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A Paris aligned 1.5 °C mitigation pathway for the chemical industry based on 100% renewable energy and novel production technologies

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Abstract
With renewables growing at an unprecedented pace and critical carbon budget deadlines approaching, research is shifting to the new frontier of Paris aligned 1.5 °C mitigation pathways for hard-to-abate sectors, including the chemical industry sector. This is a significant challenge with chemical products such as plastics, fertilizers and many more products intertwined with today's society and with CO_2 emissions originating both from energy and from chemical conversions. This paper presents a detailed bottom-up production-based energy and emission calculation to make a 1.5 °C compatible scenario for the chemical industry based on three main measures compared to a business-as-usual scenario. This research found that the holistic combination of demand and supply measures is critical to reduce the different types of emissions in the sector (energy and non-energy process emissions). An overall reduction of 82% of CO_2 emissions in 2050 is calculated with a decrease in base chemical production growth (− 21%), 100% renewable energy for heat and electricity (− 50%) and the introduction of novel electrical-based and biomass-based production technologies for ethylene, propylene, methanol and ammonia (− 10%). Critical system developments include slowing chemical demand growth with recycling and circularity best practices, advanced electrification of heat supply and the substantial market penetration of the current most advanced sustainable production technologies for methanol, ammonia, and ethylene based on their reasonable technology maturation trajectories. Here, green methanol and ammonia will require 381 TWh in 2030 and 3232 TWh in 2050 for green hydrogen electrolysis, which will represent 1% and 4% of global electricity demand.

Article Highlights

- A holistic 1.5 °C chemical sector pathway requires both demand and supply measures.
- Far-reaching electrification is crucial for industrial heat. Synfuels, hydrogen and biomass fulfil remaining demand.
- Green production technologies are crucial to reduce non-energy CO_2 emissions.

Keywords Chemical industry · Green chemicals · 1.5 °C pathways · Circularity · Carbon budget · 100% renewables

Abbreviations

BAU	Business-as-usual
BAT	Best available technology

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BECCS	Bioenergy with carbon capture and storage
BTX	Benzene, toluene and xylene
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
DAC	Direct air capture
E-methanol	Electrical based methanol
FOAK	First-of-a-kind
IEA	International energy agency
MTA	Methanol to aromatics
MTO	Methanol to olefins
NOAK	*N*th-of-a-kind
OECM	One Earth climate model

1 Introduction

In 2020, the chemical industry was responsible for 2.4 Gt of CO_2 emissions, compared to a global total of 31.8 Gt of energy related CO_2 emissions [1]. In the last 10 years the chemical industry has grown significantly in production. Chemicals form the base material for a wide range of products used by the world population and therefore the industry follows the socio-economic growth of the world population. Key examples here include plastic products and fertilizers. However, the current global growth rate for chemical production will not be compatible with a 1.5 °C emission scenario [2, 3].

Despite a considerable share of global emissions, the chemical industry receives less attention, than for instance the power sector. As one of the hard-to-abate industries, sustainability in the sector is difficult and complex. The simple reason behind this is that it is harder to reduce greenhouse gas emissions from the chemical industry, due to four main factors. Firstly, the industry is notorious for its process emissions from chemical conversion of feedstock (not originating from combustion for heat or electricity). Secondly, most of the heat used in the sector is high temperature heat (> 500 °C), which is required to drive chemical reactions. This makes it more challenging to replace these energy sources with renewables than in other sectors. Thirdly, the chemical sector consists of tens of thousands of unique processes that interact in a complex web of interactions. Finally, long lifetimes of infrastructure and a fossil-fuel based feedstock make a sustainable transition for the industry even more complex.

All these factors make the existence of sound energy transition sectorial pathways until 2050, with clear targets, crucial for the chemical sector. Comprehensive energy transition pathways would include energy estimations based on chemical production data, calculation of overall CO_2 production, the integration of sustainable chemical production technologies, renewable energy, and considerations for key interventions such as circular economy, product stewardship and extended producer responsibility, that are likely to impact future demand for virgin polymers and other chemical industry inputs. Moreover, there is a need for global and country-specific pathways to steer investments and policy-making.

Currently, there are several industry reports from the International Energy Agency (IEA) and McKinsey and Meng et al. [3–6] and regional studies for Europe, India, China [7–11]. Recent work from Meng et al. described planet-compatible pathways for the sector with a range of circularity interventions and carbon capture and storage (CCS) solutions [3]. In addition, Lopez et al. explored a full implementation of electrical based chemicals produced with carbon capture and utilization (CCU) for the sector—while excluding bio- based chemicals [12]. There are however remaining critical research gaps that have not been addressed by the current body of scientific literature. There is a need for detailed transparent technical scenarios on a global and on a regional level, with links to chemical production levels, circularity and other sustainability practices, 100% renewable energy and upcoming green production technologies (both synthetic and bio-based). This paper will answer the first research question of what the detailed energy demand projection for the chemical industry is up to 2050 in a business-as-usual scenario and in a scenario compatible with a 1.5 °C carbon budget with a novel expansion of a production based methodology for calculating the energy demand (including electricity estimation based on chlorine production). In addition, the novelty of the presented research in this paper includes that chemical industry sustainable pathways have not been examined in a holistic manner before, regarding carbon neutral 100% renewable energy, green feedstock and trajectories for novel sustainable production technologies. Resulting research can be used for informing net-zero target setting in general policy and sustainable finance.

To achieve a sustainable chemical industry, the industry will have to rely on three pillars of sustainable measures: reducing growth of production and demand, a renewable energy mix and novel production technologies. By reducing the future use of plastic products such as packaging, increasing best practices such as circularity and recycling and implementing sustainable agriculture practices, the required growth of chemical production can be decreased [13–15]. Furthermore, replacing the fossil-fuel based energy used for heat and electricity by 100% renewable energy will reduce the energy related carbon emissions. Lastly, novel technologies will reduce the non-energy related carbon emissions. In the following paragraphs, latest developments will be described for the three pillars, finally leading to the introduction of our second research question regarding their impact.

