



This document is an excerpt of the
3rd Roadmap of the Kopernikus project P2X.
You can find the full (German) version
on the project's website:

<https://www.kopernikus-projekte.de/projekte/p2x/#roadmaps>



*3rd Roadmap
of the Kopernikus project P2X
Phase II*

OPTIONS FOR A SUSTAINABLE ENERGY SYSTEM WITH POWER-TO-X TECHNOLOGIES

Transformation – Applications – Potentials

Editors:
Florian Ausfelder
Hanna Dura

SPONSORED BY THE



Federal Ministry
of Education
and Research

KOPERNIKUS

P2X

PROJEKTE

The Future of Our Energy

PREFACE

Dear reader,

under the 2015 Paris Agreement, an international treaty was concluded with the goal of limiting global warming in 2050 to 1.5°C relative to pre-industrial levels. This shall prevent the climate from reaching irreversible tipping points, such as the melting of the permafrost or the weakening of the Gulf Stream. Efforts have been made since the Kyoto Protocol to reduce greenhouse gas emissions, but the budgets are based on limiting the global temperature increase to 2°C. The preferable goal of containing global warming below the mark of 1.5°C means a significant tightening of the target and requires fast and more comprehensive measures.

The recent decision of the German Federal Constitutional Court (BVG) on the Climate Protection Act is expected to significantly impact the policy. The court ruling states that it is not acceptable to shift the responsibility for tackling climate change to the next generation. The upcoming generations already have much less room for error since current measures lack impact or are unsatisfactory. Climate change, if not stopped, could pose a serious threat to freedoms guaranteed by the Basic Law. The BVG's ruling represents a turning point. It justifies the need to implement measures with significant greenhouse gas reduction potential more quickly and comprehensively than previously planned. Ultimately, the ruling is based on the fact that an emission saved today is more valuable than one saved tomorrow.

For the classification of the possible use of Power-to-X technologies (PtX) in Germany, this ruling of the Federal Constitutional Court will therefore be of considerable importance, as the legislator will likely have to react and change the future framework conditions. For the power supply, this could include an expansion of renewable power generation and the specification of sector-specific targets for the reduction of greenhouse gases, which would create pressure for a faster implementation of CO₂-neutral technologies. This will result in new framework conditions for the sustainability and techno-economic analyses in the Kopernikus P2X project – key basic assumptions for the analyses (e.g., concerning the electricity model used) may change significantly.

Ultimately, all work in the Kopernikus Project P2X must reflect the necessary acceleration of the technologies that are essential for achieving the climate targets. In this regard, it is important to note that at the time of the publication of the BVG's ruling, all work for this roadmap had already been completed; accordingly, none of the analyses depict the target year of 2045 for climate neutrality.

The power sector has made considerable progress in the last two decades regarding the reduction of CO₂ emissions, with over 50% of the annual electricity volume in Germany coming from renewable energy sources. This development will be driven further by the coal phase-out. At the same time, the direct electrification of further fields of application is an important key to achieving decarbonization. This is particularly true where electric processes also promise a significant increase in efficiency compared to conventional processes, e.g., electric vehicles or the use of heat pumps.

In the past, a purely electric energy supply, i.e., an "electric-only" world, was sometimes propagated. For steel production, chemical industry, aviation, or freight transport, however, direct electrification is either impossible or would require a great deal of effort. PtX technologies offer the possibility of harnessing renewable energies and raw materials through indirect use of clean electricity, such as for energy supply and feedstock in the chemical industry.

Carbon-based energy sources and chemicals will continue to play an important role in the future, but they will have to be provided differently and preferably in a climate-neutral way. As such, they will be no longer based on crude oil, natural gas, or coal, as they have been until now. Thus, we speak of defossilization in this context. Alternatives like biomass and carbon obtained from the recycling of plastics, are limited by the availability of the respective raw materials. PtX technologies complement this portfolio, e.g., with the electrolytic production of hydrogen or the co-electrolysis of CO₂, just to name a few. PtX-technologies form important bridges between renewable electricity and material products and open up new production chains, intending to combine climate neutrality with high added value.

CO₂ will play an important role as a carbon source. Assuming that fossil-fired power plants as the largest point sources to date will cease to exist in the next 10 to 20 years, industrial emissions that will continue to be unavoidable in the future will have to be tapped. These are mainly raw material-related emissions in the cement, lime, and glass industries. In addition to these industrial sources, CO₂ can also be produced in biogenic processes (production of biogas or bioethanol or thermal use of wood and straw) or directly obtained from air (Direct Air Capture – DAC).

Some PtX technologies are ready for a global deployment (100,000 to several million tons per year). The necessary chemical technologies are available in the form of Fischer-Tropsch (FT) processes for the synthesis of saturated and unsaturated hydrocarbons based on synthesis gas, for which examples are already available in South Africa and Qatar, where the starting material is coal and natural gas, respectively. For another FT-process, which is based on methanol-to-olefins and starting from synthesis gas as well, experience is available in a project in the People's Republic of China. For an overall establishment as a PtX technology, however, the political will is required which needs to set the framework conditions accordingly so that investors can become involved. To establish them as PtX technology, it requires political will to set the corresponding framework conditions and so that investors can get involved. As such, a quota system for the uptake of fuel could be implemented like in Iceland. For a rapid ramp-up, existing syngas-based production plants could be linked with necessary photovoltaic or wind power parks in the (already realized) scale of 1 TWh and larger via electrolyzer stations as a central link.

