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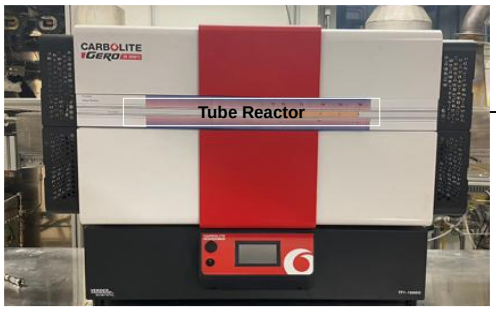
The reverse water-gas shift reaction

Investigation of the reaction with nickel and perovskite based catalysts

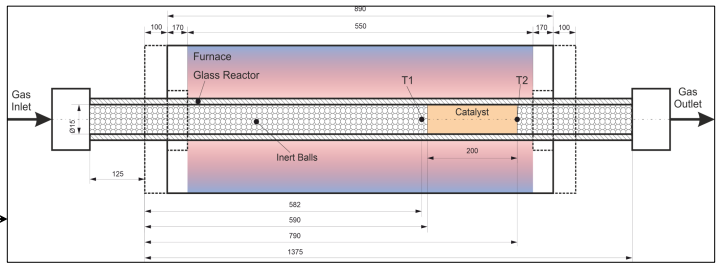
The reverse water-gas shift (rWGS) reaction is a key technology in Power-to-liquid (PtL) processes, converting carbon dioxide and hydrogen into synthesis gas for the production of chemicals or fuels. At the Chair of Process Technology and Environmental Protection, the rWGS reaction is investigated on a laboratory scale with various catalysts, in collaboration with the Chair of Physical Chemistry for catalyst development.

Experimental setup

The experimental setup consists of a catalytic medium filled quartz glass tube reactor positioned in a tubular furnace, a cooler and a gas analysis unit.



Furnace

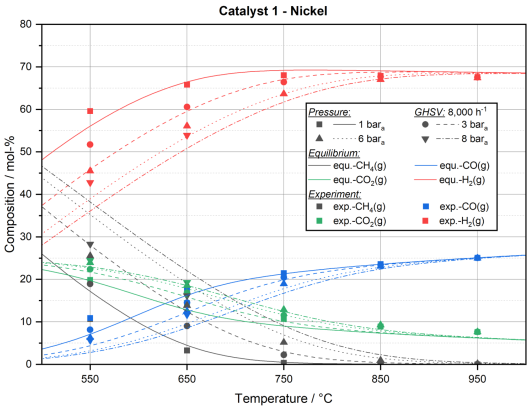


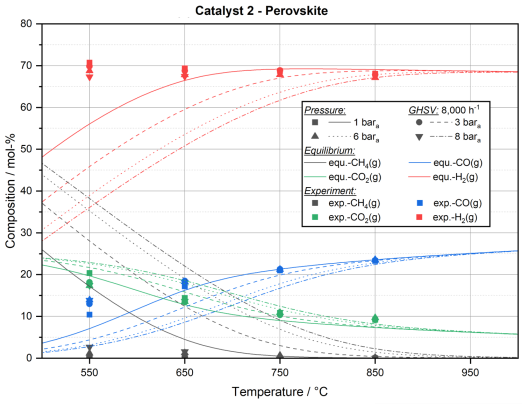
Operation conditions:

- 8 bara for T = 550 and 650 °C
- 6 bara for T = 750, 850 and 950 °C
- GHSV of 8000 and 20 000 h^{-1}

GHSV ... Gas hourly space velocity

The influence of the operating conditions on the product gas composition, the selectivity of carbon monoxide formation, as well as the occurrence of undesirable side reactions, were compared for a Ni/Al_2O_3 and perovskite-based catalyst.





Results and discussion

For the Ni/Al_2O_3 catalysts, undesired methane formation occurs notably at low temperatures of up to 650 °C and 1 bara, whereas this unwanted reaction is mostly suppressed on perovskite catalysts. At 8 bara and 550 °C, perovskite catalysts exhibit comparatively low methane formation, maxing out at 2.7 vol.-%, in contrast to nickel catalysts with approximately 28 vol.-%.

The results show that perovskite catalysts exhibit great potential for rWGS reactions related to Power-to-liquid processes, leading to further investigations in an upcoming project.

Chair of Process Technology and Environmental Protection

Research devision: Energy Process Engineering

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Comparative Techno-Economic Assessment of CO_2-Based SAF Pathways: Fischer-Tropsch, Methanol-to-Jet and Ethanol-to-Jet Across Three Global Regions: EU, USA and Middle East

Severin Sendlhofer, Willy Duan, Raphael Allgäuer, Markus Maly[a], Robert Paulnsteiner[a], Dominik Wimmer[a], Christoph Markowitsch

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Introduction

Aviation accounts for around 2.4% of global CO_2 emissions, and demand is expected to grow significantly by 2050. Although sustainable aviation fuels (SAFs) are considered a key mitigation strategy, comparative techno-economic insights across different production pathways and regions remain limited. This study provides a harmonized techno-economic assessment (TEA) of three power-to-liquid (PtL) routes for e-kerosene production: Fischer-Tropsch synthesis (FTS); methanol-to-jet (MtJ), with two variants: syngas-based via reverse water-gas shift (MtJ-1) and direct CO_2 hydrogenation (MtJ-2); and ethanol-to-jet (EtJ) via direct CO_2 gas fermentation. All pathways were modelled in Aspen Plus V14® with subsequent upgrading to kerosene-range hydrocarbons and a custom TEA tool was used for techno- economic evaluation. Regional scenarios were assessed for Europe, the USA and the Middle East.