As a first primary component of a sustainable 1.5 °C pathway, the demand of chemical products will change in character and in overall magnitude. Tulus et al. presented that over 99% of all current chemicals exceed planetary boundaries, thereby indicating the need for an overall system change [16]. Globally there are a range of external drivers that are likely to impact the status quo of the chemical industry, both from a policy and economic landscape. Current developments include the EU's 2020 strategy phasing out of chemicals linked with environmental and health impacts, changes in circularity best practices across the value chain and the push for higher plastic recycling rates [17, 18]. Chemicals of concern are particularly problematic in toys, electronics, cosmetics, textiles, and food packaging [19]. Some examples are the highly toxic and environmentally persistent PFAS (perfluoroalkyl and polyfluoroalkyl substances) that have been known to leech from products including non-stick cook wear and textiles onto furniture and food packaging along numerous points in the supply chain; legacy chemicals accumulating in the natural environment; toys using recycled black plastics from electronic waste containing levels of toxic chemicals comparable to those found in hazardous wastes, such as ash from incinerators. However, it should be noted that even though phasing-out of chemicals of concern is highly desirable, it does not automatically translate to CO_2 emissions and energy use reduction, because the use of alternative materials may still require other chemicals whose impacts are not fully known or regulated. Despite this, circular economy regulation is likely to impact demand for chemicals throughout different stages of the product lifecycle: production, consumption, and post-consumption end-of-life. The production stage encompasses material choice, design, and manufacturing. Here, regulations addressing the use of less synthetic/more natural materials in products are likely to impact chemical demand. E.g., Plastic polymers used in food contact packaging, microbeads banned in cosmetic products and clothing. Circularity during the consumptions stage relates to use, reuse, repair, and retail. Regulations such as the Right to Repair are targeted at making products more durable and in use for longer [20]. In addition, the sharing economy and second-hand sales markets also enable longer life and reuse. The post-consumption stage refers to end-of-life management and resource recovery of chemicals. Some opportunities for recovery of chemical industry byproducts exist (e.g., spent acid to chemical gypsum in cement or acid in textile and dye industries) and an overall increase in global recycling rates. Overall, these positive trends are likely to impact the average lifespans of products, encouraging consumers to use products longer before discarding and finally drive down a future growth in demand for chemical products.

A second component of a 1.5 °C compatible pathway will apply renewable energy wherever possible and the research in this paper will align with the field of 100% renewable energy systems [21]. In the field of 100% renewables, accepted energy supply sources are solar, wind, hydropower, bioenergy, geothermal energy and ocean energy and this excludes nuclear energy or fossil-fuel based energy with carbon capture and storage [21]. Here, a high share of heat demand of industry can be electrified, and high temperature renewable heat will have to be come from biomass, hydrogen and advanced electrification methods [22–24]. Here, Madeddu et al. established that 78% of industrial processes in the European Union can be electrified with available technologies and 99% with technologies currently under development [24]. Some highly heat intensive processes such as ethylene steam cracking will become electrified, thereby opening the possibility for more renewable energy integration where previously fossil-fuel based high temperature heat was used [25, 26].

The final part of the current non-energy related emissions reduction for the chemical industry will have to come from the emergence of green production technologies for chemicals. In the chemical industry, almost all chemicals are made from the base chemicals (ethylene, propylene, methanol, benzene, toluene, xylene and ammonia), therefore by replacing the technologies in the first layer of the petrochemical industry and ammonia production, the non-energy emissions of entire chemical industry can be reduced. Green production technologies are moving through the technology readiness levels towards commercialisation, which will make complete implementation by 2050 challenging. However, in recent years, two green chemical production technologies have witnessed substantial scaling-up, these are green methanol and green ammonia. Early in 2023, Carbon Recycling International announced starting production of 110 kt/annum of green methanol [27]. In addition, global green methanol is and will be supplemented with biobased sourced methanol. Green ammonia plants are under construction up to 270 kton (Unigel-Brazil) [28]. As two green chemical electrical production technologies that are closest to commercialisation, green methanol and green ammonia can have far-reaching impact on the sustainable pathways for the industry. These electrical-based chemicals can be supplemented with bio-based chemicals, where the global limit of 100 EJ for all sectors must be considered [29].

The second main research question in this paper will calculate the impact of the three main sustainability measures for the chemical industry, to meet the total emissions for a 1.5 °C budget. For this purpose, the framework of the One Earth Climate Model (OECM) will be utilised to address this. The OECM is an integrated assessment model with a framework developed to calculate global, individual country/region and industry scenarios that fit within a 1.5 °C (60% likelihood) carbon budget of 425 Gt CO_2 (2020–2050).

Section 2 presents the methodology for the bottom-up production-based energy and emissions calculations for the chemical industry sector. Moreover, it contains the parameters used for the 1.5 °C compatible and business-as-usual scenarios. This leads to Sect. 3 with results and discussions for the validated energy calculation for the industry and energy and emission projections up to 2050, and the 1.5 °C detailed scenario and the contribution of each of the three measures. Finally, Sect. 4 presents the conclusions and recommendations for further research.

2 Methodology

2.1 Energy demand calculation for the chemical industry

The chemical sector consists of a complex web of thousands of interconnected processes, which make a complete production-based bottom-up energy assessment for all chemicals an insurmountable operation. Therefore, most prior assessments for the chemical sector consider top-down data collected for individual countries based on the International Energy Agency.

However, a bottom-up energy evaluation is possible, because key base chemicals (ethylene, propylene, ammonia, benzene, toluene, xylene and methanol) make-up 74% of the energy use excluding electricity use of the sector [30]. By combining production data in Mt/a for these key base chemicals with the Best Practice Energy Values (see Table 1), energy excluding electricity for the entire sector is calculated. Figure 1 presents the methodology of the energy calculation, using production data (see Fig. 2), energy values for each chemical (see Table 1) and the division of energy and non-energy energy from the IEA (see Tables 2, 3).

This is an established methodology by Saygin et al. from a methodology report for the International Energy Agency, which was developed in 2009 [31, 45]. A key addition introduced in this paper is the calculation of the electricity demand based on the global production of chlorine (17.5% of all electricity use in the base year 2020—validated with IEA data) [44]. The reason for this is that the major key base chemicals are not the highest users of electricity in the chemicals sector and are therefore not suitable as a predictor of the sector's electricity use. Instead, the majority of electricity demand in the sector is from chlorine production and auxiliary use such as pumps, tanks and other supporting operations [31]. Thus, the calculation of electricity demand based on the global production of chlorine is a key methodological addition made in this paper.

