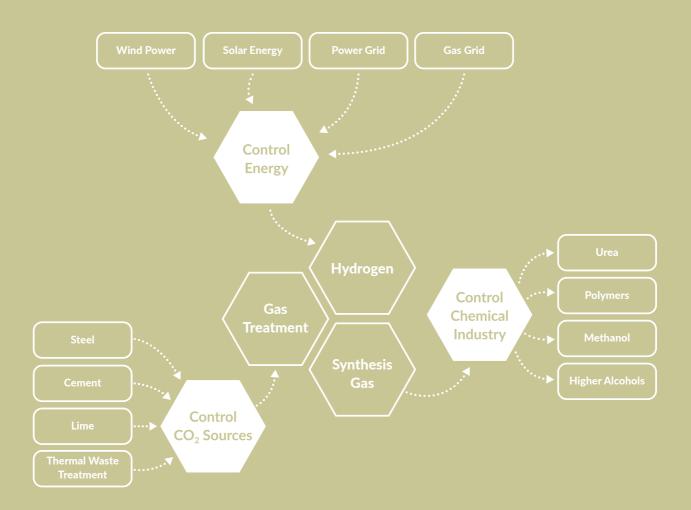


CARBON2CHEM® A KEY BUILDING BLOCK FOR THE CLIMATE PROTECTION





Dear readers,

Climate neutrality is our explicit goal. We will need innovative technologies to achieve it in the near future. It seems best to start where our action has the greatest impact, for example in steel production. Emissions are still particularly high in heavy industry. At the same time, this sector is a pillar of our prosperity.

Carbon2Chem[®] is such an innovative solution. The project shows how to successfully steer a new course in the steel industry by recovering CO_2 from blast furnace gas on an industrial scale, which can then be converted into base materials and fuels using green hydrogen. I was instantly fascinated by this prospect when I first heard of it. And what is more: these innovations can even be transferred to other energy-intensive plants such as lime works and waste incinerators. This is what I call real progress.

Another aspect of Carbon2Chem[®] also appeals to me. The interdisciplinary collaboration brings together technology leaders and research institutions and thus ensures close links between research and the transfer of its results. In this way, the project opens up new prospects for climate protection and at the same time offers promising opportunities for technology exports. For me, Carbon2Chem[®] is an outstanding example of how we can use research and innovation to provide for a sustainable future.

Projects like Carbon2Chem[®] will enable us to ensure climate-neutral prosperity in future. I hope you will enjoy reading this brochure.

B. Rech-Waterner

Bettina Stark-Watzinger Member of the German Bundestag Federal Minister of Education and Research

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Federal Ministry of Education and Research

Motivation

The goal of the Paris Climate Agreement is to limit global warming to 1.5 degrees Celsius compared to pre-industrial times. This makes the reduction of greenhouse gas emissions a key component of achieving this target. For the European Union, this means a 55 percent reduction in carbon dioxide (CO_2) emissions by 2030 and climate neutrality by 2050.

However, during this transition to climate neutrality, the raw materials industry, in particular, is facing major challenges. Carbon dioxide is not only produced when the required energy is supplied but is also generated in the course of production processes. So decarbonization of the processes will not be successful in all areas during the energy transition. Industrial processes will still continue to emit carbon dioxide in the future, like those involving the production of steel, cement or lime, as well as thermal waste treatment. On the other hand, there is a great demand for non-fossil carbon in the manufacture of chemical products. The question about how to capture unavoidable CO_2 from industrial point sources and utilize this for the chemical industry lies at the heart of the Carbon2Chem[®] joint project. The answer is: via Carbon Dioxide Capture and Utilization (CCU). A key element in ensuring success is the defossilization of the processes by transforming industrial production processes during the energy transition. The consortium involved in the Carbon2Chem[®] project is working on cross-industrial production networks whose modular design will enable process-related carbon dioxide to be captured and utilized in connected structures at existing industrial sites. The products are used as raw materials in the production of synthetic fuels, plastics or other basic chemicals.

