Black and gray H_2 refer to CO_2-intensive coal gasification or Steam Methane Reforming (SMR), and represents most of today's production. Blue H_2 refers to a modification of gray H_2 production using CCS technologies (discussed in Section 3.2) to reduce the associated CO_2 emissions. Turquoise H_2 is produced through fossil fuel pyrolysis, yielding carbon black as a byproduct. Purple hydrogen is obtained from water electrolysis powered by nuclear energy. Last, white hydrogen is a natural form of hydrogen (also called native hydrogen) produced through various phenomena (redox reactions with ferrous ions, water radiolysis…).

As of yet, production of green hydrogen (median cost 3.64 $ per kg) is more expensive than production of gray hydrogen (median cost 1.66 $ per kg for steam reforming of methane without CCUS).[81] Several projections phase out gray hydrogen by 2050,[82] but with non-fossil H_2 production remaining below 50% of total hydrogen production. The scientific literature does not unanimously agree on the benefits of transitioning through blue H_2 due to limitations in CCS technologies (see Section 3.2), and arguments have been advanced for greater investment in renewables (*i.e.*, green hydrogen) in the midterm.[81]

The IEA roadmap[24] anticipates an explosive rise in blue and green H_2 demand from about 0.3 Mt in 2021 to about 420 Mt in 2050, with 13% of this demand coming from the energy sector, 30% from industry, 26% from transportation, and 26% for use as feedstock in the production of other low-carbon fuels. In this scenario, hydrogen would represent a 20% share of the yearly global energy supply. This scenario contrasts with another projection set out in the same IEA report, the Stated Policies Scenario (STEPS), which is based on a trajectory modeled on today's global policy settings. The latter predicts a lower demand for blue and green H_2 of only 24 Mt by 2050. This illustrates the gap to be bridged if we are to transition to a green hydrogen economy capable of net-zero CO_2 emissions. For comparison, current demand for H_2, which is met by gray H_2, is about 95 Mt.

3.3.2 Hydrogen as an energy vector. While hydrogen has sometimes been presented as a key fuel for the energy transition, recent roadmaps, including the IPCC report, tend to downplay this vision and emphasize the efficiency of using electricity (over H_2 fuel) for buildings energy needs and light-duty vehicles. Hydrogen fuel cell vehicles have been substantially overshadowed by the rise of electric vehicles (EV), the lack of infrastructure for H_2-based vehicles being a significant obstacle. Indeed, 1.3 million refueling stations were available globally for EV in 2020, compared to just 530 for H_2-powered vehicles.[48,83] The market for H_2-fueled vehicles is also hampered by the price and stability of fuel-cells requiring platinum catalysts. Potentially game-changing innovations could still emerge for H_2-fueled internal combustion engines, thus providing a significantly extended range compared to EVs: the focus on fuel cell development is shifting towards heavy-duty trucks.[84] Hydrogen remains a more convincing option than electrification for other heavy-duty transport such as the marine and aviation sectors, either directly or through synthetic fuels (power to liquid technology, ammonia, *etc.*).[85]

As the electrification of the chemical industry progresses, the IPCC scenarios envisage hydrogen primarily as an energy carrier. The limited development of a hydrogen infrastructure, compared to the electricity grid, supports this trend. Nevertheless, green hydrogen may be adopted by some large industrial sectors, for example as fuel for furnaces in the glass industry, which need very high temperatures and stable operation conditions.[86]

Overall, the role of hydrogen as a fuel in the IEA global energy picture is projected to have a relatively low impact. Thus, in the NZE 2050 scenario, that is "Net Zero Emissions by 2050" scenario (one of the more optimistic scenarios when it comes to fossil resource and H_2 use), H_2 will account for a total share of roughly 6% by 2050.[87]

3.3.3 Hydrogen as a chemical for industry. While its future application as an energy vector is somewhat nuanced, there seems to be a clear advantage of switching out gray H_2 for green H_2 in chemical processes, in particular for the production of steel (through hydrogen-based direct reduced iron), ammonia, methanol, or chemical feedstock from biogenic sources. In one specific example, Dechema presents methanol production from captured CO_2 and green H_2 as the cornerstone of a low-carbon strategy to synthesize complex organic compounds. This alternative to traditional petrochemical pathways involves mature methanol-to-olefin and methanol-to-aromatics processes.

3.3.4 Green H_2 production infrastructure. The 2050 targets proposed for green hydrogen production require the rapid and large-scale development of a new global park of industrial electrolyzers. According to the IEA, if all projects announced as of September 2022 are completed, the global electrolyzer capacity could rise from 1 GW (currently) to 134–240 GW by 2030.[88] This estimation is double that from the previous year, which highlights the difficulty in predicting future green H_2 production. To meet this growth, electrolyzer production must reach 65 GW per year by 2030. Various existing and emerging electrolyzer technologies are foreseen to achieve this objective (see ESI, Section SI-4†).

3.3.5 Green H_2 transport infrastructure. Repurposing natural gas pipelines for long-range H_2 transport appears economically viable, with a potential 50 to 80% reduction in initial investment compared to building new pipelines according to IEA. Two conditions must be met: (i) avoiding interference with existing natural gas demand, and (ii) having a market of large hydrogen consumers nearby. Nevertheless, retrofitting poses technological challenges. The IPCC report mentions issues like steel embrittlement and seals degradation: H_2 leakage is likely to be even more prevalent than natural gas leakage, raising safety concerns (although not a GHG, H_2 is explosive). These concerns are further compounded by the expected atmospheric reactivity of leaked dihydrogen with hydroxyl radicals, ultimately leading to a longer atmospheric methane lifetime, enhanced production of tropospheric ozone (GHG with 2000 CO_2 equivalent power over 100 years), increased production of stratospheric water (GHG), and influence on aerosol formation and behavior.[89] No convincing approach to address this issue, which already plagues the methane infrastructure, has yet been proposed. Repurposing liquefied natural gas (LNG) infrastructure seems even more unlikely due to the high cost of H_2 liquefaction (−253 °C) compared to methane (−162 °C).

3.3.6 Conclusion on H_2-related scenarios. We have attempted to highlight the most salient features for the future of hydrogen, focusing on the economic and technological data available in the open literature. While H_2 is expected to be able to support the defossilization of many industrial processes, from the chemical to the transportation sectors, the development of safe and easy-to-scale infrastructures to allow H_2 transport and storage remains challenging. The ongoing development of electrolyzing technologies makes the evolution of green hydrogen difficult to predict.

3.4. Dominant projected future for methane

Methane is attributed a particular role in energy transition in cases where existing infrastructure can be easily switched from coal to gas.[90] In the Net-Zero-Emission scenario by 2050, a 75% reduction of energy-related emissions is projected by 2030, down to 30 Mt, and reaching 10 Mt in 2050. Indeed, due to the increased global warming potential of methane (80 times that of CO_2 in a 20 years timeframe), its emissions must be substantially reduced in the near future by diminishing fossil fuel consumption, applying new emission-reduction measures throughout the fossil technology supply chain,[91] and implementing leak-detection programs impacting on fossil methane's climate footprint.[90] Measures to reduce these leaks and rapidly phase out all non-emergency flaring are included in all the scenarios, as they address both the strained gas markets (prone to geopolitical tension) and the need to reduce GHG emissions. According to Shell Sustainability Report 2021,[92] routine flaring contributed to 7% of Shell's global GHG emissions in 2021 (4.5 $MtCO_{2eq.}$); and it was reduced by 33% from 2020 to 2021 (0.2 Mt).

3.4.1 Technologies for methane use and production. In the context of society's transition towards decentralized technologies, the exploitation of fossil or biomass-derived methane feedstock to produce energy-dense and more easily transportable chemicals (*e.g.*, higher hydrocarbons and methanol) is attractive to maximize efficient use of energy resources. Yet, this remains a scientific and industrial challenge.

Methane could be used as a low carbon-footprint feedstock for hydrogen production during its controlled thermal decomposition.[25] Synthetic natural gas (SNG) production from CO_2 could be considered as a means to store energy, if green H_2 is employed to reduce CO_2. Using CO_2 in this way could help with the transition from fossil fuels to sustainable and renewable fuels, in accordance with the Paris Agreement and the SUNRISE Technological Roadmap for the development of negative emissions technologies (NETs), which are supposed to be optimized by the 2030s.[26]

Methane and fuels in general could also be produced by reducing CO_2 in photoelectrochemical devices, which should allow a more versatile, local, and thoughtful on-demand production. Working with autonomous systems that only depend on sunlight would obviously represent a great advantage.[26]

3.4.2 Biomethane as a turning point in the energy transition. Biomethane can be defined as renewable methane, and is today mainly produced from biomass, in the form of municipal solid waste, animal manure, crop residues, and wastewater. These materials need to be anaerobically digested to produce biogas (mainly CH_4/CO_2), which can then be converted to biomethane by removing CO_2: 90% of biomethane is currently produced this way.[93] The second route produces biomethane by direct gasification of biomass (*e.g.* forestry residues), followed by methanation.

Even though in 2020 biomethane only accounted for 0.1% of methane demand, sustainable biomethane production could be a turning point in the context of circular use of energy resources. Since it is chemically equivalent to fossil-derived methane, biomethane can be used directly to produce electricity and heat, and is fully compatible with natural gas infrastructures and gas-powered vehicles.[94] Around 60% of plants are currently operational or under conversion to include biomethane in the gas distribution network.[94] Biomethane combines the advantages of natural gas with a lower carbon footprint.[90] It is thus a valuable tool to harness agricultural/

municipal waste, since it can generally be produced in small-scale plants located near the end-use site. Adoption of biomethane could require a drastic modification of the distribution network to allow for the injection of excess biomethane produced in summer into the underground reserves as well as a change in production scale, from large to smaller, in particular for rural and farming communities. Such a change could limit transportation issues and geopolitical tensions. Hence, the benefits of biomethane might extend even beyond the defossilization issue.