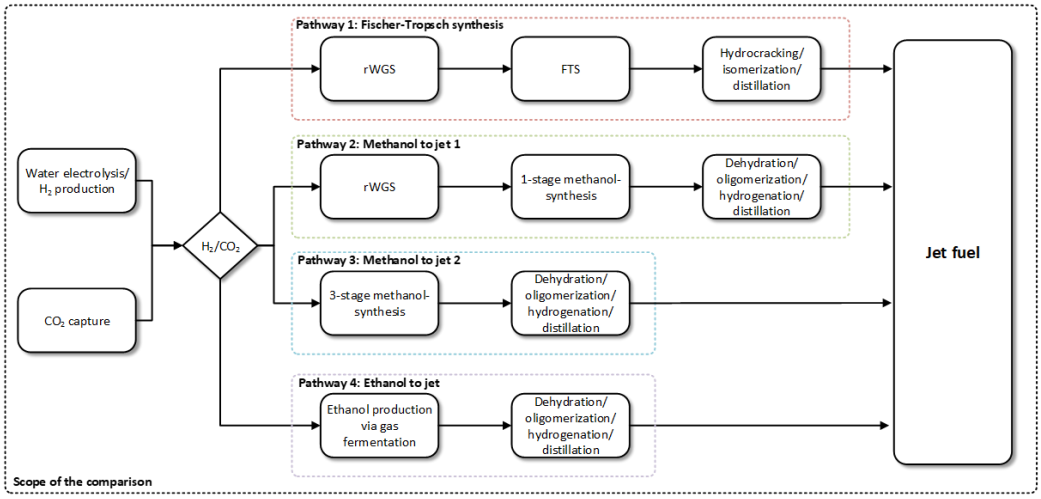

Figure 1 - Scope of the comparison and overview of the investigated pathways

Results

The results show that electrolysis accounts for 55-80% of capital expenditures, rendering hydrogen production a decisive cost driver. Net production costs (NPCs) range from 2.8 to 8.2 USD per kg of SAF across all pathways and regions, exceeding the cost of fossil Jet A-1 fuel (approximately 1 USD per kg) by at least a factor of three.

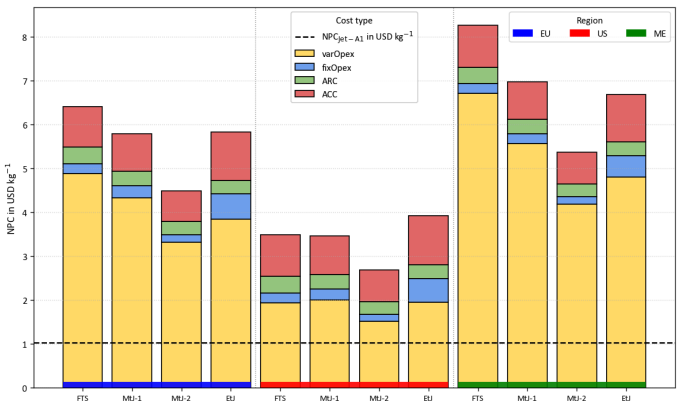

Figure 2 - Cost breakdown of the NPC for all scenarios

MtJ-2 consistently emerges as the most cost-efficient pathway, with NPCs of around 2.8 to 5.3 USD per kg, while FTS performs worst due to extensive tail gas recycling loops and low single-pass CO conversion. EtJ exhibits intermediate performance, but faces uncertainties linked to large-scale gas fermentation. The carbon and energy efficiencies con-firm this trend, at 56-63% and 48-54% respectively for alcohol-based routes versus 42% and 50% for FTS.

Conclusion

In summary, the study shows that the choice of pathway is less important than the cost of green hydrogen. Nevertheless, pathway complexity matters. MtJ and EtJ involve multiple conversion steps, whereas FTS is structurally simpler, but suffers from low selectivity and high recycle demands.

Supportive policies and financial instruments remain crucial. While the US Inflation Reduction Act offers tax credits for low-carbon hydrogen and SAF, the EU focuses more on quota obligations (RED III) and direct subsidies (Innovation Fund, IPCEI Hydrogen). In both cases, PtL-SAF can only become cost-competitive with fossil jet fuel if electricity prices decrease and electrolysis technology matures.

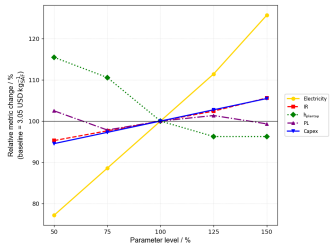

Figure 3 - Sensitivity analysis of the key parameters conducted for the MtJ-2 US case

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VTiU Verfahrenstechnik des industriellen Umweltschutzes

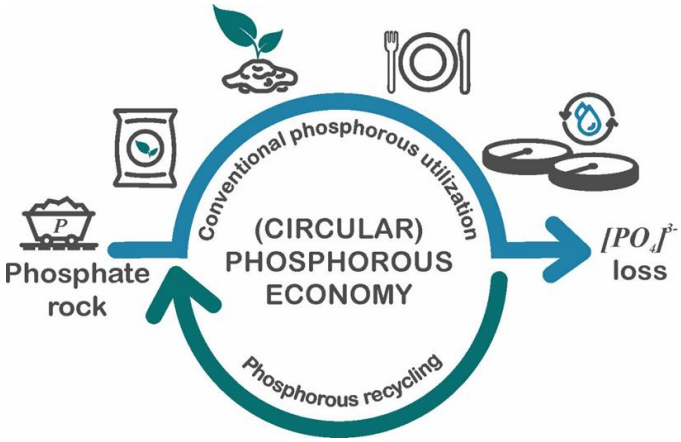
Mining Phosphorus from Wastewater

Biogenic Waste Streams as a Sustainable Resource for Critical Raw Materials

Recovery rates of more than 90% from effluents reveal a great potential for future phosphorus recycling in addition to conventional mining, energy-intensive efforts based on sewage sludge ash recycling and struvite precipitation!