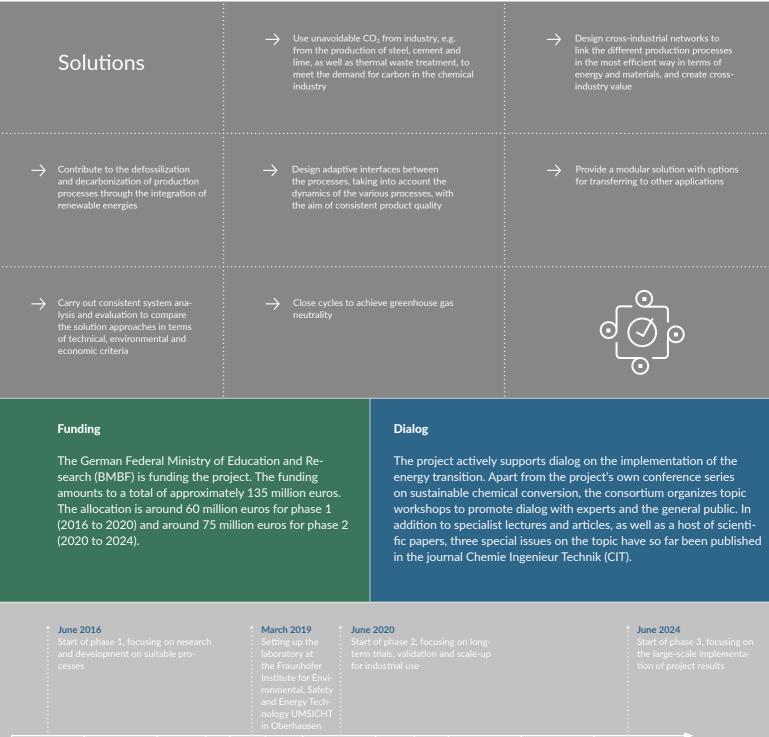
In addition to making technical progress, combining climate protection and competitiveness and dialoging with the scientific community and society, forms an integral part of the project. The results produced by the project are expected to make a tangible contribution to reducing emissions from greenhouse gases and using fossil raw materials in the industry by 2030. The feasibility of the technical solutions and their positive impact have been successfully demonstrated by the project consortium during the first phase of the project.

The consortium firmly believes that **Carbon2Chem®** represents a key building block for the climate protection.

Overall objective of the project

To provide technical solutions for implementing the transformation process in the industry as part of the energy transition that is aimed at achieving the climate goals

Carbon2Chem[®] at a glance



September 2018

Setting up of the technical center at thyssenkrupp's steel mill in Duisburg

Startup of the methanol

June 2019

August 2021

Continuous methanol pro-duction in the demonstra-tion plant over a period of five weeks



Key milestones

Structure as a success factor

The Carbon2Chem[®] project is divided into five sub-areas based on the processes involved:

The system integration process ties the results of all partners to an overall concept. The system integration process evaluates and optimizes the solution approaches developed with the help of various modeling and simulation tools. The starting point is the potential **sources** of CO_2 and the associated infrastructure - current status and future development. The key element is **gas treatment**, which includes gas conditioning in addition to gas cleaning. A variety of products can be conceived based on CO_2 . With a view to prompt implemen-tation and the potential leverage effect, the Carbon2Chem[®] project is working on solutions for the **synthesis** of methanol, urea, higher alcohols and polymers. The form and requirements of the **applica-tion** in terms of quality, quantity and availa-bility of the products essentially determine the upstream process steps and the overall balance, which is why it is part of the project

A science and industry consortium is working in partnership on the project in several subprojects. One vital aspect in this regard is the clear focus on the largescale implementation of the technical solutions by 2030. All subprojects are therefore headed up by industry experts. This means that much more direct consideration is given to operational aspects.

The interaction between the subprojects is facilitated by the overall coordination activity. In addition, within the project there are expert communities on interdisciplinary topics, such as process design, simulation, sustainability assessment, as well as the laboratory and technical center. Multi-layered dialog between science and industry experts from different disciplines has become established during the project and is now a factor that contributes to the project's success in developing cross-industrial solutions.





