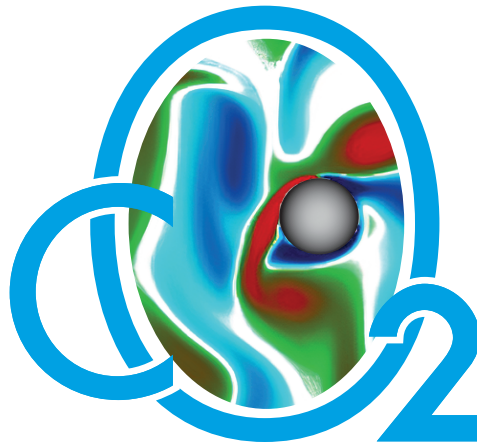


CRC/Transregio 129 "Oxyflame"

Development of Methods and Models to Describe Solid Fuel Reactions within an Oxy-Fuel Atmosphere

**Overview of scientific publications resulting from the
Collaborative Research Centre 129 "Oxyflame"**

RWTH Aachen University
Ruhr-Universität Bochum
Technische Universität Darmstadt



2025

edited by
Stefan Pielsticker, Anna Maßmeyer, Reinhold Kneer

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1 Project summary

In oxy-fuel combustion, air as an oxidiser is replaced by oxygen. The flue gas then consists almost entirely of CO₂ and H₂O with minor pollutants. Condensing H₂O and removing pollutants yields a CO₂-rich stream for efficient CO₂ capture. Despite the extra energy demand for oxygen production, oxy-fuel with carbon capture, utilisation, and storage (CCUS) enables near carbon-neutral operation. Combined with biomass (BECCUS), it can even create a net carbon sink.

1.1 Motivation

To keep global warming within 1.5 °C – consistent with the Paris Agreement – anthropogenic CO₂ emissions must reach net zero by ~ 2055. As 79% of CO₂ originates from power generation and industrial production, mitigation must prioritise these sectors. Because fossil fuels will remain a substantial energy source through 2040, CCUS is essential. Achieving this requires major process changes or retrofits, for which several technologies have been developed, with oxy-fuel combustion representing an advanced option.

Today, the cement industry pursues 100% oxygen atmospheres, whereas most applications use mixtures of roughly 30% oxygen with 70% recycled flue gas. Consequently, combustion occurs in O₂/CO₂/H₂O atmospheres.

1.2 Objectives

Replacing the N₂ fraction of air with the more chemically reactive and radiatively absorbing CO₂ and H₂O fundamentally alters reaction rates, gas-phase transport, and radiative heat transfer relative to air combustion. Designing reliable, large-scale oxy-fuel systems therefore requires a deep, multi-scale understanding across length scales from $\mathcal{O}(10^{-10} \text{ m})$ to $\mathcal{O}(10^1\text{--}10^2 \text{ m})$ and time scales from $\mathcal{O}(10^{-9} \text{ s})$ to $\mathcal{O}(1 \text{ s})$.

As a foundation for this understanding, the CRC/TRR 129 "Oxyflame" pursued the development of:

- A comprehensive understanding of mechanisms governing combustion of solid, pulverised fuels in O₂/CO₂/H₂O atmospheres.
- Generalised, validated models for combustion and transport in oxy-fuel environments that capture the relevant effects on each scale.
- Physics-based, efficient simulation methods for the design of oxy-fuel combustion chambers, enabling model-based design, optimisation, and sensitivity analysis.

These goals were reached by the combined theoretical and experimental expertise in solid-fuel and gas combustion, chemistry, thermodynamics, and fluid mechanics at RWTH Aachen University (RWTH), Ruhr-Universität Bochum (RUB), and Technische Universität Darmstadt (TUDA).

1.3 Structure of the CRC/TRR 129

To pursue these goals, the CRC/TRR 129 was organised in three thematic areas. The system complexity and scale increased from **A** to **C**, while the investigated level of detail decreased. The close interconnections of the projects and the project areas are displayed in Figures 1.1 to 1.3.

In project area **A**, the physico-chemical fundamentals were investigated and incorporated into kinetic fuel conversion models. The primary goal of project area **A** was to deepen the understanding of chemical and physical phenomena at the single-particle level to develop sophisticated conversion

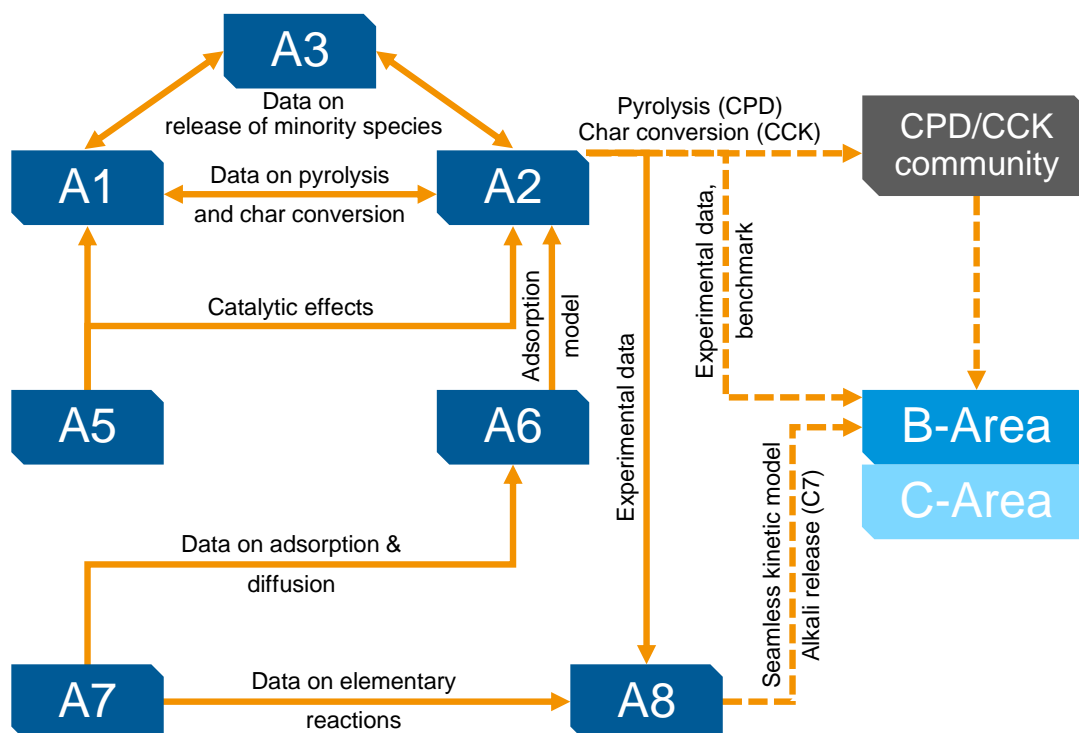


Figure 1.1: A area: Physico-chemical fundamentals and incorporation into kinetic fuel conversion models.

models. These models encompassed all relevant effects that influenced pyrolysis and char conversion processes, a challenging task due to the complexity of solid fuel structures, the wide variety of feedstocks, and the numerous chemical reactions involved. The complexity necessitated a balance between model accuracy and computational cost. To support the development of these models, experimental reference data were collected under various boundary conditions. Furthermore, atomistic multiscale simulations provided crucial data. The **A** area strategy is summarised as follows:

- **A1** and **A2** provided complementary data on kinetics and products during pyrolysis and char conversion. **A1**'s fluidised bed test rig allowed observation of the entire conversion. **A2** focused on shorter timescales using laminar flow reactors. **A1** and **A2** managed the advanced pyrolysis and char conversion models: Chemical Percolation Devolatilisation (CPD) for pyrolysis and Char Conversion Kinetics (CCK).
- **A3** examined the release of minority species from solid fuel and the subsequent conversion of these species in the gas phase. Also, nitrogen species (NO_x precursors) and alkalis were included.
- **A5** investigated the catalytic effect of minerals on char conversion, while **A6** analysed sorption effects in porous fuel particles.
- **A7** contributed to understanding the elementary reactions of carbon with reactive gases (O_2 , CO_2 , H_2O) using atomistic simulations.
- **A8** developed a seamless conversion model based on the CRECK-S approach, which captures the effect of pyrolysis conditions on initial char reactivity – an effect the step-separate CPD/CCK approach does not cover.

Project area **B** focused on non-homogeneous flow and combustion processes. Building upon the knowledge gained in project area **A**, the central goal of project area **B** was to study, understand, and model the interaction of these phenomena with reactive flows. Relevant aspects investigated included gas-phase chemistry, the mutual impact of flow and turbulence on particles, turbulence/chemistry

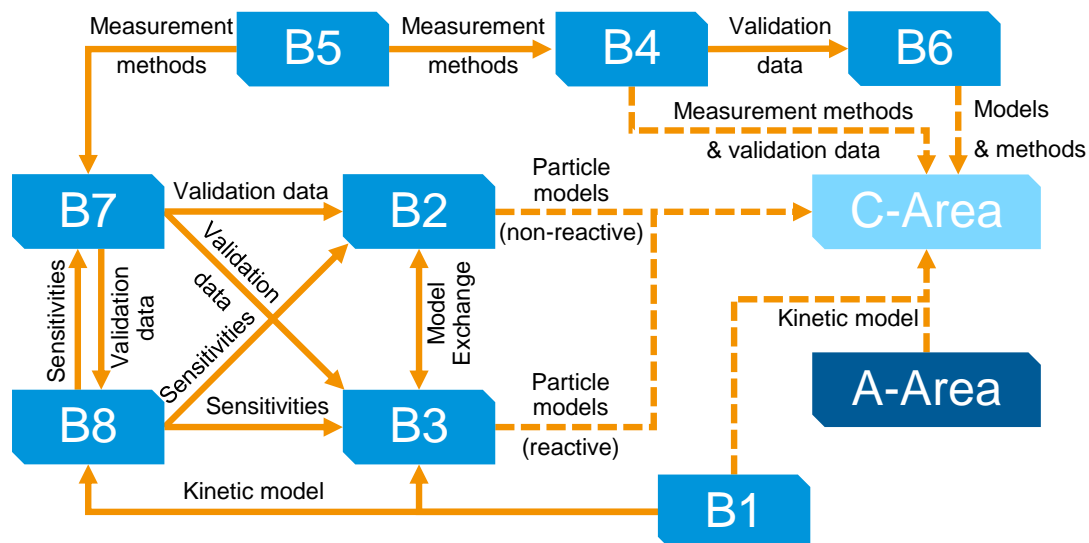


Figure 1.2: B area: Non-homogeneous flow and combustion processes.

interactions, and particle-particle interactions. A crucial parallel effort was the development of experimental techniques. Particle models and models for turbulence/chemistry interactions were formulated and validated for pulverised biomass combustion under oxy-fuel conditions within projects **B2** and **B3** (jointly with **C2**). These models were then incorporated into the OpenFOAM simulation environment OxySim-129 by **C2**. The model development efforts were supported by adjoint-based sensitivity analysis in **B8**. The single projects in the **B** area contributed as follows:

- **B1** studied gas-phase chemistry using a laminar counterflow burner.
- **B2** and **B3** (jointly with **C2**) formulated and validated particle models and models for turbulence/chemistry interactions.
- **B4** investigated a swirl-burner configuration with optical access, allowing for detailed velocity and temperature measurements.
- In **B5**, robust laser-absorption-based measurement techniques were developed and their functionality was demonstrated in the pilot-scale system.
- In project **B6**, models and methods for the LES-based Oxy-Sim 129 model were developed and validated against the experiments conducted in **B4**.
- Project **B7** provided the experimental basis for studying the effects of particle interactions on flame ignition and devolatilisation.
- **B8** assisted model development using adjoint-based sensitivity analysis.

In project area **C**, coupled processes were investigated. Project area **C** successfully addressed three core objectives: a deeper understanding of coupled subprocesses, including radiation, the integration of mathematical models from project areas **A** and **B** into a comprehensive model, and the validation of this comprehensive model. The resulting comprehensive model, OxySim-129, established the bridge to practical application, enabling a more predictive design. Validation covered a sequence of flow processes across different scales. Project area **C** was structured into projects focusing on the pilot-

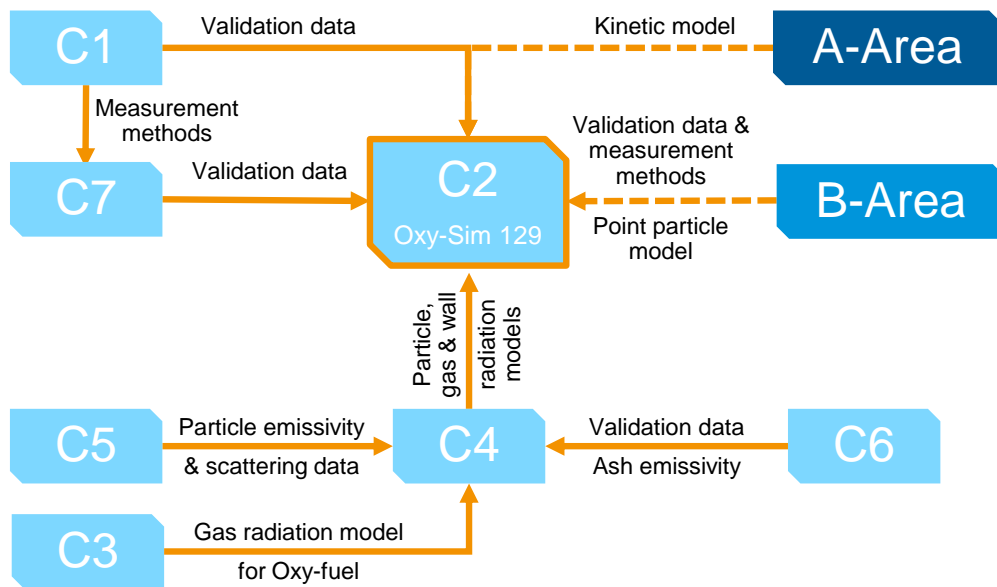


Figure 1.3: C area: Coupled processes and syntheses of model development in Oxy-Sim 129.

and large-scale experiments (**C1**, **C7**), the overall model (**C2**), and radiation processes (**C3**, **C4**, **C5**, **C6**).