The potential scope of the applications of PtX technologies cannot be comprehensively represented by a single project. Instead, the Kopernikus P2X project has examined relevant aspects from various application areas in depth, without claiming to exhaustively present the various options in the application field. For example, the issue of iridium content in PEM electrolyzers is being investigated as an example of the challenges of resource-efficient mass production, and modular and flexible production units are being developed that can be optimally adapted to different site conditions. The transport of hydrogen via liquid organic hydrogen carriers (LOHC) represents an option that can be linked to industrial applicati-

ons, e.g., glass production or supply mobility concepts. The use of PtX technologies to produce polymers is also addressed, as is the linking of industrial value chains for butanol production, by combining electrochemical with microbiological processes.

In this sense, the seeds of the Kopernikus project P2X have been sown to address numerous central aspects and to demonstrate their development potential. These aspects are expanded and deepened in many ways in the research and development projects initiated by the National Hydrogen Strategy. The BMBF's hydrogen lead projects, supplemented by fundamental research, address the mass production of electrolyzers (H₂Giga), the transfer of electrolyzers and PtX technologies to an offshore environment (H₂Mare), and transport options for hydrogen (TransHyDE). The BMWi's regulatory sandboxes on hydrogen and sector coupling transfer PtX technologies to relevant industrial environments and are supported in a comprehensive and structured manner (Trans4ReaL), while hydrogen technologies are recorded and classified across sectors (H₂-Kompass).

The overall structure of the Kopernikus project P2X is divided into three phases, which provide the technical development strands from fundamental and applied research to technical demonstration in the relevant environment. Currently, the Kopernikus P2X project is in the middle of the second phase. The technologies must now be developed to the point where a technical demonstration can be carried out in the next phase. P2X will therefore continue to actively shape future research and development work in the field of PtX technologies through its own contributions.

A critical aspect of the deployment of PtX technologies is the specific CO₂ emissions of the electricity used. Once the electricity mix is sufficiently decarbonized, the use of PtX technologies will have a positive climate impact compared to the use of the corresponding fossil references. This is not yet the case with the current electricity mix in Germany. Decentralized plants consisting of renewable energies and PtX plants at favored locations would be a general option. From a cost perspective, only offshore wind farms are likely to be considered due to the higher number of full load hours in Germany.

As a consequence, PtX technologies must also be considered from a global perspective, leading to a shift and an expansion shift of perception of the above-mentioned aspects. Nevertheless, PtX technologies open up opportunities for new players to supply Germany with renewable energy sources. The decisive factors will then be the respective local conditions for the use of PtX technologies, including the potential for renewable energies, instead of the availability of fossil resources. In this context, the concept of energy partnerships with selected countries is interesting. With the research and development work in the Kopernikus project P2X, important contributions must be made to ensure that products with PtX technologies will still be "Made in Germany" and "P2XINSIDE". As such, PtX technologies are not an element for the retreat from a global world, but rather a global contribution to climate protection and international trade. At the same time, innovative products will open new opportunities for the export-oriented German apparatus and plant engineering industry in analogy to environmental technologies alike.

Within the framework of roadmapping as an integral part of the Kopernikus P2X project, the second phase focuses on the entire production chains of PtX technologies and not solely examines individual technologies regarding their sustainability and acceptance. These value chains and their technologies will be investigated by a series of different evaluation procedures, listed in the following.

To classify the PtX technologies and their contribution to the energy transition and climate protection, detailed scenario analyses are carried out for Germany. In the background, scenario analyses will model the availability of electric power in Germany and the demand for raw materials and energy, considering greenhouse gas limitations. Thus, it can be derived how high the demand and contribution of PtX products are and might be, as well as in which application sectors they are primarily used. Of course, the model results depend on the assumptions made, so different scenarios cover a spectrum of assumptions, from which the sensitivities of the corresponding parameters then become apparent.

Life Cycle Assessment (LCA) is an integrated method for determining the relative environmental sustainability of a process compared to a reference. In this process, the environmental impacts are recorded over the entire process chain, i.e., including the upstream processes of the raw materials and their respective disposal. The result is a comprehensive description of the processes in terms of their environmental impact.

The techno-economic analysis (TEA) estimates the expected costs of the processes and products investigated based on the data from the project. Here, a comparison is made with the corresponding conventional reference substances or processes.

The implementation of new technologies also depends on a "social license to operate (SLO)". Therefore, investigations of the social acceptance of PtX technologies are of particular importance. The already mentioned intergenerational challenge which exemplarily manifested in the "Fridays for Future" movement, is considered by a special approach ("Invisible Kids"). Adolescents, who currently have little opportunity to participate in political decision-making, are subject to acceptance studies. For the lives of this generation, PtX technologies will either play an important role, or they are expected to participate in their large-scale technical implementation, but they currently have little opportunity to participate in political decision-making.

The development and deployment of PtX technologies in a country is limited by the availability of renewable energy, especially renewable electricity, and water, but also by other factors such as infrastructure needs. Such an analysis must also ensure that the energy needs of the local population should be met first. To consider these aspects consistently, the methodology of a potential analysis is developed and firstly validated on the example of Germany. Afterwards, different countries and regions can be evaluated by this methodology regarding their potentials for implementing PtX technologies.

In the present work, the aim is to achieve the highest possible internal consistency of the results. Thus, the assumptions and results of the scenario analysis are included as parameters in the evaluation procedures. However, this means that the individual results of the investigated technologies can only be compared with the evaluation results of the previous roadmaps after considering possible different assumptions within each roadmap.