Overall coordination

Another feature of the project is the cooperation between basic research, applied research and industry, managed as part of the overall coordination activity. This is the only way to ensure that the path from concept to implementation is achieved in the three established phases of the project. The three areas are represented as follows:

Applied research

As an institute whose guiding principle is "Production without raw materials", we are an excellent fit for this project. The Fraunhofer Institute for Environmental, Safety and Energy Technology UMSICHT has been conducting research for several years in projects that have set themselves the goal of both achieving further reductions in CO₂ emissions and phasing out the use of fossil raw materials and instead using "waste products", such as steel mill gases, which are inevitably emitted during steel production, for the production of chemicals such as methanol. This is why we want to use Carbon2Chem® to recycle the carbon so that it is not released but instead reused sustainably after being produced on site.

Prof. Dr. Görge Deerberg Project Coordinator

Industry

thyssenkrupp is the first industrial company to engage in pioneering work in this area, together with the scientific community and other partners from industry. This effort is not about devising a single solution, but about developing a modular system of solutions that can also be used by other steel mills and industries. The ultimate result is that it should be possible to link all the technology modules together. The first industrial-scale application has been developed in the steel industry - an extremely CO₂-intensive industry. We are therefore doing the groundwork in the industrial environment to enable us to roll out the modules to other industrial sectors, which we again benefit from as a diversified group.

Dr. Markus Oles Project Coordinator

Basic research

At the Max Planck Institute for Chemical Energy Conversion, we are finding ways to efficiently convert energy into storable and usable forms. We are primarily looking for suitable catalysts to use for the necessary chemical reactions. In general, industry tries to save CO₂ by not using it. In fact, German industry is already operating with a minimum use of carbon. However, it is not possible to avoid using it completely. The Carbon2Chem[®] project enables us to develop a modular principle for these industries, generating modules that can be used for implementing the energy transition.

Prof. Dr. Robert Schlögl Project Coordinator



Our research representatives

In the scientific field, the consortium covers a wide range of areas with the research representatives involved and their expertise. The direct collaboration to this extent between basic and applied research is an essential feature of the Carbon2Chem[®] project. During the project, methods, tools and skills offered by the partners have been gradually linked together. In phase 1 of the project, basic research provided important insights regarding technology selection and concept development. A key element of this was the analytical skills which were developed as part of the project as needed.

"Basic research is the bedrock of any future feasibility. Investigating the influence of constantly changing parameters in steel mill flue gases is an essential prerequisite before large-scale plants can be built in the Carbon2Chem® project."

> Julian Schittkowski Max Planck Institute for Chemical Energy Conversion

"The particular challenge presented by the project is how to produce methanol with gas mixtures that are not used so much nowadays."

> Andreas Menne Fraunhofer UMSICHT

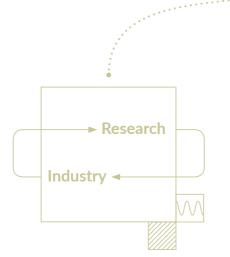
Although established technologies have been selected in the form of methanol and urea synthesis, there was and still exists a need for research and development. One reason for this is that up to several hundred different trace substances can be found in the process gases produced by industry. The different dynamics of the processes must also be fully taken into account in links and from an economic perspective. This is an aspect that can be resolved jointly by the collaboration of basic and applied research.

Abandoning the use of fossil raw materials as part of the defossilization of industrial processes also generates a requirement for new processes that enable the utilization of carbon dioxide. In particular, an innovative combination of process components is required to establish a circular carbon dioxide economy. Partners from the participating universities and institutes pool the expertise from their different departments.



In collaboration with industry, the research partners used their process engineering and mathematical skills to develop the necessary models to describe the processes and their technical components. The different detail levels of the models support needs-based simulation and optimization. In combination with the experimental investigations, it is possible to provide statements on the long-term behavior of various components and aggregates.

In addition to transferring established technologies and processes to be applied in the project, the research partners are also working on the development of new processes and components to create further options for CCU applications in industry. The successfully evaluated technologies in phase 1 will be further scaled up for industrial implementation in phase 2 of the project. The transition from the laboratory to the technical center is an essential step. During evaluation of the results, there is a close interaction between research and industry.



"Models and simulations are tools that make it possible to illuminate complex relationships. Long-term behavior is observed in the blink of an eye and critical processes are investigated thoroughly. This makes it possible to compare scenarios and identify the best parameters."