- **C1** provided considerable validation data by investigating flames up to 180 kW_{th}, bridging the gap between laboratory and semi-industrial scales.
- **C2** developed the comprehensive model OxySim-129 and integrated the large number of sub-models from areas **A** and **B**.
- **C3** advanced the modeling of gas radiation and its integration into the comprehensive model.
- **C4** developed advanced models for particle radiation, radiation transport, turbulence-radiation interaction, and ash/deposit influence.
- **C5** established the experimental investigation for radiation and scattering behavior of coal particles as well as aspherical particles, and also investigated multiple scattering.
- In project **C6**, the spectral emissivity of real and synthetic fuel ash for key mineral groups was determined.
- In **C7** flames with 1 MW_{th} were investigated, allowing for a critical examination and understanding of subprocess changes at a larger scale.

1.4 Key findings

The CRC/TRR 129 project aimed to investigate and enhance the understanding of oxy-fuel combustion processes, particularly concerning solid fuels. The overarching goal was to develop reliable models and simulation tools that could be applied in industrial settings to improve energy efficiency and reduce carbon emissions.

A comprehensive experimental database was established that focused on pyrolysis and char conversion kinetics under high heating rates for various solid fuels. This database included results from both

– solid sampling and gas-phase analysis, as well as optical measurements that provided insights into single particle temperatures and their evolution during combustion. The influence of catalytically active minerals (e.g., Fe, K, Na) on pyrolysis gas yields was examined, confirming their relevance in enhancing reaction rates under oxy-fuel conditions. Detailed measurements were conducted using time-of-flight mass spectrometry in counterflow diffusion flames. These studies investigated different fuel blends representing volatile gases in both air and oxyfuel atmospheres. The findings led to the development of validated, detailed kinetic models for the gas-phase kinetics of volatiles derived from coal and biomass, which are crucial for accurate combustion modeling.









Research into coupled reaction-transport processes utilised direct numerical simulations (DNS) alongside canonical experiments to explore how particle-laden two-phase flows behave. DNS modeling revealed interactions between flow fields and particles, providing new insights into drag correlations necessary for point particle approaches. Additionally, experimental studies showed changes in flame topology when transitioning from individual particle combustion to group combustion. Cascaded experiments were performed in optically accessible combustors operated with various O_2/CO_2 mixtures to investigate flame shape changes depending on oxidiser concentration. Unique data sets were compiled that not only validated existing solid fuel flame models but also aided interpretations relevant for larger-scale industrial combustors with limited optical access.

Recognising the importance of thermal radiation effects – especially when high concentrations of H_2O and CO_2 are present – the project developed a weighted-sum-of-grey-gases (WSGG) model. This model accounted for wavelength-dependent radiative properties of both – gas phase and particle phase – leading to improved predictions of heat transfer within large-scale combustors.

The CRC/TRR 129 overall modeling framework was created as an advanced 3D computational fluid dynamics (CFD) tool specifically designed for predicting pulverised carbonaceous solid fuels' behavior under oxy-fuel conditions. This framework integrates detailed kinetic models for both the solid phase and turbulent reacting gas phase interactions while incorporating fully coupled radiation models. Committed to open science principles, the CRC/TRR 129 ensured that its RANS simulation tools are available as open-source software, while plans are underway for releasing OxySim-129 similarly.

Collaborative efforts extended beyond academia into industry applications, particularly within the cement sector, where oxyfuel technology has gained traction. This led to the successful initiation of a transfer project, based on research outcomes. The CRC/TRR 129 project has significantly advanced knowledge regarding oxy-fuel combustion through extensive research output, innovative experimental methodologies, robust modeling frameworks, and successful industry collaborations aimed at reducing carbon emissions while improving energy efficiency across various sectors.






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- [4] Blume, N. G. "Supercontinuum Absorption Spectroscopy for Combustion Diagnostics". PhD thesis. Technische Universität Darmstadt, 2019. [www](#) [@](#)
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4 Project overviews

4.1 A1 – Experimental investigations of pyrolysis and char conversion kinetics in a well-stirred reactor under atmospheric and pressurised conditions

4.1.1 Project members

a) Project leader(s)

- Kneer, Reinhold

b) Scientific project workers

- Askarizadeh, Hossein
- Gövert, Benjamin Maximilian
- Hatzfeld, Oliver
- Kreitzberg, Thobias
- Lotfinia, Mahshad
- Pielsticker, Stefan


4.1.2 Project summary

Project **A1** developed and validated detailed kinetic models for volatile release (pyrolysis) and heterogeneous char conversion (combustion and gasification) across all fuels investigated in the CRC/TRR 129. A redesigned batch fluidised bed reactor with time-resolved online FTIR provided well-stirred conditions, effectively unlimited particle residence times, and exceptionally short response times, enabling char conversion measurements in air and oxy-fuel at higher temperatures and O₂ concentrations. Improved FTIR quantification resolved up to 22 pyrolysis-gas species, supporting parameter estimation and rigorous model calibration/validation. After elucidating boundary condition effects (notably H₂O and high O₂ partial pressures), the focus shifted to biomass pyrolysis of cellulose, hemicellulose, and lignin. CPD-based modeling was advanced and linked to intra-particle transport (**A6**) and catalytically active minerals (**A5**). Char-conversion kinetics for mixtures of O₂, CO₂, and H₂O were pursued in close collaboration with **A2**. The program delivered a new pressurised reactor system and deeper insights into high-heating-rate, moderate-temperature pyrolysis, alongside studies of char morphology and pyrolysis products. Results from **A2** complemented **A1**, yielding comprehensive TGA, FBR, and DTR datasets that underpinned improved network models and their validation. The established CPD (pyrolysis) and CCK (char conversion) frameworks facilitated knowledge transfer to **A8** and enabled implementation in large-scale CFD simulations.







4.1.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **Askarizadeh, H.**, Lotfollahzadeh, A., Wolfersdorf, C., **Pielsticker, S.** and **Kneer, R.** "An Equilibrium Calculation Tool with Development Potential for Predicting Phosphorus Recovery from Sewage Sludge in Entrained-Flow Gasifiers". *Chemical Engineering Research and Design* 197 (2023), 53–64. 

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- [15] **Pielsticker, S., Gövert, B., Kreitzberg, T.**, Habermehl, M., **Hatzfeld, O.** and **Kneer, R.** "Simultaneous Investigation into the Yields of 22 Pyrolysis Gases from Coal and Biomass in a Small-Scale Fluidized Bed Reactor". *Fuel* 190 (2017), 420–434. [doi](#)
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- [20] **Pielsticker, S.** and **Kneer, R.** "Modeling Pyrolysis Kinetics of Extracted Biomass Components with the Bio-Chemical Percolation Devolatilization Model". *Fuel* 360 (2024), 130454. 
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- [23] **Pielsticker, S.**, Schlögel, K. U., **Kreitzberg, T.**, **Hatzfeld, O.** and **Kneer, R.** "Biomass Pyrolysis Kinetics in a Fluidized Bed Reactor: Measurements and Plausibility Verification for Reaction Conditions". *Fuel* 254 (2019), 115589. 





Conference papers

- [24] **Askarizadeh, H.**, Lotfollahzadeh, A., Wolfersdorf, C., **Pielsticker, S.** and **Kneer, R.** "Modeling of a Pilot Plant for Entrained Flow Gasification of Fuel Mixtures Containing Sewage Sludge". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.
- [25] **Askarizadeh, H.**, **Pielsticker, S.**, Nicolai, H., **Kneer, R.**, Hasse, C., Özer, B. and Maßmeyer, A. "Numerical Study on the Influence of Devolatilisation Kinetics on Pulverised Solid Fuel Turbulent Swirling Flames Under Oxyfuel Conditions". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.
- [26] Gfall, K., **Kneer, R.** and **Pielsticker, S.** "Determination of PMMA Pyrolysis Kinetics and the Role of Heat Transfer Limitations". *13th Mediterranean Combustion Symposium*. Corfu, Greece, 2025.
- [27] **Kreitzberg, T.**, Bormann, C., **Pielsticker, S.**, **Hatzfeld, O.** and **Kneer, R.** "Thermal Deactivation of Biogenic and Fossil Fuels: Experimental Investigation and Modeling Approaches". *Energy Procedia* 158 (2019), 2025–2030.  
- [28] **Pielsticker, S.**, **Gövert, B.**, Möller, G. H., **Hatzfeld, O.** and **Kneer, R.** "Impact of Torrefaction on Flash Pyrolysis Products of Biomass and Comparison to Fossil Fuels". *11th Asia-Pacific Conference on Combustion*. Sydney, Australia, 2017.  
- [29] **Pielsticker, S.**, Hendricks, K. and **Kneer, R.** "Experimental Determination of Quantitative Yields from Polymethyl Methacrylate (PMMA) Flash Pyrolysis in a Fluidized Bed Reactor". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.











b) Other publications (non peer-review)



Book chapters

- [62] Berkel, L., Debiagi, P., **Pielsticker, S.**, Tarlinski, D., Senneca, O., Faravelli, T., Scherer, V., **Kneer, R.** and Hasse, C. "Kinetic Modelling of Thermochemical Conversion of Solid Fuels". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and **Pielsticker, S.** Springer, 2025.  









- [63] **Pielsticker, S.**, Freisewinkel, E., Böttger, J., Cerciello, F., Senneca, O., König, D., Scherer, V., Muhler, M., Epple, B. and **Kneer, R.** "Pyrolysis Products and Kinetics". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and **Pielsticker, S.** Springer, 2025.  
- [64] Tarlinski, D., **Pielsticker, S.**, **Kneer, R.**, Schiemann, M. and Scherer, V. "Char Conversion Kinetics". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and **Pielsticker, S.** Springer, 2025.  

Conference papers



- [30] **Askarizadeh, H.**, Nicolai, H., Zabrodiec, D., **Pielsticker, S.**, Hasse, C., **Kneer, R.** and Maßmeyer, A. "Numerische Untersuchung zur Relevanz von Teilmodellen für Pyrolyse und Koksabbrand in turbulenten drallbehafteten Flammen unter Oxyfuel-Bedingungen". *30. Deutscher Flammentag*. Hannover, Germany, 2021.  
- [31] Debiagi, P., Ontyd, C., Heuer, S., **Pielsticker, S.**, Schiemann, M., Faravelli, T., **Kneer, R.**, Scherer, V. and Hasse, C. "Solid Fuel Kinetics for Oxy-Fuel Conditions". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [32] **Gövert, B.**, **Pielsticker, S.**, **Hatzfeld, O.** and **Kneer, R.** "Bestimmung der Koksabbrand-Kinetik in einem Wirbelschichtreaktor am Beispiel einer kolumbianischen Steinkohle". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017.  
- [33] **Gövert, B.**, **Pielsticker, S.**, Vorobiev, N., Heuer, S., **Hatzfeld, O.**, **Kneer, R.**, Schiemann, M. and Scherer, V. "Examination of Pyrolysis and Char Burnout in Oxyfuel Atmosphere Using Plug Flow and Well Stirred Reactor Type Systems". *18th IFRF Members conference*. Freising, Germany, 2015.  
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- [35] **Kreitzberg, T.**, **Gövert, B.**, **Pielsticker, S.** and **Kneer, R.** "CO₂ and H₂O Gasification Under Chemically and Diffusion Controlled Conditions". *33rd Annual International Pittsburgh Coal Conference*. Cape Town, South Africa, 2016.
- [36] **Kreitzberg, T.**, Haustein, H. D., **Gövert, B.** and **Kneer, R.** "Investigation of Gasification Reaction of Pulverized Char Under N₂/CO₂ Atmosphere in a Small-Scale Fluidized Bed Reactor". *40th International Technical Conference on Clean Coal & Fuel Systems*. Clearwater, Florida, USA, 2015.
- [37] **Kreitzberg, T.**, Phounglamcheik, A., Bormann, C., **Kneer, R.** and Umeki, K. "The Change in Size of Char Particles During Combustion and Gasification in Regime II". *11th Mediterranean Combustion Symposium*. Tenerife, Spain, 2019.
- [38] **Kreitzberg, T.**, **Pielsticker, S.**, **Hatzfeld, O.** and **Kneer, R.** "Reactivity of Biochar Gasification in Atmospheres of Steam, Carbon Dioxide and Their Mixtures". *Joint Meeting the German and Italian Sections of the Combustion Institute*. Sorrento, Italy, 2018.  
- [39] Krusch, S., Scherer, V., Solimene, R., Ruoppolo, G., Cerciello, F., **Pielsticker, S.**, **Kneer, R.**, Schlögel, K. U. and Senneca, O. "Comparison of Different Diagnostic Techniques for the Assessment of Coal Pyrolysis Rate". *Joint Meeting the German and Italian Sections of the Combustion Institute*. Sorrento, Italy, 2018.  
- [40] **Pielsticker, S.**, **Gövert, B.**, **Kreitzberg, T.**, Habermehl, M., **Hatzfeld, O.** and **Kneer, R.** "Theoretical and Experimental Evaluation of a Fast Fluidized Bed Reactor for the Investigation of Combustion Reactions". *10th Mediterranean Combustion Symposium*. Naples, Italy, 2017.