Current worldwide bio-LNG and synthetic LNG production is 2.2 bcm per year (0.07 EJ per year, 2.3×10^{10} kW h per year). Biomethane potentials are in fact much higher and, in principle, could provide nearly 60 bcm per year (2 EJ per year, 6.3×10^{11} kW h per year) in the EU-27 for production only through thermal gasification.[95] This value has almost doubled compared to the data provided for 2019, in line with the REPowerEU 2030 target plans.[96] Biomethane potentials in EU-27 by 2030 are estimated at 41 bcm per year (1.3 EJ year, 4.3×10^{11} kW h per year), considering both biomethane produced from anaerobic digestion and from thermal gasification.[96] Even if biomethane is more expensive than natural gas, its cost-effectiveness and competitiveness could increase over time. Nevertheless, it is quite difficult to evaluate the CO_2 footprint of biomethane because it depends on the region, type of biomass and technology used. The IEA Sustainable Development Scenario underlines that consuming biomethane will avoid the emission of around 1000 Mt of GHG in 2040, including CO_2 emissions related to natural gas and CH_4 emissions from biomass decomposition.[90]

3.4.3 Conclusion on CH_4-related scenarios. To conclude, methane emerges as a promising energy and chemical vector due to its lower CO_2-to-energy production compared to fossil fuels, provided that the leaks of this potent green house gas could be limited (see Section 2.4). Fossil methane would need to be completely replaced by green or biomethane to allow defossilization. This will probably entail the development of decentralized infrastructures in most cases – *i.e.*, for agriculture-derived biomethane – and wider development of CCUS solutions. However, the energy transition must be supported by policies coordinating the various aspects involved, namely waste management, environmental issues, and agricultural, energetic and transportation sectors.[90]

3.5. Dominant projected future for ammonia

The amount of anthropogenic reactive nitrogen species (Nr) has increased constantly since the Haber–Bosch process was initially developed in the early 20th century as a result of its use for agriculture (see Section 2.5). Production will accelerate in the near future if NH_3 use is extended to energy applications.

3.5.1 CO_2-mitigation scenarios. Mitigation strategies linked to fossil-based ammonia production strongly focus on CO_2 emissions related to the Haber–Bosch process. Due to an inherent low conversion rate and economies of scale, Haber–Bosch plants are large facilities, typically producing ammonia in the order of kt per day. In addition, latest-generation steam reforming ammonia plants operate close to the exergy limit. As a result, modern Haber–Bosch plants have a process-related carbon footprint of *ca.* 30% of the total carbon footprint, as reported in eqn (1) of Fig. 4, for total and stoichiometric ammonia production-related CO_2 emissions, respectively, in steam reforming-based Haber–Bosch plants.

Therefore, overall efficiencies do not leave much room for improvement on that front, and indeed they have remained largely constant over the last two decades. In fact, most of the carbon footprint of the Haber–Bosch process is linked to H_2 production *via* natural gas reforming (Fig. 4).[97] A modern methane-powered Haber–Bosch process generates at best around 0.6 tNH_3/tCO_2. It is less in practice, resulting in effective global emissions of 450 Mt per year of CO_2. This makes current industrial ammonia a fossil chemical in all but name.

Current decarbonation approaches are based on the deployment of carbon dioxide capture and storage technologies at ammonia plants (blue ammonia) or use of decarbonized H_2 from water electrolysis powered by renewable electricity (green ammonia) (Fig. 4).

3.5.2 Ammonia as an energy vector. Ammonia is being advanced as a prime candidate carbon-free energy vector (or hydrogen vector). The 2022 World Energy Outlook[87] states that to achieve NZE by 2050, NH_3 should be co-fired in coal power plants in the short-term, and later on used as the primary long-distance hydrogen vector (representing 85% of planned hydrogen transportation capacity for projects announced). Furthermore, ammonia is expected to represent as much as 45% of fuel for shipping by 2050 in the NZE framework. Similar projections for industrial ammonia use are included in roadmaps presented by energy suppliers, such as Shell. Many current projections rely on the use of low-carbon hydrogen (green, blue, turquoise, *etc.*, see Fig. 4) as part of a more sustainable Haber–Bosch process and on a reduction in the energy costs of producing ammonia. The advances required to transform ammonia into an energy vector in terms of technology, energy efficiency, and infrastructure are substantial and far from guaranteed for deployment at the proposed massive scales.[99]

3.5.3 Scenario considerations other than the carbon-intensity of ammonia and its use as an energy vector. Little is mentioned with respect to ammonia production for fertilizers other than the need to lower the CO_2 footprint, which is likely due to the fact that most scenarios analyzed are skewed toward energy transition. Instead, the topic is dominated by the potential use of ammonia as an energy or hydrogen carrier. The few scenarios addressing the topic of poor nitrogen use efficiency (NUE) in agricultural practices relying on ammonia focus strongly on variations in agricultural practices (nutrient recycling, agroforestry, cover crops, hydroponics) and very little on chemistry-related levers (*e.g.*, slow-release ammonia fertilizers combined with precision farming).

3.6. Dominant projected future for plastics

In the roadmaps studied here, the impact of plastic production and use in relation to Earth system processes is almost

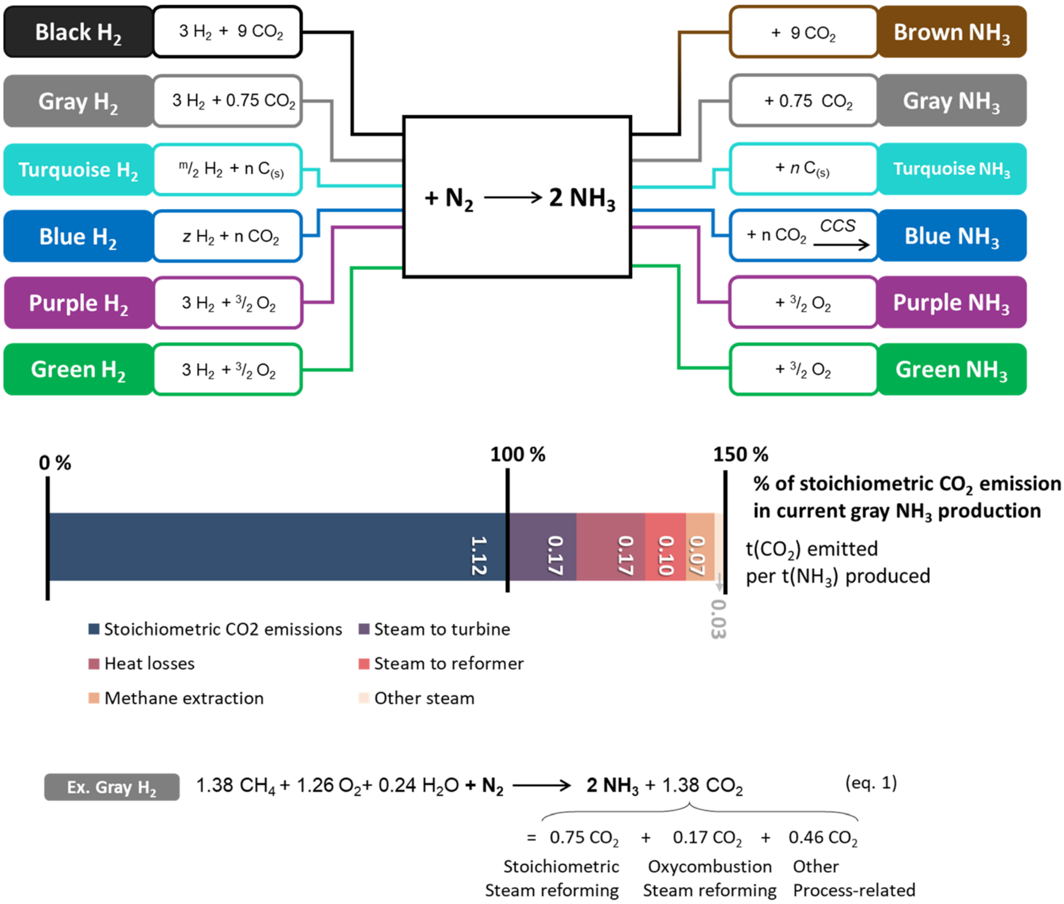


Fig. 4 Upper panel: schematic representation of current fossil-based and projected ammonia synthesis processes with decreasing CO_2 emissions (top to bottom) and respective ammonia "color". The CO_2 reported is only the stoichiometric quantity. See Scheme 1 for hydrogen syntheses. Since in ammonia plants, on-site hydrogen production is integrated with ammonia synthesis, the two hydrogen routes in Scheme 1 and here differ. Lower panel: differences between stoichiometric quantity (blue) and additional process-related CO_2 emissions (other colors) expressed in tCO_2/tNH_3 in modern optimized methane-powered Haber–Bosch processes for gray ammonia, leading to overall eqn (1) (see more on eqn (1) in Scheme SI-1†).[98]

exclusively tied to the high CO_2 emissions generated by the production of monomers by oil cracking in refineries. To mitigate this issue, three main low-carbon-emission circular alternatives are advanced. (i) Producing bioplastics from biomass, the largest reservoir of contemporary carbon, by breaking down and refining biopolymers into biosourced monomers. Dechema suggests that this path should be preferentially followed to obtain monomers that maintain the functional units of the feedstock molecules, (*e.g.*, oxygen-rich and carbonated molecules), rather than hydrocarbons such as ethylene or propylene, due to the low efficiency of biomass use for the production of the latter. Biomass is also recommended for the production of methanol and ethanol for further exploitation. (ii) Using CO_2 and green hydrogen as feedstock to produce syngas, followed by Fischer–Tropsch inspired production of olefins. This route should reduce CO_2 emissions, but can be energy intensive. (iii) Alternatively, CO_2 can be hydrogenated to produce methanol, which can then be converted into light olefins or aromatic compounds through established catalytic "methanol-to-olefins" and "methanol-to-aromatics" processes.

