Carbon2Chem®

The Carbon2Chem® Communities

PRE-PROCESSING Simulation | ENGINEERING Process Design | POST-PROCESSING GWI Analysis | POST-PROCESSING Cost Estimation

Simulation Community Developing Cross-industrial Networks

Carbon2Chem® Simulation Community represented by
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If several industrial plants are connected to form a CCU network with the goal of CO_2-reduction, new questions arise regarding their operation. The Carbon2Chem® Simulation Community applies numerical tool chains to predict (1) the production of methanol, urea and other basic chemicals from (2) an unsteady supply of steel mill gases, as well as (3) an unsteady supply of H_2 from renewable energy. A paramount input for the design of such networks is (4) the projection of needed external H_2 and (5) of achieved CO_2 reduction; both are calculated from simulation results. Last but not least simulations deliver (6) the key parameters for techno-economic evaluations.

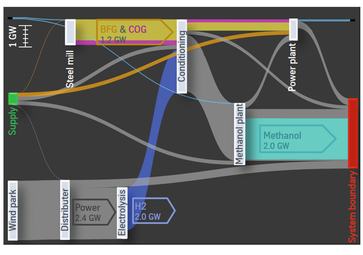
COMMUNITY OF MODELING & TECHNOLOGY EXPERTS

The simulation of networks needs a network of experts. In this spirit, the Carbon2Chem® project has founded four communities working together at different levels of the problem. The Simulation Community actual pools 28 people from scientific and industrial institutions with expertise in:

- Scientific modeling and simulation of process engineering systems, dynamics and control
- Gas cleaning and separation
- Methanol, ammonia and urea processing
- Experimentally based reaction engineering

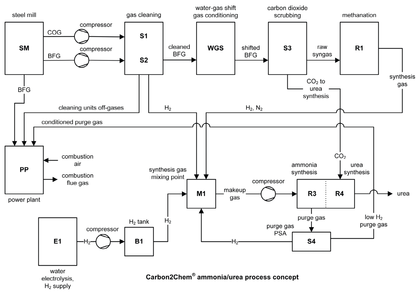
The network simulation model is built from higher level process engineering models, which are parameterized and validated against detailed, precise simulation models, company know-how and experimental data. The simulation community coordinates the expert's activities:

- Collection of data from process design models
- Collection of experimental validated data
- Approval of company know-how and IP
- Discussion and validation of simulation results



Effective energy flow of an example Carbon2Chem® network (from Büker et al.: Verbundvorhaben Carbon2Chem®-L0: System-integration - Teilvorhaben thyssenkrupp AG: Schlussbericht 2020, TIB).

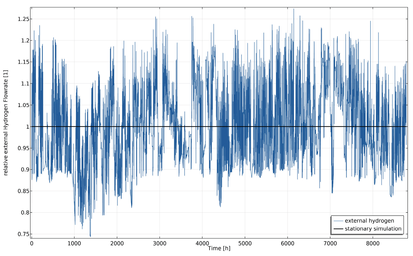
SIMULATION OF THE CROSS-INDUSTRIAL NETWORKS



Simulated cross-industrial network – simplified example

Direct simulation and co-simulation are applied for predicting essential process data:

- Availability and volatility of gas and energy flows
- Design of cleaning, conditioning and compression units
- Utilization of internal H_2 and demand for external H_2
- Advantageous energy and heat integration with steel mill
- Chemical syntheses for several competing products
- Power plant operation and off-gas combustion
- Ecologically and economically optimal distribution of mass and energy utilization in production year



Methanol process – demand of external H_2 in simulated production year, related to the H_2 demand from the stationary simulation case.

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A KEY BUILDING BLOCK FOR THE CLIMATE PROTECTION

CO_2 reduction by cooperation of process industrial sectors