- [41] **Pielsticker, S.** and **Kneer, R.** "Modelling Pyrolysis Kinetics of Extracted Biomass Components with the Bio-CPD Model". *12th Mediterranean Combustion Symposium*. Luxor, Egypt, 2023.
- [42] **Pielsticker, S., Kreitzberg, T., Hatzfeld, O.** and **Kneer, R.** "Using the Chemical Percolation Devolatilization Model for Analysis of Pyrolysis Kinetics in a Fluidized Bed Reactor". *11th Mediterranean Combustion Symposium*. Tenerife, Spain, 2019.
- [43] **Pielsticker, S.,** Schlögel, K. U., **Kreitzberg, T., Hatzfeld, O.** and **Kneer, R.** "Measurement of Beech Wood Pyrolysis Kinetics in a Fluidized Bed Reactor". *Joint Meeting the German and Italian Sections of the Combustion Institute*. Sorrento, Italy, 2018.  
- [44] **Pielsticker, S.,** Senneca, O., **Kreitzberg, T.,** Cerciello, F., **Hatzfeld, O.** and **Kneer, R.** "Comparability and Validity Range of Pyrolysis Kinetics from Chinese Coals Obtained with Different Experimental Setups". *9th International Symposium on Coal Combustion*. Qingdao, China, 2019.
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- [46] Solana Gómez, R., Streier, R., **Pielsticker, S.,** Scherer, V. and **Kneer, R.** "Experimentelle Bestimmung der Pyrolysekinetik von Ersatzbrennstoffen". *31. Deutscher Flammentag*. Berlin, Germany, 2023.

Data sets

- [47] **Askarizadeh, H., Pielsticker, S.,** Nicolai, H., Özer, B., **Kneer, R.,** Hasse, C. and Maßmeyer, A. *Influence of the Devolatilisation Kinetics on the Numerical Simulation of Pulverised Fuel Swirl Flames Under Oxyfuel Conditions – Supplementary Dataset*. 2025.  
- [48] Koch, M., Tarlinski, D., **Pielsticker, S.,** Scherer, V. and **Kneer, R.** *Dataset to "Coupling Radiative Properties with Detailed Char Conversion Kinetics"*. 2024.  
- [49] **Pielsticker, S.,** Debiagi, P., Cerciello, F., Hasse, C. and **Kneer, R.** *Comparative Analysis of Pyrolysis Models Including SFOR, CRECK, and Bio-CPD to Predict Reaction Kinetics and Products from Extracted Biomass Components – Supplementary Dataset*. 2024.  
- [50] **Pielsticker, S., Gövert, B.,** Umeki, K. and **Kneer, R.** *Flash Pyrolysis Kinetics of Extracted Lignocellulosic Biomass Components: Supplementary Data Set*. 2021.  
- [51] **Pielsticker, S.,** Hendricks, K., Knevels, C., Lehnertz, M., Palkovits, R. and **Kneer, R.** *Experimental Determination of Quantitative Yields from Polymethyl Methacrylate (PMMA) Flash Pyrolysis in a Fluidized Bed Reactor via Online FTIR Gas Analysis – Supplementary Dataset*. RWTH Aachen University. 2025.  
- [52] **Pielsticker, S.** and **Kneer, R.** *Modeling Pyrolysis Kinetics of Extracted Biomass Components with the Bio-Chemical Percolation Devolatilization Model: Supplementary Dataset*. 2023.  
- [53] **Pielsticker, S.,** Schlögel, K. U., **Kreitzberg, T., Hatzfeld, O.** and **Kneer, R.** *Biomass Pyrolysis Kinetics in a Fluidized Bed Reactor: Measurements and Plausibility Verification for Reaction Conditions: Supplementary Data Set*. 2019.  

Presentations and Posters

- [54] Berkel, L., Debiagi, P., Nicolai, H., Cerciello, F., **Pielsticker, S.,** Senneca, O., **Kneer, R.,** Faravelli, T. and Hasse, C. "Walnut Shell Pyrolysis: Feedstock Characterization and Kinetics Considering Hemicellulose-Lignin Interactions (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 10–11.  

- [55] Debiagi, P., **Pielsticker, S.**, Cerciello, F., Scherer, V., **Kneer, R.**, Faravelli, T. and Hasse, C. "Development of a Comprehensive Kinetic Model of Biomass Conversion in Inert, Air and Oxy-Fuel Conditions (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [56] **Gövert, B.**, **Kreitzberg, T.**, **Pielsticker, S.** and **Kneer, R.** "A1 – Experimental Investigation of Pyrolysis and Char Burnout Kinetics in a Well-Stirred-Reactor Under Flames and Burnout Conditions (Poster)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.  
- [57] Koch, M., **Pielsticker, S.**, Tarlinski, D., Scherer, V. and **Kneer, R.** "Coupling Radiative Properties with Detailed Char Conversion Kinetics (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [58] **Kreitzberg, T.**, **Pielsticker, S.** and **Kneer, R.** "Einfluss von erhöhtem Druck bei Pyrolyse, Abbrand und Vergasung alternativer Brennstoffe (Presentation)". *Jahrestreffen der ProcessNet-Fachgruppe Wärme- und Stoffübertragung*. Erfurt, Germany, 2020.
- [59] **Kreitzberg, T.**, **Pielsticker, S.** and **Kneer, R.** "Influence of Oxygen and Water Vapor on the Thermochemical Conversion of Fossil, Biogenic and Surrogate Fuels (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.  
- [60] **Pielsticker, S.**, Berkel, L., Debiagi, P., Senneca, O., Hasse, C. and **Kneer, R.** "Consideration of Interacting Biomass Components in Sophisticated Pyrolysis Network Models (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 7–8.  
- [61] **Pielsticker, S.**, Debiagi, P., Cerciello, F., Coppola, A., Hasse, C. and **Kneer, R.** "Prediction of Pyrolysis Kinetics with Models of Different Complexity for Isolated Biomass Components (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.2 A2 – Experimental investigations of pyrolysis and char conversion kinetics in plug flow configurations with a focus on the ignition and early char burnout phase

4.2.1 Project members

a) Project leader(s)

- Scherer, Viktor

b) Scientific project workers

- Freisewinkel, Erik
- Heuer, Sebastian
- Hilse, Nikoline
- Ontyd, Christian
- Schiemann, Martin
- Tarlinski, David
- Valentiner, Sarah
- Vorobiev, Nikita

4.2.2 Project summary



















Project **A2** delivered comprehensive oxy-fuel datasets and models for pyrolysis and char conversion, using laminar plug-flow reactors with gas/solid sampling versus residence time and optical diagnostics for single-particle ignition and char conversion, complementary to **A1**'s fluidised-bed studies. It quantified oxy-fuel (CO₂) effects on post-pyrolysis char porosity and reactivity (coal, biomass), derived two-step pyrolysis models with distributed activation energies, validated them with combined optical/sampling datasets (coal, miscanthus), and evaluated particle fragmentation against enhanced models. Focusing on biomass, **A2** showed how minerals control product spectra (char, gas, tar, soot) and govern molten-like amorphous versus thermally annealed, graphitic-like carbon formation. Links to feedstock properties and pyrolysis conditions were established, catalytic contributions to flame-temperature char conversion were quantified, and requirements for statistically robust population datasets were defined. Pyrolysis results underpinned model development in **A1** and **A8**, while CCK was optimized with statistical particle-diameter representations, thermal annealing, catalytic effects (**A5**) and sorption (**A6**). A fast-quench sampling probe and CFD-assisted residence-time/temperature determination enabled atmosphere-effect analyses and CFD-ready two-step pyrolysis models. The impacts of H₂O and CO₂ on coal combustion kinetics were assessed, and CCK capabilities for catalytically active minerals were improved.











4.2.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Apicella, B., Senneca, O., Russo, C., **Heuer, S.**, Cortese, L., Cerciello, F., **Scherer, V.**, **Schiemann, M.** and Ciajolo, A. "Separation and Characterization of Carbonaceous Particulate (Soot and Char) Produced from Fast Pyrolysis of Coal in Inert and CO₂ Atmospheres". *Fuel* 201 (2017), 118–123. [doi](#)
- [2] Bareschino, P., Urciuolo, M., **Scherer, V.**, Chirone, R. and Senneca, O. "Effect of O₂/CO₂ Atmospheres on Coal Fragmentation". *Fuel* 267 (2020), 117145. [doi](#)
- [3] Becker, A., **Schiemann, M.**, **Scherer, V.**, Shaddix, C. R., Haxter, D. and Mayer, J. "Comparative Ignition Tests of Coal Under Oxy-Fuel Conditions in a Standardized Laboratory Test Rig". *Fuel* 208 (2017), 127–136. [doi](#)
- [4] Cerciello, F., Allouis, C., Russo, C., **Freisewinkel, E.**, **Tarlinski, D.**, Apicella, B., **Schiemann, M.**, **Scherer, V.** and Senneca, O. "Thermoplastic Phenomena and Morphological Changes Upon Fast Pyrolysis of Biomass and Model Compounds". *Molecules* 30.3 (2025). [doi](#) [orcid](#)
- [5] Cerciello, F., **Freisewinkel, E.**, Coppola, A., **Ontyd, C.**, **Tarlinski, D.**, **Schiemann, M.**, Senneca, O., Salatino, P., Allouis, C., **Scherer, V.** and Fletcher, T. H. "Xylan Fast Pyrolysis: An Experimental and Modelling Study of Particle Changes and Volatiles Release". *Fuel* 357 (2024), 129983. [doi](#)
- [6] Debiagi, P., **Heuer, S.**, **Ontyd, C.**, **Schiemann, M.**, Faravelli, T., Hasse, C. and **Scherer, V.** "Differences in Formation and Oxidation of Colombian Coal Chars in Air and Oxy-Fuel Atmospheres". *Chemical Engineering Transactions* 74 (2019), 151–156. [doi](#) [orcid](#)
- [7] Debiagi, P., **Ontyd, C.**, Pielsticker, S., **Schiemann, M.**, Faravelli, T., Kneer, R., Hasse, C. and **Scherer, V.** "Calibration and Validation of a Comprehensive Kinetic Model of Coal Conversion in Inert, Air and Oxy-Fuel Conditions Using Data from Multiple Test Rigs". *Fuel* 290 (2021). [doi](#)
- [8] Düdder, H., Wütscher, A., **Vorobiev, N.**, **Schiemann, M.**, **Scherer, V.** and Muhler, M. "Oxidation Characteristics of a Cellulose-Derived Hydrochar in Thermogravimetric and Laminar Flow Burner Experiments". *Fuel Processing Technology* 148 (2016), 85–90. [doi](#)
- [9] Eckhard, T., Pflieger, C., Russo, C., **Freisewinkel, E.**, Eisenbach, T., Böttger, J., Senneca, O., Apicella, B., **Schiemann, M.**, Span, R., **Scherer, V.**, Muhler, M. and Cerciello, F. "Mineral Effects on Chemical and Physical Transformations of Fast Pyrolysis Products of Cellulose-Based Model Fuels in N₂ and CO₂". *Fuel* 340 (2023), 127477. [doi](#)
- [10] Eckhard, T., Pflieger, C., Schmidt, S., Böttger, J., Senneca, O., **Schiemann, M.**, **Scherer, V.**, Muhler, M. and Cerciello, F. "Catalytic Effects for Cellulose-Based Model Fuels Under Low and High Heating Rate in Air and Oxy-Fuel Atmosphere". *Fuel* 324 (2022), 124437. [doi](#)
- [11] Farazi, S., Sadr, M., Kang, S., **Schiemann, M.**, **Vorobiev, N.**, **Scherer, V.** and Pitsch, H. "Resolved Simulations of Single Char Particle Combustion in a Laminar Flow Field". *Fuel* 201 (2017), 15–28. [doi](#)
- [12] **Freisewinkel, E.**, Eisenbach, T., Weise, V., **Tarlinski, D.**, Pörtner, L., Cerciello, F., Wedler, C., **Schiemann, M.**, Span, R., Senneca, O. and **Scherer, V.** "Porosity Measurement of Biomass Char by a Novel Combination of Adsorption Measurements and an Optical Method". *International Journal of Energy for a Clean Environment* (2025). [doi](#)
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- [40] **Ontyd, C.**, **Freisewinkel, E.**, Wedler, C., Eisenbach, T., Span, R., Senneca, O. and **Scherer, V.** "Flash Pyrolysis of Walnut Shells and Poplar in N₂ and CO₂: Pyrolysis Kinetics, Pore Evolution and a Model for Evaluation of Pyrolysis Species". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.






b) Other publications (non peer-review)

Book chapters

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Conference papers







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- [46] Debiagi, P., **Ontyd, C.**, **Heuer, S.**, Pielsticker, S., **Schiemann, M.**, Faravelli, T., Kneer, R., **Scherer, V.** and Hasse, C. "Solid Fuel Kinetics for Oxy-Fuel Conditions". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
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- [48] Farazi, S., **Schiemann, M.**, **Vorobiev, N.**, **Scherer, V.**, Kang, S. and Pitsch, H. "A New Variable Transport Coefficient Single-Film Model for Char Combustion". *8th European Combustion Meeting*. Dubrovnik, Croatia, 2017.
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- [51] **Heuer, S.**, **Schiemann, M.** and **Scherer, V.** "Determination of Devolatilization Kinetics in Inert and CO₂-Enriched Atmospheres in a Plug Flow Reactor". *32nd Annual International Pittsburgh Coal Conference*. Pittsburgh, Pennsylvania, USA, 2015.
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- [57] Senneca, O., Cerciello, F., Cortese, L., **Heuer, S., Schiemann, M.** and **Scherer, V.** "Effects of Oxy-Fuel Conditions on Walnut Shells Pyrolysis in a Drop Tube Reactor". *10th Mediterranean Combustion Symposium*. Naples, Italy, 2017.
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- [59] **Tarlinski, D., Freisewinkel, E.,** Eisenbach, T., Span, R., **Schiemann, M.** and **Scherer, V.** "Char Burnout of Walnut Shells Using Optical Measurement Techniques and First Comparison of the Experimental Data to the CCK Model". *46th International Technical Conference on Clean Energy*. Clearwater (USA), 2022.
- [60] **Tarlinski, D.,** Yao, D., Chang, Y., Levendis, Y. A., **Schiemann, M.** and **Scherer, V.** "Optical Measurements of Pulverized Pine Needles Burning in a Drop Tube Furnace". *48th International Conference on Clean Energy*. Clearwater, USA, 2024.
- [61] **Vorobiev, N., Schiemann, M.,** Wirtz, S. and **Scherer, V.** "Pyrometrische Bestimmung von Koksabbrandkinetiken unter Oxyfuel-Bedingungen". *27. Deutscher Flammentag*. Clausthal-Zellerfeld, Germany, 2015.
- [62] Wütscher, A., Apicella, B., Russo, C., Stanzione, F., Ciajolo, A., **Heuer, S., Scherer, V.,** Muhler, M. and Senneca, O. "Characterization of Tar Produced from Walnut Shells Pyrolysis". *40th Meeting of the Italian Section of the Combustion Institute*. Rome, Italy, 2017.  

