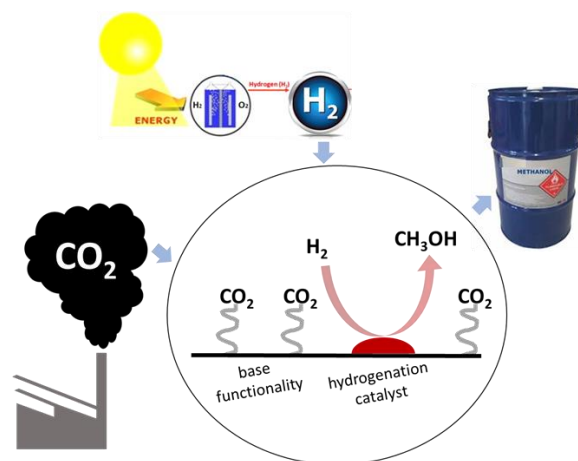


Hydrogenation of CO₂ to Methanol under Dynamic Reaction Conditions: A Novel Concept for Carbon Capture and Utilization

Background: Carbon Capture and Utilization (CCU) will be one of the concepts required in the future to limit the CO₂ emission from the combustion of fossil fuels for a sustainable energy supply. For coal fired power plants (due to the high levels of CO₂ in the flue gas as the C/H ratio is the highest among all fossil fuels) sorption concepts are currently under investigation, which are based on amine functionalized liquid and solid sorbents. The hydrogenation of CO₂ by using hydrogen produced by renewable electricity is an attractive approach for the chemical recycling of CO₂ to energy carriers or chemicals.



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Project: The concept proposed allows to directly convert CO₂ into fuel components and large scale bulk chemicals. H₂ will be used to regenerate the solid, base functionalized sorbent and will be directly converted with the liberated CO₂ from the sorption unit to MeOH. This intrinsically dynamic process will be followed via two concepts: (i) CO₂ bound/activated as carbamates on the basic sites of the sorbent will be directly converted to MeOH or (ii) CO₂ will be thermally removed from the solid sorbent and then converted in a separate, downstream reactor using a low temperature MeOH synthesis catalyst. Both approaches are inherently dynamic on two time scales: One is the periodic switching between loading and releasing CO₂ from the sorber columns (minutes). The other process is the dynamic availability of the CO₂, which is coupled to the electricity demand from fossil fuel based power plants in the electric grid, in the time scale of hours or even days. Our research focus on the kinetic modeling of the methanol synthesis over the selected catalyst that will lead to detailed elementary-based within the mean field approximation that can successfully predict the catalyst performance under dynamic conditions. Additionally, combined experiments of sorption/desorption-reaction using the hybrid material (sorbent-catalyst) under relevant conditions lead to the investigation of the coupling of the kinetics of the two processes (desorption and catalytic reaction). The rates of reaction, transport and sorption under dynamic conditions will be related to facilitate an effective conversion of CO₂ and H₂ to methanol. A critical point for the success of this concept is the tailoring of the sorption strength of CO₂ on the base sites with respect to the reactivity as the CO₂ should not be released from the basic sorption sites before it is converted to methanol. On the other hand binding should not be too strong to limit the reactivity. Thus, the development of accurate kinetic models of the sorption-desorption of CO₂ as well as of the catalytic conversion to methanol is required. Furthermore, the consideration of mass and heat transport is critical in the successful description of the combined process.

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