Table 1 Best practice energy values for key base chemicals, based on data from [31]

Chemical	Production method	Primary feedstock	Unit	Electricity	Feedstock	Fuel	Steam	Total excl. electricity
Ethylene	Steam cracking	Naphtha	GJ/tonne	0.3	45	13.1	− 1.4	56.7
Propylene	Steam cracking	Naphtha	GJ/tonne	0.3	45	13.1	− 1.4	56.7
Ammonia	Haber–Bosch	Natural gas	GJ/tonne	0.3	20.7	10.9	− 3.9	27.7
Ammonia	Haber–Bosch	Coal	GJ/tonne	3.7	20.7	17.3	− 1.3	36.7
Benzene	Aromatic extraction	Naphtha	GJ/tonne	0.1	45	–	2	47.0
Toluene	Aromatic extraction	Naphtha	GJ/tonne	0.1	22.5	–	2	24.5
Xylene	Aromatic extraction	Naphtha	GJ/tonne	0.1	45	–	2	17.0
Methanol	Natural gas based	Natural gas	GJ/tonne	–	20	–	8.5	28.5
Methanol	Coal based	Coal	GJ/tonne	–	20	–	12.8	32.8
Chlorine	Electrochemical	Salt	GJ/tonne	10	–	–	1.9	n.a

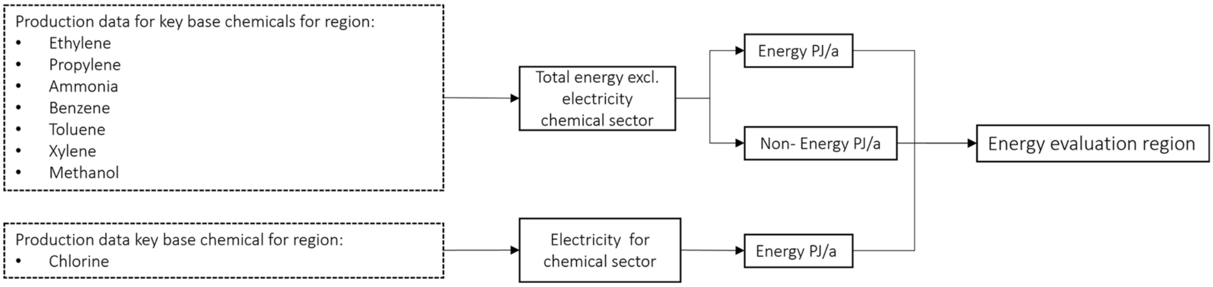

Fig. 1 Methodology for total energy demand estimation for the chemical industry

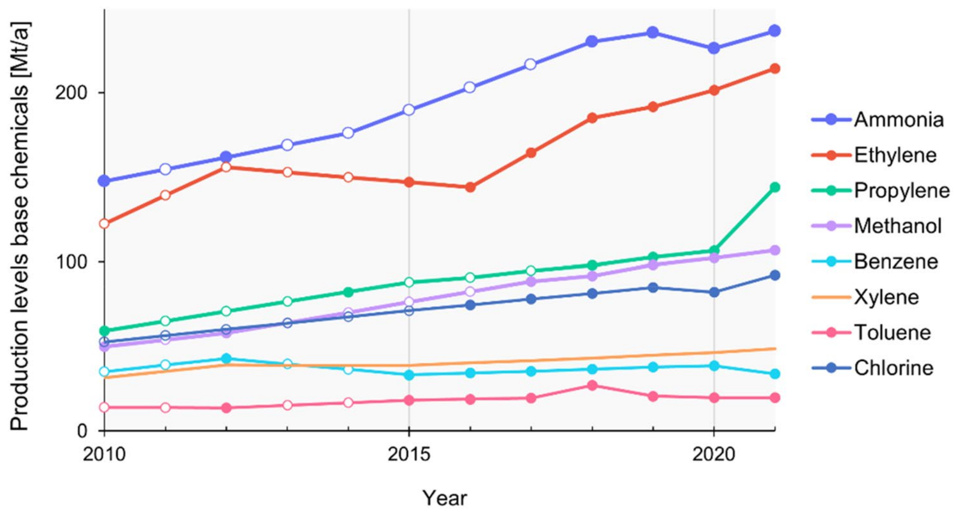

Fig. 2 Production numbers based on publicly available information. Closed markers indicate production data and open markers indicate an interpolation of data. Ethylene: [5, 32, 33], propylene: [34], ammonia: [5, 35, 36], benzene: [5, 37, 38], toluene: [38, 39], xylene: [38, 40], methanol: [5, 41, 42], chlorine: [43]. Regional production numbers are documented in the Supplementary information S4

Table 2 Division of non-energy energy and energy for the chemical industry, data from a paid IEA data package [44]

Year	2015	2016	2017	2018	2019	2020
Non-energy energy/energy in IEA statistics [%]	57	56	57	58	58	59

This percentage is kept constant in projections up to 2050

Table 3 Energy supply input for the chemical industry in the 1.5 °C compatible scenario

Energy supply form	Unit	2020	2030	2040	2050
Coal	[%]	33%	19%	0%	0%
Oil	[%]	14%	3%	0%	0%
Gas	[%]	36%	22%	14%	0%
Renewable heat (biomass, biomass derived fuels, geothermal, solar thermal)	[%]	9%	21%	17%	20%
Electricity for heat	[%]	1%	28%	59%	68%
District heating	[%]	7%	6%	6%	6%
Hydrogen and synthetic fuels	[%]	0%	1%	5%	7%

The BAU scenario considers the 2020 values to remain constant up to 2050. Source 2020 data: [44]

Chemical production data is hard to acquire due to the competitive nature of the industry. For this research, publicly available data was used from a range of sources, most notably the University subscription to the statistical service, Statista (see Fig. 2). Global published production data can vary between different sources and the quality of the granular information will vary (this includes production facility type, feedstock type and commercial owner of the process—see the Supplementary information for more info on temperature split, feedstock split and regional differences). Therefore, annual IEA statistics were used to verify the methodology [44].

2.2 Emissions of the chemical industry

To convert the total energy demand of the chemical industry to the sector's emissions, the framework of the One Earth Climate Model is used. The OECM is an integrated assessment model with a framework developed to calculate global, individual country/region and industry scenarios that fit within a 1.5 carbon budget. For historic energy numbers it utilizes the IEA statistics, while the energy and emission calculations up to 2050 are executed in a bottom-up manner [44]. This methodology is widely documented in several scientific resources and publications [46–49]. For the energy related emissions, this is a linear combination of calculated energy demand (see Sect. 2.1), energy supply per source (see Table 3) and emission intensities per source (see Table 4). The emission calculations are presented in Fig. 3. Moreover, for additional information on the non-energy emissions, information from the International Energy Agency and other relevant publications are utilized [50, 51]. Parameters for calculation of non-energy emissions of traditionally fossil-fuel based chemicals are presented in Table 5.