Data sets

- [63] Koch, M., **Tarlinski, D.,** Pielsticker, S., **Scherer, V.** and Kneer, R. *Dataset to "Coupling Radiative Properties with Detailed Char Conversion Kinetics"*. 2024.  

Presentations and Posters

- [64] Cerciello, F., **Ontyd, C.,** Russo, C., **Freisewinkel, E.,** Oliano, M. M., Senneca, O., **Scherer, V., Schiemann, M.,** Muhler, M. and Apicella, B. "Biomass Pyrolysis: Critical Issue on Tar Analysis (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [65] Dadduzio, R., Penati, M., Bini, L., Rogora, M., Valenzano, M., Saponaro, A., Senneca, O., Cerciello, F., **Ontyd, C.,** Brand, D. J., Uzair, A. and Torresi, M. "BE4G Ultra-Low Emissions Biomass Burner: Modelling Procedure and Full-Scale Test Results (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [66] Debiagi, P., Pielsticker, S., Cerciello, F., **Scherer, V.,** Kneer, R., Faravelli, T. and Hasse, C. "Development of a Comprehensive Kinetic Model of Biomass Conversion in Inert, Air and Oxy-Fuel Conditions (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [67] Eckhard, T., Pflieger, C., Russo, C., Böttger, J., Senneca, O., Apicella, B., **Schiemann, M., Scherer, V.,** Muhler, M. and Cerciello, F. "Mineral Effects on Chemical and Physical Transformations of Cellulose-Based Model Fuels in N₂ and CO₂ Atmospheres (Poster)". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.

- [68] Eckhard, T., Pflieger, C., Russo, C., Böttger, J., Senneca, O., Apicella, B., **Schiemann, M.**, **Scherer, V.**, Muhler, M. and Cerciello, F. "Mineral Effects on Chemical and Physical Transformations of Cellulose-Based Model Fuels in N₂ and CO₂ Atmospheres (Poster)". *23rd edition of the International Conference on Analytical and Applied Pyrolysis*. Ghent, Belgium, 2022.
- [69] Eckhard, T., **Valentiner, S.**, Pflieger, C., Lotz, K., **Schiemann, M.**, **Scherer, V.** and Muhler, M. "The Catalytic Influence of Doped Metals on the Pyrolysis Product Distribution and Resulting Chars of Hydrothermally Derived Model Fuels (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [70] Farazi, S., Attili, A., **Heuer, S.**, **Schiemann, M.**, **Scherer, V.** and Pitsch, H. "Modeling and Simulation of Coal Ignition and Combustion Under Oxy-Fuel Condition (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [71] **Freisewinkel, E.**, Cerciello, F., **Tarlinski, D.**, **Schiemann, M.**, **Scherer, V.** and Senneca, O. "Role of Holocellulose on Thermal Annealing and Morphology of Biomass (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 17–18.  
- [72] Koch, M., Pielsticker, S., **Tarlinski, D.**, **Scherer, V.** and Kneer, R. "Coupling Radiative Properties with Detailed Char Conversion Kinetics (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [73] **Ontyd, C.**, Senneca, O., **Schiemann, M.** and **Scherer, V.** "A2 – Influence of Water Vapour on Tar and Gas Formation During Biomass Pyrolysis Under N₂ and CO₂ Atmosphere in a Drop Tube Reactor (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [74] Pörtner, L., Koch, M., **Freisewinkel, E.**, Pielsticker, S., **Schiemann, M.**, Kneer, R. and **Scherer, V.** "Investigations on Solid Fuel Particle Porosities and Their Influence on the Particle Radiation Interaction (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [75] Senneca, O., **Vorobiev, N.**, Wütscher, A., Cerciello, F., **Heuer, S.**, Wedler, C., Span, R., **Schiemann, M.**, Muhler, M. and **Scherer, V.** "Assessment of Combustion Rates of Coal Chars for Oxy-Combustion Applications (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
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- [77] **Tarlinski, D.**, **Freisewinkel, E.**, **Scherer, V.** and **Schiemann, M.** "Metal Fuels Reacting in Oxy-Fuel Flue Gas Mixtures (Poster)". *Renewable Metal Fuels Symposium*. Rapperswil, Switzerland, 2025.
- [78] **Tarlinski, D.**, **Freisewinkel, E.**, **Schiemann, M.** and **Scherer, V.** "Combustion and Pyrolysis of Aluminum and Magnesium Particles in Oxy-Fuel Atmosphere (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 57–58.  
- [79] **Vorobiev, N.**, **Schiemann, M.** and **Scherer, V.** "Optical Investigation of Char Combustion Kinetics Under Oxy-Fuel Conditions (Presentation)". *IFRF 2018 Conference*. Sheffield, United Kingdom, 2018.
- [80] Weber, K., Wang, L., **Heuer, S.**, **Scherer, V.**, Li, T., Skreiberg, Ø. and Løvås, T. "CO₂ Gasification of Biomass Chars Derived from Fast Pyrolysis of Birch Bark and Forest Residues (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [81] Wedler, C., **Ontyd, C.**, **Schiemann, M.**, **Scherer, V.**, Richter, M. and Span, R. "Evolution of Micro- and Mesopore Structure During Pyrolysis of Coal and Biomass in Different Atmospheres (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.

4.3 A3 – Experimental determination of reaction kinetics for the release of chlorine and sulphur species and for the conversion of these species in the gas phase

4.3.1 Project members

a) Project leader(s)

- Epple, Bernd

b) Scientific project workers

- Frigge, Lorenz
- Schmidt, Dominik
- Ströhle, Jochen
- Yildiz, Coskun
- von Bohnstein, Maximilian

4.3.2 Project summary

A3 investigated the release and conversion of S-, Cl-, and N-species in oxy-fuel combustion with exhaust-gas recirculation, where negligible N₂ and elevated CO₂ concentrations are present, the volatile-phase chemistry is altered, and corrosion risks are enhanced. Complementary TGA (intrinsic, low heating rate) and EFR (high heating rate, high temperature) measurements delivered model-ready datasets across fuels and atmospheres. Instrumentation was advanced from GC to GC-MS for highly reactive S/Cl compounds with higher temporal resolution, MS channels for CS₂ and CH₃SH as well as an FTIR spectrometer for NH₃ and HCN detection.












Starting from coal and extending to biomass (poplar, walnut shells; miscanthus), **A3** derived two-step pyrolysis models with distributed activation energies and developed mechanistic descriptions of S and Cl release and conversion, including mineral transformation and subsequent gas-phase reactions. These models were transferred to the CRC/TRR 129 CFD framework **C2** via **A8**, and kinetic schemes were extended to S devolatilisation and S-char conversion while advancing Cl release and N conversion. Cross-reactor comparisons with **A1** and **A2** established heating-rate consistency for walnut-shell pyrolysis. Pyritic-S behavior was inferred using **A5** synthetic fuel. The campaigns revealed strong temperature dependence of S, Cl, and N release, clarified temperature- and atmosphere-driven changes in bound S and Cl, fuel-specific shifts when switching from N₂ to CO₂, and the formation and conversion of NO_x.

4.3.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Debiagi, P., Yildiz, C., Richter, M., Ströhle, J., Epple, B., Faravelli, T. and Hasse, C. "Experimental and Modeling Assessment of Sulfur Release from Coal Under Low and High Heating Rates". *Proceedings of the Combustion Institute* 38.3 (2021), 4053–4061. [doi](#)
- [2] Debiagi, P., Yildiz, C., Ströhle, J., Epple, B., Faravelli, T. and Hasse, C. "Systematic Evaluation and Kinetic Modeling of Low Heating Rate Sulfur Release in Various Atmospheres". *Fuel* 289 (2021), 119739. [doi](#)

- [3] **Frigge, L.**, Elserafi, G., **Ströhle, J.** and **Epple, B.** "Sulfur and Chlorine Gas Species Formation During Coal Pyrolysis in Nitrogen and Carbon Dioxide Atmosphere". *Energy & Fuels* 30.9 (2016), 7713–7720. 
- [4] **Frigge, L.**, **Ströhle, J.** and **Epple, B.** "Release of Sulfur and Chlorine Gas Species During Coal Combustion and Pyrolysis in an Entrained Flow Reactor". *Fuel* 201 (2017), 105–110. 
- [5] Ontyd, C., Pielsticker, S., **Yildiz, C.**, Schiemann, M., Hatzfeld, O., **Ströhle, J.**, **Epple, B.**, Kneer, R. and Scherer, V. "Experimental Determination of Walnut Shell Pyrolysis Kinetics in N₂ and CO₂ via Thermogravimetric Analysis, Fluidized Bed and Drop Tube Reactors". *Fuel* 287 (2021), 119313. 
- [6] **Schmidt, D.**, **Yildiz, C.**, **Ströhle, J.** and **Epple, B.** "Release of Nitrogen, Sulfur and Chlorine Species from Coal in Carbon Dioxide Atmosphere". *Fuel* 284 (2021), 119279. 
- [7] **von Bohnstein, M.**, Langen, J., **Frigge, L.**, Stroh, A., **Ströhle, J.** and **Epple, B.** "Comparison of CFD Simulations with Measurements of Gaseous Sulfur Species Concentrations in a Pulverized Coal Fired 1 MW_{th} Furnace". *Energy & Fuels* 30.11 (2016), 9836–9849. 
- [8] **von Bohnstein, M.**, **Yildiz, C.**, **Frigge, L.**, **Ströhle, J.** and **Epple, B.** "Simulation Study of the Formation of Corrosive Gases in Coal Combustion in an Entrained Flow Reactor". *Energies* 13.17 (2020), 4523.  
- [9] **Yildiz, C.**, Richter, M., **Ströhle, J.** and **Epple, B.** "Release of Sulfur and Chlorine Gas Species During Combustion and Pyrolysis of Walnut Shells in an Entrained Flow Reactor". *Energies* 16.15 (2023), 5684.  
- [10] **Yildiz, C.**, Richter, M., **Ströhle, J.** and **Epple, B.** "Pollutant Formation Under Nitrogen and Carbon Dioxide Atmosphere of Torrefied Poplar in an Entrained Flow Reactor". *Energy & Fuels* 38.9 (2024), 8157–8167.  



b) Other publications (non peer-review)

Conference papers

- [11] Debiagi, P., **Yildiz, C.**, **Ströhle, J.**, **Epple, B.**, Faravelli, T. and Hasse, C. "Validation of a Comprehensive Kinetic Mechanism for Sulfur Release During Pyrolysis of Solid Fuels". *9th International Symposium on Coal Combustion*. Qingdao, China, 2019.
- [12] **Frigge, L.**, **Ströhle, J.** and **Epple, B.** "Sulfur and Chlorine Gas Species Formation During Temperature-Programmed Coal Air- and Oxy-Fuel Combustion". *13th International Conference on Energy for a Clean Environment*. Ponta Delgada, Portugal, 2017.

Presentations and Posters

- [13] Debiagi, P., **Yildiz, C.**, **Ströhle, J.**, **Epple, B.**, Faravelli, T. and Hasse, C. "Systematic Evaluation and Kinetic Modeling of Low Heating Rate Sulfur Release in Pyrolysis and Oxidation in Various Atmospheres (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [14] **Frigge, L.**, **Ströhle, J.** and **Epple, B.** "Modification of a Model for Sulfur Release During Coal Pyrolysis to Account for Oxy-Fuel Conditions (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [15] **Schmidt, D.**, **Yildiz, C.**, **Ströhle, J.** and **Epple, B.** "Experimental Assessment of the Release of Nitrogen, Sulfur and Chlorine Species During Pyrolysis of Coal and Biomass in CO₂ Atmosphere (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.

