Subproject L-KK

COORDINATION AND COMMUNICATION

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

The aims of the L-KK sub-project are the provision of needs-appropriate support for the overall project coordination, ensuring an exchange of information between the subprojects, communication of the results of the overall project externally, and a discussion of the necessary framework conditions.

In addition, work is being conducted on concepts that enable necessary skills to be acquired in training with the support of suitable learning modules.

The presentation and discussion of the project results outside the consortium should be particularly reinforced with a communication concept and various measures.

PROJECT CONTENT

As part of the overall project coordination, the project coordinators support the subproject in terms of coordination with the project consortium. This includes, among other things, preparing meetings concerning several subprojects as maintaining the information transfer in the consortium.

Overall, the implementation of the project results requires broad support that should be acquired with a suitable communication strategy. The necessary communication concept is developed and implemented for this.

The "Conference on Chemical Conversion in Industry" series launched in the first project phase is continued by the subproject. Alongside the conferences designed for a wide audience, technical workshops on selected themes are planned with business, science and politics. The partnership with other R&D projects should also be intensified.

MILESTONES

- Conferences 2020 to 2024
- Participation ACHEMA 2022
- Communication concept
- Technical workshops 2021 to 2024
- Draft and discussion of regulatory framework conditions
- Further education modules

PROJECT PARTNERS

- Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT (coordinator)
- Max Planck Institute for Chemical Energy Conversion (MPI CEC)
- thyssenkrupp AG (associated partner)

Subproject L-0

SYSTEM INTEGRATION

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

The aim of the second phase is to expand the previously developed concepts for purifying metallurgical gases, which are used to synthesize various chemicals and, in particular, for system integration, in such a way that industrial implementation is realized following the project phase and the robustness of the solution can be demonstrated.

Methanol and higher alcohols are primarily considered here as starting materials for synthetic fuels, as well as urea as a starting material for artificial fertilizers. In addition, the individual technology modules are combined and adapted in such a way that they can also be used to implement greenhouse gas neutrality in other sectors. The system boundaries are extended beyond the metallurgical plant in the second project phase, so that all technology modules can ultimately be linked to new cross-industrial interlinked productions. Possible target areas include, for instance, the cement and lime industry or the recycling of residual materials, in addition to the steel industry. With regard to steel production, the "hydrogen route", which is considered in parallel by thyssenkrupp, is included in the system analysis and compared with the Carbon2Chem® path.

PROJECT CONTENT

In the second phase, the process concepts that were developed in the first phase and assessed as economically and ecologically beneficial are further refined for the metallurgical plant at the Duisburg site. Solutions are developed in detail for technical hurdles and the coupled processes are optimized. Using this as a basis, analyses are conducted on the transferability of previously developed concepts to further sources of carbon dioxide (CO_2) and metallurgical plants at other sites and the integration of other procedural/chemical processes is investigated. Taking into account a comprehensive system approach, possible technological transformation paths are developed and assessed.

The previously developed methods are used here, in particular the Carbon2Chem® simulation and the previous experimental tests. The methods of simulation and the subsequent assessment are gradually expanded according to the new requirements. In addition to this wide-ranging approach, the industrial implementation and the preparations that are necessary for this take priority in the second project phase.

MILESTONES

Several milestones are planned in the second phase of the project. The clear goal of having developed and optimized the Carbon2Chem® technology to such an extent at the end of the second funding phase that an industrial implementation can be begun is based on the third level of consideration of subproject L-0. The introduction of the technology on the market is explicitly driven forward and relates to the establishment of a Carbon2Chem® system on an industrial scale at the Duisburg site using the metallurgical gases from the metallurgical plant of thyssenkrupp Steel Europe AG. In order for it to be possible to implement this project in 2025, basic engineering is prepared as far as possible as early as the second project phase.

PROJECT PARTNERS

- thyssenkrupp AG (coordinator)
- Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT
- Max Planck Institute for Chemical Energy Conversion (MPI-CEC)
- Siemens Energy AG

Subproject L-I

CO_2 SOURCES AND INFRASTRUCTURE

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

The solutions and concepts on the use of carbon dioxide (CO_2) in the joint project Carbon2Chem® should be transferred to other sources of CO_2. A roll-out thus takes place to other industries with unavoidable CO_2 emissions, such as the lime industry or waste incineration plants. This means that CO_2 emissions are minimized across sectors.