Table 4 Emission intensity energy sources in the 1.5 °C compatible scenario. The BAU scenario considers the 2020 values to remain constant up to 2050

Energy form:	Unit	2020	2030	2040	2050
Renewable electricity share [1]	[%]	28	75	95	100
Electricity [1]	[g CO_2/kWh]	456	133	23	0
Hard coal [47, 52]	[kt CO_2/PJ]	← 93.0 →			
Lignite [47, 52]	[kt CO_2/PJ]	← 111.0 →			
Oil [47, 52]	[kt CO_2/PJ]	← 75.0 →			
Natural gas [47, 52]	[kt CO_2/PJ]	← 56.0 →			

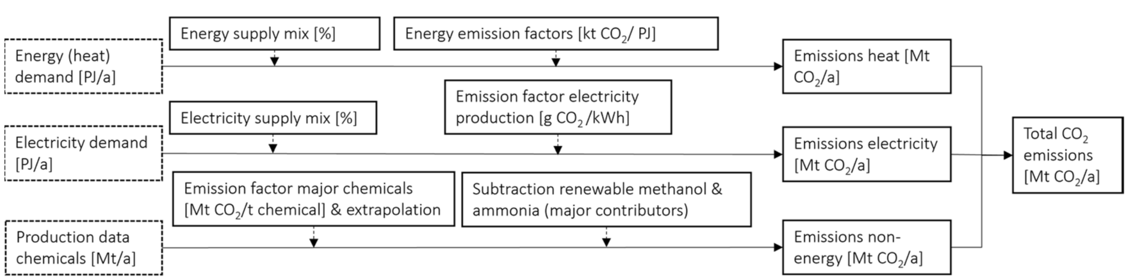

Fig. 3 Methodology for CO_2 emission calculation chemical industry

Table 5 Non-energy emission intensity for fossil-fuel based chemicals

Chemical:	Unit	Value
Primary chemicals [50]	Mt CO_2/t chemical	1.29
Ammonia [51]	Mt CO_2/tonne ammonia	1.8
Methanol [51]	Mt CO_2/tonne methanol	1

2.3 Sustainability measures for a 1.5 °C scenario

To form and explore a 1.5 °C pathway, first a business-as-usual (BAU) trajectory for the chemical industry will be calculated. This will take the average production growth for individual chemicals between 2010 and 2020 to calculate the energy and emission values for a continued growth scenario for the chemical industry in the OECM. By keeping the 2020 energy supply of the industry constant this calculation will represent a worst-case/uncontrolled growth scenario. Subsequently, this scenario will be converted to a 1.5 °C compatible scenario using three previously introduced measures: (1) a decrease in production growth rates; (2) transitioning to renewable energy for heat and electricity; and (3) the introduction of novel green production technologies.

A variety of sustainability measures would contribute to a decrease in growth rates for the base chemicals. For instance, plastic products are major downstream products of the chemical base products ethylene and propylene. Therefore, reduction of the use of plastic packaging, general plastic products, implementation of circular economy and improved recycling can decrease the growth rates for these base chemicals. To make this quantitative, Meng et al. estimated that resource efficiency and circular economy can result in 23–33% reduction in overall demand [3] Fig. 4 presents the chemical production numbers for the business-as-usual (BAU) scenario versus the decreased chemical production numbers as used in the calculation for the 1.5 °C scenario. On average, chemical production is decreased by 27% between the BAU and the 1.5 °C scenario.

For the second main measure, the energy supply for heat and electricity in the sector will have to be converted to a renewable energy supply. Table 3 presents the shift from traditional fossil fuel energy sources such as coal, oil and gas to renewable sources for heat and electricity.

The introduction of novel chemical production technologies forms the last of the three main measures. The technology development timeline presented in Fig. 5 and Table 6. These trajectories are used as input for the 1.5 °C compatible pathway. New technologies will follow a development pathway where they are consequentially tested on a laboratory scale, benchtop scale, unit operating under industrial conditions, pilot plant, demonstration plant and then a first mature sized facility. The US National Energy Technology laboratory describes the first mature sized facility as a First-of-a-Kind (FOAK) [53] Each scaling-up step takes many years to complete and key lessons need to be learned before the next step. This is a known limiting factor in technology development and these trajectories have a direct effect on 1.5 °C pathways for the chemical industry. After a FOAK and following build facilities, the technology development can build towards the *N*th-of-a kind plant [53, 54]. At this stage, lessons learned have resulted in the first cost reductions and moving forward a technology can progress towards a considerable market-share.

Table 4 presents the energy emission intensities for each energy source used for the calculations. The initial 2020 numbers in Table 3 come from the purchased IEA data. [44]. A high degree of electrification is considered for heat demand, supported by literature [24]. This is a methodological choice, where both options of either a high degree of electrification or the implementation and development of alternative heat sources such as synthetic fuels/hydrogen/

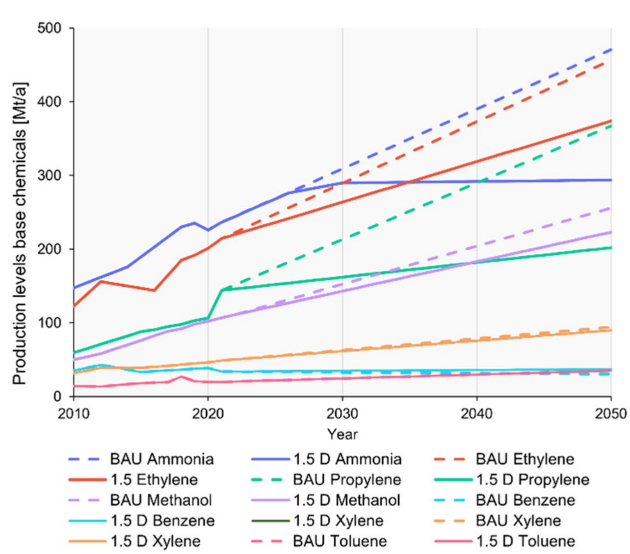

Fig. 4 Input base chemical production numbers for a business-as-usual (BAU) scenario versus a 1.5 °C compatible scenario

