

Final Report

Interaction of catalytic chemistry and transport inside and around porous catalyst pellets for CO₂ methanation under enforced dynamic operation

1 General Information

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Project title: Interaction of catalytic chemistry and transport inside and around porous catalyst pellets for CO₂ methanation under enforced dynamic operation

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2 Summary / Zusammenfassung

This collaborative research project aimed to fundamentally study the dynamic interaction of catalytic chemistry, heat and mass transport within and around porous catalyst pellets during CO₂ methanation under enforced dynamic operating conditions. To elucidate this behavior at the pellet scale, *in-situ* experiments using a novel Single-Pellet Profile Reactor (SPPR) were combined with detailed particle-resolved Computational Fluid Dynamics simulations (PRCFD).

The experimental contribution (Horn group, TUHH) included the construction of a lab-scale SPPR, which for the first time enabled the simultaneous measurement of radial concentration profiles with a movable capillary and the surface temperature via infrared (IR) thermography under industrially relevant conditions up to 400 °C. Initial findings with Ni/γ-Al₂O₃ pellets revealed significant internal CO₂ concentration gradients despite stoichiometric inlet conditions, while H₂ profiles were flatter due to higher diffusivity. Axial temperature gradients on the pellet surface were detected, attributed to the surrounding boundary layer and external heat transfer resistance to the gas. In a final test, the ability to resolve concentration profiles under dynamic feed modulation was demonstrated and an amplification of the hydrogen oscillation amplitude was revealed.

The CFD modeling and simulation studies (Wehinger group, KIT) focused on developing and validating a 3D-PRCFD model that explicitly couples external flow with reaction-diffusion inside the pellet. During the reactor design phase, the influence of confining walls and the reactor length were examined. The final SPPR design was adopted in the PRCFD model and enables steady-state simulations of the reactor by taking the narrow borehole and the capillary geometry into account. Due to the excessive computational cost of full-transient 3D simulations over a broad parameter space, the dynamic analyses of the system behavior were performed using a transient 1D pellet model, to which dynamic feed boundary conditions are coupled by film theory.

This project combined the development of a novel SPPR reactor with 3D-PRCFD simulations to reveal significant internal concentration and temperature gradients in catalyst pellets during CO₂ methanation. Additionally, a coupled transient 1D pellet model enabled dynamic analysis at feasible computational cost and the reactors capability of resolving intra-pellet gradients under transient feed modulation was demonstrated. The developed methodology of combining SPPR experiments with PRCFD is directly transferable to other dynamically operated, strongly exothermic reaction systems governed by intra-pellet transport limitations.

Dieses kooperative Forschungsprojekt hatte zum Ziel, das dynamische Zusammenspiel von katalytischer Chemie, Wärme- und Stofftransport innerhalb von und rund um poröse Katalysatorpellets während der CO₂-Methanisierung unter erzwungenen dynamischen Betriebsbedingungen grundlegend zu untersuchen. Um dieses Verhalten auf Pellet Ebene zu untersuchen, wurden *in-situ* Experimente an einem neuartigen Single Pellet Profile Reaktor (SPPR) mit detaillierten partikelaufgelösten Computational Fluid Dynamics Simulationen (PRCFD) kombiniert.

Der experimentelle Beitrag (Arbeitsgruppe Horn, TUHH) umfasste den Aufbau eines SPPR im Labormaßstab, welcher erstmals die simultane Messung radialer Konzentrationsprofile mittels verfahrbarer Kapillare sowie die Messung der Oberflächentemperatur mittels Infrarot(IR) Thermografie unter industrienahen Bedingungen bis 400 °C ermöglichte. Erste Ergebnisse an Ni/γ-Al₂O₃ Pellets zeigten trotz stöchiometrischer Eingangsbedingungen deutliche interne CO₂-Konzentrationsgradienten, während die H₂-Profile aufgrund der höheren Diffusivität flacher ausfielen. Auf der Pelletoberfläche wurden axiale Temperaturgradienten festgestellt, die auf die umgebende Grenzschicht und den äußeren Wärmeübergangswiderstand zum Gas zurückgeführt werden konnten. In einem abschließenden Test wurde die Fähigkeit demonstriert, Konzentrationsprofile unter dynamischer Feed Modulation aufzulösen, wobei eine Verstärkung der Amplitude der Oszillation von Wasserstoff festgestellt wurde.

Die CFD Modellierungs- und Simulationsarbeiten (Arbeitsgruppe Wehinger, KIT) konzentrierten sich auf die Entwicklung und Validierung eines 3D-PRCFD Modells, das die äußere Strömung mit der Reaktion und Diffusion im Inneren des Pellets koppelt. Während der Phase des Reaktordesigns wurde der Einfluss der begrenzenden Wände sowie der Reaktorlänge untersucht. Das finale SPPR-Design wurde in das PRCFD Modell übernommen und ermöglicht stationäre Simulationen des Reaktors unter Berücksichtigung der engen Bohrung und der Kapillargeometrie. Aufgrund des hohen Rechenaufwands vollständig transients 3D-Simulationen über einen breiten Parameterbereich wurden die dynamischen Analysen des Systemverhaltens mit einem transienten 1D-Pelletmodell durchgeführt, an das dynamische Feed Randbedingungen über die Filmtheorie gekoppelt sind.