The European Green Deal includes a plan on increased regulations regarding the use and production of microplastics, and highlights the need for risk assessments to include the entire life cycle of materials, which is relevant to remaining within the planetary boundary related to Novel Entities. Importantly, the EU also voiced concerns with the global trade of plastics, and in particular the export of plastic waste. This strategy has led to plastic waste accumulation in landfills in South-East Asia, progressively contaminating freshwater sources, and ultimately large ocean areas in the form of a loosely agglomerated floating mass three times the size of France. This mass was infamously named the "seventh continent".[100] A recent European Green Deal[101] act implements stricter measures on plastic consumption, adopting a reduce-reuse-recycle strategy. Attention is drawn to a more transparent labeling system, especially with regard to the use of "bioplastics" terminology, making consumers active players in the energy transition.

Among the scenarios analyzed, the main solutions proposed for the manufacture of sustainable and defossilized plastics include the macro-topic of bioplastics to replace conventional plastics and the use of CO_2 to produce building blocks as part of a sustainable polymer industry. Less emphasis is placed on end-of-life of synthetic polymers, which is linked to the issue of environmental accumulation. When tackling this aspect, scenarios often encourage investment in the recycling chain, and only touch on biodegradability, even though this is a hot topic in polymer research. Furthermore, replacement of conventional plastics with biodegradable plastics has been proposed or is under implementation in several countries.[102]

3.7. Conclusion on the scenarios section

In summary, the five European/UN/OECD scenarios reviewed share some viewpoints. The existence of climate change and its consequences are central: the aim is to develop energy systems that are more carbon-sober. This system should be scaled to respond to projected increases in demand in most economic and industrial sectors. While all the scenarios generally agree that the energy transition envisioned should be powered by low-carbon electricity, different technical solutions, or distributions over various solutions are proposed. The general consensus is that some new or currently low-maturity technologies will be needed, and must be deployed at scale to reach some of the goals. This vision shapes most research-orienting frameworks and research-funding opportunities at the chemistry/energy nexus.

Open questions remain, as pointed out in the IPCC report, for example: “most models and studies fail to address the systemic impacts of the widespread development of new technology” including “material and resources”. “Systemic solutions are also not being sufficiently discussed, such as low-carbon materials; making buildings, transport, and industrial equipment lighter-weight; promoting a circular economy, recyclability and reusability, and addressing the food-energy-water nexus”.[23]

4. Interdisciplinary considerations

The scenarios presented above set out scientific and technological orientations mostly informed by engineering and data processing tools (such as techno-economic analysis, life cycle analysis, *etc.*). In addition, the scenarios have been almost exclusively elaborated to address the transgression of the planetary boundary causing climate change, with little to no mention of possible ripple effects impacting other Earth system processes. In this section, through selected examples, we will attempt to show that extension toward other fields of knowledge (game-theory, history, ethics, ecology, earth systems, *etc.*) can help bring to focus aspects that the scenarios might appear to overlook but that remain relevant when seeking to assess the sustainability of the proposed research directions.

We will showcase six examples related to the substances discussed above and some other underlying concepts mobilized by the energy transition/chemistry/Earth system processes nexus addressed in this manuscript:

- CO_2: how (economics-derived) game-theory considerations moderate the hopes that research into the use of CO_2 with a view to industrial transfer will substantially contribute to mitigating climate change.

- CH_4 and H_2: how political science can bring forward the tensions and potential conflicts surrounding the use of land and water resources for the deployment of methane- or hydrogen-based “energy transition solutions”.

- NH_3: how Earth system analysis, based on the planetary boundaries framework, raises questions as to the suitability of ammonia as a major contributor to the energy transition.

- Plastics: how decolonial studies can bring into focus the dynamics of waste recycling at a global scale.

- Related issue of the requirement for materials: how cultural studies of science can help deconstruct part of the implicit model in the scenarios proposed, whereby access to natural resources is taken for granted.

- Within the overarching concept of the energy transition: how history raises questions on the use of the term “transition” subsuming the scenarios proposed.

4.1. CO_2 as a raw material: can we really scale up?

The direct catalytic conversion of CO_2 to valuable chemicals has attracted considerable research interest over the past few years.[103] As detailed above, from a fundamental research perspective, like for many other challenging reactions, there is a curiosity-driven interest in understanding how such a stable and relatively inert molecule can be activated in an energy-efficient way to selectively produce carbon-based molecules.[104] In a more climate-related context, any such process could also theoretically contribute to reducing atmospheric CO_2 concentrations – either by replacing fossil fuels with CO_2-derived “solar” and “e-fuels,” or by producing useful fossil-free carbon-based chemical – thus helping to “close the carbon cycle”.[105] These approaches are often referred to by acronyms such as “CCU”, “CCUS” and “CDU” (for, respectively, “carbon capture and utilization”, “carbon capture, utilization and storage” and “carbon dioxide utilization”). Furthermore, these “emerging” technologies/processes can be viewed as possible contributors to the value chain in the chemical industry.[75,106] Carbon capture technologies are thus represented both as an economic opportunity and as an environmental solution, with verification of total global warming impact provided by life cycle analysis (LCA).[107]

Even if the current technological hurdles could be overcome, substantial economic and social obstacles might arise.[108] Game-theory can be an interesting tool to help analyze and understand how decision-making is influenced on a global scale. In public economics, two criteria are generally used to characterize goods: rivalry and exclusion. Rivalry refers to the fact that a product can only be consumed once. Exclusion refers to the fact that some individuals may not have access to the market. Based on these criteria, four categories of goods are defined: private goods, club goods, common goods, public goods (Table 2).

In this economic framework, the reduction of CO_2 emissions can be considered a public good, as it counteracts a public menace – CO_2 emissions – that has a negative impact on climate stability. The reduction of CO_2 emissions is subject to what

Table 2 Matrix of economic goods and simple examples

	Rivalry	Non-rivalry
Exclusion	**Private goods** *e.g.*, open-market products	**Club goods** *e.g.*, products accessible only to a restricted group of individuals
Non-exclusion	**Common goods** *e.g.*, fish or game stocks in freely-accessible fishing/hunting grounds	**Public goods** *e.g.*, public lighting, broadcasted radio programs, open-access scientific literature

economists call free riding: the tendency of individuals to benefit from collective efforts without having to contribute to them. Within this analysis, to mitigate climate change, every country tends to make the minimum effort. In game-theory, economists also refer to a sub-optimal equilibrium, or Nash equilibrium: the resulting strategy is that each country keeps polluting, whereas, the optimal strategy would be to reduce emissions (Table 3).

Research aiming to reduce CO_2 through chemical transformation could be included in these public good-oriented activities. In our current situation, it is difficult to imagine the potential scale-up of CO_2-based industry. Indeed, in the case of free riding, unless the technological solutions found are price-competitive in the current (possibly subsidized, more below) market, they will not be adopted.

Even assuming an absence of free riding (if, for example, a binding international climate agreement were adopted), the success of CO_2-based chemicals would not be guaranteed if fossil-based materials and fuels remained cheaper and widely available. The argument that CO_2-based chemicals have a double advantage – of creating new value and reducing the amount of CO_2 in the atmosphere – could be strengthened by quantifying what economists call the co-benefits of a policy. Co-benefits refer to subsidiary gains from a policy initially targeting a specific objective. In environmental policy, co-benefits are commonplace: *e.g.*, the promotion of active forms of transport (walking, cycling) not only reduces polluting motorized traffic but also has long-term health benefits.[109] In the case of CO_2-emission reduction, the co-benefits of CO_2-based chemicals could be measured by estimating the values of carbon emissions – there are many estimates of the social value of carbon that reflect the economic and social gains associated with reducing emissions.[110] This social value could then be added to the private value of the chemicals, and this might actually reverse the co-benefit comparison relative to fossil-derived chemicals. To achieve this reversal, the co-benefits must not only be theoretically quantified, but strong political measures are needed to support them, *e.g.*, forcing fossil-based products to bear an additional cost through a carbon tax. However, the economics literature shows that the capacity of industrial and political trade-offs to take into account the co-benefits associated with environmental measures remains weak for the moment.[111] Hindrances and obstacles, including lobbying, are important, and difficult to quantify. It is therefore far from certain that the environmental co-benefits associated with the development of CO_2-based chemicals would tip the balance in favor of these products, especially as a full assessment would also include potential drawbacks or hidden costs of these products, such as the risks of rent capture by a few private actors, like industrial companies capable of deploying the technology at the targeted scale, to the detriment of social welfare.