Closing the Loop…

Conventional phosphate sources are significantly detrimental to the environment and lead to economic and political dependencies of the European Union on third party countries where it is mined. On the other hand, phosphorus passes through our value chain only once before it is lost to the environment again via wastewater leading to severe eutrophication or has to be disposed of with sewage sludge at considerable expense.

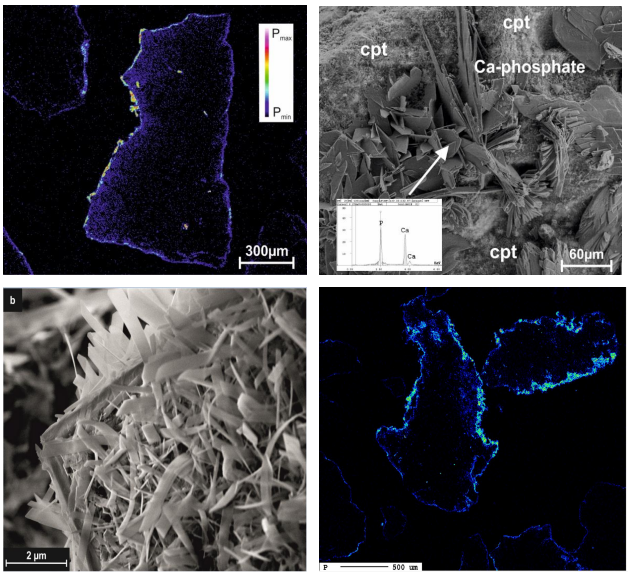


The final strategy has not yet been found…

Various approaches to prevent phosphate losses along the value chain are still under investigation, and no definitive solutions have yet been established. Recycling technologies like burning sewage sludge and leaching P from its ashes require high energy demands and are currently far from reasonable costings. Struvite precipitation depends strongly on phosphorus concentration and requires high chemical input to modify the entire wastewater stream.

The Process…

A novel process to selectively recover PO_4^{3-} without interfering wastewater treatment processes was developed. In a 20' container plant the wastewater is contacted with modified natural zeolites (cpt) during which zeolitic Ca precipitates with the phosphate on the zeolite's surface, facilitating easy recovery by acid flushing. The zeolites are alternately loaded and acid-flushed to gain a sustainable and concentrated phosphate solution.



Highlights…

- **low energy demand** – just ambient temperatures
- **low chemical input** – no influence on wastewater
- **safe product handling** – liquid product
- **minimal waste** – zeolites are regenerable
- **minimal operation requirements**

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Learning from Earth processes to engineer sustainable ones!

Pyrolysis behavior comparison of wood samples using simultaneous thermal analysis

Simon Moll[1], Elias Vigl[1], Jasr Negm[2], Nina Schlemmer[3], Fritz Kittinger[1]

Abstract

Slow pyrolysis behaviour of different mid-european wood samples is compared with bamboo samples by thermogravimetric analysis (TG) and differential scanning calorimetry (DSC). Significant differences in the heat of reaction during the main pyrolysis stage were observed for the coniferous wood and the bamboo samples. To investigate a potentially catalytic effect of inorganic constituents on bamboo pyrolysis, the corresponding ashes were chemically analyzed, and spruce samples were impregnated with selected salts and subsequently subjected to thermal analysis. The results provide indications that sodium and potassium ions and/or chloride ions may indeed catalyze the pyrolysis process in bamboo.

Methodology

Different mid-european wood samples (larch, pine [Pinus cembra, Pinus nigra], spruce, beech) are compared with bamboo samples (moso [Phyllostachys pubescens], tonkin [Arundinaria amabilis], tutul [Bambusa maculata], wulung [Gigantochloa atroviolacea]) regarding their slow pyrolysis behavior. Analysis material is extracted from the sapwood area. Lamellae of 3±1 mm thickness are cut from the bulk with a circular saw. Disks of 5 mm diameter are punched out of the lamellae and used for the pyrolysis investigation. Experiments are performed in a simultaneous thermal analysis setup (TG/DSC) of type Netzsch STA 449 C in alumina crucibles without lid. Experimental conditions are identical for each sample run: a continuous nitrogen gas flow of 60 mL/min (20 mL/min protective gas + 40 mL/min purge gas, purity 5.0), a heating rate of 20 K/min to 105 °C, followed by a holding time of 1 h (so that each sample is pyrolyzed from its dry state) and lastly a ramp of 20 K/min to 850 °C (pyrolysis end temperature).

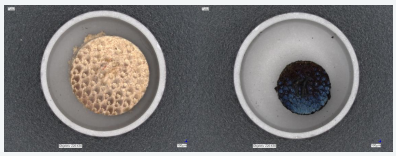

Fig.1: Exemplaric photographs before and after STA of tutul bamboo

Results

The analysis results are split into the mid-european and the bamboo samples (figure 2). The temperature ranges from 150—550 °C. In the first row, the mass loss and in the second row the DSC signals are given for each sample, respectively. While the main pyrolysis phase is endothermic in the case of all coniferous wood samples, beech wood and all bamboo species studied exhibit exothermic behavior with two stages.