Dieses Projekt verband die Entwicklung eines neuartigen SPPR-Reaktors mit 3D-PRCFD-Simulationen, um deutliche interne Konzentrations- und Temperaturgradienten in Katalysatorpellets während der CO₂-Methanisierung aufzudecken. Zusätzlich ermöglichte ein gekoppeltes transientes 1D-Pelletmodell dynamische Analysen bei vertretbarem Rechenaufwand. Außerdem wurde die Fähigkeit des Reaktors, intrapartikuläre Gradienten unter transients Feed-Modulation aufzulösen, demonstriert.

3 Progress Report

3.1. Background and Objectives

Dynamic operating conditions and flexible load changes are becoming increasingly important for the future operation of catalytic reactors in many process applications. A central Power-to-X technology in which catalytic fixed bed reactors are operated in dynamic modes is the hydrogenation of carbon oxides to methane (methanation).



Due to the strong exothermicity, this reaction system responds particularly sensitive to changes in temperature and composition of the feed gas. Previous literature studies, however, often focused on macroscopic reactor models or simplifying assumptions on intra-pellet transport [1,2]. In particular, the influence of external perturbations on local temperature and concentration fields within a single catalyst pellet and the induced interaction with the surrounding flow have not been investigated previously. To close this knowledge gap, the original concept consisted of the following working packages:

Experimental (Horn group)

- E.I: Development and construction of a single-pellet profile reactor
- E.II: Systematic investigation of steady-state and dynamic pellet behavior
- E.III: Extension of the experimental setup for studies on particle arrays

Modeling (Wehinger group)

- M.I: Development of a validated, stationary single-pellet CFD model
- M.II: Extension of the CFD model for dynamic operating conditions
- M.III: Development of a CFD model for an array of particles
- M.IV: Investigation of dynamic behavior using system identification tools

In aim *E.I* the novel reactor should be developed, assisted by CFD results from the Wehinger group. *M.I* aimed at developing a steady-state model, validating it with the experiments and to study the influence of the capillary on the measured concentration profiles. In *M.II* and *E.II*, dynamic operating conditions by concentration forcing should be investigated by simulations and experiments, respectively. Finally, to elucidate the influence of surrounding particles on the pellet behavior, an array of several neighboring particles should be studied in aims *M.III* and *E.III*. To systematically study and predict the pellet response, *M.IV* aimed at applying system identification methods. The project work was coordinated between the two groups. While the experimental group (TUHH) constructed the reactor and performed experimental

campaigns, the modelling group (KIT) focused on simulation of the setup taking the coupling of transport phenomena with reaction into account.

3.2. Project-specific Results

The present work and initial project planning was based on an existing prototype developed in a previous research project [3]. The novel version of the single pellet profile reactor was developed in collaboration between both working groups. This included numerical design studies from the modeling group to assist in equipment sizing. To leverage existing workflows within the modeling group, the CFD simulations were performed with Siemens Simcenter STAR-CCM+ version 21.02.007.

3.2.1. Stationary Operating Conditions (*E.I.*, *M.I.*)

In the first phase of the project, a second-generation single pellet profile reactor (SPPR) was developed. It combined the single pellet concentration sampling approach by [3] with the IR thermography approach developed by [4]. The combination of these two techniques enabled new combined insights by measuring the concentration profiles and surface temperature distribution simultaneously under reaction conditions. It could be operated at up to 400 °C and 10 L_N/min. To perform the CO₂ methanation reaction, a cylindrical pellet with 5x5 mm was placed in the reactor. It was held in place with three needles to reduce the holders influence on the