Table 3 Representative example of cooperative failure in a simplified two-country coalition (two-player game) for public goods (or bads) like country-wide greenhouse gas emission reductions policies. The sub-optimal Nash equilibrium is in bold.[7] In each cell of the table, "*X*,*Y*" should be read X = economic gain for country A, and Y = economic gain for country B, $X + Y$ = total gain for the system. The maximum total gain for the system is equal to 10 (5 + 5), when countries A and B both reduce their emissions (cooperation). The minimum total gain for the system, equal to 6 (3 + 3), is when both countries do not engage in country-wide greenhouse gas emission reductions policies. The intermediary situation is when only one country, either A or B, engages in gas emission reductions policies. This would lead to collective gains of 8 (6 + 2 or 2 + 6). In this case, the country reducing its emissions would bear alone the whole cost of the collective improvement (gain of only 2), while the other country-the free rider-would reap most of the benefits (gain of 6). Therefore, both countries would tend not to engage, and thus lead to cooperative failure and remain in the sub-Nash equilibrium of status quo, with total gain of 6 (3 + 3)

Relative gains	Country B reduces	Country B pollutes
Country A reduces	5, 5	2, 6
Country A pollutes	6, 2	**3, 3**

At the same time, the co-development of waste-handling strategies (*e.g.*, geological storage, CO_2-based carbon cap-and-trade programs, synthesis of stable CO_2-based molecules as a form of long-term chemical storage, *etc.*) are already underway. The emerging players for the most part respond to the dynamics of market economies (large established industrial groups, start-up companies whose business model revolves around CCUS-related services, *etc.*). These players have therefore found solvent markets for their activity. Without going into the open question raised by the possible rebound effect, also known as Jevons effect, of a downstream "solution" to emissions, it can be relevant to connect that these solvent payers are mostly public bodies. The cost of such remediation actions is therefore to be borne by public assets. Noteworthy, the private profits made by the oil sector over the last 50 years is estimated at 3 billion dollars a day over 50 years,[112] with no foreseeable substantial and specific redistribution of such private wealth. It is also in this context, that the interest in carbon capture and re-use policies to safeguard fossil production and trading-related profits can be analyzed, especially in the case that fossil assets were to become stranded assets due to fuel extraction bans.[113]

In summary, some elements of economics (like the sub-Nash equilibrium linked to the risk of cooperation failure and the fragility of schemes requiring environmental co-benefit profits), suggest that chemical research aimed at industrialization of CO_2-mitigating solutions as a means to tackle climate change might face the same market-driven economic pressures as research that has no such CO_2-mitigating ambitions, such as the requirement that they be cheaper, possibly after public subsidy, than fossil-based solutions in order to displace them.

4.2. Methane and hydrogen: are conflicts over control and usage taken into consideration?

4.2.1 Methane and armed conflicts. The potential for conflicts around the use and control of methane sources, like those for fossil fuels, is well-established in political science. While the correlation between abundant oil and conflict areas is not bijective, it remains strong, and armed conflict can be considered to closely mirror land usage conflict. The chemical community has started to integrate the relevance of armed conflict among its points of attention. For example, the European Chemical Society has labeled carbon among its conflict elements (Fig. 5). Wars are fought over the control of carbon-source fossil fields, and revenues collected from fossil fuel production are used to fight wars.[114,115] This correlation is not expected to disappear when the role of methane increases with respect to other fossil sources, as proposed in some scenarios. Nevertheless, increased use of biomethane could help address these concerns, since biomethane generated from agricultural practices should be less sensitive to geographical land usage conflicts. At the same time, all the scenarios produced so far consider biomethane as a minor contributor to the energy transition, thus it will not completely address the conflicts of usage.

The technical, social and political issues around hydrogen were already questioned by R. S. Cherry in 2004 in a paper entitled "A hydrogen utopia?".[116] Cherry stressed that most of the issues related to the development of hydrogen as an energy carrier were centered on three main topics, *i.e.*, safety, storage and cost, while externalities (side-effects) were very rarely considered. For example, he mentioned energy equity, where remote and less populated areas may encounter difficulties in accessing a competitive hydrogen infrastructure. Indeed, most projects involving a hydrogen society focus on two major bottlenecks: economy (price of hydrogen) and technology (production efficiency). This approach masks other aspects and sources of potential conflicts that nevertheless need to be addressed. Here, we will take two examples: land use and water impact.

4.2.2 Hydrogen and land use conflicts. Hydrogen production through electricity generated by photovoltaics (PV) will have an impact on the space needed to deploy solar panels. The surface area required for green hydrogen is significantly larger than that necessary for gray hydrogen. Ewan and Allen[117] showed that compared to PV-powered production, the production of hydrogen from high-density energy sources (*i.e.*, natural gas) requires an area about 40 times smaller per MW of hydrogen produced. If one considers that 4% of the land area in the United Kingdom can be devoted to PV, with a captured energy efficiency of 15%, only half of the average power requirement of the country could be covered (300 GW). However, recent data are more optimistic. Taking into account

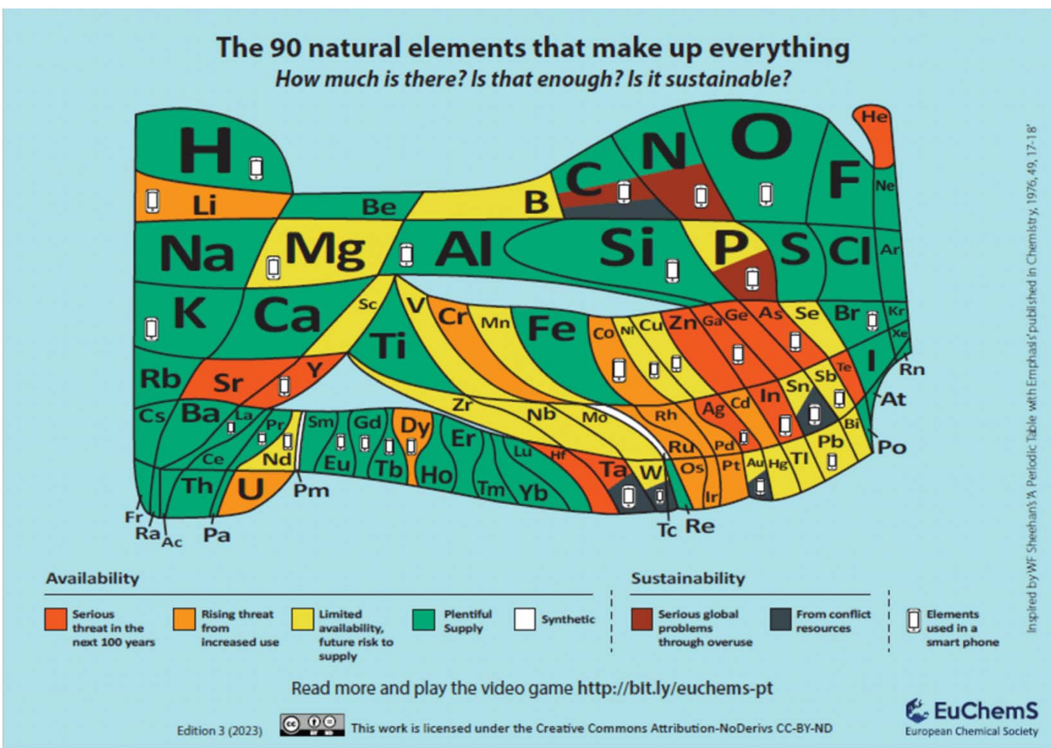


Fig. 5 The 2024 EuChemS periodic table of elements depicts element sustainability and causes of concern for future availability, including increased use and production from conflict resources, and impact on Earth system processes ("Serious global problems through overuse"). CC-BY-ND licence.

a 2050 scenario for the EU28, van Wijk[118] planned that the production of 70 Mt of hydrogen in Europe would require 0.2% of total European land area for PV, 0.5% for onshore wind and 1.1% of sea area for offshore wind. An additional 150 Mt of H_2 would be needed from North Africa, Norway, and Ukraine, with PV occupying 0.7% of the land area in North Africa.[118] These types of extra-territorial (extra-European) scenarios have obvious geopolitical ramifications linked, for example, to the installation and access to the PV panels, or to hydrogen production and transport infrastructures.

If 70 Mt of hydrogen were produced by PV in Europe alone, the land area required would increase to 22 500 km^2 (*i.e.*, about 0.5% of the total land covered by EU28, or about 4% of mainland France). Despite the apparent modesty of these figures, it should be kept in mind that, in densely populated areas, or in places where agriculture and forestry are already vying for space, adding large PV harvesting stations might be problematic, and the difficulty should not be underestimated. For this reason, the Sunergy technological roadmap targets higher solar-to-hydrogen conversion efficiencies of 30%. Recent social and political setbacks in the Netherlands related to the objectives for renewable installation at the local level[119] illustrate the potential conflicting situations arising from high hydrogen-production goals. Occupation of land may also lead to poor social acceptance, due to inequalities and non-inclusive development processes for renewable energies, leading to unwanted land uses, unfair compensation for expropriation or forced relocations. History shows that these would particularly affect vulnerable and marginalized communities (such as indigenous communities), and examples abound in Morocco, Mexico, and South Africa, where local communities were exposed to a power imbalance with energy developers.[120] Land use is definitely a place where technology development must interact with the social sciences to ensure independent local assessment of the impact of massive renewable energy projects.

4.2.3 Hydrogen and water usage conflicts. Regarding the impact on water, based on projections of a massive production of 2.3 Gt of hydrogen per year in all sectors,[121] and on a stoichiometric electrolysis reaction, the process can be estimated to consume 20.5 Gt of water (*i.e.*, 20.5 billion m^3) per year.[122] This amounts to 1.5 ppm of all the freshwater available on Earth, and is 50 times less than the volume consumed by agriculture. It should be noted that other scenarios may encompass a different energy mix, and thus project a lower demand for green hydrogen (for instance about 420 Mt by 2050 in the IEA scenario).