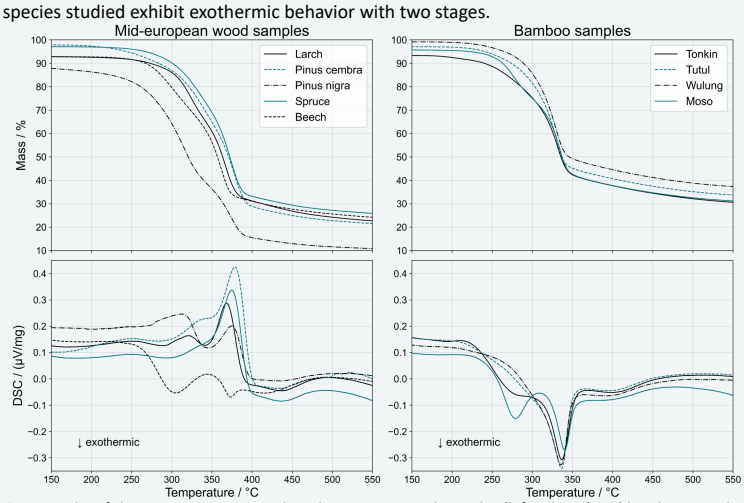

Fig.2: Results of the STA experiments with mid-european wood samples (left column) and bamboo samples (right column). First-row: TG signal; second row: DSC signal.

References

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Investigation on possibly pyrolysis-catalyzing compounds

To further investigate the reasons for the differing thermal behaviour of coniferous wood and bamboo samples, spruce samples have been impregnated with inorganic salts, that were selected based on the bamboo and spruce wood elemental composition. The loss on ignition (LOI) of the samples was determined (LOI_{spruce} = 99.76%; LOI_{tutul} = 97.91%), followed by analysis of the resulting ashes using energy-dispersive X-ray spectroscopy (figure 3).

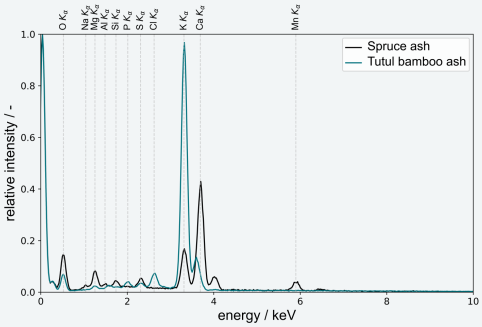

Fig.3: Normalized energy-dispersive x-ray spectra of the spruce (black) and tutul (green) ashes obtained in a SEM-EDS (Tescan Vega 1)

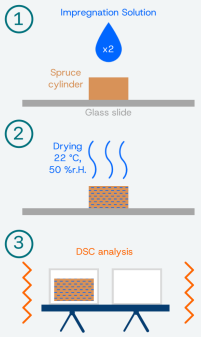

Fig.4: Schematic illustration of experiment conduction

Cylinders of spruce wood (23±1 mg) have been impregnated with 48±4 mg of solutions containing 10 g/L KCl, 8 g/L NaCl (equimolar to KCl; cation substitution), 1 g/L K_2HPO_4 and 0.8 g/L KH_2PO_4 to mimic the bamboo chemistry (step 1 in figure 4). To check, if a halide anion substitution has an effect, another sample was impregnated with 22 g/L KI (equimolar to KCl). After drying at room conditions (step 2), DSC analyses have been performed (step 3). TG and DSC results of the pyrolysis experiments (same conditions as the initial experiments, deviating only in the heating rate of 10 K/min) are shown in figure 5. It is evident, that the potassium and sodium halides are responsible for the trend reversal in the heat of reaction.

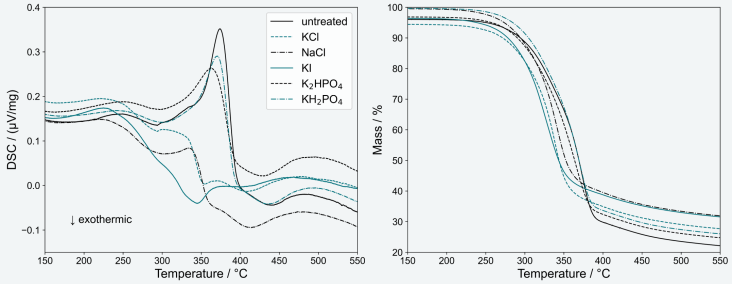

Fig.5: Results of the STA experiments with salt-impregnated spruce samples.

Discussion and Conclusion

Considering the inverse thermal behaviour (endo– vs. exothermal reaction) in the pyrolysis between 225—450 °C of the investigated conifers against the bamboo samples and beech (fig 2), the underlying mechanism of pyrolysis must be substantially different.

As the experiments are performed without lid and thus, the volatile products readily leave the furnace to the gas cuvette, secondary heterogenous carbonation reactions do not seem responsible for the exothermic bamboo pyrolysis. The reason for the difference in heat of reaction could be found in the variation of hemicellulose, cellulose and lignin content of the wood samples, as each of the compounds show differing behavior during pyrolysis [1].

Former studies [2,3] link a catalyst dependent exothermicity of the cellulose pyrolysis to an enhanced char formation, this trend can also be observed in figure 5; samples with higher exothermicity in the DSC show lower mass losses in the TG signal. Basic compounds like NaOH and Na_2CO_3 have frequently been shown to favor char formation [2]. Due to the high hygroscopicity of this compounds, excess water might play a major role in the regarding pyrolysis mechanism.