- [16] **Yildiz, C.**, Richter, M., **Ströhle, J.** and **Epple, B.** "Release of Nitrogen Gas Species During Combustion and Pyrolysis of Walnut Shells in an Entrained Flow Reactor (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.4 A5 – Kinetic investigations of the effect of catalytically active minerals in biomass-derived solid fuels on pyrolysis and char conversion under oxy-fuel conditions

4.4.1 Project members

a) Project leader(s)

- Cerciello, Francesca
- Muhler, Martin

b) Scientific project workers

- Böttger, Jannik
- Düdder, Hendrik
- Eckhard, Till
- Lotz, Katrin
- Pflieger, Christin
- Wütscher, Annika
- Zakgeym, Dina

4.4.2 Project summary


A5 systematically quantified how biomass-relevant minerals catalyze pyrolysis and char-conversion kinetics under oxy-fuel atmospheres, resolving dependencies on mineral identity, loading, counterions, and interactions while tracking speciation changes during thermal conversion. A cellulose-derived model fuel with lignite-like oxidation and multi-doped model fuels spanning mineral-free to natural coals isolated single-mineral and interaction effects across O₂, H₂O, and CO₂. Thermogravimetric and flow-through fixed-bed kinetics, heated-strip-reactor product analysis, and multidimensional pyrolysis-GC/MS-GC/TCD (with high-temperature injector and carrier-gas CO₂/H₂O) quantified product spectra, char-structure evolution, and apparent activation-energy shifts. Boiler-relevant heating rates were achieved via a flat-flame burner with **A2**.

The installation of a magnetic suspension balance enabled controlled O₂/CO₂/H₂O environments. Well-defined mixtures from hydrothermal carbonization and fast pyrolysis with typical minerals, together with leached/doped biomass components, established structure-reactivity relationships. The resulting datasets and parameters supported incorporation of catalytic effects into CPD, CCK, and CRECK-S-B and were correlated with combustion data (**A1**, **A2**), sorption (**A6**), and atomistic modeling (**A7**), yielding a systematic, quantitative description of mineral-catalyzed conversion in natural biomass and fossil fuels under oxy-fuel conditions


















4.4.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers






- [1] Apicella, B., Russo, C., Ciajolo, A., Cortese, L., **Cerciello, F.**, Stanzione, F., **Wütscher, A.**, **Muhler, M.** and Senneca, O. "High Temperature Pyrolysis of Lignite and Synthetic Carbons". *Fuel* 241 (2019), 264–272. 

- [2] **Böttger, J., Eckhard, T., Pflieger, C., Senneca, O., Muhler, M. and Cerciello, F.** "Green Coal Substitutes for Boilers Through Hydrothermal Carbonization of Biomass: Pyrolysis and Combustion Behavior". *Fuel* 344 (2023), 128025. [doi](#)
- [3] **Cerciello, F., Allouis, C., Russo, C., Freisewinkel, E., Tarlinski, D., Apicella, B., Schiemann, M., Scherer, V. and Senneca, O.** "Thermoplastic Phenomena and Morphological Changes Upon Fast Pyrolysis of Biomass and Model Compounds". *Molecules* 30.3 (2025). [doi](#) [a](#)
- [4] **Cerciello, F., Apicella, B., Russo, C., Cortese, L. and Senneca, O.** "Effects of Pressure on Lignocellulosic Biomass Fast Pyrolysis in Nitrogen and Carbon Dioxide". *Fuel* 287 (2021), 119604. [doi](#)
- [5] **Cerciello, F., Freisewinkel, E., Coppola, A., Ontyd, C., Tarlinski, D., Schiemann, M., Senneca, O., Salatino, P., Allouis, C., Scherer, V. and Fletcher, T. H.** "Xylan Fast Pyrolysis: An Experimental and Modelling Study of Particle Changes and Volatiles Release". *Fuel* 357 (2024), 129983. [doi](#)
- [6] **Düdder, H., Lotz, K., Wütscher, A. and Muhler, M.** "The Influence of Iron Oxide on the Oxidation Kinetics of Synthetic Char Derived from Thermogravimetric Analysis and Fixed-Bed Experiments Under Isothermal and Temperature-Programmed Conditions". *Fuel* 201 (2017), 99–104. [doi](#)
- [7] **Düdder, H., Wütscher, A., Stoll, R. and Muhler, M.** "Synthesis and Characterization of Lignite-Like Fuels Obtained by Hydrothermal Carbonization of Cellulose". *Fuel* 171 (2016), 54–58. [doi](#)
- [8] **Düdder, H., Wütscher, A., Vorobiev, N., Schiemann, M., Scherer, V. and Muhler, M.** "Oxidation Characteristics of a Cellulose-Derived Hydrochar in Thermogravimetric and Laminar Flow Burner Experiments". *Fuel Processing Technology* 148 (2016), 85–90. [doi](#)
- [9] **Eckhard, T., Pflieger, C., Böttger, J., Telaar, P., Cerciello, F. and Muhler, M.** "The Catalytic Effect of Iron and Alkali and Alkaline Earth Metal Sulfates Loading Series on the Conversion of Cellulose-Derived Hydrochars and Chars". *ACS Omega* 8.11 (2023), 10629–10639. [doi](#) [a](#)
- [10] **Eckhard, T., Pflieger, C., Russo, C., Freisewinkel, E., Eisenbach, T., Böttger, J., Senneca, O., Apicella, B., Schiemann, M., Span, R., Scherer, V., Muhler, M. and Cerciello, F.** "Mineral Effects on Chemical and Physical Transformations of Fast Pyrolysis Products of Cellulose-Based Model Fuels in N₂ and CO₂". *Fuel* 340 (2023), 127477. [doi](#)
- [11] **Eckhard, T., Pflieger, C., Schmidt, S., Böttger, J., Senneca, O., Schiemann, M., Scherer, V., Muhler, M. and Cerciello, F.** "Catalytic Effects for Cellulose-Based Model Fuels Under Low and High Heating Rate in Air and Oxy-Fuel Atmosphere". *Fuel* 324 (2022), 124437. [doi](#)
- [12] **Eckhard, T., Wütscher, A. and Muhler, M.** "Simultaneous Analysis of Light Gases and Heavy Pyrolyzates Evolved from Lignite and Hard Coal by Pyrolysis–GC/MS–GC/TCD". *Journal of Analytical and Applied Pyrolysis* 149 (2020), 104833. [doi](#)
- [13] Eisenbach, T., Farhadi Jahromi, B., Angenent, V., **Pflieger, C., Muhler, M., Schmid, R., Wedler, C. and Span, R.** "Linking Experimental H₂O Vapor Adsorption on Biomass Char with Physicochemical Char Properties and MD Simulation". *Fluid Phase Equilibria* 597 (2025), 114460. [doi](#) [a](#)
- [14] Freisewinkel, E., Eisenbach, T., Weise, V., Tarlinski, D., Pörtner, L., **Cerciello, F., Wedler, C., Schiemann, M., Span, R., Senneca, O. and Scherer, V.** "Porosity Measurement of Biomass Char by a Novel Combination of Adsorption Measurements and an Optical Method". *International Journal of Energy for a Clean Environment* (2025). [doi](#)
- [15] Graeser, P., **Wütscher, A., Cerciello, F., Muhler, M.** and Schiemann, M. "Emissivity Comparison Between Chars and Demineralized Coal Chars Under Oxycombustion Conditions". *Chemical Engineering & Technology* 41.7 (2018), 1490–1496. [doi](#)
- [16] Heuer, S., Senneca, O., **Wütscher, A., Düdder, H., Schiemann, M., Muhler, M.** and Scherer, V. "Effects of Oxy-Fuel Conditions on the Products of Pyrolysis in a Drop Tube Reactor". *Fuel Processing Technology* 150 (2016), 41–49. [doi](#)

- [17] **Lotz, K., Wütscher, A., Düdder, H.,** Berger, C. M., Russo, C., Mukherjee, K., Schwaab, G., Havenith, M. and **Muhler, M.** "Tuning the Properties of Iron-Doped Porous Graphitic Carbon Synthesized by Hydrothermal Carbonization of Cellulose and Subsequent Pyrolysis". *ACS Omega* 4.2 (2019), 4448–4460.  
- [18] **Pflieger, C., Eckhard, T., Böttger, J.,** Schulwitz, J., Herrendorf, T., Schmidt, S., Salamon, S., Landers, J., Wende, H., Kleist, W., **Muhler, M.** and **Cerciello, F.** "The Catalytic Effect of Iron Oxide Phases on the Conversion of Cellulose-Derived Chars in Diluted O₂ and CO₂". *Applied Energy* 353 (2024), 122068. 
- [19] **Pflieger, C., Eckhard, T.,** Schmitz, G., Angenent, V., Göckeler, M., Senneca, O., Schmid, R., **Cerciello, F.** and **Muhler, M.** "Thermicity of the Decomposition of Oxygen Functional Groups on Cellulose-Derived Chars". *ACS Omega* 7.51 (2022), 48606–48614.  
- [20] **Pflieger, C., Lotz, K.,** Hilse, N., Berger, C. M., Schiemann, M., Debiagi, P., Hasse, C., Scherer, V. and **Muhler, M.** "Catalytic Influence of Mineral Compounds on the Reactivity of Cellulose-Derived Char in O₂-, CO₂-, and H₂O-Containing Atmospheres". *Fuel* 287 (2021), 119584. 
- [21] Pielsticker, S., Debiagi, P., **Cerciello, F.,** Hasse, C. and Kneer, R. "Comparative Analysis of Pyrolysis Models Including SFOR, CRECK, and Bio-CPD to Predict Reaction Kinetics and Products from Extracted Biomass Components". *Fuel* 371 (2024), 131867.  
- [22] Senneca, O., Apicella, B., Russo, C., **Cerciello, F.,** Salatino, P., Heuer, S., **Wütscher, A.,** Schiemann, M., **Muhler, M.** and Scherer, V. "Pyrolysis and Thermal Annealing of Coal and Biomass in CO₂-Rich Atmospheres". *Energy & Fuels* 32.10 (2018), 10701–10708. 
- [23] Senneca, O. and **Cerciello, F.** "Kinetics of Combustion of Lignocellulosic Biomass: Recent Research and Critical Issues". *Fuel* 347 (2023), 128310.  
- [24] Senneca, O., **Cerciello, F.,** Russo, C., **Wütscher, A., Muhler, M.** and Apicella, B. "Thermal Treatment of Lignin, Cellulose and Hemicellulose in Nitrogen and Carbon Dioxide". *Fuel* 271 (2020), 117656. 
- [25] Senneca, O., Vorobiev, N., **Wütscher, A., Cerciello, F.,** Heuer, S., Wedler, C., Span, R., Schiemann, M., **Muhler, M.** and Scherer, V. "Assessment of Combustion Rates of Coal Chars for Oxy-Combustion Applications". *Fuel* 238 (2019), 173–185. 
- [26] Wedler, C., **Lotz, K.,** Arami-Niya, A., Xiao, G., Span, R., **Muhler, M.,** May, E. F. and Richter, M. "Influence of Mineral Composition of Chars Derived by Hydrothermal Carbonization on Sorption Behavior of CO₂, CH₄, and O₂". *ACS Omega* 5.19 (2020), 10704–10714.  
- [27] **Wütscher, A., Eckhard, T.,** Hiltrop, D., **Lotz, K.,** Schuhmann, W., Andronesco, C. and **Muhler, M.** "Nitrogen-Doped Metal-Free Carbon Materials Derived from Cellulose as Electrocatalysts for the Oxygen Reduction Reaction". *ChemElectroChem* 1 (2018), 16064. 
- [28] **Wütscher, A.,** Wedler, C., Seibel, C., Hiltrop, D., Fieback, T., **Muhler, M.** and Span, R. "On the Alternating Physicochemical Characteristics of Colombian Coal During Pyrolysis". *Journal of Analytical and Applied Pyrolysis* 123 (2017), 12–19. 





Conference papers

- [29] **Böttger, J., Eckhard, T., Pflieger, C.,** Senneca, O., **Muhler, M.** and **Cerciello, F.** "Green Coal Substitutes for Boilers Through Hydrothermal Carbonization of Biomass". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.
- [30] **Cerciello, F.,** Russo, C., Freiswinkel, E., Oliano, M. M., Ontyd, C., Senneca, O., Scherer, V. and Apicella, B. "Chemical Investigation of Heavy Condensed Products from Biomass Pyrolysis". *13th Mediterranean Combustion Symposium*. Corfu, Greece, 2025.



- [31] Eisenbach, T., Duarte, H. A., Wedler, C., **Pflieger, C., Muhler, M.** and Span, R. "Experimental Investigations on the Adsorptive Behavior of H₂O Vapor on HTC Char Particles". *14th International Conference on Applied Energy*. Bochum, Germany, 2022.  
- [32] **Lotz, K.**, Berger, C. M. and **Muhler, M.** "Catalytic Effect of Iron Phases on the Oxidation of Cellulose-Derived Synthetic Char". *Energy Procedia* 158 (2019), 694–699. 
- [33] **Pflieger, C., Eckhard, T., Böttger, J.**, Schulwitz, J., Schmidt, S., Salamon, S., Landers, J., Wende, H., **Muhler, M.** and **Cerciello, F.** "The Catalytic Effect of Iron Oxide Phases on the Conversion of Cellulose-Derived Chars". *14th International Conference on Applied Energy*. Bochum, Germany, 2022.  



b) Other publications (non peer-review)

Book chapters



- [71] **Böttger, J., Eckhard, T., Pflieger, C., Lotz, K.**, Scherer, V., **Cerciello, F.** and **Muhler, M.** "Catalytic Effects". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  
- [72] Pielsticker, S., Freisewinkel, E., **Böttger, J., Cerciello, F.**, Senneca, O., König, D., Scherer, V., **Muhler, M.**, Epple, B. and Kneer, R. "Pyrolysis Products and Kinetics". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers















- [34] **Böttger, J., Eckhard, T., Pflieger, C., Muhler, M.** and **Cerciello, F.** "Hydrothermally Carbonization of Biomass: Influence of the Cellulose, Hemicellulose and Lignin Content". *31. Deutscher Flammentag*. Berlin, Germany, 2023.
- [35] **Cerciello, F.**, Freisewinkel, E., Coppola, A., Ontyd, C., Schiemann, M., Salatino, P., Allouis, C., Scherer, V. and Senneca, O. "Xylan Fast Pyrolysis: An Experimental and Modelling Study of Particle Changes and Volatiles Release". *12th Mediterranean Combustion Symposium*. Luxor, Egypt, 2023.
- [36] **Eckhard, T., Lotz, K., Pflieger, C.**, Vorobiev, N., Valentiner, S., Scherer, V. and **Muhler, M.** "Hydrothermal carbonisierte mikrokristalline Cellulose als aschefreier Modellbrennstoff für Flachflammenbrenner". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [37] Freisewinkel, E., Eisenbach, T., Weise, V., Tarlinski, D., Pörtner, L., **Cerciello, F.**, Schiemann, M., Span, R., Senneca, O. and Scherer, V. "Porosity of Biomass Char: A Novel Determination Method and Changes in Walnut Shell with Progressing Pyrolysis". *48th International Conference on Clean Energy*. Clearwater, USA, 2024.
- [38] Kreitzberg, T., **Eckhard, T.**, Pielsticker, S., **Muhler, M.** and Kneer, R. "Änderung von Struktur und Reaktivität durch Pyrolyse fester Brennstoffe". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [39] **Pflieger, C., Eckhard, T., Böttger, J., Cerciello, F.** and **Muhler, M.** "Catalytic Influence of Minerals on Cellulose-Based Model Fuels and Model Chars in Oxidation and Gasification". *30. Deutscher Flammentag*. Hannover, Germany, 2021.
- [40] Senneca, O., Apicella, B., Russo, C., **Cerciello, F.**, Cortese, L., Stanzione, F., Salatino, P., **Wütscher, A., Muhler, M.** and Scherer, V. "Effects of CO₂ on Pyrolysis of Walnut Shells at High Temperature and Heating Rate in a HSR". *Joint Meeting the German and Italian Sections of the Combustion Institute*. Sorrento, Italy, 2018.  