The Sunergy analysis[26] – focused on Europe – calculated that if the current hydrogen production was to rely entirely on water electrolysis, this would demand 3700 TWh of electricity annually, and the freshwater requirement would amount to 630 Mt per year. This is 0.7% of the annual EU28 freshwater consumption, and remains lower (one third) than the volume of freshwater used by the service industry (2400 Mt per year). Considering that the demand for hydrogen in Europe is about 15% of the global demand, the Sunergy analysis appears to confirm that the use of freshwater is not a major barrier to the development of hydrogen through electrolysis. This figure may be underestimated: additional water may be needed due to the other processes involved in water electrolysis, such as cooling of the electrolyzers, or treatment of the input water to meet the purity standards for electrolyzers, furthermore, this is a global scale analysis, and care must be taken in areas where freshwater is not easily accessible. Desalination could be an option, and in this case Beswick *et al.*[122] calculated that the energy and cost additions would be minimal. However, desalination adds penalties in terms of (i) CO_2 emissions when the required energy is produced from fossil fuels, and (ii) brines (salt-rich mixtures potentially contaminated with chemicals), which must be disposed of in the oceans, and that may impact the marine ecosystem. Other options, still at the research level, would be to use ambient humidity for hydrogen production.[123] In addition, water stress (the ratio between the fresh water withdrawals and the total renewable freshwater resources) will need to be assessed locally as it varies considerably from one country to another (Fig. 6). The IRENA (International RENewable Agency) foresees that more than 70% of

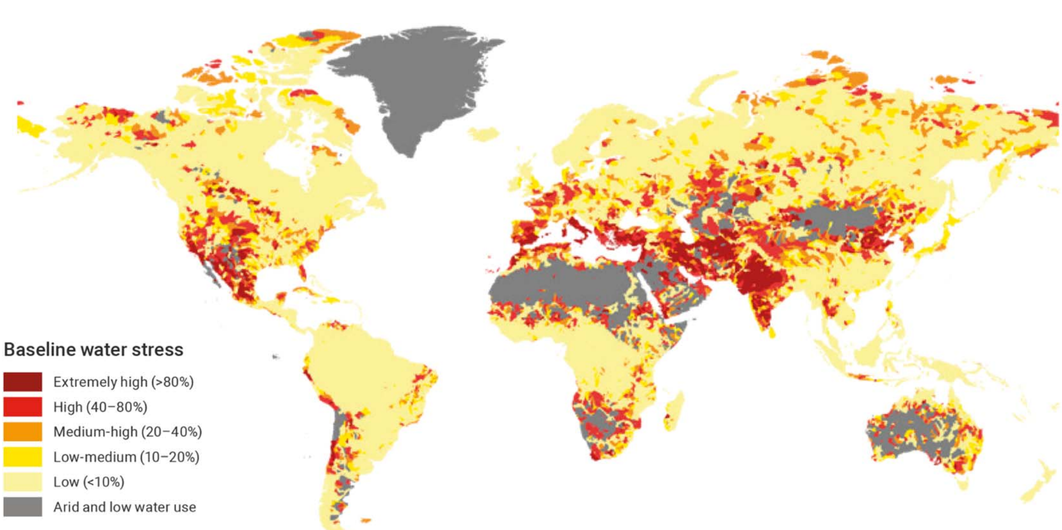


Fig. 6 Annual baseline water stress. Source: WRI (2019). Licence Creative Commons Attribution 4.0 International (CC by 4.0).[128]

planned electrolyzer projects will be in water-stressed regions, with most water provided through desalination.[124] Again, conflicts of usage over water and other resources will not be easy to resolve if they arise at the local level. In 2022, social struggles over water reservoirs for agriculture[125] and the cooling of nuclear plants in Southern France[126] show that local obstacles due to limited water supply that the generalization of large-scale hydrogen production could induce locally should not be underestimated. The NOOR I solar thermal power plant in Ouarzazate (Morocco) is another example where the constraints on water resources were experienced as a negative impact for the local communities.[127] Attempt to scale H_2 production must therefore be analyzed also in the context of practices' fairness.

In summary, this quick overview of possible increasing conflicts linked to land and water usage upon deployment of scenarios relying heavily on hydrogen or methane-based solutions reveals non-zero risks of creating or reinforcing existing geopolitical tensions, as well as triggering local social unrest.

4.3. Ammonia: should a molecule which is today a major environmental burden be scaled up and become an important energy vector in the future?

Ammonia is advanced in the scenarios analyzed as a green hydrogen carrier, or even a fuel in itself, mostly for the maritime sector (see Section 3.5). Replacing the current use of diesel for shipping by ammonia would consume approximately an additional 586 million tons of ammonia per year, *i.e.*, four times the current annual production.[99] For comparison, the planetary boundary for reactive nitrogen species is estimated at around 62 million tons per year at most.[12] Wolfram *et al.* recently pointed out that overstepping this boundary to power maritime shipping will necessarily cause major disruption in the global nitrogen cycle.[99] Moreover, they estimated that if just 0.4% of ammonia fuel were converted and released into the atmosphere as N_2O, it would completely offset the GHG emission benefits resulting from switching from diesel fuel. They point out that it is likely that leakage in extended NH_3 supply lines will result in additional N_2O emissions through natural denitrification, which will likely prove difficult to monitor and mitigate.

Beyond the projected usage, currently ammonia is mainly converted to urea and nitrates, for use as fertilizers. The scenarios reviewed identify two main approaches: blue and green ammonia (see Fig. 4). These approaches consider ammonia production through the Haber–Bosch process as an item to be improved, mostly at the level of upstream CO_2 emissions (see eqn (1) in Fig. 4), rather than as a major disruptor in ecological cycles. As a result, these approaches fail to address the severe ecological issues linked to disproportionate ammonia dispersion in the environment.[12,129]

Because of the N_2O emissions linked to poor Nitrogen Use Efficiency (NUE), even just from a climate change mitigation perspective, "green and blue" approaches are not a suitable answer when the full impact is considered. While the IPCC report points toward ways of improving NUE through nutrient recycling, or changes in agricultural practices (agroforestry, cover crops, hydroponics), it also points out that climate change is having a negative effect on the protein content of crops, leading to a compensatory increase in fertilizer use.

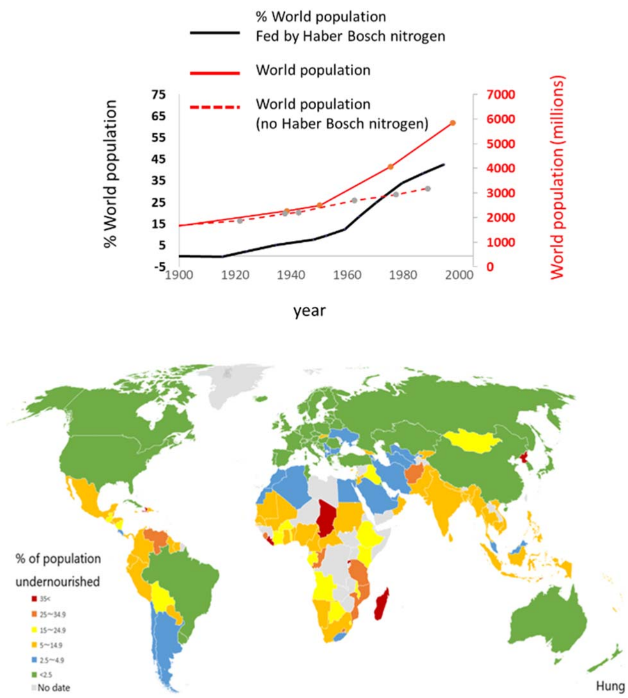


Fig. 7 Top: Evolution of world population over time (historical data) and projected world population without the development of the Haber–Bosch process, adapted from J. W. Erisman, *et al.*[62] Right: the Food Hunger Map provided by the Food and Agricultural Organization of the United Nations.[130] Global data make a clear causality link between the use of fertilizers and a growing population, but inequalities in access to food remain nonetheless. If ammonia really does feed "half of the world", which half would that be?

The argument that "ammonia feeds half of the world"[62] is regularly used to help justify the magnitude of our current reliance on it, but the argument loses some of its power and becomes tainted with condescendence in the context of global North-South food inequality (Fig. 7). The next question could be phrased: if ammonia really does feed "half of the world", which half would that be? This serves to exemplify the recurring deception that global world-average statistics can induce with respect to disparities, geographical or other. Meaningful disparities can become invisible under such global averages.

By questioning the chemical strategy linking ammonia to fertilizers, it is interesting to note that the reduction of elemental nitrogen (N^0 in N_2) to NH_3 (N^{III-}) consumes costly dihydrogen to ultimately oxidize it to N^{V+} in nitrates through the NO_x-emissive Ostwald process. It was the most efficient way to secure reactive nitrogen in Europe when the continent could no longer easily access South-American guano at the dawn of the 20th century.[131] At the time, CO_2 emissions and the downstream environmental impact of nitrogen use were almost completely ignored. But in the current framework of Anthropocene leading to the crossing of planetary boundaries related to most of the Earth system processes, this choice calls for a wider multidisciplinary assessment.

In summary, some elements taken from the scenarios for the possible role for ammonia in the energy transition combined with the current transgression in terms of reactive nitrogen release raise serious questions: Do these projections account for perturbation of the nitrogen cycle at a global scale? How could a ten-fold increase in ammonia production not have major environmental consequences, when even today – before any such increase – the environment appears severely compromised by the current production and usage?