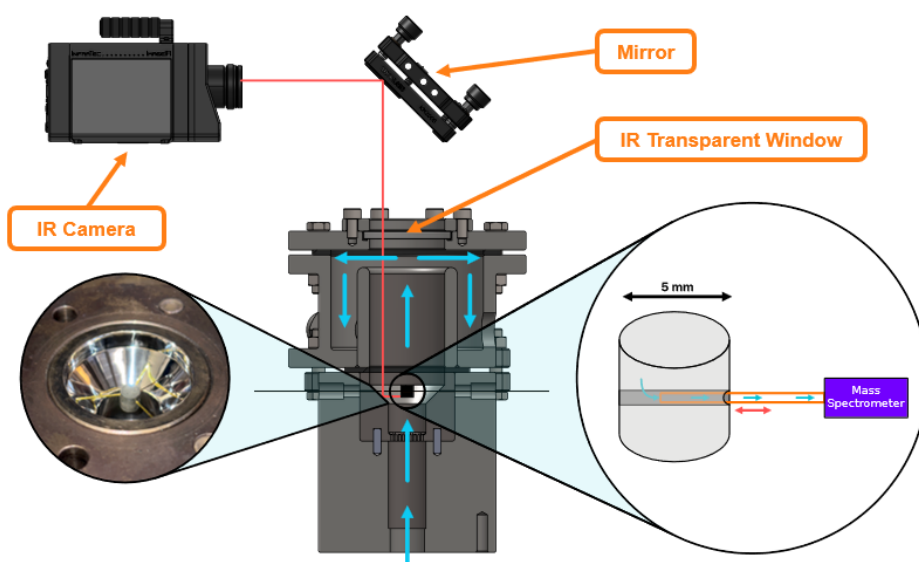


Fig. 1: Schematic of the reactor setup as used in the presented experiments. It shows the reactor in the center as well as the capillary sampling technique on the right and the infrared camera on the top. [P9] pellet perturbation. The pellet itself was surrounded by a conical mirror similar to the setup of [4] to capture not only the top of the pellet but also its sides. An IR transparent sapphire window

was used as the reactor lid to allow for optical access. A movable 363x10 μ m capillary was inserted through the sides of the reactor into a 400 μ m channel that was drilled into the pellet. Through its tip, a small flow rate could be sampled and was transferred to a mass spectrometer using a transfer capillary. The reactor setup can be seen in Figure 1. Using this setup allowed for measuring the concentration of methane, carbon dioxide, carbon monoxide and hydrogen while water had to be calculated. In total, 16 final experiments were performed during this first experimental stage. The feed composition was varied between CO₂:H₂ = 1:4 and CO₂:H₂ = 1:1 and feed temperatures between 290 °C and 380 °C. The resulting concentration profiles are shown in Figure 2.

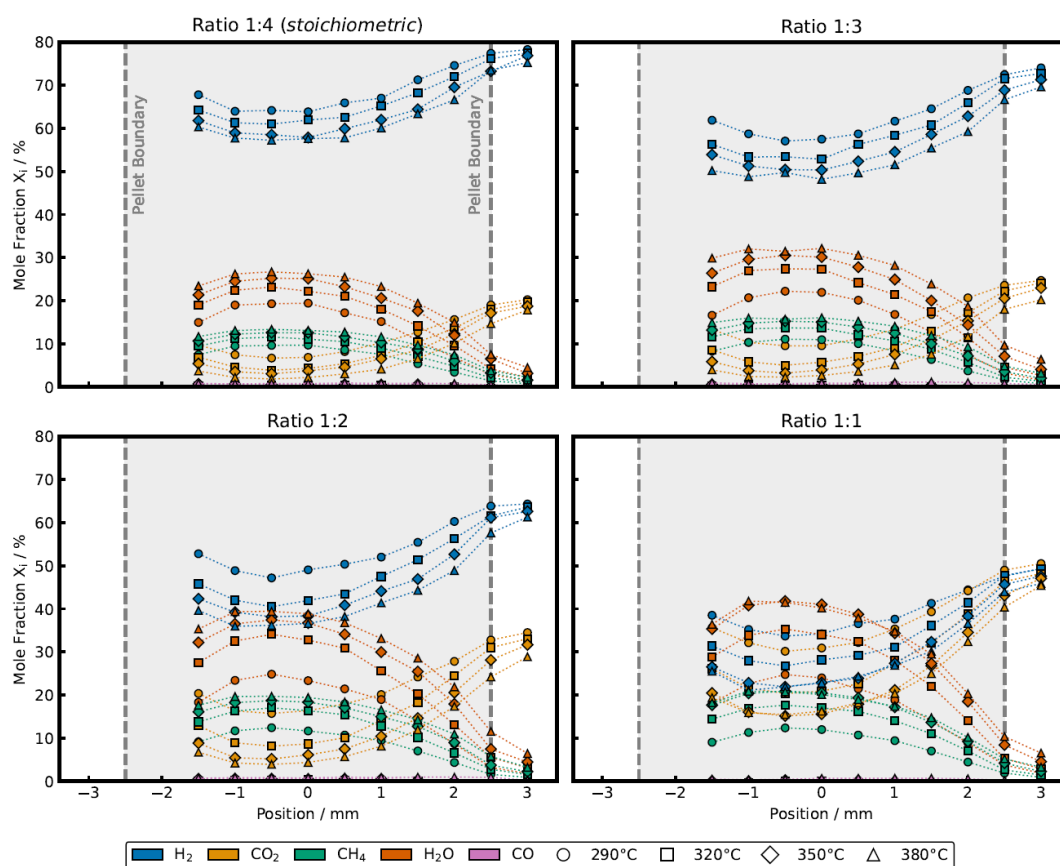


Fig. 2: Molar concentration profiles of reactants during CO₂ methanation inside the Ni/ γ -Al₂O₃ pellet at different feed temperatures and CO₂ to H₂ feed ratios. The region inside the pellet is indicated by the grey area and corresponding dashed lines [P2].