The Kopernikus project P2X brings together 42 partners from science, industry, and civil society. Each of these partner organizations brings its own perspective on PtX technologies into the project and actively develops them further through the project work. The exchange of ideas and concepts regarding the possible applications of PtX technologies and the necessary boundary conditions is an important part of the Kopernikus P2X project. In addition to the partners, the honorary advisory boards, as well as project externals are involved with their views through workshops and other interactions. In the context of this interplay, the idea of PtX technologies is continuously evolving. This document takes up and presents the current discussions in the project without claiming to be exhaustive. Rather, it is a momentary summary of the associated knowledge gained. The roadmap will also intensively accompany the further development of the project, which will be documented in further publications.

This roadmap provides a snapshot of the Kopernikus P2X project. The findings and the state of discussion remain preliminary. The roadmapping team and all authors wish you, dear reader, an experience that you will come to appreciate and that will give you plenty of material for questions and discussions. With this in mind, we hope you will read the document critically and we welcome your feedback.



Florian Ausfelder



Hanna Ewa Dura

EXECUTIVE SUMMARY

The aim of the Kopernikus P2X project is to develop the technological basis for solutions that harness renewable energy to produce chemical energy storage systems, energy carriers and chemical products – tailored to economic and social requirements – for applications in the key markets of energy, transport and industry. In the first phase, researchers were able to closely align the content and structure of the different action and application areas, enabling a range of promising options to be identified.

On the basis of these results, two energy vectors were identified, hydrogen and synthesis gas, which can be used as a basis for creating dedicated value chains for the three application areas of transport, industry and base chemicals from electrolysis to the end product and/or end application (see **Figure 0.1**)

In the second phase of the Kopernikus project P2X (P2X II), 42 partners are further developing the technologies in the different value chains with the aim of bringing these to market maturity. This development process is continually supported and evaluated by the joint roadmapping process, together with the partners, documents and analyses the

technological progress of the research and development work and places it within the context of the energy system. This Roadmap 3.0 is the continuation of the previous publications released in the first phase and documents the current status of the second phase of the Kopernikus project P2X.

An integrated energy model was developed to give uniform basis for the roadmapping process. This model combines a demand model with its detailed hydrogen (H₂) and power-to-X (PtX) products and pathways from the former satellite project SPIKE with the energy model outlining the expansion and operational planning of power plants created by the Technical University of Munich (TUM). The latter was also used to create the previous Roadmaps 1.0 and 2.0. The results of Roadmap 1.0 and Roadmap 2.0 cannot be directly compared with the results presented here because the underlying energy model has been significantly improved and is modified. However, the key benefit of this integrated approach outweighs any drawbacks, as it has created a consistent foundation across all analyses for the first time, ensuring that the results of Roadmap 4.0 will be consistent and comparable. The energy model enables a uniform

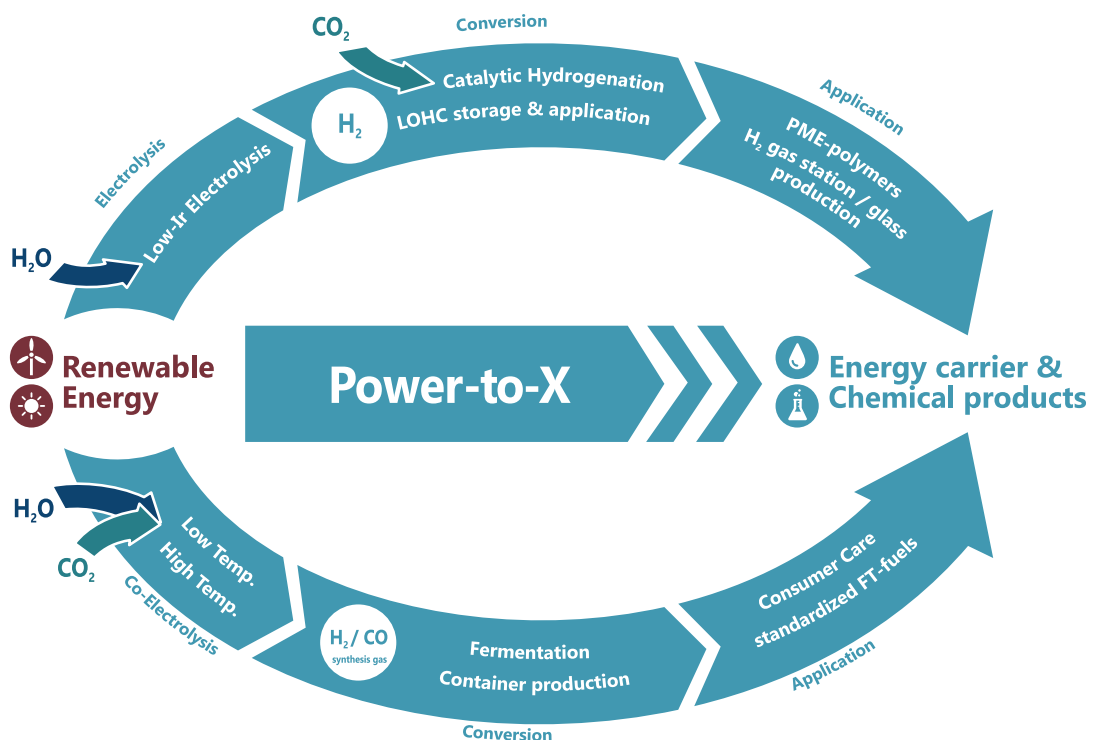


Figure 0.1 Overview of the project structure of the second phase of Kopernikus P2X.