4.4. Plastics: are we really prepared to take the consequences in our own back yards?

By contrast to CO_2, which is diluted and invisible, plastic waste is more visible and easily identifiable. It has thus elicited waste-handling strategies. Even though plastic waste trade involves a complicated network, the general flow can be identified. Worldwide waste has been transferred from Europe and North America toward Asia since the late 1980s, and China's ban in 2017 shifted the destination toward Southeast Asian countries.[132] This practice was considered as a win–win policy where the exporter gets rid of their waste, while the importer gains access to valuable material to enrich their economy,[133] resulting in an overall saving of energy and resources.[134] This type of commercial exchange, where one group's waste is sent across the world can be considered a NIMBY ("not in my backyard") attitude according to social science. One could say that, besides the plastic waste itself, the object of the commercial transaction is to shift formal responsibility for plastic pollution. The plastic waste trade, among other things, moves the burden of responsibility from the actual users and producers of waste (exporters) to the final collector.

In 2019, The European Green Deal acknowledged the issue by suggesting "that the EU should stop exporting its waste outside of the EU". The report stated that this would be tackled by revisiting "the rules on waste shipments and illegal exports", which by 2020 still accounted for more than 10% of all plastic waste produced (3.789 Mt out of 37.068 Mt).[135] Since 2021, the shipment of unsorted and hazardous waste from the EU to non-OECD countries has been banned, and only clean, non-hazardous waste can be exported for the specific purpose of recycling.[136] However, is it really sustainable, and fair, to export (even part of) our plastic waste to other parts of the planet? Regarding sustainability, the consequences of the Anthropocene will ultimately affect the global North, notwithstanding the original destination of the waste. Moreover, regarding fairness, from the importers' point of view, plastic waste trade can be considered an unwanted remnant of colonial ideology, contributing to the exploitation of populations in the global South.[137]

A partial solution to this situation, the third R of the "Reduce, Reuse and Recycle" strategy is to create new waste treatment facilities within our borders, on a scale compatible with the size of the problem to be treated. In other words, one more technology-intensive industrial infrastructure must be added to European material needs (steel, cement, metals, *etc.*) to handle its transition to better waste-handling.

The production of bio-sourced conventional bioplastics will not solve the recycling question, as these plastics are still in large part non-biodegradable and not always easy to recycle. On the other hand, a fraction of bioplastics are also biodegradable. This difference must be highlighted to avoid confusion caused by the prefix "bio". However, biodegradability remains a general concept. Biodegradable materials are defined as those that break down into natural elements or small molecules under the influence of microbial activity in a relatively short timeframe and in naturally occurring conditions.[138] Although it is mostly accepted that the ultimate products of such degradation processes are water, CO_2, methane and biomass,[139,140] biodegradable biopolymers are quite often only broken down into oligomers, called metabolites, which then enter the catabolism of nature.[141] Assuming that the eventual biodegradation of plastics in the amounts currently produced would not cause imbalance in the ecosystem is a risky bet. The open questions on the end-of-life effects of bio-sourced plastics on the environment remain.

4.5. What does the scalability requirement say about cultural representations?

The need to scale-up emerging technologies is central to the vast majority of "Net-Zero-Emissions" roadmaps. The benefits of this intensification are clearly presented in terms of reduced GHG emissions and through the traditional levers of the economy of scale to power the energy transition and the electrification of the chemical industry, with the related costs and hurdles generally being also partly discussed.

Solar and wind energy, while ubiquitous, are naturally intermittent, low-density sources of energy. Consequently, collecting and storing them will take up much more space and require far more units than current power plants.[142,143] Moreover, direct electrification has been prioritized due to the excellent energy yield it offers (especially for transportation with electric vehicles). At the same time, transport and storage of electricity will require considerable construction of novel infrastructure, which explains in part the projected increases in mineral resource consumption.[144] Even replacing fossil fuels with "green fuels", such as hydrogen, relies on significant critical metal availability (see ESI, Section SI-5†). This rampant increase in resource consumption is not new. In fact, it has been a defining aspect of the Anthropocene, and it remains a dynamic on which the energy transition is being constructed. Indeed, the IEA forecasts a six-fold increase in mineral demand by 2040 to meet the target of NZE by 2050, mostly driven by steel, rare earths, graphite, copper, aluminum, zinc, cobalt, nickel, silicon, and lithium.[144] The extraction of these resources is mainly performed in open-pit mines with a high land footprint and causing extensive ecosystem disruption.[145–147] Moreover, extracting these non-renewable resources will itself consume significant energy, and generate substantial pollution at the site of extraction. Is it reasonable to keep labeling some scenarios as "sustainable solutions", notwithstanding these (generally less addressed) aspects (with respect to carbon footprint, for example)?

Associated with this increased demand for mineral resources is the fact that in our current globalized world, the targeted elements from the mineral resources are often not used where they are produced. North America and Europe exhibit by far the highest domestic material consumption per capita, but Europe in particular generates the lowest amount of ore per capita, with the exception of West Asia.[148] For instance, the vast majority of the world's cobalt comes from the Democratic Republic of Congo, while nickel is mainly produced in Indonesia, Iran, and the Philippines, and the biggest producer of copper is Chile.[144,149] Much like with plastic waste management, the outsourcing of metal supply directly transfers pollution to places where environmental and health fallouts are less controlled and regulated, particularly in the context of the increasing development of artisanal mining operations.[150–152] In addition, the scale of disruption expected for the energy transition is enormous, as fossil resource mining operations are expected to shut down, while exploitation of other resources is expected to surge rapidly.[153,154] Due to the urgency imposed by the accelerating climate crisis, such a drastic and fast-paced shift is bound to lead to numerous "casualties" on the social and human front.[155,156] How are the interdependencies between countries and their dramatically different circumstances taken into account? Is it a mistake to continue to adopt a neutral and universal viewpoint when describing the problems and their possible solutions? Is considering the Earth in terms of "resources" part of the problem?

Overall, it appears to us that the proposed pathways toward a low-carbon economy are essentially built on most of the same mechanisms and dominant beliefs that led to the very advent of the Anthropocene: consuming ever-increasing amounts of energy, ultimately requiring most likely increasing natural resources that are incompatible with Earth system processes, while at the same time failing to set the social implications of the desired transition as a guiding principle. It is notable that, historically, the interests of indigenous peoples have suffered as a result of large-scale resource extraction or energy production projects. There seems to be high probability of conflicts that will emerge from the intensification of resource extraction and the building of large-scale installations. Some of the places concerned are already the most threatened by the ongoing climate crisis, and socio-political problems have already started, such as forced migrations or unconsidered health problems, for example caused by mining. Is the projected energy transition really going to be "clean"? Does this transition deal with different cultural representations?

4.6. Does the notion of energy transition really make sense? And if so, how?

The common narrative associated with the history of energy transitions is a succession of dominant energy sources and regimes, particularly since the advent of the Industrial Revolution at the end of the 18th century. Western society moved from an organic energy regime, based on photosynthesis and brute (animal) force, to a fossil energy regime, the consolidation of which occurred in the 19th century. Starting with coal, then petroleum and natural gas, societies underwent successive energy changes, especially following the development of electricity in the 20th century. According to this narrative, the energy transition in the 21st century would constitute a new, albeit ambitious, phase in history, with the replacement of dominant CO_2-emissive energy sources by renewables and other non-emissive sources.

However, this narrative is hardly correct: our modern energy scenario has not so much evolved through transitions and shifts, as through addition and accumulation.[157] The massive development of coal extraction in the 19th century did not lead to the disappearance of so-called organic sources of energy, especially animal strength. During the 19th century, the number of horses in France increased by 50% and water and wind mills continued to meet the need of a large part of the European population.[158,159] In the mid-20th century, the rapid increase of oil supply did not lead to an equivalent decline in coal extraction; nor did the later development of nuclear power. Today, according to the IEA, the world's coal, oil, and natural gas supply is at more than 490 000 000 TJ, more than ever before in modern history.[160]

Furthermore, these energy layers have not been added as mere juxtapositions. Energy sources have, throughout history, been combined with each other, and with material resources. An example is provided by the massive use of wood in the coal age, to consolidate mine shafts, build railway tracks, as cable supports for the emerging telegraph, *etc.* Thus, coal only developed thanks to the parallel use of wood and steel. This is what has been called energy and material "symbioses".[161]

Through this historical lens, the challenges for the 21st-century energy transition increase immeasurably: the complete replacement of CO_2-emissive energies by non-CO_2-emissive energies would be unprecedented. It will not be simple to achieve as it will require significant reconfiguration of current energy and material symbioses – see the need for rare earths or lithium for batteries intended for electric, low-carbon mobility.[144]

In chemical terms, it is therefore hardly possible to tackle today's challenges by reasoning in silos, molecule by molecule, without considering from the outset that molecules combine, not only in the literal, microscopic sense – through catalysis, for example – but also in the figurative, macroscopic sense, in material and socio-technical configurations that must be kept in mind. To produce NH_3 with low GHG emissions, we need to think about green hydrogen and about all the materials needed to store and transport it. We also need to think about all the energy and material combinations on which this NH_3 and hydrogen could be grafted, to be sure that they will not support other GHG-emissive technologies or symbioses – a major issue that is not really addressed in the scenarios mentioned above. This will require chemists to constantly broaden how they view their own field of specialization.

History also teaches us that energy is never only a matter of source or technology. Indeed, energy systems have always required infrastructure (*e.g.*, distribution networks such as pipelines),[162] business models (*e.g.*, large *vs.* small companies, rent distribution, marginal pricing strategies for electricity),[163,164] institutional rules (*e.g.*, anti-trust laws, energy policies),[165] and even cultural representations and practices (*e.g.*, pressing a button to get light in no way resembles switching on a paraffin lamp and having to ensure the availability of fuel).[166] If the notion of transition might be meaningful from a historical perspective, it is not just in relation to energy sources or technologies *per se*, but when energy systems as a whole are considered.