- [41] **Wütscher, A.**, Apicella, B., Russo, C., Stanzione, F., Ciajolo, A., Heuer, S., Scherer, V., **Muhler, M.** and Senneca, O. "Characterization of Tar Produced from Walnut Shells Pyrolysis". *40th Meeting of the Italian Section of the Combustion Institute*. Rome, Italy, 2017.  

Data sets

- [42] Pielsticker, S., Debiagi, P., **Cerciello, F.**, Hasse, C. and Kneer, R. *Comparative Analysis of Pyrolysis Models Including SFOR, CRECK, and Bio-CPD to Predict Reaction Kinetics and Products from Extracted Biomass Components – Supplementary Dataset*. 2024.  

Presentations and Posters

- [43] Berkel, L., Debiagi, P., Nicolai, H., **Cerciello, F.**, Pielsticker, S., Senneca, O., Kneer, R., Faravelli, T. and Hasse, C. "Walnut Shell Pyrolysis: Feedstock Characterization and Kinetics Considering Hemicellulose-Lignin Interactions (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 10–11.  
- [44] **Böttger, J.**, **Cerciello, F.** and **Muhler, M.** "Pyrolysis of Hydrochars Derived from Co-Hydrothermal Carbonization of PVC and Biomass (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, p. 9.  
- [45] **Böttger, J.**, **Eckhard, T.**, **Pflieger, C.**, **Muhler, M.** and **Cerciello, F.** "Hydrothermal Carbonization of Biomass: Influence of Cellulose, Hemicellulose and Lignin (Poster)". *23rd edition of the International Conference on Analytical and Applied Pyrolysis*. Ghent, Belgium, 2022.
- [46] **Böttger, J.**, **Eckhard, T.**, **Pflieger, C.**, Senneca, O., **Muhler, M.** and **Cerciello, F.** "Influence of Minerals on the Pyrolysis of Hydrothermally Carbonized Biomass (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [47] **Cerciello, F.**, Ontyd, C., Russo, C., Freisewinkel, E., Oliano, M. M., Senneca, O., Scherer, V., Schiemann, M., **Muhler, M.** and Apicella, B. "Biomass Pyrolysis: Critical Issue on Tar Analysis (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [48] Chagtmi, R., Maaoui, A., **Cerciello, F.**, Ben Hassen Trabelsi, A., Apicella, B., Stanzione, F., Migliaccio, R., Olliano, M. M., Urciuolo, M. and Senneca, O. "Effects of Pyrolysis Reactor Types on the Bioproduct Compositions of Tannery Fleshing Waste (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [49] Dadduzio, R., Penati, M., Bini, L., Rogora, M., Valenzano, M., Saponaro, A., Senneca, O., **Cerciello, F.**, Ontyd, C., Brand, D. J., Uzair, A. and Torresi, M. "BE4G Ultra-Low Emissions Biomass Burner: Modelling Procedure and Full-Scale Test Results (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [50] Debiagi, P., Pielsticker, S., **Cerciello, F.**, Scherer, V., Kneer, R., Faravelli, T. and Hasse, C. "Development of a Comprehensive Kinetic Model of Biomass Conversion in Inert, Air and Oxy-Fuel Conditions (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [51] **Düdder, H.**, **Wütscher, A.** and **Muhler, M.** "Catalytic Influence of Minerals on the Combustion Behavior of a Cellulose-Derived Solid Fuel (Poster)". *48. Jahrestreffen Deutscher Katalytiker*. Weimar, Germany, 2015.
- [52] **Düdder, H.**, **Wütscher, A.** and **Muhler, M.** "Kinetic Analysis of Temperature-Programmed and Isothermal Hydrochar Oxidation Experiments (Poster)". *European Symposium on Chemical Reaction Engineering*. Fürstfeldbruck, Germany, 2015.
- [53] **Eckhard, T.** "Pyrolysis-GC/MS-GC/TCD: Analysis of Broad Product Distributions Evolving During Coal Pyrolysis (Presentation)". *Pyrolysis GC-MS User Meeting*. Duisburg, Germany, 2019.

- [54] **Eckhard, T., Lotz, K., Wütscher, A.,** Berger, C. M. and **Muhler, M.** "Kinetic Investigations on Catalytic Properties of Mineral Matter in Oxy-Fuel Combustion (Poster)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [55] **Eckhard, T., Pflieger, C.,** Russo, C., **Böttger, J.,** Senneca, O., Apicella, B., Schiemann, M., Scherer, V., **Muhler, M.** and **Cerciello, F.** "Mineral Effects on Chemical and Physical Transformations of Cellulose-Based Model Fuels in N₂ and CO₂ Atmospheres (Poster)". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.
- [56] **Eckhard, T., Pflieger, C.,** Russo, C., **Böttger, J.,** Senneca, O., Apicella, B., Schiemann, M., Scherer, V., **Muhler, M.** and **Cerciello, F.** "Mineral Effects on Chemical and Physical Transformations of Cellulose-Based Model Fuels in N₂ and CO₂ Atmospheres (Poster)". *23rd edition of the International Conference on Analytical and Applied Pyrolysis*. Ghent, Belgium, 2022.
- [57] **Eckhard, T.,** Valentiner, S., **Pflieger, C., Lotz, K.,** Schiemann, M., Scherer, V. and **Muhler, M.** "The Catalytic Influence of Doped Metals on the Pyrolysis Product Distribution and Resulting Chars of Hydrothermally Derived Model Fuels (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [58] Eisenbach, T., **Pflieger, C.,** Wedler, C., **Muhler, M.** and Span, R. "Correlation of Chemical and Structural Pore Properties and H₂O Vapor Adsorption in Biomass Char Particles (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [59] Eisenbach, T., Wedler, C., Quast, C., Angenent, V., **Muhler, M.,** Schmid, R. and Span, R. "Untersuchung der Korrelation von Wasserdampfadsorption und chemischen und strukturellen Eigenschaften von Biomassekoksen (Presentation)". *Thermodynamik-Kolloquium*. Hannover, Germany, 2023.
- [60] Freisewinkel, E., **Cerciello, F.,** Tarlinski, D., Schiemann, M., Scherer, V. and Senneca, O. "Role of Holocellulose on Thermal Annealing and Morphology of Biomass (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 17–18.  
- [61] **Lotz, K., Wütscher, A., Eckhard, T.** and **Muhler, M.** "The Impact of Mineral Matter on the Evolved Pyrolysis Gases (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [62] **Lotz, K., Wütscher, A.** and **Muhler, M.** "The Influence of Iron Oxide on the Oxidation Kinetics of Synthetic Char (Poster)". *50. Jahrestreffen Deutscher Katalytiker*. Weimar, Germany, 2017.
- [63] Maaoui, A., Chagtmi, R., **Cerciello, F.,** Apicella, B., Migliaccio, R., Stanzione, F., Oliano, M. M., Ben Hassen Trabelsi, A. and Senneca, O. "Fast Pyrolysis of Biomass of Different Type and Origin: Effect on Bio-Oil and Char (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [64] Maaoui, A., Chagtmi, R., **Cerciello, F.,** Ben Hassen Trabelsi, A., Urciuolo, M., Stanzione, F., Migliaccio, R., Senneca, O. and Apicella, B. "Use of Egg Shells Wastes for Catalytic Pyrolysis of Lignocellulosic Biomass (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [65] **Pflieger, C., Eckhard, T., Böttger, J.,** Telaar, P., Schulwitz, J., Schmidt, S., **Cerciello, F.** and **Muhler, M.** "The Catalytic Effect of Iron on the Oxidation of Cellulose-Derived Chars (Poster)". *55. Jahrestreffen Deutscher Katalytiker*. Weimar, Germany, 2022.
- [66] **Pflieger, C., Lotz, K., Eckhard, T.** and **Muhler, M.** "Reactivity of Mineral-Free and Doped Synthetic Chars in O₂-, CO₂-, and H₂O-Containing Atmospheres (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [67] Pielsticker, S., Debiagi, P., **Cerciello, F.,** Coppola, A., Hasse, C. and Kneer, R. "Prediction of Pyrolysis Kinetics with Models of Different Complexity for Isolated Biomass Components (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

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- [68] Senneca, O., Vorobiev, N., **Wütscher, A.**, **Cerciello, F.**, Heuer, S., Wedler, C., Span, R., Schiemann, M., **Muhler, M.** and Scherer, V. "Assessment of Combustion Rates of Coal Chars for Oxy-Combustion Applications (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [69] **Wütscher, A.**, **Düdder, H.** and **Muhler, M.** "Detailed Investigations on Particle Related Effects in Oxy-Fuel Coal Combustion: Pyrolysis, Char Burnout and Release of Sulphur and Chlorine Components (Presentation)". *1st International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2016.
- [70] **Wütscher, A.**, **Düdder, H.** and **Muhler, M.** "Synthetic Lignite-Like Fuel for Oxy-Fuel Combustion (Presentation)". *49. Jahrestreffen Deutscher Katalytiker*. Weimar, Germany, 2016.

4.5 A6 – Determination of excess-sorptive kinetics and equilibrium loadings of oxy-fuel gas components on solid fuels

4.5.1 Project members

a) Project leader(s)

- Fieback, Tobias
- Richter, Markus
- Span, Roland

b) Scientific project workers

- Eisenbach, Tim
- Seibel, Christopher
- Wedler, Carsten



4.5.2 Project summary

A6 quantified diffusion-driven sorption and pore-structure evolution in chars to mechanistically link pore-scale transport with solid-fuel conversion kinetics. Advanced gravimetric and volumetric measurements delivered extensive datasets on pore-surface evolution during pyrolysis and char conversion and on adsorption/desorption kinetics for chars from biomass, coal (lignite to bituminous), and **A5** model fuels. High-temperature sorption equipment enabled equilibrium loadings up to reaction onset, including components of oxy-fuel atmospheres (O₂, CO₂, H₂O). Sensitivity upgrades resolved low-affinity species, and an online gas chromatograph quantified selectivity for condensing components. Guided by these data, a selective sorption model was developed that distinguishes pore regimes and provides closed-form diffusion fluxes via partial derivatives with respect to time, temperature, and pressure; a complementary pore-surface evolution model captures structural changes with temperature and conversion progress. Together, they yield regime-specific effective diffusion coefficients and equilibrium parameters for macro/meso-, micro-, and ultramicropore domains, suitable for embedding in detailed pyrolysis and char-conversion frameworks (CPD, CCK). Validation across multiple chars and gas species was initiated, with parameter generalization based on surface/pore characterization and fuel composition. Collaboration with **A2** supported model implementation, cooperation with **A5** extended sorption studies on synthetic fuels, and joint work with **A7** provided links to molecular-scale simulations.

4.5.3 Published project results

a) Publications with scientific quality assurance (peer-review)






Journal papers

- [1] Eckhard, T., Pflieger, C., Russo, C., Freisewinkel, E., **Eisenbach, T.**, Böttger, J., Senneca, O., Apicella, B., Schiemann, M., **Span, R.**, Scherer, V., Muhler, M. and Cerciello, F. "Mineral Effects on Chemical and Physical Transformations of Fast Pyrolysis Products of Cellulose-Based Model Fuels in N₂ and CO₂". *Fuel* 340 (2023), 127477. 
- [2] **Eisenbach, T.**, Farhadi Jahromi, B., Angenent, V., Pflieger, C., Muhler, M., Schmid, R., **Wedler, C.** and **Span, R.** "Linking Experimental H₂O Vapor Adsorption on Biomass Char with Physico-chemical Char Properties and MD Simulation". *Fluid Phase Equilibria* 597 (2025), 114460. 

