TLK-Thermo GmbH

TLK ENERGY

From Hydrogen Production to Synthetic Fuels
Modeling and Simulation Along the Process Chain

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Motivation

In the context of the energy transition, a wide variety of technical solutions along the entire value chain of CO_2-based Fuels and Chemicals are currently being researched and developed. Using **model-based design, analysis and optimization**, application-specific and efficient solutions can be developed in line with requirements. This work shows how **model-based analysis can efficiently support the development of those systems** regarding the design of components, the optimization of system topologies and the identification of operating parameters. The exemplary system models and simulation results presented have been created in **Modelica** using the **TIL Suite** and **PSL** modeling libraries developed by TLK.

Co-Electrolysis with a SOEC-Stack

Figure 1 shows a simplified Modelica flow diagram of **a SOEC system operated in Co-Electrolysis mode**. The **stack model** is designed such that an **easy adaption of the considered (electro-)chemical reactions**, the transport phenomena in the fluid channels and the membrane-electrode-assembly (MEA) is possible. Models for pure **water-electrolysis** or the **Co-Electrolysis** can be realized. As well, different approaches (**equilibrium and kinetic**) for the reverse water-gas-shift-reaction (WGSR) and the reverse methanation (SMR) are implemented.

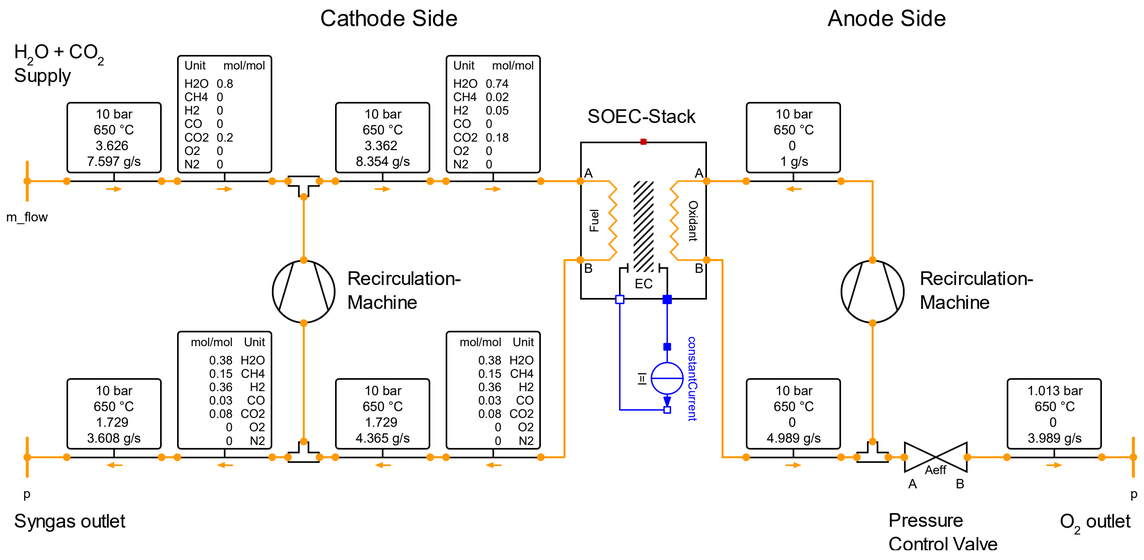

*Figure 1: At the fuel supply, a gas mixture of **CO_2 and H_2O** with a molar mixing ratio of 1:4 flows into the system. At the given mass flow rate, about 1 g/s of CH_4 could be obtained from a perfect methanation of CO_2 and H_2O. In the **SOEC stack** the catalytic **reverse SMR/WGSR** is calculated from an equilibrium reaction model. The electro-chemical reaction (HER/OER) in the SOEC is modeled based on a **Butler-Volmer-Kinetic**. In addition to the **syngas** produced on the fuel side, **highly pure O_2** can be obtained on the oxidant side. Here, a recirculation loop is utilized and uses the produced O_2 itself as sweep gas.*