For researchers in chemistry, this has two further implications. First, it means that when working on a molecule or a specific reaction, chemists do not work only on specific materials or related technologies; they also indirectly tap into broader components of the energy or material system, including infrastructure, business models, and policies, but also cultural representations, and habits.[167] For instance, turning CO_2 into a raw material would certainly change what is now a waste product into a valuable material, but it would also mean changing the representations associated with CO_2. Why should we strive to reduce emissions if CO_2 is now a "good" thing? This might have detrimental effects if as a result emissions remain too high – no longer being avoided, with the public thinking that a high atmospheric CO_2 concentration is no longer an issue – compared to the absorption and transformation capacities of new technologies.[75] This threat can be exemplified by the recent German request to postpone the termination of commercialization of internal combustion engine vehicles, set by the EU for 2035, on the basis, among other considerations, that by that time we will be able to produce CO_2-neutral e-fuels.[168] It is therefore legitimate for chemists to wonder about the systemic effects of the chemical processes they work out and to act so that no misleading or detrimental cultural representations emerge or is strengthened thanks to their discoveries.

The second implication is that in energy systems the difficulties with changing long-lasting technological trajectories and habits – or path dependencies – have not only material (or chemical) and economic (related to profitability) explanations, but also institutional and cultural ones. This might seem obvious, but it may not be so obvious when faced with social demand for (technical and profitable) solutions to the ecological crisis from fundamental and applied sciences, as if the technological lever was the cornerstone of future changes. It is worth remembering that levers other than technology exist (*e.g.*, energy demand modulation, new spatial planning, reduced packaging, better sharing of existing resources) to ensure the transition to a non–CO_2–emissive energy system.

4.7. Discussion

4.7.1 On the scientific method. New research avenues expected to lead to operational technologies for the energy transitions are projected as a necessary part of the solution, with a massive scale-up that should be deployed fast. In Section 3, we reviewed the consensus that the low-maturity of some of these technologies raises doubts about whether scale-up is technically feasible. This section of the paper (Section 4), focused on interdisciplinary elements, shows that such technical uncertainty is compounded by risks linked to environmental, geopolitical, and social effects, even when novel technologies were to be technically available at scale.

As a first example of the just mentioned risks, focused on potential environmental impacts, several Earth system processes, which are connected to the interdependencies outlined (*e.g.* freshwater Earth system process for hydrogen and water conflicts, and Land Use Earth system process for hydrogen and land use conflicts, Novel Entities Earth for the section on plastics) are generally either ignored or overlooked by the scenarios analyzed. Returning within some of the identified planetary boundaries is not explicitly stated as a goal of the scenarios, and little evidence is provided to project that the transgression of these boundaries could eventually be reversed. While the main focus of the scenarios we have chosen is, by construction, one particular Earth system process (*i.e.*, dominance of climate change-tailored actions through the recurrent notion of the carbon footprint), other interconnected consequences of a move away from fossil fuels are seldom adequately treated (*e.g.*, land, water and resource management connected to the energy transition; effect on biodiversity; consequences of the introduction of novel entities). On the contrary, in some cases, the energy transition scenarios analyzed carry a serious risk of further exacerbating the overstepping of a planetary boundary, even when the situation is already dire (*e.g.*, ammonia).

As a second example of the possible risks, focused on the potential geopolitical and social impacts of the proposed scenarios, (some) people are overlooked by scenarios. Many of the proposed strategies are blind to North-South inequalities, and the scenarios may contribute to maintaining or even exacerbating conflicts linked to extractivism, productivism, commodification of resources, and waste management (*e.g.*, through extra-European mining activities connected with metal resources required to establish fossil fuel-decoupled European mobility).

Concurrently, this interdisciplinary analysis of scenarios, examined through the prism of five molecular substances at the energy-chemistry nexus, also highlights one invariant between the present time and the projected transition(s): the hierarchy of values.

Even though the triple-bottom line of sustainability – the "three Ps", People, Planet, and Profit, *i.e.*, economically viable, socially just, and ecologically sound – is mentioned throughout some scenarios and prospective sustainability exercises, these are generally established and projected in a hierarchical order. Profitability appears as a necessary condition, with scalability and commodification being the main – if not the only– reasonable strategy, while at the same time *de facto* omitting important aspects of the Planet and People bottom lines.[155,169] This will potentially have problematic consequences in terms of environmental and social justice.

Notwithstanding possible intrinsic limits to the efficiency of some industry-targeted research, as discussed in the context of proposed energy-transition-related solutions (*e.g.*, sub-optimal Nash equilibria), the strategies analyzed overwhelmingly retain private profit as a necessary principal driver. This driver has a structural tendency to increase production and/or exclude less profitable beneficiaries, thus echoing and substantiating the two aspects of concern highlighted above: supply the world with commodities beyond its planetary limits and/or prosper by excluding or exploiting some groups of people or resources. Consequently, the trajectory associated with the development and scaling-up of several novel technologies could potentially mimic some aspects of the dynamics that led to the Anthropocene in the first place. For this review, we considered scenarios requiring the creation of and need for new entities, with an expectation of a dramatically-expanding market: non-fossil fuels and technologies, and commodities, infrastructure, *etc.*, associated with their production. We are poised to see a considerable acceleration of new variables, potentially representing additional energy sources rather than complete substitutions for current fuels. The question relates less to the common objective (to decrease fossil fuel consumption) and the possible means to achieve it (alternative energy sources, increased efficiency, *etc.*) than to the overall arc traced by these scenarios, and the method(s) that will reveal it. This question is further complexified by the fact that through interdisciplinary dialog, we are able to catch a glimpse of the non-scientific – some philosophers have used the term "imaginary"[170] in contexts akin to the one under study here – dimensions underlaying our scientific developments. This interdisciplinary dialog has helped show that, in order to build up and justify our scientific choices, we rely on "cultural axioms", that we mostly do not question nor explicitly mention.

We propose that including inter/transdisciplinary thinking as part of a broader and more systemic vision of the energy transition, relying not only on productivity and CO_2 emission numbers, could produce more balanced and equitable roadmaps (see ESI, Section SI-1.3† for our distinction between interdisciplinarity and transdisciplinarity). For instance, established and measurable global descriptors, such as planetary boundaries, could be used to assess and teach[171,172] the impact of any proposed approach, along with systems thinking. In addition, notions of social and environmental justice, that go beyond the use of measurable descriptors, could be included when considering societal organization, resource use, and waste disposal. In ecological economics for instance, *i.e.* a research arena gathering both economists and environmental scientists, some initiatives do exist to cross indicators and recommendations for a more sustainable future, with varying degree of heuristics power. Kate Raworth's doughnut economics, combining social thresholds and ecological ceilings, is one example.[173] Richard Norgaard's coevolutionary economics, examining the interrelation between socio- and eco-systems, is another one.[174]

Developing transdisciplinary tools to explore and analyze the complex ramifications of the global shift in economic, social, and technological models represented by the energy transition appears to us not only beneficial, but necessary, to break the hegemonic view currently put forward and to generate novel paradigms for the chemistry-energy nexus. We note that alternatives have been and continue to be proposed.[175] The relevance of non-hegemonic frameworks may need to be assessed to widen the narrow and potentially dangerous path currently set out by the dominant scenarios analyzed. We mentioned Profit, Planet and People: examples of existing scientific and minoritarian frameworks in non-mainstream economics (ecological economics, degrowth/post-growth, political ecology) and in critiques of dominant power structures, including economic ones, are all relevant in this quest to deconstruct the current implicit hierarchy of values that could very problematically guide the future of research at the chemistry-energy nexus.

In summary, the take-home message is two-fold: the path offered by the scenarios is narrow and is associated with numerous pitfalls. This suggests that alternatives based on a broader, transdisciplinary method of analysis with closer attention to historically overshadowed – or politically suppressed – theories can be revisited by chemists as a source of inspiration.

4.7.2 On the timeframe. Even among scenario proponents (with no attention to Planetary boundaries or the North-South divide), doubts on their own feasibility exist given the scale and timeframe. Scenario after scenario, the timeframe is shrinking. The solutions proposed in scenarios published some time ago are not being picked up, but updated scenarios essentially propose more of the same over a shorter period (despite the previous failure to adopt). Goals are re-evaluated every five years. "Progress needs to be faster" and yet little has been achieved so far in light of the magnitude and speed of the global changes unfolding.

In 1972, twelve scenarios were presented by Meadows' team, in the "limit to growth" report,[176] regarding the trends for five key interconnected indicators (resources, population, food per capita, pollution, industrial output per capita) between 1900 and 2100. Modeling their interdependencies and carve system-based scenarios were termed "wicked problems" by the Club of Rome. In 2021, almost 50 years later, current analyses[156] after a 30 years update[178] suggest that among all the scenarios considered, the one that is statistically the furthest from empirical data is the "Stabilize the World" scenario (see Fig. 8). While this scenario contributed to the UN "sustainable development" definition that still permeates some current discourse, other scenarios like "Business As Usual" and "Comprehensive Technology" are on the contrary the most compatible with current data (see ESI, Fig. SI-4†). Pointedly, the "comprehensive technology" scenario assumes "exceptionally high technological development and adoption rates". This, compounded with the feasibility doubts mentioned by technology-driven proponents mentioned above, show that there is an active possibility for a path to the most unstable future which entails brutal collapse of population and resources (see "business as usual" models, Fig. SI-4†).