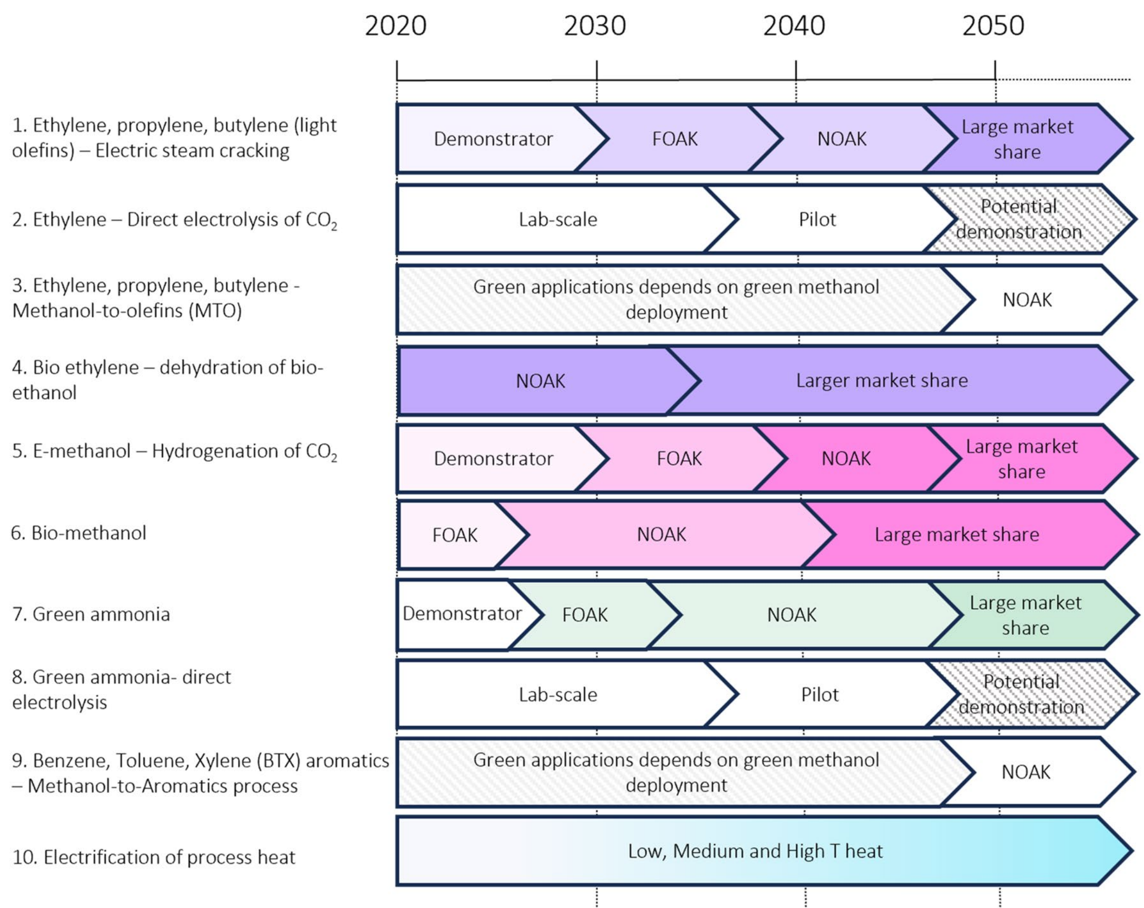

Fig. 5 Methodological input for development trajectories of major green chemicals (see Table 6 for a detailed description)

biomass would require new technology development. For heat, there are different temperature and heat load levels that are required. According to IEA statistics, 48% of the heat demand will be 500–1000 °C and 12% requires over 1000 °C (see Supplementary information S1) [44] In addition to temperature level, the heat load is another critical consideration, where the heat load represents the rate of heat transfer required. Typically, fossil fuel-based heat sources can provide a high heat transfer rate, which must be taken into consideration when replaced with renewable energy sources such as biomass [22] A solution here is to use fuels derived from biomass for providing the energy for the chemical processes. A large impact can be made for the chemical industry by transitioning the highest heat demand for the industry, originating from the process of steam cracking to produce ethylene and propylene, to an electrical based process. Here, steam cracking accounts over 37% of the heat demand of the chemical industry and therefore new production technologies for the light olefins ethylene and propylene can convert a major part of the heat supply to a sustainable form [30] Here, Electric cracking is a technology development that is currently tested at demonstration scale by BASF and this technology is integrated in this paper supplemented with bio-ethylene [25].

The introduction of novel chemical production technologies forms the last of the three main measures. The technology development timeline presented in Fig. 5 and Table 6. These trajectories are used as input for the 1.5 °C compatible pathway. New technologies will follow a development pathway where they are consequentially tested on a laboratory scale, benchtop scale, unit operating under industrial conditions, pilot plant, demonstration plant and then a first mature sized facility. The US National Energy Technology laboratory describes the first mature sized facility as a First-of-a-Kind (FOAK) [53] Each scaling-up step takes many years to complete and key lessons need to be learned before the next step. This is a known limiting factor in technology development and these trajectories have a direct effect on 1.5 °C pathways for the chemical industry. After a FOAK and following build facilities, the technology development can build towards the Nth-of-a kind plant [53, 54]. At this stage, lessons learned have resulted in the first cost reductions and moving forward a technology can progress towards a considerable market-share.

Table 6 Development trajectories for green production technologies base chemicals

	Chemical and production process	TRL	Indicative commercial/technological development	Ref
1	Ethylene, propylene, butylene (light olefins)—*Electric steam cracking*	8/9	BASF demonstration plant for electrical heated steam cracker (ethylene & propylene) finished construction in September 2023. Production levels for the demonstrator will be around 32 kton of processed hydrocarbons per year. In comparison, a mature steam cracker facility can produce 320 kton of ethylene and 175 kton of propylene each year	[25, 55, 56]
2	Ethylene—*Direct electrolysis of CO_2*	1–4	In the direct electrolysis of CO_2 to produce ethylene, the electrons are directly used to produce the final product (instead of first producing hydrogen). This technology is in the early stages of technology development, often performed in lab-scale equipment. Furthermore, the potential of the technology is hindered by the amount of electrons needed per molecule of ethylene (12 electrons for one molecule of ethylene), low conversions, low selectivity and material performance. These factors result in high operational cost and large/costly equipment	[57]
3	Ethylene, propylene, butylene—Methanol-to-olefins (MTO)	n.a	While MTO plants are relatively mature (operating up to 833 kton/a), this development strongly depends on the development of green methanol as an input feedstock in order to produce sustainable olefins. MTO development is therefore put on a later point in the timeline to properly present this green methanol dependency to produce sustainable olefins	[58, 59]
4	Bio ethylene—via dehydration of bio-ethanol	10	Bio-ethanol can be converted into ethylene via a dehydration process and around 0.3% of global ethylene production uses this process. Here, the feedstock includes 1st and 2nd generation biomass resources for bioethanol production. The technology is mature and there are commercial processes in India and Brazil, currently producing around 200 kton/a	[60, 61]
5	E- methanol—*Hydrogenation of CO_2 (green H_2 and sustainable CO_2)*	8/9	Demonstration plant for green methanol started production of 110 kt CO_2 to methanol/year in 2023. For reference, a commercial methanol plant produces around 440 kt/annum	[27, 62, 63]
6	Bio-methanol	10	Bio-methanol is currently produced up to 2 Mt/a by OCI, with commercial plants in the Netherlands and Canada. A gradual production increase is planned up to 6 Mt by 2028	[63, 64]
7	Green ammonia—produced from green hydrogen	9	Unigel's green ammonia plant is under construction, with start of production planned for the end of 2023. Initial production is 60 kton/a, scaling up to around 600 kton/a in 2027. For reference, a commercial ammonia plant produces around 1 Mt/a	[28]
8	Green ammonia—direct electrolysis	1/2	Direct production of ammonia through electrochemical reduction is still facing several lab-scale challenges	[65]
9	Benzene, toluene, xylene (BTX) aromatics—methanol-to-aromatics process	n.a	While there are pilot facilities (up to 30 kt/a in China) for the MTA technology, this development strongly depends on the development of green methanol as an input feedstock in order to produce sustainable aromatics. MTA development is therefore put on a later point in the timeline to properly present this dependency to produce sustainable olefins	[66]

