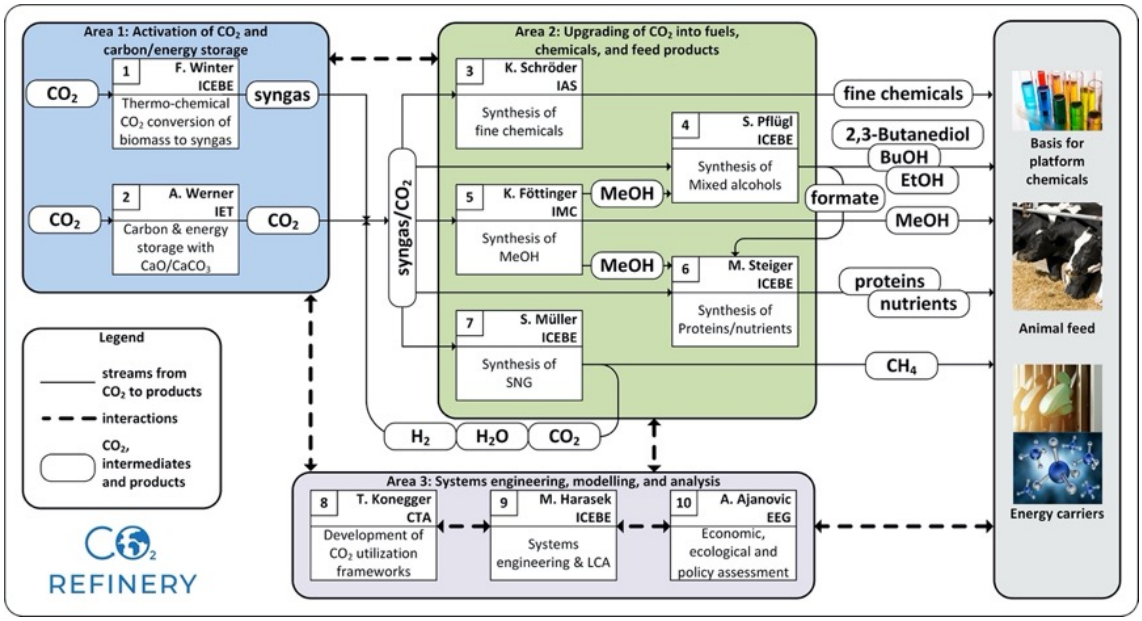
Open Position PhD #9: Systems engineering and life cycle assessment

General

The TU Wien doctoral school **CO_2Refinery** covers a wide range of methods and will integrate multiple disciplines required to implement a fully functional facility for refining and upgrading CO_2 on a technical center scale. With its integrated research and training program, the doctoral school targets to train "**one carbon engineers**" will work together on the development of technologies to efficiently utilize CO_2 as a carbon source to make a broad variety of products using chemical and biological catalysts. In addition to synthesis of products from CO_2, **CO_2Refinery** will focus on the activation of CO_2 for utilization as a carbon source in synthesis processes. Moreover, using renewable resources such as biomass and energy, and energy storage with CO_2 as the scaffold will be investigated. The strategy of **CO_2Refinery** is complemented by research on systems engineering, modelling, and analysis to provide the framework of the individual unit operations. Additionally, life cycle analysis will be used as a powerful tool to evaluate performance of the refinery on an economic scale. The research topics are structured into three research areas as shown below.



Within the proposed research framework, the members of the TU Wien doctoral school will be trained interdisciplinary to obtain a unique skillset. Graduates are envisioned to work at the forefront of groundbreaking research, but also to implement the concepts and ideas of a CO_2 refinery in industry. **CO_2Refinery** offers excellent scientific research, combined with a multi- and interdisciplinary curriculum (lectures and lab rotation) and a dedicated supervision and mentoring program. The PhD students are in the center of attention and their training and scientific advancement is the key to a successful implementation of this program. Research training will be obtained through work embedded into high-quality scientific research environments provided by supervisors that are internationally recognized experts in their fields and the close support through junior faculty members.

Project description:

Process simulation allows the steady state or dynamic representation of complex multistage process routes at unit operation level. Considering thermodynamics of separation and reaction processes, material and energy balances are calculated to find optimal combinations of process units. In the context of **CO2refinery**, upstream processes to produce CO_2, reaction processes to convert CO_2 to valuables, and downstream processes to separate the valuables including recycles and by-product treatment have to be implemented into the process simulator. Due to frequent temperature changes along the process routes, energy integration is a key success factor for the selection of favourable process routes reducing energy consumption and/or energy storage needs. With key process parameters, the material and energy balances at hand, the environmental impact of process routes from cradle to gate or even from cradle to grave can be calculated. Usually, life cycle analysis fed with balancing data from process simulation or experiments is the common approach in this context.

For technologies in stages of early development (low technology readiness level, TRL) as targeted in the proposed PhD works #1 to #7 of **CO2Refinery**, special care must be taken in LCA studies, since most reference technologies are mature and have been optimized over decades. In contrast, low TRL processes usually have higher energy demand or solvent consumption because of not yet established heat integration and/or process optimization.

Key goals and tasks:

PhD #9 will integrate and scale-up all **CO2Refinery** routes into flow sheeting tools to provide consistent material and energy balances for economic and sustainability analysis in close interaction with PhDs #1 to #7. In particular, relevant process steps from providing feedstock streams to conversion steps to products including by-product formation, waste-streams, recycles shall be considered to generate zero-waste process routes and suggestions for circular economy approaches. To follow an open-source software strategy, process simulation and LCA should be implemented into open-source tools, e.g. DWSIM and OpenLCA.

Experience and skills:

- Master level degree in technical chemistry, chemical engineering, physics, mechanical engineering or related discipline.
- Basic experience and interest in process simulation, chemcial thermodynamics, life cycle analysis and/or C/C++/python programming.
- Excellent written and verbal communication skills, and a safe command of English
- Personal skills: independence, creative thinking, systematic and structured work approach, hands-on mentality, team player
- Willingness to participate in teaching and supervision of students
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Supervisors:

Michael Harasek / Bettina Mihalyi / Walter Wukovits