To return to the topic of this paper, there is still a chance that the common elements of the five "energy transition" scenarios discussed above (Section 3.7) could be enacted, if the incessant, increasing, and here-to-fore only very partially addressed calls for substantial changes were finally met. However, even if these calls were met, some of the flaws consubstantial with the scenarios mentioned above would become a reality (*e.g.*, recurrent disregard of the global South and disregard of Earth system processes (other than CO_2)-related problems).

Therefore, the urgency is evident: we must make sure that we have the appropriate tools to avoid the aforementioned failure to

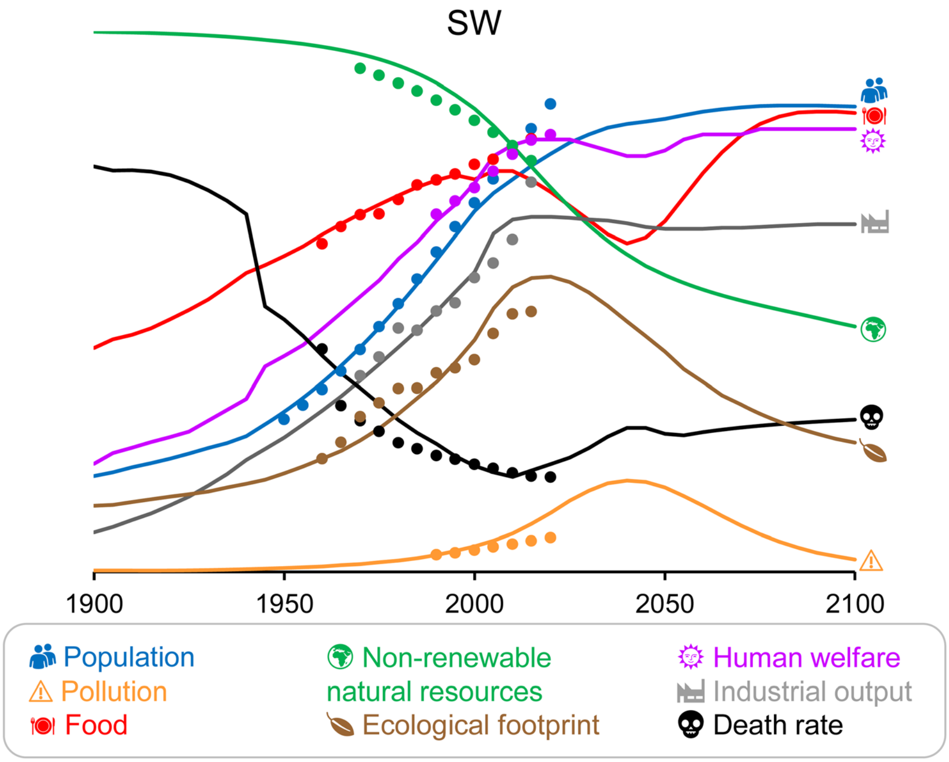


Fig. 8 SW (stabilize the world) scenario for the projected evolution of population (blue line), pollution (orange line), food per capita (red line), non-renewable resources (green line), ecological footprint (brown line), human welfare (pink line), industrial output (gray line), and death rate (black line), and comparison with corresponding empirical data (dots), adapted from Herrington[177] and Meadows.[178] SW is referred as the sustainable model: indicators are stabilized on the long-term thanks to meaningful policy changes. Data for three other scenarios (Business As Usual and Comprehensive Technology) are available in ESI, Section SI-6 and Fig. SI-4.†

change, but we must also make sure that we have the appropriate tools to avoid the risks associated with implementation of some aspects of the dominant scenarios discussed above.

5. General conclusion and perspectives

5.1. Broader scenarios needed

We are living in the Anthropocene, and as such the quality of human life on Earth is jeopardized by certain choices, and modeled and institutionalized under some ideas of how we should inhabit Earth. These choices and ideas permeate the research horizons and the specific research subjects we as scientists must treat.

One of the pervasive messages surrounding the energy transition, included in the chemistry-oriented responses analyzed through the pivotal molecules dealt with in this paper, is that the energy transition is designed to avoid future crises that remain to be faced. However, this minimizes the fact that the planet is already in crisis. We further showed that this crisis was potentially caused by some aspects that are still present in some of the responses that are currently proposed as solutions to implement the energy transition. We also showed that this crisis presents multiple aspects that are not addressed by the response specifically tailored to the energy transition challenge. We therefore propose as first conclusion to this paper that there is a potential incongruity between the problem stated and several of the scientific research avenues proposed in the scenarios analyzed here.

The second conclusion is based on the disciplinary fragmentation we face in our academic practice. This is a complicating factor when trying to address such types of incongruity. In contrast, transdisciplinarity appears to help circumvent deadlocks emerging from proposing disciplinary approaches to systemic problems. Indeed, one lead from this paper is that a radically interdisciplinary dialog – between the natural and social sciences – must be explored. Progress in natural science has the power to facilitate a change in society, just as much as the pressures exerted by a changing society or politics can lead to intensified efforts in some specific areas of research in natural science. Echoing a classification proposed by German philosopher Dilthey,[179] chemistry is a science that focuses on mastering how transformations occur, while social sciences and humanities describe and interpret why transformations occur. This is not to say that social sciences can explain why the transformation of matter and energy occurs in physical or chemical terms, but that, since the transformation of technologies and production processes also has social motivations and implications, social scientists provide critical information about the connection between, on one side, these motivations and implications and, on the other side, the technological and material change itself: What are the social motivations and implication that contribute to the chemists being asked to search for CO_2-based materials? What sort of (social and economic) hypotheses are implicitly embarked in their research? *etc.* As a consequence, social scientists should be involved in chemistry projects, not as side contributors but more granularly throughout the projects. In a sense, the project that led to this paper explored precisely this suggestion. Intertwining aspects of the chemical sciences, relevant to the transformation of matter at the energy-chemistry nexus, through the prism of five molecular substances, with aspects of social sciences and philosophy, connected to transformations of societies at the same nexus, seems to offer a relevant perspective on the transition scenarios during the Anthropocene crisis.

The third conclusion to this work relates to the utility of turning to wider scientific approaches that have been historically/politically suppressed (non-orthodox economics, decolonial and post-colonial studies, gender studies, see Section 4) and of investigating their capacity to inspire chemistries beyond the currently hegemonic one which is, at least partly, problematic. For example, academic chemists' agenda is for now mostly framed, often implicitly, by economic and political ideas such as, for instance, priority given to research likely to lead to economic growth and profitability and toward the quest for groundbreaking technological progress. By looking at other economic, social, and political framings, inspired for instance by ecological economics[173] and post-growth theories,[180,181] or decolonial studies,[182,183] chemists could become inspired in investigating other, less conventional research avenues. For example, community energy projects that could exemplarily contribute to mitigation strategies while inspiring the rise of other energy communities elsewhere,[184] as well as low-tech and nature-inspired approach developed in the global South using a non-hegemonic framing,[185] could inspire global North initiatives to develop low-tech as a way to rethink technology for sobriety, conviviality, and sustainability, options in academia,[186] there included in chemistry research.

5.2. How do research topics align with researchers' values?

Beyond interdisciplinarity and transdisciplinarity interactions with other disciplines, as well as devoting attention to suppressed portions of disciplines, the questioning can be further extended to the forms of knowledge themselves. The production of knowledge that by academic construction rewards and sustains a narrow path (with problematic invariants) is also part of the equation. What values collectively lead us to define research excellence, or, on the contrary, irrelevance? What values are encouraged, allowed or suppressed by the scenarios shaping our research projects? Do these reflect our personal values, and ensure Earth will remain habitable while emphasizing the need for social justice?

In the context of the Anthropocene, this leads to an immediate overarching question: What is our responsibility with respect to the research horizons and the specific subjects we treat as scientists, when we suspect such incongruity? Some may think this has nothing to do with our job as scientists and that we should leave the problem to international organizations, or governments – that we can act only as individuals with individual responsibilities. On the contrary, following in the footsteps of eminent thinkers (Box 1), we believe that there is a social dimension of responsibility. Quoting the ethical group advising the CNRS, the largest French research body, "the specific purpose [of research], which is to produce knowledge in the service of society, confers on research[ers] the particular responsibility of also questioning the use that can be made of their contributions […] and the way that this use can help respond positively to the problems encountered by society or, on the contrary, perpetuate or even aggravate them." We also believe, although we each have our own specialization, that we bear an ethical responsibility for the consequences of our acts, which often lead to consequences well beyond our disciplines. Do our research and the knowledge it produces respond to, perpetuate, or aggravate the problems raised?

> *"I believe that scientists have absolute responsibility for thinking about the use of their creations, even the abuses by others"* — Roald Hoffmann, 1981 Chemistry Nobel Prize winner
>
> *Box 1*

To explore our own invitation to mobilize concepts produced in the global South as a source of inspiration, the problem might be less related to what we know and what we can do, but more to what we do not know and what we are willingly ignoring.[187–189] We suggest that overcoming disciplinary isolation, paying attention to critical scientific theories and reaching out to knowledge-producing activities beyond academic circles should be explored to help deflect the ominous course of the Anthropocene through our research activities. Even if we are scientists, the Anthropocene is neither just a matter of academic discussion nor a question of agreement or disagreement. Our posture cannot be that of academic practitioners undertaking compartmentalized disciplinary research based on scenarios that only partially reflect our values.

Author contributions

More information on the authors' contributions can be found in section "SI-1.2 Our Authorship policy" of the ESI.†

Conflicts of interest

We have no conflict of interests to declare. In spirit of transparency, we wish to mention here that VA contributed to the Sunergy technological roadmap discussed in Section 3.

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