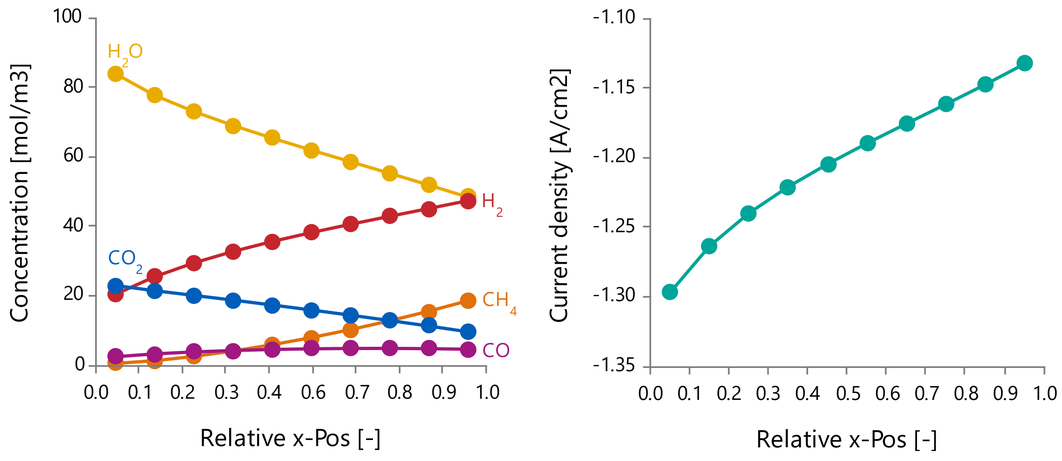

*Figure 2: **Spatially resolved evolution** of the **gas composition** In flow direction of the fuel side channel (left). The corresponding **local current density distribution** (right). The SOEC is operated at 10 bar and 650 °C*

The model **enables studies, for example, of syngas composition dependency** on the feed gas composition, operating pressure and temperature, current densities as well as geometric parameters of the SOEC-Stack. Therefore, it allows for a **model-based optimization of design parameters and operating conditions**.

Direct Air Capture

Direct Air Capture (DAC) is a technology that reduces atmospheric CO_2 levels by capturing it directly from the air. The **captured CO_2** can then be used as a raw material in processes like **methanol synthesis**.

One method for DAC is the adsorption of CO_2 on **amine-functionalized solid adsorbents** in **temperature-vacuum swing adsorption (TVSA)** processes. Current research focuses on reducing the energy consumption and enhancing the adsorption rate of this process to reduce the cost per captured ton of CO_2.

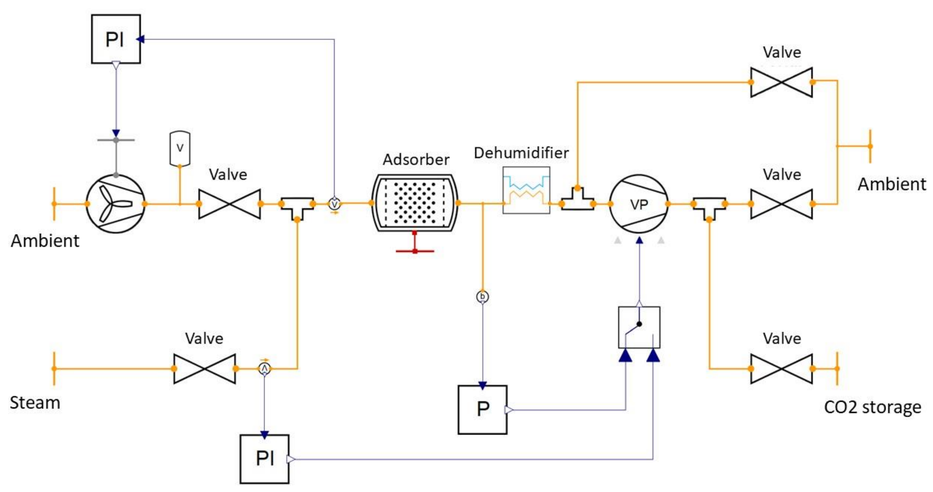

*Figure 3: Flow diagram of the **temperature-vacuum swing adsorption (TVSA) direct air capture** process implemented in Modelica*

Dynamic system simulation helps optimizing the process, by enabling the analysis of various parameters on the process performance. For example, varying the adsorber length while keeping the volume and adsorbent mass constant can reveal optimal configurations. As shown in Figure 4, longer adsorbers offer higher adsorption rates but require more energy compared to shorter ones.

These **insights allow for selecting an optimal adsorber length** based on specific needs, balancing efficiency and energy use.