- [3] **Eisenbach, T., Wedler, C. and Span, R.** "Experimental Investigation and Modeling of Mass Transport Properties of O₂ in Biomass Chars". *Chemical Engineering Science* 287 (2024), 119735. [doi](#) [a](#)
- [4] Freisewinkel, E., **Eisenbach, T.**, Weise, V., Tarlinski, D., Pörtner, L., Cerciello, F., **Wedler, C.**, Schiemann, M., **Span, R.**, Senneca, O. and Scherer, V. "Porosity Measurement of Biomass Char by a Novel Combination of Adsorption Measurements and an Optical Method". *International Journal of Energy for a Clean Environment* (2025). [doi](#)
- [5] Heuer, S., **Wedler, C.**, Ontyd, C., Schiemann, M., **Span, R., Richter, M.** and Scherer, V. "Evolution of Coal Char Porosity from CO₂-Pyrolysis Experiments". *Fuel* 253 (2019), 1457–1464. [doi](#)
- [6] **Seibel, C. and Fieback, T.** "New Sample Carrier Systems for Thermogravimetric Analysis Under Forced Flow Conditions and Their Influence on Microkinetic Results". *Review of Scientific Instruments* 86.9 (2015), 095104. [doi](#)
- [7] **Seibel, C., Wedler, C., Vorobiev, N., Schiemann, M., Scherer, V., Span, R. and Fieback, T.** "Sorption Measurements for Determining Surface Effects and Structure of Solid Fuels". *Fuel Processing Technology* 153 (2016), 81–86. [doi](#)
- [8] Senneca, O., Vorobiev, N., Wütscher, A., Cerciello, F., Heuer, S., **Wedler, C., Span, R.**, Schiemann, M., Muhler, M. and Scherer, V. "Assessment of Combustion Rates of Coal Chars for Oxy-Combustion Applications". *Fuel* 238 (2019), 173–185. [doi](#)
- [9] Tarlinski, D., Freisewinkel, E., **Eisenbach, T., Span, R.**, Schiemann, M. and Scherer, V. "Combustion of Single Walnut Shell Particles in a Laminar Flow Reactor Under Oxy-Fuel Conditions: Optical Measurements and Particle Sampling". *Fuel* 369 (2024), 131613. [doi](#) [a](#)
- [10] **Wedler, C., Lotz, K., Arami-Niya, A., Xiao, G., Span, R., Muhler, M., May, E. F. and Richter, M.** "Influence of Mineral Composition of Chars Derived by Hydrothermal Carbonization on Sorption Behavior of CO₂, CH₄, and O₂". *ACS Omega* 5.19 (2020), 10704–10714. [doi](#) [a](#)
- [11] **Wedler, C. and Span, R.** "A Pore-Structure Dependent Kinetic Adsorption Model for Consideration in Char Conversion – Adsorption Kinetics of CO₂ on Biomass Chars". *Chemical Engineering Science* 231 (2021), 116281. [doi](#)
- [12] **Wedler, C. and Span, R.** "Micropore Analysis of Biomass Chars by CO₂ Adsorption: Comparison of Different Analysis Methods". *Energy & Fuels* 35.10 (2021), 8799–8806. [doi](#)
- [13] **Wedler, C., Span, R. and Richter, M.** "Comparison of Micro- and Macropore Evolution of Coal Char During Pyrolysis". *Fuel* 275 (2020), 117845. [doi](#)
- [14] Wütscher, A., **Wedler, C., Seibel, C., Hiltrop, D., Fieback, T., Muhler, M. and Span, R.** "On the Alternating Physicochemical Characteristics of Colombian Coal During Pyrolysis". *Journal of Analytical and Applied Pyrolysis* 123 (2017), 12–19. [doi](#)



Conference papers

- [15] **Eisenbach, T., Duarte, H. A., Wedler, C., Pflieger, C., Muhler, M. and Span, R.** "Experimental Investigations on the Adsorptive Behavior of H₂O Vapor on HTC Char Particles". *14th International Conference on Applied Energy*. Bochum, Germany, 2022. [doi](#) [a](#)
- [16] **Fieback, T. and Span, R.** "High Temperature Sorption Measurements for Determining Surface Effects of Solid Fuels". *Energy Procedia* 61 (2014), 1501–1504. [doi](#) [a](#)
- [17] Ontyd, C., Freisewinkel, E., **Wedler, C., Eisenbach, T., Span, R., Senneca, O. and Scherer, V.** "Flash Pyrolysis of Walnut Shells and Poplar in N₂ and CO₂: Pyrolysis Kinetics, Pore Evolution and a Model for Evaluation of Pyrolysis Species". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.
- [18] **Wedler, C., Arami-Niya, A., Xiao, G., Span, R., May, E. F. and Richter, M.** "Gas Diffusion and Sorption in Carbon Conversion". *Energy Procedia* 158 (2019), 1792–1797. [doi](#) [a](#)



- [19] **Wedler, C., Eisenbach, T., Schwarz, J. and Span, R.** "A First Parameterization of the Pore-Structure Dependent Kinetic Adsorption Model for O₂ Adsorption in Biomass Conversion Modeling". *13th International Conference on Applied Energy*. online, 2021. 
- [20] **Wedler, C., Richter, M. and Span, R.** "Integration of Sorption Kinetics in Carbon Conversion Modeling for the Description of Oxyfuel Combustion Processes". *Energy Procedia* 142 (2017), 1361–1366.  
- [21] **Wedler, C., Seibel, C., Richter, M., Fieback, T. and Span, R.** "Oxyfuel Combustion – Experimental Investigation of Sorption Effects on Coal Char". *Energy Procedia* 105 (2017), 1847–1851.  

b) Other publications (non peer-review)



Book chapters

- [39] **Eisenbach, T., Wedler, C. and Span, R.** "Sorption Effects". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers

- [22] Freisewinkel, E., **Eisenbach, T.**, Weise, V., Tarlinski, D., Pörtner, L., Cerciello, F., Schiemann, M., **Span, R.**, Senneca, O. and Scherer, V. "Porosity of Biomass Char: A Novel Determination Method and Changes in Walnut Shell with Progressing Pyrolysis". *48th International Conference on Clean Energy*. Clearwater, USA, 2024.
- [23] Schiemann, M., Vorobiev, N., Scherer, V., **Wedler, C., Richter, M. and Span, R.** "Effektive Diffusionskoeffizienten in Kokspartikeln aus Oxyfuel-Feuerungen". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017, pp. 395–406.  
- [24] Tarlinski, D., Freisewinkel, E., **Eisenbach, T., Span, R.**, Schiemann, M. and Scherer, V. "Char Burnout of Walnut Shells Using Optical Measurement Techniques and First Comparison of the Experimental Data to the CCK Model". *46th International Technical Conference on Clean Energy*. Clearwater (USA), 2022.
- [25] **Wedler, C.**, Angenent, V., Yönder, Ö., Hättig, C., Schmid, R., **Span, R. and Richter, M.** "Adsorption und Diffusion bei der Oxyfuel-Verbrennung von Festbrennstoffen: Vergleich von Experiment und MD-Simulation". *29. Deutscher Flammentag*. Bochum, Germany, 2019.

Presentations and Posters

- [26] **Eisenbach, T.**, Duarte, H. A., **Wedler, C. and Span, R.** "Experimental Investigation on the Adsorptive Mass Transfer of H₂O Vapor on HTC Char Particles (Poster)". *1st International Workshop on Reacting Particle-Gas Systems*. Bochum, Germany, 2022.
- [27] **Eisenbach, T.**, Duarte, H. A., **Wedler, C. and Span, R.** "Experimental Investigations on the Adsorptive Mass Transfer of H₂O Vapor on Biomass Char Particles (Poster)". *Thermodynamik-Kolloquium*. Chemnitz, Germany, 2022.
- [28] **Eisenbach, T.**, Pflieger, C., **Wedler, C.**, Muhler, M. and **Span, R.** "Correlation of Chemical and Structural Pore Properties and H₂O Vapor Adsorption in Biomass Char Particles (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [29] **Eisenbach, T. and Span, R.** "Adsorption Measurements: An Experimental Basis for the Determination of Pore Structure and Mass Transport Properties (Presentation)". *Workshop on thermophysical properties and related topics*. Prague, Czech Republic, 2023.

- [30] **Eisenbach, T.** and **Span, R.** "Modeling Mass Transport Properties of Oxyfuel Species in Solid Biomass Fuel Particles (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 37–38.  
- [31] **Eisenbach, T.**, **Wedler, C.**, Quast, C., Angenent, V., Muhler, M., Schmid, R. and **Span, R.** "Untersuchung der Korrelation von Wasserdampfadsorption und chemischen und strukturellen Eigenschaften von Biomassekoksen (Presentation)". *Thermodynamik-Kolloquium*. Hannover, Germany, 2023.
- [32] **Fieback, T.** "Hochtemperatur-Sorptionsmessungen für die Bestimmung von Oberflächeneffekten an Festbrennstoffen". *Thermodynamik-Kolloquium 2014*. Stuttgart, Germany, 2014.
- [33] Senneca, O., Vorobiev, N., Wütscher, A., Cerciello, F., Heuer, S., **Wedler, C.**, **Span, R.**, Schiemann, M., Muhler, M. and Scherer, V. "Assessment of Combustion Rates of Coal Chars for Oxy-Combustion Applications (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [34] **Wedler, C.**, Angenent, V., Yönder, Ö., Hättig, C., Schmid, R., **Span, R.** and **Richter, M.** "Adsorption and Diffusion in Oxyfuel Combustion – Linking Experiment and MD Simulation Through Graphite Structures as a First Example (Poster)". *Diffusion Fundamentals 8*. Erlangen, Germany, 2019.
- [35] **Wedler, C.**, Arami-Niya, A., Xiao, G., **Span, R.**, May, E. F. and **Richter, M.** "Sorption Kinetics of CO₂, CH₄ and O₂ on Cellulose-Based Hydrochars for Carbon Conversion Modelling (Presentation)". *Thermodynamik-Kolloquium 2018*. Kassel, Germany, 2018.
- [36] **Wedler, C.**, Ontyd, C., Schiemann, M., Scherer, V., **Richter, M.** and **Span, R.** "Evolution of Micro- and Mesopore Structure During Pyrolysis of Coal and Biomass in Different Atmospheres (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [37] **Wedler, C.**, **Richter, M.** and **Span, R.** "Sorptive Determination of Effective Diffusion Coefficients for Integration in Carbon Conversion Models (Poster)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [38] **Wedler, C.**, **Span, R.** and **Richter, M.** "Adsorption und Diffusion bei der Oxyfuel-Verbrennung: Graphit als Türöffner zur Verknüpfung von Experiment und MD-Simulation (Poster)". *Jahrestreffen der ProcessNet-Fachgruppen Adsorption und Hochdruckverfahrenstechnik*. Freiberg, Germany, 2019.

4.6 A7 – Atomistic multiscale simulations of char conversion

4.6.1 Project members

a) Project leader(s)

- Hättig, Christof
- Schmid, Rochus

b) Scientific project workers

- Angenent, Vanessa
- Dürholt, Johannes
- Schmitz, Gunnar
- Schnieder, Bastian
- Warczinski, Lisa (born Götte)
- Yönder, Özlem
- Farhadi Jahromi, Babak


4.6.2 Project summary
















A7 delivered ab initio kinetics and molecular-transport data to close gaps in semi-global mechanisms for char conversion beyond experimental reach. Quantum electronic-structure calculations provided rate constants for elementary surface reactions in char oxidation, and molecular dynamics (MD) yielded adsorption isotherms and diffusion coefficients for O₂, CO₂, and H₂O in nanometer-scale pores. A multiscale protocol for char conversion was established by generalizing an automated kinetic-model workflow from small molecules to complex char fragments and validating efficient screening methods. Mesoscopic char structures were constructed from elemental analysis, density, infrared, and solid-state NMR data and used to study adsorption on graphitic surfaces with varied terminations (periodic slabs) and transport in atomistic char models; model construction assimilated structural constraints from **A5** and **A6** (e.g. HR-TEM, pore-size distributions). Methods were extended to heteroatoms (S, N, P) and biochar-relevant ions (Na⁺, K⁺, Ca²⁺). Biochar models templated from cellulose, hemicellulose, and lignin captured defect-rich PAH networks with aliphatic bridges and non-six-membered rings. Accurate kinetic parameters for these motifs were tabulated for direct incorporation into CRECK-S-B in **A8**. Sorption and diffusion results supported the transport model in **A6**, and gas-phase pathways for OPAHs, NPAHs, and fuel-NO_x were provided to **B1**. Integration and cross-validation with **A1**, **A2**, **A5**, **A6**, and **B1** ensured consistency across scales and facilitated transfer via **A6** and **A8** to areas B and C.