Christian Geitner Fraunhofer UMSICHT

"As the raw materials industry undergoes restructuring towards greenhouse gasneutral production, carbon dioxide and hydrogen will be two key components that must be transported, stored and processed safely and in compliance with the law."

Ulrich Seifert Fraunhofer UMSICHT



Our industry representatives

"Our product portfolio is already making significant contributions to sustainability and environmental protection in various applications. It is time now to also think about the lime production process in terms of climate neutrality."

> Thomas Perterer Lhoist Germany

"There are a great many projects and initiatives promoting climate protection and a sustainable future for the chemical and steel industry, with plenty of interesting ideas, concepts and ambitions. The Carbon2Chem[®] project will turn the visions into a practical reality and demonstrate their feasibility directly in the industrial environment."

> Matthias Krüger thyssenkrupp Industrial Solutions

The structure of the consortium's industry representatives reflects the key sectors of the planned cross-industrial production networks. Companies actively contribute their expertise as leading representatives of their respective markets to their daily project work. Their expertise is used to evaluate the technical, economic and environmental feasibility of the solutions in the Carbon2Chem[®] project. After evaluating the feasibility of CCU solutions based on the example of the steel mill in Duisburg, representatives of other sectors – from the lime industry and the circular economy – were also successfully brought onboard as partners at the end of phase 1.

Since the start of the project, activities involving the planning and implementation of measures to introduce climate protection into industry have gained significant momentum. Existing integrated systems, such as the integrated steel mill, need to be rethought. Companies contribute current developments and provide strategic direction from tangential industries to the project work. This means that work plans and development approaches can be repeatedly tailored to suit the developments in the project's environment. Long-term implementation of the solution concepts means that modular building blocks need to be supplied, making it possible later to adapt implementation in the form of cross-industrial production networks to different production plants.

The development of new process systems is more than possible with the combining of research and industry in the consortium. The expertise of the partners from industry constantly provides the necessary benchmark for development activities. This close collaboration can not only ensure the development of the processes, but also the opportunity to test them on different scales.



Two elements are key to the success of the CCU solutions. The first is a facility for providing a suitable synthesis gas for synthesizing the target products. Compared to the conventional processes currently used, this requires additional steps for capturing, cleaning and conditioning CO_2 . As for the second element, a sustainable effect by the concepts can only be achieved with the integration of renewable energies. The efficient use of energy and resources is a key aspect of the process design, which is why opportunities for sector links are being explored in this project.

Developments in the project are opening up to the chemical industry one option for defossilizing its processes. Compatible technical, economic and environmental criteria must be devised. CCU solutions must be designed dynamically to ensure consistent product quality alongside fluctuating input gases.

Looking ahead to phase 3 of the project, additional partners will be needed who can use their expertise to support and implement the development of cross-industrial networks.

The implementation phase (phase 3) requires further expertise and more partners. "Hydrogen — regardless of whether it is produced regeneratively or recovered from industrial processes — will play a key role in the future energy landscape. Regeneratively generated energy can be transported and stored using hydrogen. Furthermore, the option of linking sectors, for example, steel production and petrochemical processes, is conceivable. These are an absolute must when it comes to implementing the energy transition."

Jürgen Nowicki Linde Engineering

"This project helped create prerequisites allowing both CO and CO₂ to be integrated from the basic oxygen furnace gas into polymer production."

Stefanie Eiden Covestro Deutschland GmbH



System approach

Description

A key feature and outcome of the project is system approach. It is an essential part of the high-level work carried out in the project. System approach is used to evaluate the various process concepts on the basis of technical, environmental and economic criteria.

Technical developments

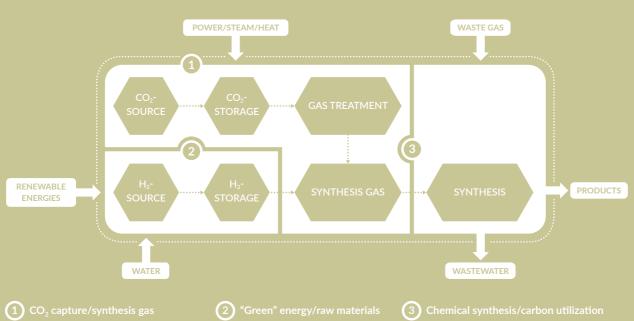
Ancillary studies on the knowledge status in the project are carried out regularly. The results from these are used to evaluate the work carried out in the project and to adjust the work plan. Current developments in the various industries moving in the direction of greenhouse gas neutrality are also taken into account in the system approach.