scenario framework that allows researchers to map out developments in the transition to a more sustainable energy system (Energiewende). A backcasting approach is applied here, whereby the achievement of climate protection goals and other conditions such as compliance with the CO₂ budget, import quantities and sufficiency measures are defined and the entire system is optimised based on the most cost-effective routes for achieving this goal (e.g. climate neutrality by the year 2050). In four different scenarios, the effects of various factors on the development of the energy transition are investigated and presented here (see Section 4.1):

- The baseline scenario corresponds to the German government's goal to reduce greenhouse gas emissions by at least 55 percent (2030), 70 percent (2040) and 80 to 95 percent (2050) of 1990 levels. No changes in consumer behaviour are taken into consideration here. Imports are defined as electricity imports and exports to cover demand for power. The baseline scenario is used as the foundation for the detailed ecological (LCA) and economic (TEA) analyses.
- In the import scenario, the system is more flexible as it allows international hydrogen pipelines to be added to the model as an alternative to electric power transmission. The remaining assumptions are the same as in the baseline scenario.
- The 1.5-degree scenario takes a different approach. Here, the starting point is the achievement of the 1.5°C target. This is then used to calculate the per-capita budget of Kyoto gases, which is used as the basis of the model.
- The sustainable transport scenario (Verkehrswende) represents an extreme scenario aimed specifically at the transport sector. It models the emissions reductions that would be possible through changes in behaviour based on a change in the modal split and a reduction in overall transport and journeys. The remaining assumptions are the same as in the baseline scenario.

Life-cycle analyses (LCA), techno-economic analyses (TEA) and social acceptance analyses will be used to investigate the ecological, economic and social advantages and disadvantages of the value chains researched in P2X II. In addition to these detailed analyses, a potential analysis will also be carried out as part of the roadmapping process. In order to structure and categorise current discussions surrounding "the potential of

PtX" more effectively, a correspondingly methodical approach is developed. This method will be validated using a specially developed tools and Germany as an example. In the further course of the project, the interdependencies of relevant criteria and their impact on the potential of PtX technologies will be investigated for other countries.

The baseline scenario is used as the basis for the detailed environmental, economic and potential analyses in the application areas of transport, base chemicals and industry. This baseline scenario is being continually developed. As such, the results of the LCA, TEA and potential analysis are still based on a yearly resolution. The next development step, which is the transition to an intertemporal view, is described in Section 4.1; however, it will not be possible to incorporate this into the other analyses until a later point in time. An intertemporal view has a number of benefits, allowing researchers, for example, to make forecasts about subsequent years. A rough comparison, however, has revealed that the differences between these two modelling types only have a minor impact on the results of the LCA and TEA in the years 2030 and 2040.

To research levels of social acceptance, a panel survey was carried out with a sample size of 1,123 young adults aged between 16 and 25 (invisible kids) and 1,134 people over the age of 25. The survey included content levels related to the evaluation of the various PtX technologies in the application areas of transport, energy and the chemicals sector as well as their intended use and sustainability focus together with other factors such as willingness to pay, level of knowledge and environmental awareness.

PLACING PTX TECHNOLOGY PATHWAYS WITHIN THE CONTEXT OF THE CHANGING ENERGY SYSTEM

The results of the energy model show that PtX technologies and products will have a vital role to play in a future defossilised energy system. However, PtX should not be used as a blanket solution in all application areas. Instead, it should be used in a targeted way in areas where more efficient, alternative technologies are not available or where carbon-based molecules are required as non-energy feedstocks. In the following sections, the different technologies are allocated to the relevant areas of application under investigation (transport, base chemicals and industry).

Demand for PtX products in the target year 2050 largely depends on the climate goals and the associated level of

defossilisation: The more ambitious the goals, the earlier PtX technology will be needed. This document assumes the use of the average German electricity generation, currently with high specific CO₂-emissions, which would be required to be largely defossilised within the governmental target for expansion of renewables, in order to implement PtX-technologies. The results of the LCA show that greenhouse gas (GHG) emissions from electricity use must be reduced to below approximately 200g of CO₂-eq./kWh (see Section 4.2) before PtX technologies can contribute positively to a reduction in GHG emissions.

Overall demand for renewable energy for primary electricity consumers and PtX technologies in the target year 2050 will exceed Germany's potential to generate renewable energy, making imports unavoidable. As such, Germany will not be self-sufficient in its supply of energy carriers and raw materials, which means that it will remain a country dependent on imports of energy carriers in future.

APPLICATION AREA: TRANSPORT

The transport sector is one of the biggest challenges for Germany's energy transition and drive to GHG neutrality as emissions have remained at a consistently high level since 1990 [1]. This is primarily due to the fact that measures aimed at making vehicles more efficient have been offset by simultaneous increases in engine power and vehicle weight as well as increased mileage. Generating 163Mt of CO₂, the transport sector currently accounts for around 25% of all energy-related CO₂ emissions in Germany. From a systematic perspective, technological measures and initiatives aimed at promoting modal shifts and reducing journeys and transport will be required to reduce emissions [2].