The various CO_2 reduction initiatives within industries will fundamentally change the CO_2 sources and their availability in the next 30 years. These changes are shown in a CO_2 matrix, which serves as the basis for investment and technology decisions involved in the transformation of industries towards climate neutrality. One example is a sensible combination of CO_2 use and hydrogen metallurgy in the steel industry.

Other areas of focus are the comparison of the availability of and need for hydrogen (H_2) and suggested solutions to balance this, e.g. with a feasibility study on a hydrogen cavern storage facility as intermediate storage.

PROJECT CONTENT

In subproject L-I, new cross-industrial networks are examined. To transfer the process concepts developed in the first phase of Carbon2Chem® to other industries, the technologies need to be adapted. This concerns the changed gas composition and also the quantity of the gases that arise. Smaller, modular concepts are thus developed in the project. These are theoretically evaluated in the first half of the project and designed in the second half of the project as demonstrators. Alongside this, CO_2 sources, including their composition and temporal availability, the necessary hydrogen and its availability, and the availability of renewable energy are analyzed.

A database is thus developed to enable sensible optimizations and a suitable setup of the necessary infrastructure for the overall system.

MILESTONES

- Creation of a CO-/CO_2 matrix (static in project month 12, forecast up to 2050 in project month 45), also comparison with the necessary H_2 (static in project month 12, forecast in project month 48)
- Geological feasibility study on H_2 cavern storage (project month 23) and the development of the associated technical requirements (project month 48)
- System concepts for CCU in the lime industry (project month 15) and the implementation of options for a pilot plant (project month 21)
- Changed process gas availability in the steel industry by using DRI and H_2 as a reducing agent (project month 21)
- Creation of framework conditions for the construction of a demonstrator (project month 30) and associated operator concepts (project month 36)
- Analysis of the gas and electricity network infrastructure (project month 21)
- First concepts for regulatory framework conditions in coordination with the subproject L-KK (project month 15)

PROJECT PARTNERS

- thyssenkrupp AG (coordinator)
- Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT
- Lhoist Germany Rheinkalk GmbH
- Thyssen Asset Management Ltd.
- REMONDIS Assets & Services GmbH & Co. KG

Subproject L-II

DYNAMIC METHANOL PRODUCTION FROM METALLURGICAL GASES

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

In order to be able to use metallurgical gases to produce methanol, it must first be shown that conventional methods are suitable for the new raw material or how these may need to be altered to suit the properties of the metallurgical gases. One area of focus in the first phase of the joint project lay, among other things, in the assessment of the scalability of the observed effects and in the creation and analysis of methanol samples to examine the formation of byproducts with different compositions of the feed gas. The relocation and integration into the Carbon2Chem® technical center in Duisburg with two testing plants was already conducted in the first phase in order to enable the very important long-term operation with real purified metallurgical gases in the second phase.

PROJECT CONTENT

To process the tasks, subproject L-II consists of various work packages on different technical and scientific questions. A work package involves the optimization of overall process concepts and economic benchmarks. The aim is to validate the dynamic simulation with data from the operation of the real systems. As part of mini engineering, a process description, an equipment list, a set of flow charts, a heat and material balance, and a costing should be created for multiple run cases. In another work package, tests take place on long-term measurement at the Carbon2Chem® technical center in Duisburg. In order to minimize the economic and technical risk of this scale increase, several thousand operating hours are necessary under realistic conditions at the Duisburg site. The various mini plant/pilot plant systems are perfectly suited to this task due to their scale, process concept, and their high level of automation. The long-term operation should demonstrate that methanol synthesis from metallurgical gases is possible.

Another work package focuses on the deactivation speed of the industrial catalyst as a function of various factors (temperature, pressure, catalyst mass, catalyst poison concentration and type) and the optimization of selectivity and productivity.

The aim of the laborious long-term studies is to create a broad kinetic database, which should be used for modelling and the preparation of potency estimates. The implementation of a digital twin at the pilot plant, the optimization of the process while taking into account economic and ecological aspects, and the scale-up of the digital twin are the content of a further work package. The last work package involves the groundwork for a complete life-cycle assessment.