Modeling and simulation

A core aspect of system approach is modeling and simulation, which can be used to map and analyze the interaction of different plant components in a crossindustrial network using an overall simulation. The concepts devised for the network are analyzed by carrying out simulations of the processes relating to their stationary and transient behavior. These simulations make an important contribution in devising a targeted design for the network group in both technical and financial terms.

As part of the project, a cross-tool simulation platform was created that makes it possible to combine an analysis of process engineering and energy technology with sustainability analysis. An extensive model library provided the basis for this.

Simulations are used for selected concepts to develop management and control concepts that ensure safe and efficient operation of the plant network. Partial simulation models supplement the data from the experiments conducted in the laboratory and technical center or provide the specifications for the experiments.



Process Engineering Simulation

Process engineering simulation

Process engineering simulations are planned in the expert communities. Depending on the simulation scenario and requirement, certain operating points can be verified and checked more precisely in highly detailed process engineering models. This kind of simulation case can include periods of up to one year to take account of seasonal effects.

Depending on the question arising from a particular simulation task, models with different levels of detail are required to obtain an appropriate answer. As a result, the model library contains multiple implementations for each module so that the most appropriate model within a given simulation context can be selected. Process simulation is based on the mathematical modeling of physical processes.

The simulated process concepts differ in terms of the synthesized product, the steel mill gases used (type and quantity) and the technical components used (e.g. gas conditioning, gas storage). Each simulation case refers to a specific combination of these points and provides a statement about the time-processed mass and energy flows. The simulation results provide a basis for environmental and financial analysis.

Process logistics simulation

A process logistics optimization model is used to perform scenario calculations in order to obtain the best possible operating schedule for the entire future plant network. The best possible schedule can be calculated according to each criterion in the target function (electricity, storage, hydrogen scenarios, etc.). When comparing the process concepts in terms of energy, aspects such as supplying hydrogen via an electrolysis plant, using buffers and storage systems, or treating process gases, etc. must be taken into account. This also includes integration routes for material and heat flows, as well as statements on the underlying energy system. In addition to the conceivable system concepts, the future development of participating markets for reagents, products, electricity and CO_2 certificates is crucial to an investment decision. These market developments are taken into account in the form of simulation scenarios. The results from process

> logistics simulations provide the basic data for performing the additional life cycle assessment calculations.

Life cycle assessment

A life cycle assessment evaluates the potential environmental effects of the various process concepts. In any case, the starting point for comparing the process concepts is the current production process, which provides a benchmark for subsequent concepts. In the case of the cross-industrial

networks in the Carbon2Chem[®] project, a standardized method for comparative life cycle assessments was developed on the basis of ISO 14040/44.

Regulatory framework

The system approach also takes into account the regulatory framework, as it significantly influences the development and subsequent implementation. The framework conditions can relate to product specifications, safety aspects, formal aspects or financial aspects.

Expert communities

There is regular dialog between the experts involved in the individual subprojects about progress, adjustments and results. Expert communities for process design, simulation and sustainability assessments coordinate the simulation cases and procedure together. The results of the system approach are available to all partners for detailed analysis.



Carbon2Chem® laboratory

Another vital aspect of the project is the Carbon2Chem[®] laboratory. It is located on the campus of Fraunhofer UMSICHT in Oberhausen, occupying an area of approx. 500 m² and equipped with around 30 office workstations. It is used in basic research in the fields of catalytic production of methanol and higher alcohols, gas cleaning and the development of analysis processes. This area is available to the consortium for carrying out joint research and development on a laboratory scale.

Researchers focus on the behavior of different catalysts and the dynamic operation of the processes. The results are used as a basis for the work carried out in the technical center. In specific terms, components and processes are scaled up, and optimum operating points, control strategies and operations are determined.