The findings of this study show that the effect of the anionic species of the catalytically active material is not neglectable. Phosphate (K_2HPO_4 and KH_2PO_4) impregnated samples show no significant exothermicity, whereas the influence of the halides (KCl, NaCl, KI) is clearly visible. Using the HSAB concept, the lewis-basicity can be arranged as follows: H_2PO^{4-} << Cl^- < I^- << HPO_4^{2-}. The basicity alone can therefore not be the reason for the resulting trend. Study [3] indicates, that the formation of the dominant primary decomposition product of cellulose, levoglucosan ($C_6H_{10}O5$), is almost totally supressed if alkaline or alkaline earth chlorides are added — even at low concentrations of 5 mmol/mol glucose-unit. Combining this information together with the findings in this study, the halide ions might be catalytically involved in a chain reaction favoring the exothermal combination of radicals to high MW products (char).

The increased chloride and potassium content in bamboo wood could therefore explain not only the exothermicity during pyrolysis, but also the higher charcoal yield. Furthermore, it is suggested, that the increased potassium content in bamboo wood catalyzes the pyrolysis and yields higher char residue (lower mass loss during tutul experiment).

Characterisation of structured packings for increased efficiency in carbon capture processes

INTRODUCTION

Carbon capture using chemical absorption represents a key technology for reducing industrial CO_2 emissions. A wide variety of structured packings is available on the market, many of which are specifically designed for absorption processes. However, reliable and comparable data describing their performance in real carbon capture systems is still limited. This leads to uncertainties in the selection and design of column internals for industrial applications.

OBJECTIVE

The aim of this work is to characterise structured packings based on standardised test systems using the pilot plant "Packed column" (see Fig. 1) and to transfer these results to real carbon capture processes. By incorporating relevant physico-chemical properties, such as diffusion coefficients and Henry constants, the actual performance of the packings in industrial absorption systems is approximated. In addition, the study seeks to identify limiting mass transfer resistances and to derive a systematic approach for selecting suitable packing structures.

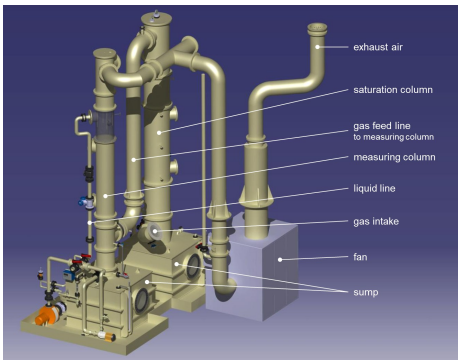

Fig. 1: Model of the pilot plant an the Montanuniversity of Leoben [1]

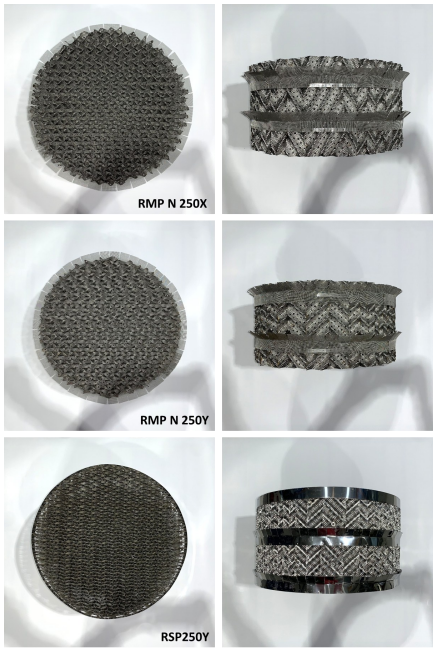

Fig. 2: Different investigated packing structures

METHODOLOGY

Three structured packings (see Fig. 2) are investigated with regard to their mass transfer performance. Experimental and literature-based data obtained from standardised systems are adapted to real absorption conditions by accounting for fluid properties and reaction kinetics. The analysis is based on established mass transfer models, in particular the two-film theory (see Fig. 3), allowing a consistent description of transport phenomena in both phases.

KEY FINDINGS

A central outcome of this work is the determination of a local resistance distribution along the packing height.

This approach makes it possible to identify the dominant mass transfer limitations within different sections of the column. It is shown that the prevailing reaction regime can change significantly over the column height, which directly influences the effectiveness of a given packing structure.

INDUSTRIAL RELEVANCE

The presented methodology enables a more realistic evaluation of structured packings under industrial conditions. By linking standardised measurements with actual process properties, it provides a practical basis for improving column design and operation. In particular, the results indicate that changes in the reaction regime may require the targeted use of different packing structures, offering new potential for increasing the overall efficiency of carbon capture processes.

CONCLUSION

The combination of experimental characterisation, property-based adaptation and resistance analysis forms a coherent framework for assessing and optimising structured packings. This approach not only enhances the understanding of mass transfer behaviour but also supports the development of more efficient and application-specific carbon capture systems.

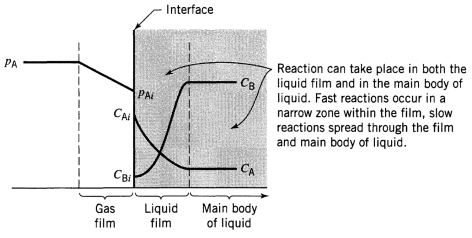

Fig. 3: Scheme of the two-film-theory in case of chemical absorption [2]

References:
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KEYWORDS

Carbon Capture
Chemical Absorption
Structured Packings
Mass Transfer
Process Optimisation

VTiU Verfahrenstechnik des industriellen Umweltschutzes

ANDRITZ

From Measurement to Comparability: Standardizing Packing Characterization Across Facilities

INTRODUCTION

Reliable mass-transfer data are essential for the design, scale-up and modelling of absorption columns. Although standardized guidelines such as VDI 2761-2 exist, significant discrepancies between datasets from different laboratories are still observed. These inconsistencies limit the transferability of experimental results and reduce confidence in simulation and design approaches.