In the underlying energy model, technology changes are the only changes assumed for the transport sector in all scenarios with the exception of the transport scenario. Sustainable transport (Verkehrswende) is a special scenario that allows to investigate the effects of modal shifts and reduced journeys on the development of the energy system and the use of PtX-technologies. The results of the energy model show that for defossilising transport, the general trend is to first turn to direct electric and hydrogen-powered modes of transport. Liquid, synthetic energy carriers will only emerge from 2040 onwards as Fischer-Tropsch (FT) synthesis becomes cheaper and more efficient, whereby the different scenarios each require different ramp-ups and quantities of H₂/PtX-fuels.

The quantities of H₂/PtX modelled in the different scenarios for the transport sector in 2050 amount to 130 up to 170 TWh.

H₂/PtX fuels are only used to a limited extent initially for passenger and private transport. In this area, defossilisation is primarily achieved through electric cars and buses as well as the electrification of rail transport up to the maximum level allowed in the energy model. FT fuels will only be needed for air passenger transport. They may also serve as an interim technology in private motor vehicles, provided that sufficient renewable energy capacity has been created in Germany.

The transition in freight transport will start around the year 2025. Wherever possible, direct electric vehicles will also be favoured in this subsector. The assumptions regarding the use of trolleytrucks and the electrification of railway lines have a highly sensitive impact on demand for PtX solutions in this transport segment as a lack of these options or their limited availability will directly increase demand for H₂ vehicles.

Synthetic fuels play a central role, however, in aviation and maritime transport as there are almost no other viable alternatives here. As a result, the detailed analyses of environmental and economic aspects in P2X II focus on the FT value chain, in particular FT kerosene for cargo aircraft. The results of the detailed analyses are outlined in Section 5.2.

The LCA covers the entire life cycle of fuels from manufacturing to combustion in the aircraft turbines and the resulting release of the CO₂ contained in the fuels. The life-cycle-based net greenhouse gas emissions (i.e. after subtracting the CO₂ used as feedstock) for 2050 in the baseline scenario amount to around one third of the emissions that would be released using fossil equivalents. The remaining emissions primarily stem from upstream chains related to power and heat generation. Plant construction only accounts for around one tenth of the life-cycle-based GHG emissions. The ecological break-even point in this value chain is around 150g of CO₂-eq./kWh of electricity.

With regard to production costs for FT kerosene, the costs for electricity and for the supply of CO₂ from direct air capture (DAC) are the biggest drivers. Other CO₂ sources, including industrial point sources or biomass are also possible options. During the transition phase until GHG neutrality has been achieved, industrial CO₂ point sources will still be available, albeit in decreasing quantities. Due to the lower CO₂ separation costs, they could contribute to a reduction in the cost of PtX products. At the same time, efficiency improvements and

technological developments could also reduce the cost of DAC technology, which is still in its infancy. Based on the assumptions made in the modelling, the production costs for FT kerosene are higher than the current prices of the fossil reference. In the long term, however, the price for fossil kerosene may change significantly, for example, due to a correspondingly high CO₂ tax.

With regard to social acceptance, the panel survey revealed strong willingness among participants to use transportation (cars, trains, plane and ships) with hydrogen or synfuel drive systems. FT kerosene is still undergoing research and development and is therefore the subject of expert discussions. As a result, measures are required to ensure that this topic is transferred openly for discussion by society. It is important that the scientific community provides clear, more easily understandable data about available potentials, taking into account the development along temporal and spatial dimensions, as a sound basis for social dialogue. Despite the uncertainty that still surrounds the assumptions, these issues are reported in an overall positive light in the media and in society. A detailed overview of the panel survey can be found in Section 5.3.

APPLICATION AREA: BASE CHEMICALS

Alongside the metal industry, the base chemicals sector is the most energy-intensive industry in Germany. One of the particular characteristics of this sector is that the energy carriers are not just used to generate energy, they are also used as feedstock (non-energy use). In fact, non-energy use exceeds use as an energy source and currently 86% of non-energy feedstocks are made of fossil raw materials, in particular mineral-oil-based raw materials. In contrast, process energy needs are primarily met with natural gas (42%) and electricity (26%) [3].

Due to the complexity and large numbers of different products and processes in the chemicals industry, the scope of the overall system analysis has been limited to base chemicals, which, overall, account for the majority of GHG emissions from the chemicals industry. These include, for example, chlorine, oxygen, ammonia, methanol, the high-value chemicals (HVCs) ethylene, propylene, butylene and butadiene as well as aromatics (BTX). All scenarios under consideration showed a rise in energy consumption as efficiency improvements are offset by the expected expansion of the industry. There are only marginal differences between the different scenarios. The main phase

of the base chemical industry's transition takes place relatively late. In 2040, for example, around half of the energy and raw materials are still obtained from fossil sources (mineral oil and natural gas). One third stems from PtX products while the remainder is sourced from biogenic raw materials and using electricity. In all scenarios, biomass and regenerative electricity are used exclusively as energy carriers and for producing feedstocks in the base chemicals sector in 2050 due to the requirement to reduce GHG emissions to 95% of 1990 levels. Overall, average energy and feedstock consumption is 425 TWh. 32 TWh of this stem from biomass, 69 TWh from electricity and 324 TWh from PtX products. In the model, the electricity required for the domestic generation of H₂/PtX products for the chemicals industry is provided by the national expansion of renewable energy plants, above all wind and solar. To produce these feedstocks in Germany, capacity must be expanded by a factor of five to six compared with today's levels. This will create the right conditions for ensuring that the entire value chain for the base chemicals industry remains vertically integrated in Germany. Alternatively, these could be imported (similar to the situation today) with potential consequences for production chains. A detailed overview of the assumptions and results used to position the chemicals sector in the energy model can be found in Section 6.1.