By changing chemical production methods to green production methods, CO_2 emissions originating from the fossil fuel feedstock and conversion for methanol and ammonia can be avoided. In current production, methanol and ammonia rely on hydrogen produced from fossil resources with steam methane reforming, which produces CO_2 as a major by-product. By introducing green technologies such as synthetic methanol (formed from captured CO_2 or bio-based methanol), these non-energy emissions can be avoided. For the deepest CO_2 reduction for green methanol, this would rely on the technology development trajectory of direct air capture (the footprint of the CO_2 influences the sustainability of the final product)—where there are currently many development concerns [67]. A similar strategy exists for green ammonia produced from hydrogen produced from renewable energy and nitrogen. Both green ammonia and green methanol are modelled to represent a 75% share of their respective markets in 2050. Moreover, electric steam cracking introduces renewable energy instead of heat produced from natural gas for the most energy intensive process in the chemical industry. This is especially impactful due to the high endothermicity, high energy use and high associated emissions of steam cracking [26].

As Table 6 presents, these technologies have hit recent major milestones with demonstration sized production plants coming in operation in 2023. Therefore, these three technologies are modelled as the dominant technology for their market segment in 2050 in the 1.5 °C scenario. Table 7 presents the definitive overview for novel production technologies included in the scenario and the introduction of renewable heat and electricity for all included technologies. Other technologies such as renewable BTX aromatics production from methanol or more specialized chemicals is slower in upscaling and has not been taken into yet for the 2050 market share. Lignin-based aromatic production has potential as a technology, however there are no pilot/demonstration plants identified that are designed to produce major chemicals such as Benzene, Toluene and Xylene. Moreover, the methanol-based pathways such as methanol-to-olefins and methanol-to-aromatics have a strong dependency on the roll-out of green methanol production. Calculation parameters for methanol, ammonia and hydrogen are presented in Table 8 [62, 68].

3 Results and discussion

3.1 Results energy demand calculation

Global energy demand of the chemical industry is calculated according to the methodology described in Sect. 2. As a first result, Fig. 6 presents the global calculated energy demand for the sector between the years 2008 and 2020, compared to historic statistics from the International Energy Agency for validation [44]. The calculated energy demand for all those years is an average of 85% of the utilized IEA statistics and for the last five years the calculated energy data approaches the IEA statistics with a 91% average.

Overall, this shows the suitability of the method of using publicly available production data for eight base chemicals and calculating the energy use of the entire chemical sector based on these processes with the highest energy demand. Because the methodology uses energy numbers for the Best Available Technology (BAT) it is logical that the calculated total energy demand is lower than the values reported by individual countries to the International Energy Agency in their annual statistics. This is because technologies used on a global scale are more inefficient than BAT technologies. In addition, the accuracy for the energy demand calculation for individual countries and regions is presented in Fig. 7. Here, the calculation accuracy is 96% of the documented IEA statistics. It is important to note the uncertainty embedded in the calculations due to the large variation in different potential feedstock and process types for each of the base chemicals, regional process efficiency performance, differences in public reporting of production statistics and other local factors. For this reason, the calculation validation with the IEA statistics presented here is essential, while considering the intrinsic ambiguity in the IEA statistics collected from individual IEA countries (each country reports energy demand in their own way, which causes reported feedstock and process energy to blend) [70].

Total calculated contribution to the energy demand of nine individual countries and regions is presented in Fig. 7. Here, China is the largest contributor on a global scale, followed by the USA and the EU-27. These three regions make up for roughly half of the global energy demand for the chemical industry. Therefore, the technology and energy choices made for these countries will have a significant influence on the energy demand and emissions for the global chemical sector. In addition, China's and India's chemical processes use coal as the primary base material, which is more CO_2 emission intensive.

Table 7 Overview of novel emerging production technologies, renewable heat and renewable electricity included or excluded from the scenario

Target chemical group	Specific production technology	Novel sustainable production technology in this scenario	Renewable heat and electricity supply introduced in this scenario
Light olefins, methanol and ammonia	Ammonia from green H_2, light olefins from electric cracking, methanol from green H_2 and CO_2 supplemented with current production bio methanol/bio ethylene)	Included	Included
	Emerging production technologies for light olefins, ammonia and methanol through electrolysis	Excluded	n.a
Downstream chemicals from olefins, methanol and ammonia (for example formaldehyde), aromatics or inorganic chemicals	Production technologies to produce conventional downstream products from olefins, methanol, ammonia aroamtics or inorganic chemicals	Excluded Due to immaturity of technologies or no longer required if the feedstock chemical is renewable	Included
Novel production technologies to produce other new chemicals from methanol	For example, novel route of methanol-to-aromatics (MTA), methanol-to-olefins (MTO) or methanol to gasoline (MTG)	Excluded First a full renewable production for methanol is needed by 2050, before production can be expanded to make additional chemicals that are now not made from methanol	n.a

Table 8 Parameters for green methanol and ammonia calculation

Green methanol synthesis: $CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$	
Required H_2/CH_3OH [mol/mol]	3/1
Required CO_2/CH_3OH [mol/mol]	1/1
Plant efficiency including Purge streams	94% [62]
Green ammonia synthesis: $2\ N_2 + 3H_2 \leftrightarrow 2NH_3$	
Required H_2/NH_3 [mol/mol]	3/2
Plant efficiencies including purge streams	98% [68]
Hydrogen electrolysis efficiency:	
2020—2050	67–76%[69]