RELEVANCE

Reliable and comparable packing data are crucial for:

- Design of absorption columns
- Validation of rate-based models
- Development of data-driven / ML approaches

The presented work provides a framework to improve data consistency and supports more reliable process design and scale-up.

MOTIVATION

What if identical packings yield different mass-transfer coefficients depending on the pilot plant used?

This question highlights a central challenge:

Comparability cannot be ensured by standards alone. Differences in experimental setups, sampling strategies and test systems continue to influence the results significantly.

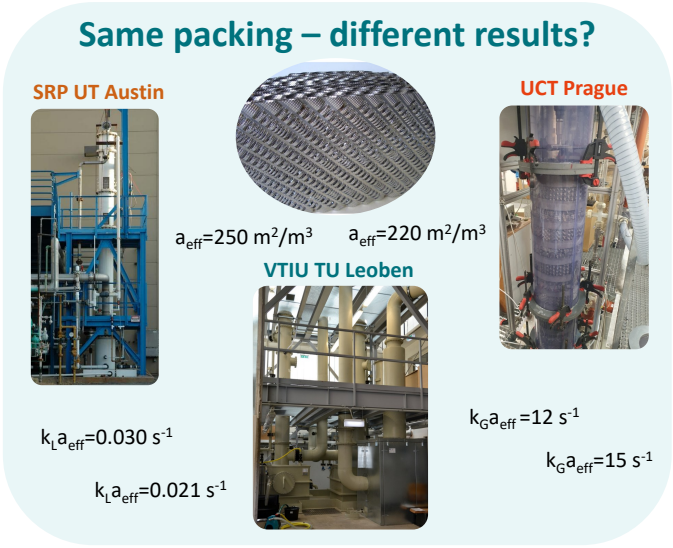

Fig.1: Even under comparable conditions, significant deviations in mass transfer parameters are observed across pilot-scale facilities.

KEY FINDINGS

The results demonstrate that even under nominally identical conditions, deviations in mass-transfer parameters persist between pilot-scale facilities. These differences are primarily caused by methodological influences, in particular:

- end effects and their treatment
- sampling location and phase accessibility
- choice of test systems
- facility-specific design and operation.

At the same time, consistent trends across all facilities confirm that comparability is achievable.

APPROACH

In this work, a systematic comparison of packing characterization data obtained at three leading pilot-scale facilities is performed:

- TU Leoben (Austria)
- SRP at UT Austin (USA)
- UCT Prague (Czech Republic)

A key aspect of this study is the harmonization of experimental procedures across facilities, supported by direct collaboration and knowledge transfer. By combining new measurements with carefully selected literature data, a consistent basis for comparison is established.

CONCLUSION

This study shows that true comparability in packing characterization requires more than standardized procedures. An integrated and transparent experimental strategy is needed to account for facility-specific influences and parameter sensitivities.

The derived recommendations contribute to improved harmonization and form a basis for future best-practice guidelines.

References:

VDI 2761-2: Chemical separation processes - Measurement and evaluation of fluid dynamics and mass transfer in packed columns - Absorption and desorption

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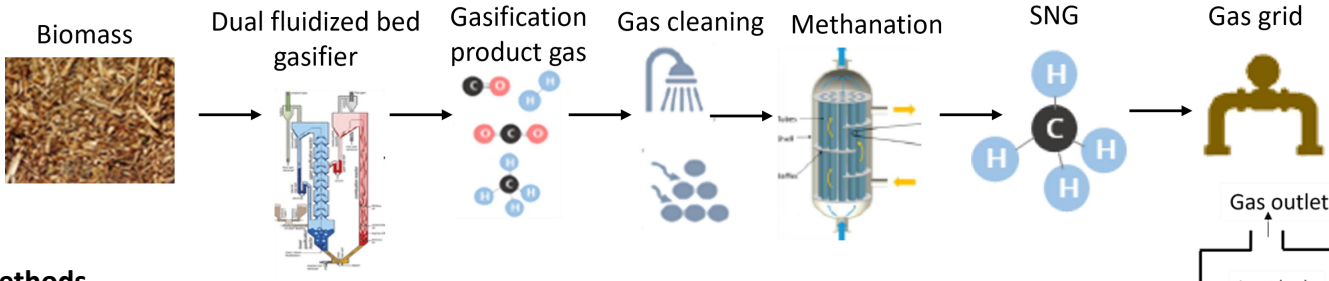
KEYWORDS

Packing Characterization
Data Comparability
Standardization
Mass Transfer
Pilot Plants
End Effects

Catalytic methanation of biomass gasification product gas - Role of lighter hydrocarbons

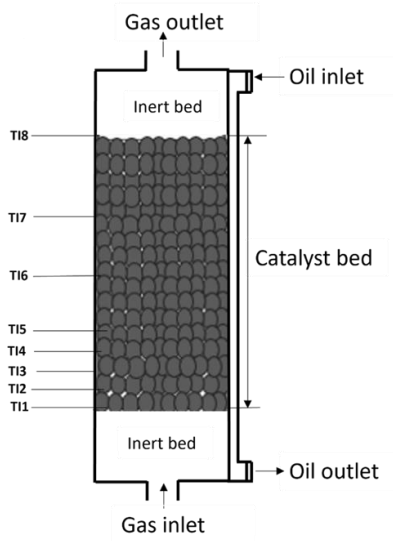
Marija Jeremić, Andreas Krammer, Markus Lehner

The production of synthetic natural gas (SNG) from biomass is a promising route for renewable energy storage and gas grid decarbonization. In a dual fluidized bed reactor (DFB), biomass is converted into syngas (H_2, CO, CO_2, CH_4, and trace components). During methanation, CO and CO_2 react with hydrogen to form CH_4 and water, releasing significant heat. This study investigates the role of lighter hydrocarbons in catalytic methanation.