In P2X II, two special value chains from the chemicals industry are analysed in detail to determine their ecological, economic and social aspects. This includes the biotechnological production of butanol based on co-electrolytically generated synthesis gas and the production of PME polymers. The ecological LCA evaluation is limited to a cradle-to-gate assessment, which means that the environmental impacts from the utilization phase and end of life are not taken into consideration.

The life-cycle-based GHG emissions from the production of butanol using electrical energy are driven by GHG emissions from the electricity mix. The break-even point is at an emissions value of around 170 g of CO₂-eq. per kWh of electricity; beneath this threshold, the PtX pathway is more beneficial than conventional synthesis. Plant construction and the fermentation and production of auxiliaries account for just a very small share of GHG emissions. A further reduction of GHG emissions in electricity generation in 2050 would even result in net negative GHG emissions for butanol fermentation within the system's boundaries as the DAC process takes more CO₂ from the surrounding air than is emitted in the process chain. However, it must be noted here that a corresponding amount of carbon is bound up in butanol (2.37 kg of CO₂ / kg of butanol) and

this may be released further downstream in the life cycle. This is not included in the cradle-to-gate assessment.

Based on the assumptions made for the TEA, the cost of manufacturing butanol using the PtX process today is around three times higher than its fossil reference. Over the period to 2050 and given the assumptions made here, the costs difference will be reduced to 1.5 times higher than the fossil reference process, which is based on propylene produced by steam cracking naphtha. Electricity costs are the main drivers here. Based on a sensitivity analysis, the price of electricity in 2050 would have to be 0.03€/kWh for the production costs of PtX butanol to be comparable with the current price of the reference process. Further details on the ecological and economic aspects, in particular other environmental impacts, are outlined in Section 6.2.

Polyurethanes are one of the most important types of plastic. They are conventionally made from three fundamental components: Isocyanates, polyols and various additives. PtX offers an alternative method for manufacturing polyols that can reduce the life-cycle-based GHG emissions associated with the plastic. Three different production pathways for synthesising the new polyols (pFA-fossil, pFA-PtX and LA-PtX) (pFA: paraformaldehyde) are researched and compared with the fossil reference. In the new PME polyol synthesis, propylene glycol and a certain amount of propylene oxide is replaced with paraformaldehyde (pFA), which can be produced from methanol. To ensure the analysis is as extensive as possible, the effects of a fossil-based (pFA-fossil) and a renewable (pFA-PtX) methanol manufacturing process are also being investigated. When comparing these production pathways, it should be noted that the linear acetal process (LA-PtX) is still at laboratory scale and the results can therefore only provide an initial estimate and scale. With regards to the life cycle analysis, the pFA-fossil route with paraformaldehyde can already reduce GHG emissions today compared with the conventional manufacturing route as the process is not based on electrical energy. If the paraformaldehyde is produced using PtX (pFA-PtX), the process is again dependent on the GHG intensity of the electricity mix; the break-even point of life-cycle-based GHG emissions is set at a GHG intensity of 80g of CO₂-eq./kWh or higher for electricity and will not lead to a reduction of GHG emissions until 2050. The estimate for the LA-PtX production path shows that linear acetal is also a promising replacement component for polyol synthesis and will be able to reduce GHG emissions to a similar extent as pFA-PtX in 2050.

The alternative synthesis of PME polyols could already be carried out cost effectively today. pFA-fossil is a good interim solution for as long as the pFA-PtX value chain remains in the development phase and the renewable energies required for generating the electrical energy are being ramped up. Raw material costs are the main cost factor in the production of PME polyols. The sensitivity analyses for natural gas, CO₂ and H₂ prices show that a break-even point between the pFA-PtX and pFA-fossil production paths will only be achieved if the price of natural gas increases while, simultaneously, prices of CO₂ and H₂ fall. The corresponding process description and detailed results on economic and ecological factors, in particular other environmental impacts, are outlined in Section 6.4.

As there are hardly any connections for the general public to engage with base chemicals in day-to-day life, current levels of social acceptance were assessed using a range of potential end products that can be manufactured using the base chemicals. These include cosmetics, mattresses, clothes and sneakers. The panel survey revealed an overall positive willingness to purchase these "PtX end products". A detailed analysis of the results of the panel survey can be found in Section 6.5.

APPLICATION AREA: INDUSTRY

The industrial sector consumes around 700 TWh of energy and is responsible for 28 percent of total energy consumption in Germany. The energy demand is dominated by primary industries such as metal production, the chemical- and mineral-processing industry and the paper industry. In total, the sector generates emissions of around 170Mt of CO₂-eq. per year. This is caused, on the one hand, by energy consumption and, on the other, by process-related emissions, that are mainly attributable to primary industries [1].

One of the biggest challenges facing the industrial sector is securing the supply of process heat at the right temperatures and amounts as well as the use of carbon energy carriers as feedstock (non-energy use). Temperatures in metal and glass manufacturing typically range from 1,000–1,600 °C. In the chemicals industry, temperatures of up to 1,200 °C are achieved. Here, however, energy carriers are often also used to create the process conditions. In the steel industry, coke is used as a reducing agent. Transitioning these processes is a huge challenge. The fact that they also use materials as feedstock also means that process-related GHG emissions will still be emitted in 2050.