It is apparent, that the methane concentration inside the pellet increased with temperature and increasing feed CO₂ concentration. The most surprising finding was that the highest methane concentration was not found under stoichiometric feed conditions but rather CO₂ excess in the feed. In close relation to this, an almost flat H₂ concentration profile was observed under stoichiometric conditions although CO₂ was almost completely depleted in the center of the pellet. The primary reason for this is the higher effective diffusivity of H₂ compared to CO₂ in the mesopores of the catalyst pellet.

During these measurements, the surface temperature distribution was recorded using the IR camera. Prior to the measurements, a background image was recorded under non-reactive flow conditions at the required feed temperature to later correct for differences in surface emissivity and reflectivity through subtraction. For this reason, all temperatures are given as a temperature difference to the non-reactive case. The IR camera recorded the lateral surface temperature of the pellet as a ring reflection from the conical mirror. Fitting the outer and inner boundary of the ring with an ellipse, followed by coordinate transform to cartesian coordinates, yielded an “unwrapped” rectangular image of the lateral surface temperature distribution. The ellipse fit was necessary to correct slight misalignment between the camera and the reactor. An example of these images is shown in the left part of Figure 3.

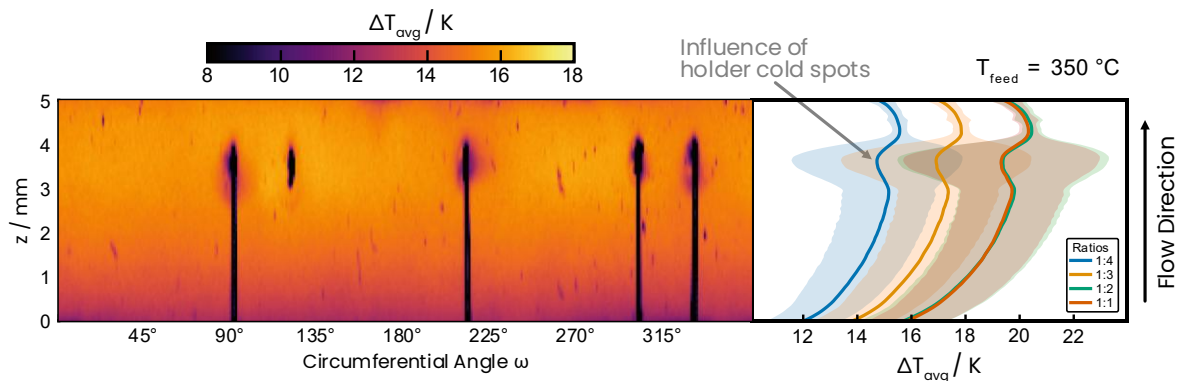


Fig. 3: Temperature distribution of for a feed temperature of 350°C and a ratio of 1:4 (left) and axial temperature profiles at 350°C and different feed ratios. [P2]

Clearly visible are the three needles holding the pellet in place and the sampling capillary. Circumferential averaging yielded the axial temperature profile in flow direction as shown in the right part of Figure 3. The profiles revealed a strong axial gradient that is caused by the convective cooling of the catalyst pellet by the feed gas. In close reference to the concentration profiles, the comparison between different feed ratios showed an increase in surface temperature with increasing CO_2 concentration up to a ratio of 1:2. This was caused by both a higher catalytic activity but also a drastic change in thermal conductivity of the feed gases and hence decreased convective cooling. The corresponding research data is available as stated in the publication [P2].

During the initial project phase, a nonreactive CFD model was developed to assist the experimental group in sizing the lab-scale reactor and investigate possible wall effects. Following a full-factorial Design of Simulation Experiments plan, the particle Reynolds number $Re_p = u_{\text{in}} \rho d_p / \mu$ was varied alongside the diameter D of the rectangular flow channel covering a broad range of values ($Re_p = 10\text{--}10^3$, $D = 4\text{--}20d_p$). The results showed that drag and heat transfer coefficients are influenced particularly by low values of Re_p and D , which can be

corrected by a proposed correlation [P1,P3]. As part of *M.I.*, a reactive 3D-PRCFD model of the SPPR was developed and validated against the experiments. State-of-the art methanation kinetics [5] were used to implement the reaction as associated source terms. Species transport within the porous phase and the interface coupling with the surrounding fluid phase are explicitly accounted for by a conjugate heat and mass transfer model [6]. Fig. 4 shows the velocity field through a midplane cross-section of the reactor. The validation with the experimental data