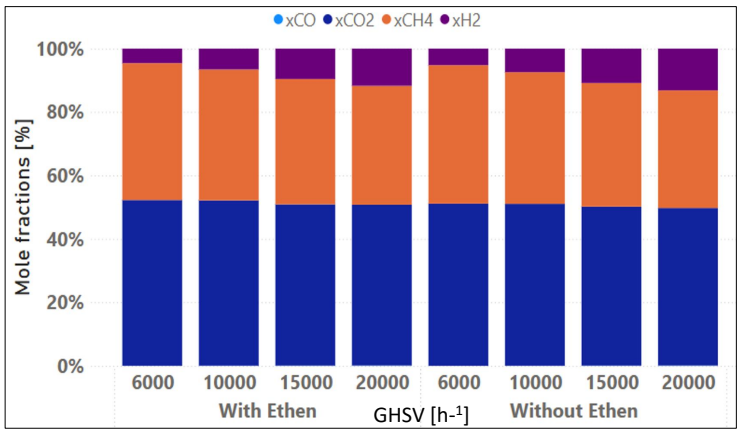
Methods

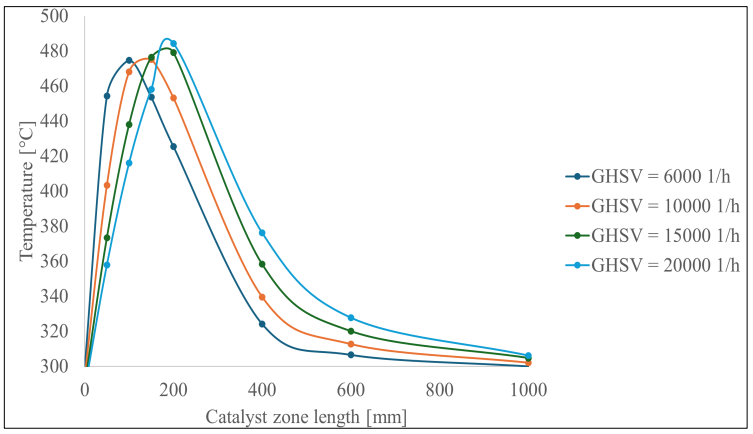
- Experimental investigations conducted in a lab-scale methanation unit with thermal oil-cooled shell-and-tube reactor
- Use of a nickel fixed-bed catalyst
- Eight thermoelements placed along catalyst zone for temperature measurement
- Variation of operating parameters such as reactor pressure, GHSV, and oil temperature



Results and Discussion

- Ethene increases methane production (due to hydrogenation of ethene)
- Temperature peaks indicate strong exothermic behavior
- Hot spot at reactor inlet
- GHSV shifts reaction zone





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VTiU Verfahrenstechnik des industriellen Umweltschutzes

Modelling a Reverse Water-Gas Shift Reactor with an Artificial Neural Network

Introduction and methodology

Process intensification of the endothermic reverse water-gas shift (RWGS) reaction as given in Equation 1, computational modelling represents a methodological approach. While detailed simulations provide valuable insights into process conditions, reactor optimization and control are often highly cost-intensive. In contrast, simplified reaction models offer reduced computational demand but at the expense of accuracy, thereby limiting their predictive capability for syngas (CO and H_2) formation and downstream applications such as sustainable aviation fuel (SAF) production via Fischer-Tropsch synthesis (FTS). As shown in Figure 1, 416 data points from a tubular rWGS fixed-bed reactor were pre-processed, scaled, and split into training (90%) and test (10%) datasets. An artificial neural network (ANN), was built with Scikit-learn in Python to predict both CO_2 conversion and CO selectivity with features: temperature, pressure, H_2:CO_2 ratio & gas hourly space velocity (GHSV)).

$$CO_2 + H_2 \leftrightarrow CO + H_2O$$
$$\Delta H_R° = 41\ \text{kJ mol}^{-1}$$