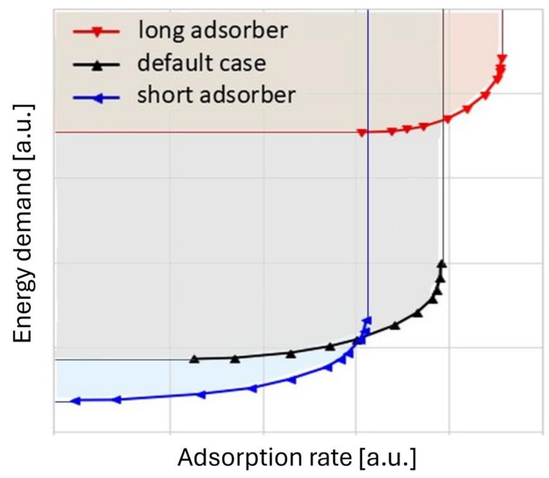

*Figure 4: **Pareto-curve of an optimized DAC** process. The trade-off between exergy consumption and adsorption rate is shown for different adsorber lengths*

Synthesis of Sustainable Fuels

Methanol serves as an **efficient liquid hydrogen carrier**, facilitating storage and transportation, and acts as a base chemical in processes like **Methanol-to-Olefins (MTO).** As future energy systems become more dynamic, flexibility in operation is crucial to enable adaption to fluctuating demands and decentralized production.

Dynamic simulation plays a vital role in understanding plant behavior under varying conditions. By considering factors such as **kinetic reaction rates**, **fluid inertia**, and **control strategies**, these simulations help optimize plant design and operation.

The insights enable the development of demand-side management strategies that ensure process performance while adapting to energy demands. This know-how is essential for designing resilient energy systems that integrate renewable sources and respond effectively to demand fluctuations.

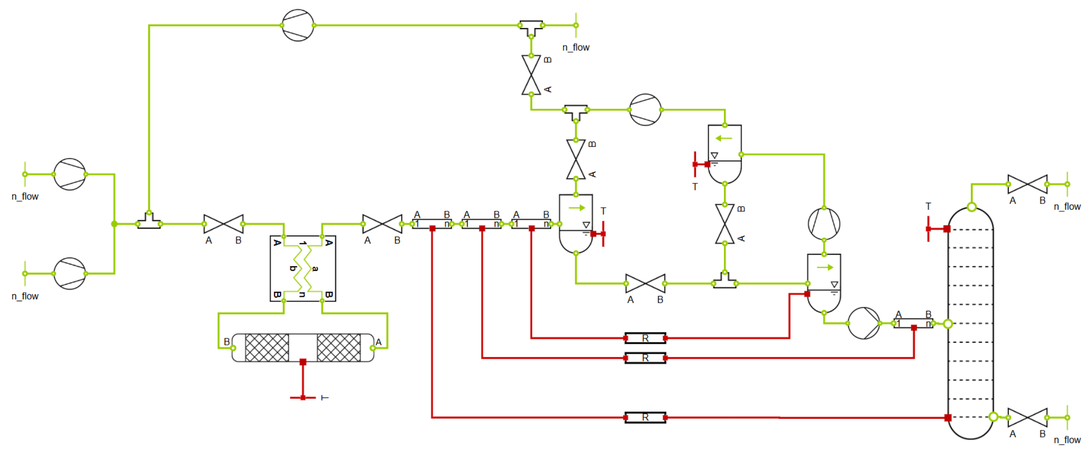

*Figure 5: Flow diagram of the **Methanol synthesis process***

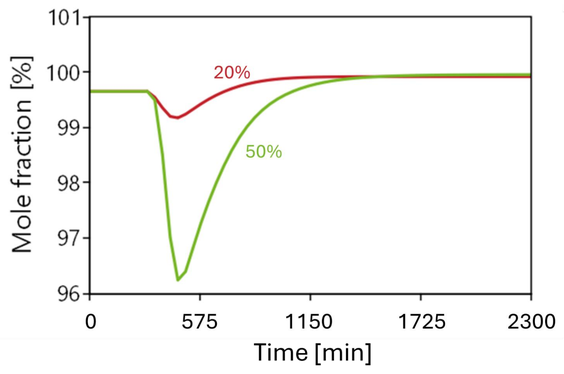

Figure 6: Impact of a feed flow rate reduction of 20% and 50% on the methanol purity at the system outlet

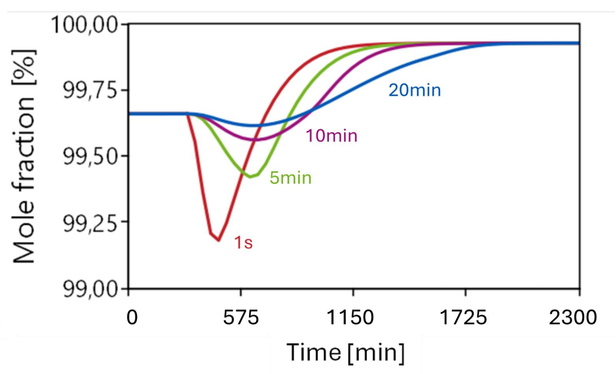

Figure 7: Impact of a feed flow rate reduction of 20% applied at different time intervals on the methanol purity at the system outlet

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