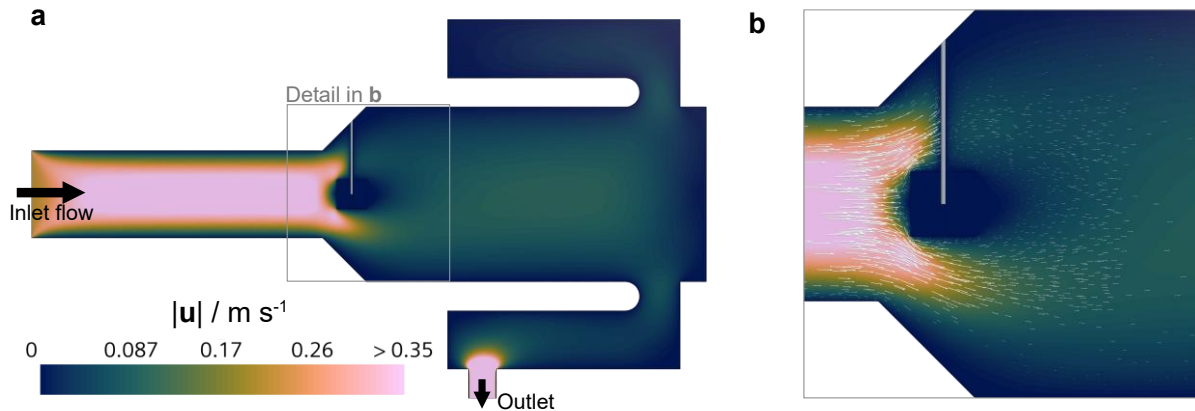


Fig. 4: Velocity magnitude $|u|$ from PRCFD through midplane at $T_{in}=350^{\circ}\text{C}$, CO_2/H_2 ratio of 1:4 and $1 \text{ L}_N/\text{min}$.

shows that the concentration profiles can be reproduced by resolving the borehole including the capillary, see Fig. 5a. Discrepancy remains, however, when comparing the pellet surface temperature to the measured IR field, shown in Fig. 5b-c for T_{in} at 290°C and 350°C . The cause of this difference is currently being investigated. However, this analysis is complicated by experimental uncertainties, e.g. IR thermography and cover-side heat loss, and uncertainties in model parameters regarding the optical properties of the surfaces. The findings of *M.I.* are currently being extended thoroughly by further studies, and a future publication is in preparation [P11] to which a Zenodo repository containing the numerical data will be linked.

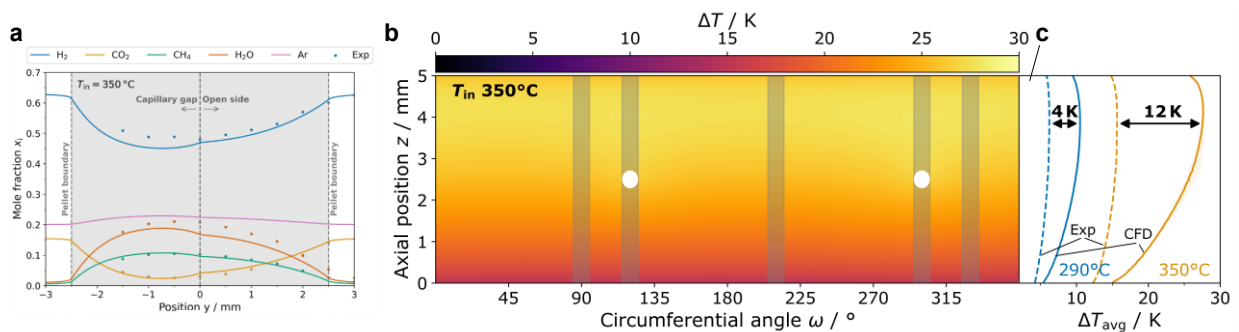


Fig. 5: PRCFD results of a) mole fraction profiles for central capillary position, b) side surface temperature rise and c) axial profiles (average excluding masked areas) for $T_{in}=290^{\circ}\text{C}$ and 350°C . [P9]

3.2.2. Catalyst Synthesis and Characterization (*E.II*)

The catalyst used for the experiments was Ni/ γ -Al₂O₃ supplied as 5x5 mm cylindrical pellets. Before impregnation, the preformed cylinders were drilled using 400 μ m tungsten carbide drills under constant water cooling to form the channel for the sampling capillary. After washing with nitric acid and deionized water to remove the drilling residue, the pellets were dried. After that, they were impregnated via incipient wetness with a nickel nitrate solution. The concentration of this solution was set aiming at a final weight loading of 10 wt.% in two impregnation steps. After each step, the pellet was carefully dried overnight in a desiccator to prevent cracking or the formation of an eggshell catalyst due to too high drying rates. Following the impregnation, the catalyst was calcined in air at 400°C to decompose the nitrate and reduced in 5% H₂ to yield the final active metallic nickel. The reduction step was performed directly in the reactor just before the experiments. To obtain the specific surface area, a BET analysis was performed. As further part of the physical characterization, mercury intrusion porosimetry measurements were performed at CVT, KIT (Micromeritics MicroActive AutoPore V 9600). Furthermore, light microscopic images of drilled pellets were taken at CVT, KIT (Leica DM6 M), see Fig. 6a. Environmental scanning electron microscopy (ESEM) and energy dispersive X-ray spectroscopy (EDXS) have been performed by the Laboratory for Electron Microscopy (LEM) at KIT (FEI Quanta FEG 650). Three pellet samples were analyzed, two of which were embedded into epoxy resin for metallographic preparation to analyze longitudinal and horizontal sections. The EDX mapping of the spectra showed that the Ni nanoparticles are homogeneously distributed throughout the porous matrix, see Fig. 6b-d. The light and electron microscopic imaging further confirmed that the drilling procedure results in a uniform borehole diameter of 400 μ m.