Analytics and gas generators

The appropriate analytics for detecting the important lead components and identified trace substances had to be developed first at the start of the project. In addition, a gas generator system was set up in the Carbon2Chem[®] laboratory to be able to simulate gas mixtures (e.g. steel mill gases) for coordinating the analytics.

The analytical capabilities achieved make it possible to identify potential impurities (catalyst toxins, etc.) even in complex structures in the ppb to ppt range, as well as to quantify and analyze critical components (e.g. fragmentation patterns). Trace compounds can be identified and quantified both in the untreated and treated steel mill gases and in liquid samples. Based on the analytics carried out, it is also possible to support parameter optimization (dilution factor, collision energy, pressure, temperature, etc.) in the laboratory.

Catalyst tests

One of the laboratory's roles is to carry out catalyst screening as part of catalyst development for the synthesis of higher alcohols. The "Spider" test system used is designed to test eight catalysts in parallel. This is an intermediate stage between a conventional individual examination and high-throughput screening. The objective is to examine the influence of important reaction parameters and to compare different generations of catalysts under identical conditions. Optimization of the operating parameters involves varying the residence times and parameter optimization (reaction temperature, reaction pressure, gas composition, etc.).

Testing trace substances

Part of the basic research is to investigate the longterm effect on the catalysts of various trace substances contained in the real gases. The effects of trace substances on product quality also forms part of the laboratory tests. This provides important insights for the design of the gas cleaning process, which in turn significantly determines the cost-effectiveness of the process concepts.

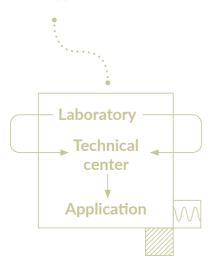


Carbon2Chem® demonstration plant

In September 2018, methanol was produced for the first time from real steel mill gases in the Carbon2Chem® technical center at the Duisburg steel mill. The Carbon2Chem® demonstration plant has been in operation at the Carbon2Chem® laboratory in Oberhausen since July 2019. The demonstration plant will be involved in further scaling up in the development of methanol synthesis. From 2022, the plant will produce up to 75 liters of raw methanol (a mixture of methanol and water) per day from real steel mill gases at the Carbon2Chem® technical center in Duisburg.

Despite the low production capacity, the plant possesses all the essential design features of a large-scale plant. The reactor tube has a diameter of 42 millimeters and a length of 6 meters, with unreacted synthesis gas being returned to the reactor after separation of the liquid products. The installed gas analyzers and the temperature measurement along the reactor axis with its 36 measuring points provide a precise insight into the process and a detailed evaluation of the catalyst activity over the entire height of the reactor.

In combination with the process engineering simulation, the plant enables the production of methanol from synthesis gas with any desired ratio of carbon dioxide and carbon monoxide. Known fluctuations in the composition of real process gases can therefore be reproduced. The plant is representative of the progressive scaling-up in the project from laboratory to technical center and then to application.







Carbon2Chem® technical center

The Carbon2Chem[®] technical center covers an area of 3,700 m². Due to its location — adjacent to the thyssenkrupp site in Duisburg, integrated into the pipeline network — it enables access to steel mill gases and therefore facilitates the technical implementation of previously developed concepts under real conditions. Since it was commissioned in September 2018, the technical center has been operating as the first demonstration of a cross-industry network with the complete process chain and providing a link between steel and chemicals.

Focus of research work: cleaning and conditioning of the real steel mill gases along with water electrolysis to provide additional hydrogen for chemical synthesis. These gases are converted into methanol, ammonia and higher alcohols in pilot plants. The analyses in the technical center are used to prove the catalyst performance and stability with synthesis gases from real steel mill gases. The structure allows the gas cleaning concept to be validated for synthesis gas production by comparing the tests with real and synthetic synthesis gases.

As with the Carbon2Chem[®] laboratory, the technical center offers project partners a unique opportunity to collaborate at a central location under uniform conditions. The expertise is networked and linking the different disciplines creates the basis for the large-scale industrial solutions.





Gas cleaning

Gas cleaning is one of the key technologies of CCU applications and therefore also of the process chain in the technical center. It can process around 240 cubic meters of steel mill gas per hour. The gas must have impurities removed so that it meets the high purity requirements for synthesis gas. The basis for operational management is provided by the results of the analysis of the impurities and the laboratory results for potential catalyst poisons.