MILESTONES

- Creation of block flow charts and mass balance calculations for all process concepts
- The compilation of the business case for selected process concepts exists.
- There is a detailed list of poisoning mechanisms and an identification of new catalyst phases and catalyst poisons.
- Establishment of kinetic models for reversible and irreversible poisoning and identification of the centers for the carbon monoxide steam conversion reaction and alkene hydrogenation
- Implementation of a digital twin
- Interfaces for the use of methanol in the fuel sector are defined and various business models determined for the use of methanol.
- The environmental effects are quantified for the coordinated scenarios.

PROJECT PARTNERS

- Nouryon Industrial Chemicals GmbH (coordinator)
- thyssenkrupp AG
- Clariant Produkte (Deutschland) GmbH
- Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT
- Fraunhofer Institute for Solar Energy Systems ISE
- Ruhr University Bochum

Subproject L-III

SYNTHESIS GAS

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

Using the example of the integrated metallurgical plant of thyssenkrupp Steel Europe AG in Duisburg, it was successfully shown in the first phase of the subproject that the gases that arise containing carbon oxide, hydrogen, and nitrogen can be used chemically. In the project, hydrogen production was also demonstrated using pressure swing adsorption (PSA) from coke oven gas. The robustness of the previously developed concepts for purifying and conditioning metallurgical cases should now be verified. These processed gases can be used to synthesize various chemicals. The findings should be transferred to the use of other CO_2 sources. Possible sources include waste incineration plants, cement works, lime grinding plants, and biogas plants.

PROJECT CONTENT

The solutions developed for purifying industrial process gases should be robust and versatile. The intensive operation of the technical center is required for further development. In the following points, the robustness of the systems should be presented:

- The operation of the technical center, gas purification, the PSA, and electrolysis should run fault-free.
- The purified and conditioned gases are made available to chemical syntheses in the laboratories.
- A further aspect is the oxygen separation from coke oven gas previously only investigated using model gases. The reactors and systems should now be operated in the laboratory and technical center with real gases.
- The synthesis of ammonia continues to be a key part of the subproject.

MILESTONES

The focus of the second phase lies on process intensification. The concepts of innovative production networks consisting of metallurgical plant and chemical production, which were created in the first phase, are developed in detail and, where applicable, expanded. Many functioning gas purification concepts are investigated in long-term experiments and optimized technologically, economically, and ecologically. The results flow into ecological and economic overall views. These represent a direct interface to the overall simulation. The testing plants for fundamental laboratory research are continuously operated with real gas.

An industrial implementation and basic engineering of the system networks should be largely feasible from a technical viewpoint after the end of the project. As part of this, technical transferability to other applications and industries, which cannot prevent CO_2 emissions in their processes in the future, is also investigated intensively. These industries must increasingly make use of a circular economy in the future and develop new technologies for this.

PROJECT PARTNERS

- Linde GmbH, Linde Engineering (coordinator)
- thyssenkrupp AG
- Clariant Produkte (Deutschland) GmbH
- Ruhr University Bochum
- Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT

Subproject L-IV

C_{2+} ALCOHOLS, C_{2+} OLEFINS, SYNTHETIC FUEL COMPONENTS

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

The aim is to develop a catalytic process for the use of a syngas consisting of purified metallurgical gases from a steelworks and sustainably produced hydrogen to create short-chain alcohols, olefins and/or synthetic fuels. The use of the alcohols and olefins as fuel and for other chemical components reduces the use of fossil raw materials. The fixation of carbon in recyclable products reduces carbon dioxide emissions from the steelworks. A large reduction in CO_2 results from the large-volume markets for the products addressed by subproject L-IV. With technological adjustments to gas purification, the syngas-based manufacturing of higher alcohols or olefins offers opportunities to transfer to other industrial process gases or CO_2 sources (e.g. from the cement and lime industry or waste incineration) and use renewable raw materials and plastic waste.