Aside from the limited potential for thermally utilising biomass and recycled plastics, PtX fuels are the only option available for making these processes greenhouse gas neutral from an energy perspective. The most energy- and emissions-intensive industries together with their processes and energy carriers are included in the energy model as individual process pathways: Cement, lime, glass, paper, steel, non-ferrous metals and base chemicals. This information can then be used to analyse industry-specific greenhouse gases, energy consumption and use of PtX fuels. In the baseline scenario, 398 TWh of PtX products are required in the target year 2050. The majority of PtX products will be used as feedstocks in the chemicals industry. However, around 43 TWh of hydrogen will also be used in the steel industry for the direct reduction of steel. In contrast, the synthetic fuels will be used across all industries to generate high-temperature heat and in particular in the glass industry and in the production of non-ferrous metals.

In the project, researchers are specifically researching and evaluating the use of hydrogen to melt the raw materials in speciality glass production. The hydrogen is created using PEM electrolysis and a number of different hydrogen transport options are being investigated as supply options: Production and use on site, transport in a liquid organic hydrogen carrier (LOHC), pipeline, transport in liquid form by truck. The analyses have revealed that the method used to transport the hydrogen is important, both from an ecological and economic perspective. Using hydrogen for heating can reduce GHG emissions by 2030. The largest reductions here were achieved with on-site production. By 2050, more than half the GHG emissions produced by the reference process can be reduced. Here, again, on-site production delivered the best results.

On-site PEM electrolysis is also the most cost-effective option from an economic perspective. This has the added benefit of eliminating the majority of costs for oxygen supplies required to improve product quality and increase energy efficiency. It also eliminates the need for hydrogen purification. Overall, however, hydrogen supply costs are closely linked to the identified hydrogen demand and the transportation distance. As a result, the supply paths may differ for production sites with different hydrogen requirements and different transport distances (200 km was specified in the project). Increased electrolyser efficiency and fluctuations in electricity prices during the period between the target years are the two main reasons for a significant drop in costs.

Research into acceptance levels for industry applications mainly focused on industry stakeholders in order to identify supporting

factors and barriers, and to obtain suggestions on how to design and operate the process. The relevant stakeholders primarily include companies in the steel and glass industry and their employees as well as stakeholders in the areas of sustainability, consumer and environmental protection and conservation. Qualitative interviews were conducted with these players. They revealed that supply security was a top priority here, specifically ensuring a continuous, disruption-free supply of energy for industrial processes. Operating costs also played a central role. This is flanked by planning security, which stems from the need to establish a reliable regulatory framework. In principle, PtX applications are seen as a positive step towards sustainability and a way to decarbonise industrial processes, provided the challenges mentioned above are adequately addressed.

TRANSPORT ALTERNATIVES FOR HYDROGEN

Transporting hydrogen efficiently and cost effectively is a challenge due to its physical properties. Molecular hydrogen can be transported in a liquid or gaseous state. Researchers are also currently investigating chemically bound hydrogen, stored either in LOHCs (liquid organic hydrogen carriers) or converted to ammonia. The P2X project is focusing on the development and evaluation of LOHC technology.

Increasing quantities of hydrogen will have to be transported in future to ensure secure supplies for everyone from major industrial consumers to remote filling stations. It is likely that different infrastructure alternatives will be used here as is the case with the transport and distribution structures used for fossil energy carriers.

LOHCs can be a sensible addition to other hydrogen transport infrastructures as it will be possible to use existing infrastructures to a large extent and simply add the corresponding hydrogenation and dehydrogenation systems.

The project analyses in more detail the impact of different options for transporting hydrogen over a distance of 200 km to supply ten filling stations that serve a fleet of buses. Four different transport options are compared: Transporting compressed, gaseous hydrogen in a pressurised tank truck (pressurised to 500 bar) and transporting LOHCs with different heat provision paths for dehydrogenation.

The results of the LCA show that the transport options are significantly affected by pressure levels and/or the heat

source used for dehydrogenation. Depending on the assumptions made, this can even necessitate a change in technology. For the LOHCs, the least environmental impact overall was achieved by using waste heat as the heat source for the dehydrogenation unit. When comparing LOHC transport (with waste heat) and compressed hydrogen transport, the compressed hydrogen achieved better results in all environmental categories provided it was compressed to 500 bar. If the hydrogen is only compressed to 250 bar, LOHC transport (with waste heat) provides more benefits in terms of climate change, summer smog and resource consumption.

The costs for transporting hydrogen in LOHCs and in a pressurised tank truck are similar under the conditions stated here and with an evaluation accuracy of ± 30 percent. The pressure of the compressed hydrogen and transport distance also play an important role here.

CLASSIFYING THE ENERGY VECTORS OF HYDROGEN AND SYNTHESIS GAS

Hydrogen and synthesis gas are currently produced and used on a large scale in the chemicals industry and in refineries. The majority of this is for captive use, which means that the hydrogen and synthesis gas are produced and processed at the same site. There are currently two insulated hydrogen pipeline networks in the Rhine-Ruhr region and in Central Germany and so the existing infrastructure is not sufficient for universal transportation. In addition to this, hydrogen has the potential to be used as a universal energy carrier in various sectors, for example, in the transport, residential and industrial sectors and for energy production. New applications will also emerge in future in the industrial sector, including, for example, the use of hydrogen as a reducing agent in primary iron production, as a fuel for high-temperature processes or in the production of base chemicals and alternative fuels. Synthesis-gas-based processes are already available on an industrial scale for these latter applications in particular. Unlike conventional synthesis gas production processes based on fossil feedstocks, these processes have to be adapted to enable synthesis gas to be manufactured from the CO₂ taken from DAC or industrial processes using hydrogen produced from electrolysis and renewable electricity and to then convert these to the desired product. These technologies provide the basis for a portfolio of processes that – from a technical perspective – can more or less substitute fossil feedstocks and energy carriers.