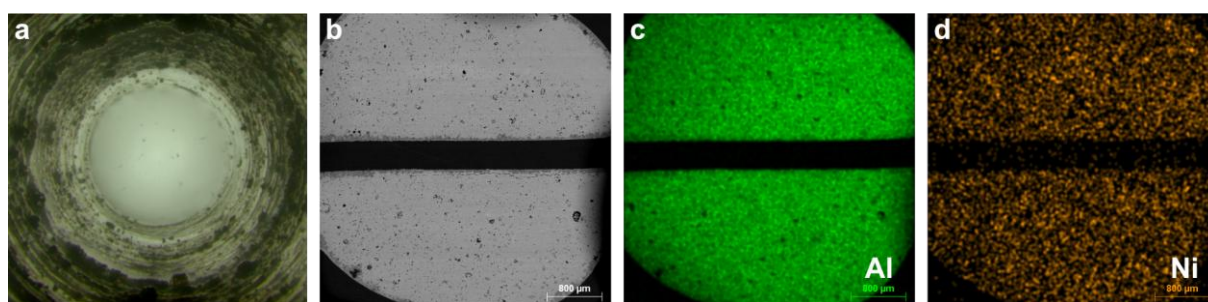


Fig. 6: a) Focus stacked image through the borehole, b) ESEM image and b) EDX mapping of aluminum (Al) and c) nickel (Ni) atoms in the horizontal pellet cross section.

3.2.3. Dynamic Operating Conditions (*E.II*, *M.II*, *M.IV*)

After the successful steady-state experiments reported above, an experimental campaign was performed to evaluate the transient behavior of the pellet under methanation conditions and

test the capabilities of the reactor. The experiments were performed at a base ratio of $\text{CO}_2:\text{H}_2$ of 1:4 and 350 °C while the feed ratio was modulated with a square wave of amplitudes of 0.1 $\text{L}_\text{N}/\text{min}$ and 0.05 $\text{L}_\text{N}/\text{min}$ and periods from 2 s to 64 s. The resulting concentrations of methane, hydrogen, carbon dioxide and carbon monoxide were evaluated at 8 points throughout the pellet and the boundary layer. To account for the strong attenuation of the signal by the sampling capillary, the transfer function between reactor and mass spectrometer was measured. By discrete Fourier transform (dFT) the measured signal was converted to the frequency domain, where the measured transfer function and the actual pellet response were deconvoluted. The resulting, deconvoluted and phase averaged concentration plots are shown in Figure 7.