Equation 1 – Reverse water-gas shift reaction and endothermic reaction enthalpy

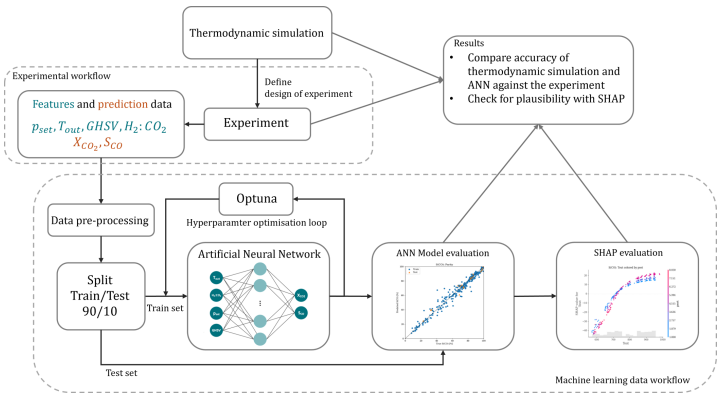

Figure 1 – Workflow for developing and interpreting a data-driven rWGS model

Results and discussion

The ANN gives model predictions with mean absolute errors (MAE) of 1.86% in training and 2.73% on the test set for both conversion and selectivity outputs. The comparison of equilibrium, ANN model, and experimental data in Figure 2 shows clear differences in prediction accuracy across the temperature range. For CO_2 conversion, the ANN reproduces the experimental trend with lower deviation than the equilibrium model, especially in the kinetically limited regime below ~750 °C. In this range, side reactions such as methanation affect the outcome. For CO selectivity, the ANN model follows data more closely than equilibrium, particularly between 600-750 °C, where equilibrium strongly overpredicts selectivity. SHAP analysis in Figure 3 identifies temperature as the dominant driver for both CO2 conversion and CO selectivity, consistent with the endothermic nature of the rWGS reaction.

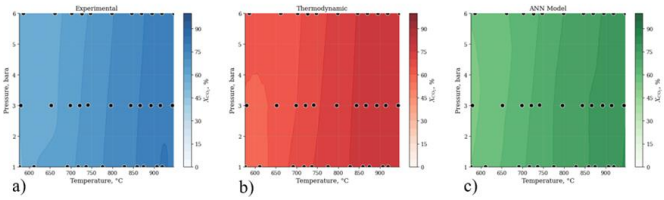

Figure 2 – Comparison of experimental data, thermodynamic equilibrium, and ANN predictions

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Research focus: The research focus lies on the development of sustainable aviation fuels (SAFs), particularly on the direct conversion of alcohols into synthetic kerosene.

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CO_2 Sequestration via Mineral Carbonation of Biomass Gasification Residues

Mineral carbonation describes the reaction of Ca- or Mg-oxides with CO_2 to form stable carbonates, providing a promising pathway for long-term carbon storage.

$$Ca/MgO + CO_2 \rightleftharpoons Ca/MgCO_3$$

A potential process route is **direct aqueous carbonation**, in which reaction kinetics are enhanced by dissolving Ca^{2+} or Mg^{2+} ions from a solid feedstock into a liquid phase, where they subsequently react with CO_2.

Due to their high content of Ca- and Mg-bearing minerals, residues from biomass gasification are among the suitable feedstocks for this process.

As biomass gasification is expected to gain importance, the CO_2 storage potential of three byproducts from dual fluidized bed gasification (DFB) of waste wood are investigated during aqueous carbonation at a CO_2 partial pressure of 5 bar.

- **Gasification fly ash (GFA):** Fly ash separated from product gas cyclone
- **Used bed material (UBM):** Mixture of olivine (Mg_2SiO_4) and lime (CaO)
- **Combustion fly ash (CFA):** Fly ash separated from flue gas downstream the DFB system

Characterization: X-Ray Florescence Analysis (XRF)
Thermogravimetric Analysis (TGA)

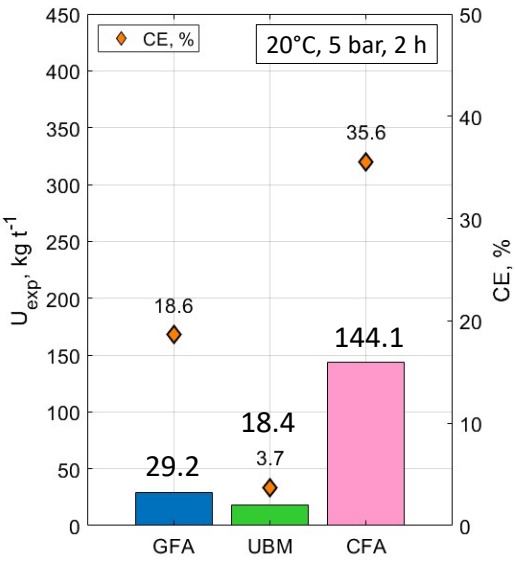

Fig. 1: Experimental CO_2 uptake (U_{exp}) and carbonation efficiency (CE), defined as the ratio of U_{exp} to the theoretically achievable maximum uptake (U_{th})

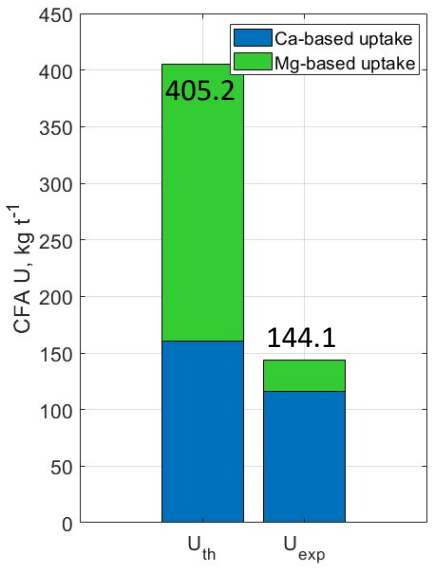

Fig. 2: Contribution of Ca- and Mg-bearing minerals to U_{th} and U_{exp} of the CFA sample

A maximum CO_2 uptake of 144 kg CO_2 per ton of feedstock is obtained for CFA at these conditions (Fig. 1). Carbonation is mainly driven by Ca-bearing phases, while Mg-bearing minerals contribute marginally (Fig. 2) due to their higher stability (e.g., olivine). Accordingly, the lower Ca-content in GFA and UBM is reflected in their reduced CO_2 uptake.

Intensified process conditions are expected to enhance Mg-phase carbonation and further increase CO_2 uptake, highlighting the need to tailor process conditions to the dominant mineral phases.

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