The P2X project is expanding the pool of available technologies for generating, transporting and utilising hydrogen and synthesis gas. This will then open up new application options at different points in the energy system and feedstock base. Based on the latest findings and the assumptions that have been made, the P2X project will closely support and extensively evaluate these technology options at every step of their journey from laboratory development to application. Like its predecessors, this roadmap provides a snapshot of the current project work, in which technological developments are completed, findings are confirmed or have to be reassessed, new questions arise and the future of the energy transition takes on a tangible shape.

- [1] **Bundesministerium für Wirtschaft und Energie (BMWi)**, „Energiedaten: Gesamtausgabe“, Berlin, Okt. 2021. Zugriffen: März 31, 2021. [Online]. Verfügbar unter: https://www.bmwi.de/Redaktion/DE/Downloads/Energiedaten/energiedaten-gesamt-pdf-grafiken.pdf?__blob=publicationFile&v=40
- [2] **J. Günther, H. Lehmann, U. Lorenz, und K. Purr**, „Den Weg zu einem treibhausgasneutralen Deutschland ressourcenschonend gestalten“, Umweltbundesamt (UBA), Dessau-Roßlau, 2019. Zugriffen: März 31, 2021. [Online]. Verfügbar unter: <https://www.umweltbundesamt.de/publikationen/den-weg-zu-einem-treibhausgasneutralen-deutschland>
- [3] **Verband der Chemischen Industrie (VCI)**, „Rohstoffbasis der chemischen Industrie“, Frankfurt, 2020. Zugriffen: Juli 27, 2021. [Online]. Verfügbar unter: <https://www.vci.de/top-themen/rohstoffbasis-chemieindustrie.jsp>

The institutions listed below are funded or associated partners in the Kopernikus project P2X II consortium. The partners have directly or indirectly contributed to the contents of this publication to different extents. Based on the technological developments in the project, the authors of the Roadmap 3.0 have developed the contents of this document based on their own work and under their own responsibility. Therefore, the opinions expressed in the texts do not reflect the position or opinion of a specific partner in the P2X consortium.

CONSORTIUM

Funded partners

Bayerisches Zentrum für Angewandte Energieforschung e.V.
Beiersdorf AG
Bund für Umwelt und Naturschutz Deutschland e.V.
Clariant Produkte (Deutschland) GmbH
Climeworks Deutschland GmbH
Covestro Deutschland AG
DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e.V.
Deutsches Zentrum für Luft- und Raumfahrt e.V.
DWI Leibniz-Institut für Interaktive Materialien e.V.
Elogen GmbH
Evonik Operations GmbH
Forschungszentrum Jülich GmbH
Framatome GmbH
Fraunhofer Gesellschaft zur Förderung der angewandten Forschung e.V.
Friedrich-Alexander-Universität Erlangen Nürnberg
Greenerity GmbH
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
Heraeus GmbH & Co. KG
H-TEC SYSTEMS GmbH
Hydrogenious LOHC Technologies GmbH
ifeu – Institut für Energie- und Umweltforschung Heidelberg GmbH
INERATEC GmbH
Institut für ZukunftsEnergie und Stoffstromsysteme gGmbH
Karlsruher Institut für Technologie
Linde AG
Ludwig-Maximilians-Universität München
Öko-Institut e.V.
Ostbayerische Technische Hochschule Regensburg
RWTH Aachen University

SCHOTT AG
Siemens Energy AG
Sunfire GmbH
Technische Universität München
Wacker Chemie AG
WWF Deutschland

Associated partners

AVL List GmbH
DB Energie GmbH
Ford-Werke GmbH
International Association for Sustainable Aviation e.V.
Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V.



FULL VERSION (GERMAN) AND TECHNICAL APPENDICES
<https://www.kopernikus-projekte.de/projekte/p2x/#roadmaps>

Made within the roadmapping activities in the Kopernikus project
P2X: Erforschung, Validierung und Implementierung
von „Power-to-X“-Konzepten sponsored by the German Federal Ministry
of Education and Research.

FKZ: 03SFK2WO-2
(DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e.V.)

IMPRINT

Editors

Dr. Florian Ausfelder
Hanna Ewa Dura

DECHEMA Gesellschaft für Chemische
Technik und Biotechnologie e.V.
Theodor-Heuss-Allee 25
60486 Frankfurt am Main
Germany

Responsible according to the German Press Law and the Media

Dr. Florian Ausfelder
DECHEMA Gesellschaft für Chemische
Technik und Biotechnologie e.V.
Theodor-Heuss-Allee 25
60486 Frankfurt am Main
Germany

Design and typesetting

Lindner & Steffen GmbH,
Nastätten

Image Credits

U1: Chokri Boumrifak, vi-studio.de
U4: EtiAmmos

Sponsored by the
German Federal Ministry of Education and Research

Supervised by
Projektträger Jülich

Published in Frankfurt am Main on May 31, 2023
1. Edition

ISBN: 978-3-89746-241-0



chance

change