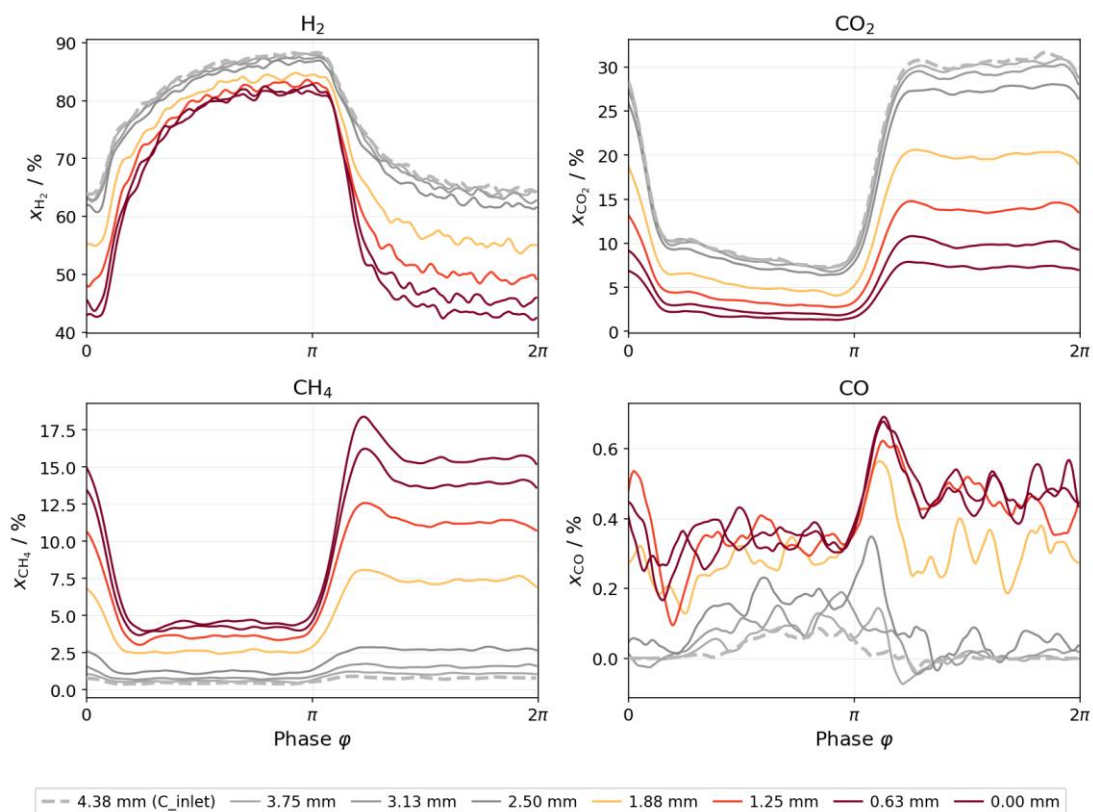


Fig. 7: Phase averaged and deconvoluted concentration profiles at a base ratio of 1:4, amplitude of 0.1 $\text{L}_\text{N}/\text{min}$ and a period of 64 s. The grey lines are outside of the pellet in the gas stream of the reactor, while the colored lines resemble the concentration inside the pellet.

The main result of these experiments was that the amplitude of H_2 grows inside the pellet compared to the outside although H_2 is consumed. Furthermore, the experiments clearly showed the limitations in temporal resolution of the setup. While the deconvolution yielded meaningful concentration profiles for periods larger than 32 s, every measurement below that was strongly attenuated by the capillary. As it is acting as a strong low pass filter, it filters all signals above a certain frequency. If the fundamental frequency of the square wave becomes smaller than the lowest passing frequency of the capillary, all transient information is lost and

only the DC response survives, and all transient information is lost. As no real transient signal survived at the end of the capillary, even dFT followed by deconvolution does not enhance the result as it cannot restore data that has never been measured in the first place. In the currently resolvable time scales, only a switching between two steady-states was observed with a methane concentration inside the pellet that always stayed below that of a steady-state operation.

Due to the excessive time demand for steady-state PRCFD simulations, as described below in section 3.2.4, transient studies were performed with a 1D pellet model developed in Python using the CasADi framework [7]. The transient 1D pellet model and variants were developed within thesis projects [8,9] and include the possibility to apply multicomponent diffusion models [9], as shown in Fig. 8a. This allows for systematic studies of the pellet studied under *E.II*, as shown exemplary in Fig. 8b-c. In addition, frequency response analyses can be employed as proposed in *M.IV*, for which a future publication is in planning. The respective model and data will be linked to a Zenodo repository [P11, P12].

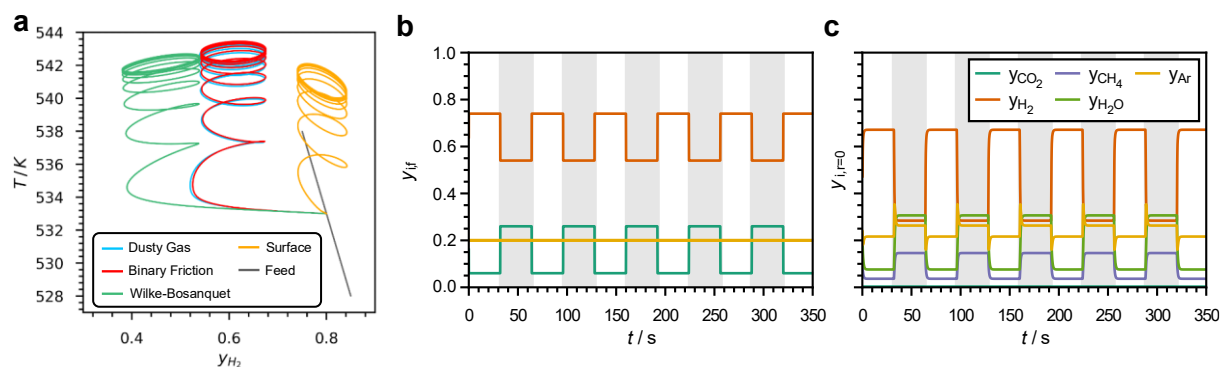


Fig. 8: a) Phase-plane for dynamic concentration forcing comparing state trajectories in the pellet center, at the surface and feed between multicomponent diffusion models [9], b) molar fractions in feed under same conditions as in the experiment (Fig. 7) and c) response at pellet center ($r=0$).

3.2.4. Deviations from the Original Concept

The steady-state 3D-PRCFD simulations that include the capillary geometry exhibited unexpectedly high computational demands. Despite parallel computing on the HPC cluster bwUni-Cluster 3.0, the elapsed computation time summed to 28 days for a single case. The cause for this is presumably a combination of resolving the capillary gap of 20 μm , low flow velocities ($Re_p < 50$) and complete depletion of CO_2 towards the pellet center. Given the prohibitive computational expense of transient PRCFD simulations, the focus was shifted toward the development of a detailed transient 1D pellet model for studying dynamic behavior in aims *M.II* and *M.IV*. The original concept included in *E.III* and *M.III* the extension of studies from the single pellet to an array of several neighboring pellets. However, the design and construction phase required additional time demand due to long delivery times of the custom-made reactor vessel

itself as well as the high precision infrared camera. Furthermore, studying particle arrays would have required building an additional reactor, which was not realizable. Therefore, it was deemed more useful to focus on single pellet experiments and simulations, following the fundamental motivation of this project. Systematic studies of the dynamic system behavior as proposed in *M.IV* were not finished within the given time frame due to the additional time demand. However, a study using the model from *M.II* is planned along with a publication referencing this DFG project.