PROJECT CONTENT

The optimization of the catalyst and reactor design for real gas operation is determined by the envisaged product mix (alcohols vs. olefins, chain lengths). Market analyses in the mobility/transport and petrochemistry sectors serve to identify market-appropriate product mixes. Product treatment takes into consideration fractionating olefins and alcohols and marketing them separately. Olefins should be hydrated/hydroformylated and the alcohol mix that arises should be marketed as a fuel component after further processing. Alcohols should be dehydrated and the olefins marketed separately after their fractionation. The CO_2 saving is additionally supported by the development of processes in which CO_2 is converted into hemiacetals with C_2-C_4 alcohols or CO_2-based methanol into iso alcohols with C-C alcohols using the Guerbet reaction. The aim is to demonstrate the process step that uses syngas while making use of the existing Carbon2Chem® infrastructure.

MILESTONES

- Milestone 1 after 24 months:
  Catalyst is available on a commercial scale, duration > 2,000 hours; productivity > 150 g/mL/h; selectivity > 55 %.
- Milestone 2 after 18 months:
  Catalyst is assessed with regard to the implementation of syngas containing CO_2.
- Milestone 3 after 20 months:
  A kinetic model describes the range of operating conditions.
- Milestone 4 after 36 months:
  The reactor model delivers realistic predictions.
- Milestone 5 after 18 months:
  A market-compatible product composition is identified and a process concept developed.
- Milestone 6 after 42 months:
  An economical procedure is developed, for which an LCA is conducted.
- Milestone 7 after 40 months:
  Demonstration of a concept to refine the product mix, CO_2 saving, process concept (continuous) exists.
- Milestone 8 after 20 months:
  The concept for renovating the methanol demonstration plant is ready.
- Milestone 9 after 48 months:
  The demonstration plant has been started up with the catalyst prototype and the developed process conditions. The feasibility of the process has been demonstrated on a larger scale.

PROJECT PARTNERS

- Evonik Operations GmbH (coordinator)
- thyssenkrupp AG
- Ruhr University Bochum
- Fraunhofer Institute for Environmental, Safety, and Energy Technology UMSICHT
- RWTH Aachen University

Subproject L-V

CARBON2POLYMERS

Project content
for the period 2020 to 2024

Carbon2Chem®

PROJECT AIMS

For the use of carbon monoxide (CO) from metallurgical gases in polycarbonate manufacturing, it should be clarified to what extent the impurities from the metallurgical gases influence two process steps that are important for polycarbonate manufacturing.
As a result, these two process steps are being researched and further developed to ensure the resource- and energy-efficient use of the CO.

The aim is, in particular, to research the catalytic mechanisms in the implementation of CO in order to develop catalysts/catalyst structures on this basis that are robust against impurities.

A further aim is to further develop a suitable reactor concept for a more energy- and resource-efficient process by incorporating renewable energies while integrating electrical heating into the process step that is currently being developed. A particular focus lies on guaranteeing a high product quality, which is an important prerequisite for the technical realization of polycarbonate production on the basis of converter gases.

PROJECT CONTENT

The research into a possible use of CO from metallurgical gases from the steel industry to manufacture high-quality plastics should take place as part of the Carbon2Polymers project specifically using the example of the manufacture of polycarbonate. The project also includes a comprehensive profitability analysis and a life cycle assessment (LCA).

In the first project phase, a laboratory facility and a technical center were established and put into operation to clarify the catalytic mechanism of CO implementation.

This is an important aspect, as catalysts can react very sensitively to traces of impurities, which impairs the yields and thus the efficiency of production. In the laboratory facility and technical center, catalysts treated with metallurgical gases are tested under various conditions.

MILESTONES

- Milestone 1 after 18 months:
  Gases that have a negative influence on a process step in PC manufacturing and must be removed were identified in a concentration of > 10 % in the CO from converter gas, and concepts were developed to remove them.
- Milestone 2 after 24 months:
  A reactor concept for the second process step in polycarbonate manufacturing was developed, and there are no critical indications that PC product qualities are impaired by impurities from the converter gas.
- Milestone 3 after 36 months:
  The use of CO from converter gas with inert gas components for polycarbonate manufacturing is possible from an ecological and economic viewpoint. The provision of CO from reforming processes, as is now standard in industrial production, forms the benchmark.

PROJECT PARTNERS

- Covestro Deutschland AG (coordinator)
- Max Planck Institute for Coal Research
- RWTH Aachen University