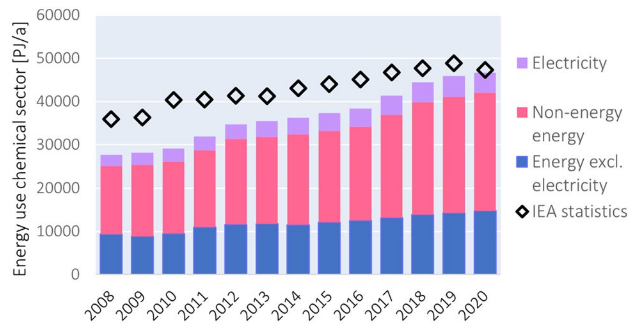

Fig. 6 Results of chemical industry energy demand calculation when compared with historic IEA data

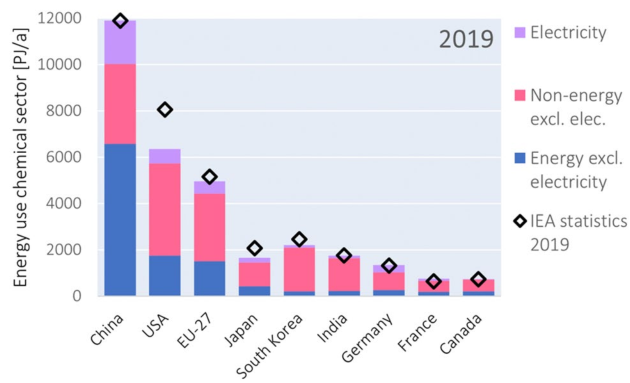

Fig. 7 Energy demand for the chemical industry by countries and regions in the year 2019

A validated calculation method for the energy demand opens the possibility to calculate a projected energy demand for the chemical industry up to 2050, and to calculate the contributions of different sustainability measures in a 1.5 °C compatible pathway.

The energy and emissions calculated up to 2050 for the business-as-usual scenario (BAU) and the 1.5 °C compatible scenario are presented in Figs. 8 and 9. Total energy used in the BAU scenario is higher than for the 1.5 °C scenario because the latter considers a decrease in production growth. Trends in energy (Fig. 8) and emissions (Fig. 9) present the decoupling of growth in energy demand for the sector and the resulting emissions in the 1.5 °C scenario. In the BAU scenario, the CO_2 emissions follow the increase in energy demand, due to the remaining fossil-fuel used energy sources for heat and electricity and the use of current technologies. The 1.5 °C compatible scenario presents a pathway with an increase in overall-energy demand, while net-zero is achieved for energy -related emissions with some remaining emissions for non-energy related sources. Here, only novel green production technologies for light olefins, methanol and ammonia will be ready to reduce non-energy emissions substantially before 2050. This does not include novel downstream production technologies or technologies that would expand the current methanol demand mix (for instance the methanol-to-aromatics pathway) and would require a substantial increase of what is reasonably achievable in terms of technological maturity and roll-out.

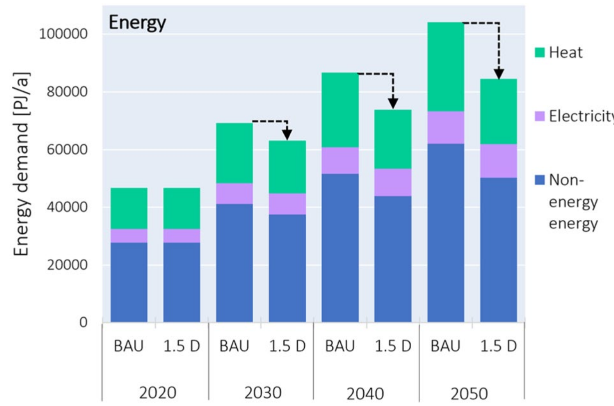

Fig. 8 Energy projection for business-as-usual scenario (BAU) and the 1.5 °C scenario (1.5 D)

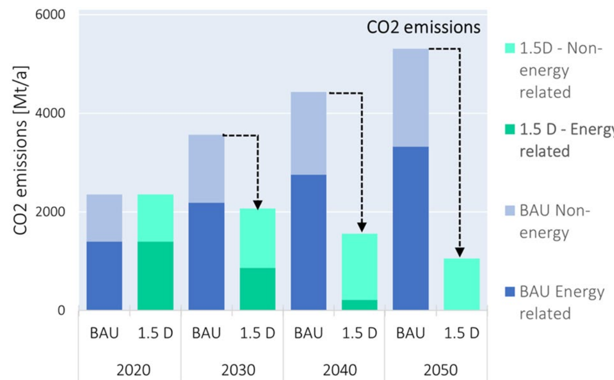

Fig. 9 Emission projection for business-as-usual scenario (BAU) and the 1.5 °C scenario (1.5 D)

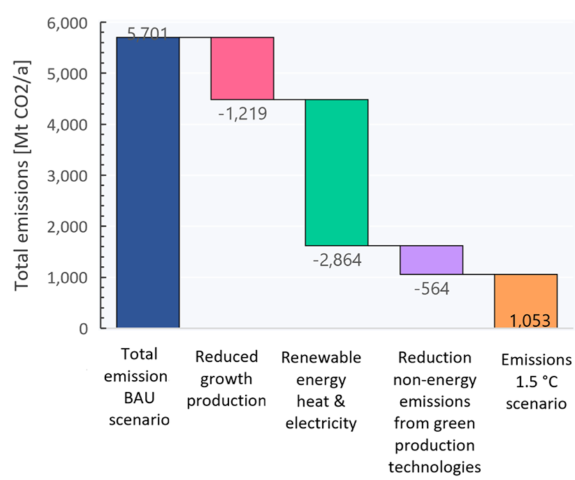

Fig. 10 Impact measures in a 1.5° C compatible pathway for the chemical industry from BAU scenario to 1.5 °C scenario

3.2 Chemical industry emissions in a 1.5 °C compatible pathway

The effect of the three main measures on the total emissions of the chemical sector is presented in Fig. 10. A reduced growth in production is the most straightforward technical solution, which targets both energy and non-energy emissions. As a sequential measure, the replacement of fossil-fuel based energy supply by renewable based heat and electricity will result in the largest reduction of total energy emissions. Finally, by introducing novel green production technologies for methanol and ammonia, the non-energy CO_2 emissions are reduced. It should be noted, that the impact from a novel technology such as electric cracking for light olefins production is part of the renewable energy CO_2 reduction, while it is in essence a novel production technology. There are remaining non-technical barriers for