In the laboratory building, additional methods for removing trace substances are being tested. The selected methods were positively validated under laboratory conditions in phase 1 of the project. The technical center offers an opportunity to scale up the processes and test them with real gases.

Laboratory facilities

The comparative analysis of the syntheses using real and synthetic synthesis gases from the Carbon2Chem[®] laboratory is carried out in the laboratory building of the technical center. In the case of methanol and ammonia, commercially available catalysts are used as a basis.

The measured catalyst performance and stability are compared with those of conventional processes. The influence of impurities in the steel mill gases and of adaptations to the catalysts is used to validate the gas cleaning concept for synthesis gas production.

The analytical methods developed in the laboratory allow the operation of gas cleaning with regard to trace substances to be controlled and monitored in the Carbon2Chem[®] technical center. The established infrastructure is characterized by continuous online measurement of the cleaned gases and identification of all primary (% range), secondary (‰ to ppm range) and trace compounds (ppb to ppt range). As a result, the analytics helps to carry out long-term campaigns and to optimize the process parameters (pressure, temperature, etc.).

Electrolysis

The integration of renewable energies in the form of green hydrogen for chemical synthesis is the second key element for the implementation of CCU applications. The core technology is water electrolysis, which produces hydrogen from water using renewable energy. A two-megawatt water electrolysis facility was built in the technical center as part of the project.

To ensure that the Carbon2Chem® project produces a positive carbon footprint, it is crucial that the electricity used for water electrolysis does not come from fossil fuels, but from renewable sources characterized by their volatility. Therefore, one focus of the development work in water electrolysis is to investigate the behavior of the facility with a fluctuating energy supply. The results will provide important insights in terms of planning the hydrogen supply for subsequent largescale implementation.



From technical center to application

Overview

The subsequent application of the products is vital for the development of the necessary processes and technologies. The market for products for CCU processes is growing and the consortium is working with potential users of the developed technologies. In addition, the requirements for the products influence the design and optimization of the product routes from the user's perspective.

Key product routes in the project are methanol, urea, higher alcohols and polymers. They are also used as basic products for the chemical industry or as raw materials for the supply of synthetic fuels.

Scaling

The project is gradually approaching an industrial scale, as planned. The demonstration plant is enabling the consortium to take the next step in scaling up the production of methanol. A few milliliters in the laboratory are turning into a few liters per day.

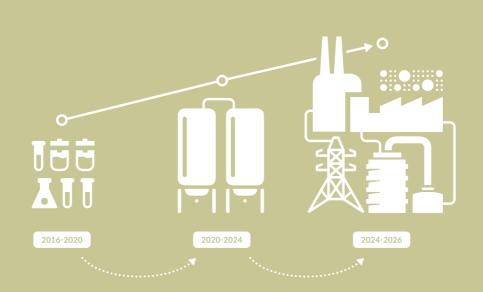
While at the outset of the project, the focus was only on the design of the process itself, now consideration is also given to the issue of optimizing and managing the processes. The dynamics at the CO_2 point source must also be taken into account. The composition and quantity of gases gained from production varies depending on the source and production cycle. The provision of renewable energies is the key element in this case. The supply of green hydrogen is part of the system analysis for each further scaling step. The import and storage of hydrogen in sufficient quantities is an integral part of the planning for the project.

Application for transport

One application is the direct use of the methanol produced for the transport sector. Obrist GmbH is working on a serial hybrid drive that, in conjunction with an electric drive, provides renewable energies in the form of produced methanol. As part of the Carbon2Chem[®] project, the team is devising the concept in the corresponding subproject, developing the specifications for the methanol, and giving a test-run to the first vehicles.

Circular economy

Raw materials and energy efficiency are key to achieving a positive overall balance in the implementation of the planned cross-industrial networks. In light of this, circular thinking is an integral part of the industrial transformation during the energy transition. With its next development steps, the project will support the implementation of a circular economy. The Carbon2Chem[®] project will be a key building block for climate protection in industry.



EDITORIAL NOTES

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#Carbon2Chem

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