3.3. Additional Bibliography

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- [8] J. Kopmann, Transient 1D Simulation of a Catalyst Particle for CO₂ Methanation, Bachelor's thesis, KIT, 2024.
- [9] R.J. Burchardt, Transient 1D Simulation of CO₂ Methanation in a Catalyst Pellet Using Multicomponent Mass Transport Models, Master's thesis, KIT, 2026.

4 Published Project Results

4.1. Category A – Articles in peer-reviewed journals, contributions to peer-reviewed conferences or to anthology volumes, and book publications

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- [P1] P. Reinold, M. Kutscherauer, G.D. Wehinger. A Numerical Study on the Influence of Confining Walls on Drag and Heat Transfer Coefficients in Single-Particle Lab-Scale Reactors. *Chemie Ingenieur Technik* 96(12), 1595-1603. 2024. <https://doi.org/10.1002/cite.202400083> (Open access)
- [P2] M. Finkeldei, P. Reinold, O. Korup, G.D. Wehinger, R. Horn. Single Pellet Profile Reactor for Measuring Concentration and Temperature Patterns on Porous Catalyst Pellets. *Chemical Engineering Journal* 549, 182393. 2026. <https://doi.org/10.1016/j.cej.2026.182393> (Open access)

4.2. Category B – Any other form of published results (selected)

- [P3] P. Reinold, G.D. Wehinger, Investigating the effect of confining walls in lab-scale single pellet reactors by CFD simulations. Poster. Annual Meeting on Reaction Engineering and Electrochemical Processes. Würzburg, 06.-08.05.2024.
- [P4] M. Finkeldei, P. Reinold, O. Korup, G.D. Wehinger, R. Horn. Measuring Concentration and Temperature Profiles in Single Porous Catalyst Pellets under Dynamic Conditions. Poster. 58. Jahrestreffen Deutscher Katalytiker. Weimar, 12.-14.03.2025.
- [P5] P. Reinold, M. Kutscherauer, G.D. Wehinger. Modeling transient CO₂-methanation in single catalyst particles with CFD and continuum models. Poster. Annual Meeting of DECHEMA / VDI specialist groups. Clausthal-Zellerfeld, 25.-27.03.2025.
- [P6] P. Reinold, M. Kutscherauer, G.D. Wehinger. Dynamic simulations of porous catalyst pellets under CO₂-methanation using CFD and continuum models. Poster. Annual Meeting on Reaction Engineering. Würzburg, 26.-28.05.2025.
- [P7] P. Reinold, M. Kutscherauer, G.D. Wehinger. Bridging Scales in CO₂ Methanation: Dynamic CFD and Continuum Modeling of Porous Catalyst Pellets. Talk. 15th European Congress of Chemical Engineering. Lisbon, Portugal, 08.-10.09.2025.
- [P8] M. Finkeldei, P. Reinold, O. Korup, G.D. Wehinger, R. Horn. Hidden Gradients in CO₂ Methanation: *In situ* Concentration Profiles and Surface Temperature Patterns in Porous Ni/γ-Al₂O₃ Pellets. Poster. 59. Jahrestreffen Deutscher Katalytiker. Weimar, 18.-20.03.2026.
- [P9] M. Finkeldei, P. Reinold, O. Korup, M. Kutscherauer, R. Horn, G.D. Wehinger. Revealing Intra-Pellet Gradients with *in situ* Measurements and Particle-Resolved Modelling of CO₂ Methanation. Tandem Talk. Annual Meeting on Reaction Engineering. Würzburg, 26.-28.05.2026.
- [P10] P. Reinold, M. Finkeldei, M. Kutscherauer, O. Korup, R. Horn, G.D. Wehinger. Spatio-temporal Analyses of Porous Catalysts for CO₂ Methanation using Particle-Resolved Modeling and Single Pellet Profile Reactors. Talk. AIChE Annual Meeting. Minneapolis, MN, USA, 08.-12.11.2026. (*accepted oral presentation*)
- [P11] P. Reinold, M. Finkeldei, M. Kutscherauer, O. Korup, R. Horn, G.D. Wehinger. Particle-resolved CFD Modeling of Single-Pellet Profile Reactors for CO₂ Methanation (*Peer-reviewed paper in preparation*).
- [P12] P. Reinold, M. Finkeldei, M. Kutscherauer, O. Korup, R. Horn, G.D. Wehinger. Modeling Single Pellets under Enforced Dynamic Conditions for CO₂ Methanation (*Peer-reviewed paper in preparation*).