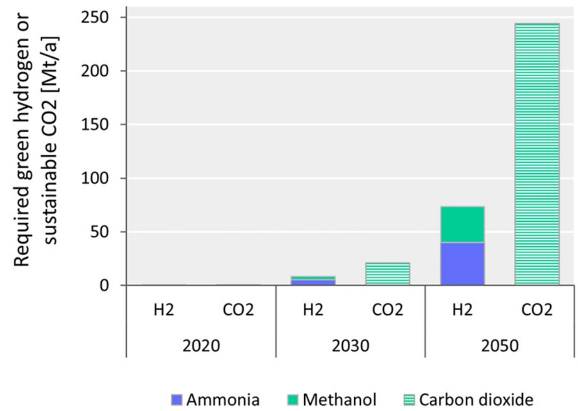

Fig. 11 Required green hydrogen and sustainable carbon dioxide for green methanol and ammonia production

Table 9 Electrical demand for hydrogen for methanol and ammonia, compared to the total demand for green hydrogen and total global electricity demand

	2030		2050	
	TWh	% Global electrical demand	TWh	% Global electrical demand
Electrical demand hydrogen power-to-chemicals	381	1	3232	4
Total demand electrolysis [1]	1822	5	17,586	19
Global electrical demand [1]	38,804	100	91,760	100

introduction of these technologies, such as competitiveness of the cost technologies. Without financial compensation schemes this be a severe obstacle to achieving the 1.5 °C scenario. As presented in Fig. 9, energy related emissions achieve net-zero, while non-energy related emissions are only slightly reduced with the introduction of the first novel production technologies. This is understandable with the fact that while methanol, ammonia and ethylene are major energy users in the industry, they are of course not the entire sector. The combination of these three measures results in a 1.5 °C scenario for the chemical industry.

The calculated required green hydrogen for green methanol and green ammonia is presented in Fig. 11. In addition, green methanol production requires a sustainable carbon dioxide feedstock. A carbon feedstock with the most suitable carbon footprint originates from Direct Air Capture (DAC) or Bio-energy derived CO_2 [67]. It is important to note that sustainable carbon dioxide is a limited feedstock and is dependent on developing technologies (and for carbon sinks the One Earth Climate model only counts on nature based systems). Current carbon dioxide captured with DAC is 0.01 Mt/a and captured with Bio-energy derived CO_2 is 2 Mt/a [71, 72].

In the One Earth Climate Model these technologies are projected to capture 1196 Mt/a CO_2 in 2050 and the available CO_2 is split over synthetic fuels and chemicals for the maritime, aviation and chemical sector, supplemented with bio-based fuels. As Fig. 11 presents around 20% of sustainable CO_2 is used as a feedstock for the chemical sector. This highlights a critical interdependency between the development of novel green production technologies and the deployment of DAC and Bio-energy derived CO_2, which are technologies still facing many challenges.

The required hydrogen for chemical production is converted to electrical demand in Table 9 and put into perspective against the global electrical demand. Here, hydrogen for chemicals only requires 1% of global electricity demand in 2030 and 4% in 2050, while total electrolysis represents 4% and 19% of total electricity in 2030 and 2050.

4 Conclusion

Decarbonising the chemical industry is a significant challenge with chemical products such as plastics, fertilizers and many more products intertwined with a range of use industries, and CO_2 emissions both from the energy and chemical conversion activities. While renewable energy is growing rapidly, limits to critical carbon budgets are still approaching and research is shifting to the new frontier of 1.5 °C compatible sustainable pathways for the hard-to-abate sectors, including the chemical industry.

This paper presents a detailed sustainable pathway for the global chemical industry with energy and emission calculations to fit within a 1.5 °C scenario. The energy demand for the chemical industry is calculated bottom-up, using global production data for eight key chemicals. To reduce the energy and non-energy CO_2 emissions of the chemical industry, the impact of three main measures is calculated: reduced growth of production of base chemicals, renewable energy for electricity and heat and the introduction of novel production technologies. These three main measures result in an overall reduction of 82% in total CO_2 emissions from the chemical industry in 2050, which is compatible with the 1.5 °C scenario in the One Earth Climate Model—a previously published energy scenario from the authors [73].

Reduced growth of chemical production by a plethora of actions (reduction of chemical products such as plastics, transitioning to a circular economy), targets both energy and non-energy emission sources in 2050. Total production of key base chemicals in Mt/a in the 1.5 °C compatible scenario is reduced by 27%, when compared to a business-as-usual (BAU) growth scenario. This reduction in production growth results in 21% less CO_2 emissions.

The largest calculated emission reduction is achieved by renewable energy mix for the heat and electricity used in the chemical industry, affecting. only the energy related CO_2 emissions. 100% renewable electricity is used for the electricity demand in 2050 and a high degree of electrification of current heat demand is implemented. Furthermore, high temperature heat is supplied with biomass or hydrogen to achieve the high temperature demand of the chemical industry. Implementing a fully renewable energy mix in 2050 results in a 50% CO_2 emission reduction. Development and implementation of sufficient electrification in the sector or alternatively developing sufficient synthetic fuels/hydrogen or biomass will be a considerable challenge, however this is what will be required to make the sector compatible to a 1.5 °C pathway.

Novel chemical production technologies, for targeting non-energy CO_2 emissions, are in various stages of technology readiness, varying from lab scale to demonstration scale (just before commercial scale operation). Green production technologies for light olefins, methanol and ammonia are the furthest in their development cycle (sourced from both biomass and renewable electricity) and are therefore given the largest share of novel green upcoming technologies. This paper calculates the emission reduction of a 75% market share for green electrical based methanol and green ammonia production, which is required to reduce the remaining non-energy CO_2 emissions to fit into the 1.5 °C carbon budget. This requires an electricity demand of 381 TWh in 2030 and 3232 TWh in 2050 for green hydrogen electrolysis for power-to-chemicals, resulting in the respective 1% and 4% of the global electricity demand. In addition, the effect of electric cracking for light olefins production is reflected in the large percentage of electrification of the overall heat supply. The change to green production technologies for methanol and ammonia in 2050 results in a further 10% CO_2 reduction compared to the BAU scenario.

Overall, this paper presents a holistic approach to fit the chemical industry to a 1.5 °C pathway, where measures for supply and demand are combined. Results of this research can inform science-based target setting for investments made by the financial sector and provide a comprehensive evidence base for governments and industry. Finally, this research opens the possibility for further exploration of 1.5 °C compatible pathways for individual regions and countries.

Author contributions Maartje Feenstra: conceptualization, data curation, formal analysis, methodology, writing—original draft preparation, visualization. Simran Talwar: conceptualization, methodology, writing—original draft preparation. Sven Teske: conceptualization, methodology, writing—original draft preparation, funding acquisition, supervision.

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Availability of data and materials The authors declare that the data supporting the findings of this study are available within the paper and its Supplementary Information files. Should any raw data files be needed in another format they are available from the corresponding author upon reasonable request.

Declarations

Competing interests The authors declare no competing interests.

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