4.6.3 Published project results

a) Publications with scientific quality assurance (peer-review)



Journal papers

- [1] **Angenent, V.**, Oelert, D. and **Schmid, R.** "Towards Realistic Structural Char Models: Generation of Stacked Graphene-Like Layers Using Constrained Reactive Molecular Dynamics Simulations". *Fuel* 372 (2024), 132064.  doi.org/10.1016/j.fuel.2024.132064

- [2] **Angenent, V.** and **Schmid, R.** "Automated Rotating TEM Simulations of Graphitic Material". *Energy Proceedings* 28 (2022).  
- [3] Chen, B., Kruse, S., **Schmid, R.**, Cai, L., Hansen, N. and Pitsch, H. "Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach". *Energy & Fuels* 35.2 (2021). 
- [4] Eisenbach, T., **Farhadi Jahromi, B.**, **Angenent, V.**, Pflieger, C., Muhler, M., **Schmid, R.**, Wedler, C. and Span, R. "Linking Experimental H₂O Vapor Adsorption on Biomass Char with Physicochemical Char Properties and MD Simulation". *Fluid Phase Equilibria* 597 (2025), 114460.  
- [5] Pflieger, C., Eckhard, T., **Schmitz, G.**, **Angenent, V.**, Göckeler, M., Senneca, O., **Schmid, R.**, Cerciello, F. and Muhler, M. "Thermicity of the Decomposition of Oxygen Functional Groups on Cellulose-Derived Chars". *ACS Omega* 7.51 (2022), 48606–48614.  
- [6] Pielsticker, S., Möller, G. H., Gövert, B., Kreitzberg, T., Hatzfeld, O., **Yönder, Ö.**, **Angenent, V.**, **Hättig, C.**, **Schmid, R.** and Kneer, R. "Influence of Biomass Torrefaction Parameters on Fast Pyrolysis Products Under Flame-Equivalent Conditions". *Biomass and Bioenergy* 119 (2018), 392–410. 
- [7] **Schmitz, G.**, **Yönder, Ö.**, **Schnieder, B.**, **Schmid, R.** and **Hättig, C.** "An Automatized Workflow from Molecular Dynamic Simulation to Quantum Chemical Methods to Identify Elementary Reactions and Compute Reaction Constants". *Journal of Computational Chemistry* 42.32 (2021), 2264–2282.  
- [8] **Schnieder, B.**, **Schmid, R.** and **Hättig, C.** "Quantum Chemical Study on the Evolution of Sulfur Functional Groups During Char Burnout". *The Journal of Physical Chemistry A* 129.14 (2025). 
- [9] **Yönder, Ö.** and **Hättig, C.** "Density Functional Theory Study of CO Formation Through Reactions of Polycyclic Aromatic Hydrocarbons with Atomic Oxygen (O(³P))". *Fuel* 241 (2019), 851–860. 
- [10] **Yönder, Ö.**, **Schmitz, G.**, **Hättig, C.**, **Schmid, R.**, Debiagi, P., Hasse, C., Locaspi, A. and Faravelli, T. "Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics". *The Journal of Physical Chemistry A* 124.46 (2020), 9626–9637. 
- [11] **Yönder, Ö.**, **Schmitz, G.**, **Schmid, R.**, **Schnieder, B.** and **Hättig, C.** "A Computational Chemistry Study on the Evolution of Oxygen Functional Groups During Char Burnout". *Fuel* 365 (2024), 131217.  

b) Other publications (non peer-review)

Book chapters











- [27] **Schnieder, B.**, **Farhadi Jahromi, B.**, **Schmitz, G.**, **Hättig, C.** and **Schmid, R.** "Atomistic Simulations". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers


- [12] **Angenent, V.**, Oelert, D. and **Schmid, R.** "In Silico Design of Atomistic Char Models of Curved Stacked Carbon Layers". *11th Mediterranean Combustion Symposium*. Tenerife, Spain, 2019.
- [13] Wedler, C., **Angenent, V.**, **Yönder, Ö.**, **Hättig, C.**, **Schmid, R.**, Span, R. and Richter, M. "Adsorption und Diffusion bei der Oxyfuel-Verbrennung von Festbrennstoffen: Vergleich von Experiment und MD-Simulation". *29. Deutscher Flammentag*. Bochum, Germany, 2019.

- [14] **Yönder, Ö., Hättig, C., Angenent, V., Schmid, R.**, Leonhard, K. and Schmalz, F. "Computational Chemistry as a Tool for Predictive Combustion Modelling". *14th International Conference on Sustainable Development of Energy, Water and Environment Systems*. Dubrovnik, Croatia, 2019.

Data sets

- [15] **Hättig, C.** and **Yönder, Ö.** *Raw Data for: "Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics"*. Zenodo. 2025.  
- [16] **Schnieder, B.**, Debiagi, P., Pelucchi, M., **Schmid, R.** and **Hättig, C.** *Raw Data to "Computational Study on the Pyrolysis of 2,5-Diketopiperazine: From Electronic Structure Calculations to Kinetic Modeling"*. 2025.  
- [17] **Schnieder, B.**, **Hättig, C.**, **Schmitz, G.**, **Schmid, R.** and **Yönder, Ö.** *Raw Data to "A Computational Chemistry Study on the Evolution of Oxygen Functional Groups During Char Burnout"*. 2024.  
- [18] **Schnieder, B.**, **Schmid, R.** and **Hättig, C.** *HyATraX*. 2024.  
- [19] **Schnieder, B.**, **Schmid, R.** and **Hättig, C.** *Raw Data to "A Quantum Chemical Study on the Evolution of Sulfur Functional Groups During Char Burnout"*. 2025.  

Presentations and Posters

- [20] **Angenent, V.** and **Schmid, R.** "Structural Char Models Including Oxygen Functional Groups (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [21] Chen, B., Kruse, S., **Schmid, R.**, Cai, L., Hansen, N. and Pitsch, H. "Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [22] Eisenbach, T., Wedler, C., Quast, C., **Angenent, V.**, Muhler, M., **Schmid, R.** and Span, R. "Untersuchung der Korrelation von Wasserdampfadsorption und chemischen und strukturellen Eigenschaften von Biomassekoksen (Presentation)". *Thermodynamik-Kolloquium*. Hannover, Germany, 2023.
- [23] **Farhadi Jahromi, B.**, Khan, M. U. and **Schmid, R.** "Atomistic Simulations of Volatile Diffusion in Char – Quantifying the Effect of the Pore Size Regime (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 35–36.  
- [24] **Schnieder, B.**, **Hättig, C.** and **Schmid, R.** "Molecular-Level Modeling of NO_x Precursor Release During the Oxy-Fuel Combustion of Biochar (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, p. 16.  
- [25] Wedler, C., **Angenent, V.**, **Yönder, Ö.**, **Hättig, C.**, **Schmid, R.**, Span, R. and Richter, M. "Adsorption and Diffusion in Oxyfuel Combustion – Linking Experiment and MD Simulation Through Graphite Structures as a First Example (Poster)". *Diffusion Fundamentals 8*. Erlangen, Germany, 2019.
- [26] **Yönder, Ö.**, **Schmitz, G.** and **Hättig, C.** "Evolution of Oxygen Functional Groups During Char Burnout (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.7 A8 – Development of a comprehensive kinetic model for the conversion of solid fuels in oxy-fuel atmospheres

4.7.1 Project members

a) Project leader(s)

- Hasse, Christian

b) Scientific project workers

- Berkel, Leon
- Debiagi, Paulo Eduardo Amaral
- Xu, Wen

4.7.2 Project summary





















A8 built a comprehensive kinetic framework for oxy-fuel thermochemical conversion of solid fuels that seamlessly couples primary pyrolysis, char conversion, and secondary gas-phase chemistry, explicitly capturing metaplast formation, thermal annealing, catalytic mineral effects, and pollutant/precursor pathways. Starting from CRECK-S, it integrated and validated data from **A1**, **A2**, **A3**, **A5**, **A7**, and **B1**, demonstrated accuracy for Colombian and high-sulphur American bituminous coals and Rhenish lignite, and extended the mechanism to oxy-fuel atmospheres with S release. A machine-learning reduced surrogate for 3D CFD was created with **C2**. Initial biomass applications (walnut shell) underscored the need for robust biochemical characterization. The finalized biomass formulation (walnut shell, miscanthus, beech wood) mirrors the coal approach with a compact set of reference species, CHEMKIN-like files, and Arrhenius parameters, covering wide temperature/heating-rate ranges, air/oxy-fuel atmospheres, and pressures. The model remains extensible to fuel-N and mineral catalysis and was deployed to **B3** and **C2**.

4.7.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Afessa, M. M., **Debiagi, P.**, Ferreiro, A. I., Mendes, M. A., Faravelli, T. and Ramayya, A. "Experimental and Modeling Investigation on Pyrolysis of Agricultural Biomass Residues: Khat Stem and Coffee Husk for Bio-Oil Application". *Journal of Analytical and Applied Pyrolysis* 162 (2022), 105435. [doi](#)
- [2] **Berkel, L.**, **Debiagi, P.**, Nicolai, H., Amjed, M. A., Stagni, A., **Hasse, C.** and Faravelli, T. "Development of a Multiphase Chemical Reactor Network Method as a Tool for Simulating Biomass Gasification in Fluidized Beds". *Fuel* 357 (2024), 129731. [doi](#)
- [3] **Berkel, L.**, Steffens, P., Nicolai, H., Gierth, S., **Debiagi, P.**, Schneider, H., Dreizler, A. and **Hasse, C.** "Comprehensive Analysis of the Effect of Oxyfuel Atmospheres on Solid Fuel Combustion Using Large Eddy Simulations". *Fuel* 380 (2025), 133449. [doi](#) [orcid](#)
- [4] Chen, Y., Stein, O. T., Kronenburg, A., Xing, J., Luo, K., Luo, K. H. and **Hasse, C.** "Analysis of Gas-Assisted Pulverized Coal Combustion in Cambridge Coal Burner CCB1 Using FPV-LES". *Energy & Fuels* 34.6 (2020), 7477–7489. [doi](#)

- [5] **Debiagi, P.**, Heuer, S., Ontyd, C., Schiemann, M., Faravelli, T., **Hasse, C.** and Scherer, V. "Differences in Formation and Oxidation of Colombian Coal Chars in Air and Oxy-Fuel Atmospheres". *Chemical Engineering Transactions* 74 (2019), 151–156.  
- [6] **Debiagi, P.**, Nicolai, H., Han, W., Janicka, J. and **Hasse, C.** "Machine Learning for Predictive Coal Combustion CFD Simulations—from Detailed Kinetics to HDMR Reduced-Order Models". *Fuel* 274 (2020), 117720. 
- [7] **Debiagi, P.**, Ontyd, C., Pielsticker, S., Schiemann, M., Faravelli, T., Kneer, R., **Hasse, C.** and Scherer, V. "Calibration and Validation of a Comprehensive Kinetic Model of Coal Conversion in Inert, Air and Oxy-Fuel Conditions Using Data from Multiple Test Rigs". *Fuel* 290 (2021). 
- [8] **Debiagi, P.**, Piazza, V., Papagni, M., Beretta, A., Frassoldati, A. and Faravelli, T. "Cellulose Pyrolysis Kinetic Model: Detailed Description of Volatile Species". *Proceedings of the Combustion Institute* 40.1-4 (2024), 105651.  
- [9] **Debiagi, P.**, Yildiz, C., Richter, M., Ströhle, J., Eppele, B., Faravelli, T. and **Hasse, C.** "Experimental and Modeling Assessment of Sulfur Release from Coal Under Low and High Heating Rates". *Proceedings of the Combustion Institute* 38.3 (2021), 4053–4061. 
- [10] **Debiagi, P.**, Yildiz, C., Ströhle, J., Eppele, B., Faravelli, T. and **Hasse, C.** "Systematic Evaluation and Kinetic Modeling of Low Heating Rate Sulfur Release in Various Atmospheres". *Fuel* 289 (2021), 119739. 
- [11] Farmand, P., Boehme, C., Steffens, P., Nicolai, H., Loffredo, F., **Debiagi, P.**, Girhe, S., Chu, H., Gauding, M., **Hasse, C.** and Pitsch, H. "Numerical Investigation and Modeling of NO_x Formation in Pulverized Biomass Flames Under Air and Oxyfuel Conditions". *Combustion and Flame* 279 (2025).  
- [12] Gao, X., Lu, L., Shahnam, M., Rogers, W. A., Smith, K., Gaston, K., Robichaud, D., Brennan Pecha, M., Crowley, M., Ciesielski, P. N., **Debiagi, P.**, Faravelli, T., Wiggins, G., Finney, C. E. and Parks, J. E. "Assessment of a Detailed Biomass Pyrolysis Kinetic Scheme in Multiscale Simulations of a Single-Particle Pyrolyzer and a Pilot-Scale Entrained Flow Pyrolyzer". *Chemical Engineering Journal* 418 (2021), 129347. 
- [13] **Hasse, C.**, **Debiagi, P.**, Wen, X., Hildebrandt, K., Vascellari, M. and Faravelli, T. "Advanced Modeling Approaches for CFD Simulations of Coal Combustion and Gasification". *Progress in Energy and Combustion Science* 86 (2021), 100938.  
- [14] Locaspi, A., **Debiagi, P.**, Pelucchi, M., **Hasse, C.** and Faravelli, T. "A Predictive Physico-Chemical Model of Biochar Oxidation". *Energy & Fuels* 35.18 (2021), 14894–14912.  
- [15] Ma, P., Nicolai, H., Huang, Q., **Debiagi, P.**, **Berkel, L.**, Stagni, A., Yang, Y., **Hasse, C.** and Li, S. "Numerical Investigation on Pyrolysis and Ignition of Ammonia/Coal Blends During Co-Firing". *Combustion and Flame* 261 (2024), 113268. 
- [16] Nicolai, H., **Debiagi, P.**, Janicka, J. and **Hasse, C.** "Flamelet LES of Oxy-Fuel Swirling Flames with Different O₂/CO₂ Ratios Using Directly Coupled Seamless Multi-Step Solid Fuel Kinetics". *Fuel* 344 (2023), 128089. 
- [17] Nicolai, H., **Debiagi, P.**, Wen, X., Dressler, L., Maßmeyer, A., Janicka, J. and **Hasse, C.** "Flamelet LES of Swirl-Stabilized Oxy-Fuel Flames Using Directly Coupled Multi-Step Solid Fuel Kinetics". *Combustion and Flame* 241 (2022), 112062. 
- [18] Özer, B., **Debiagi, P.**, **Hasse, C.**, Faravelli, T. and Kazanç, F. "An Experimental and Numerical Study on the Combustion of Lignites from Different Geographic Origins". *Fuel* 278 (2020), 118320. 
- [19] Pflieger, C., Lotz, K., Hilse, N., Berger, C. M., Schiemann, M., **Debiagi, P.**, **Hasse, C.**, Scherer, V. and Muhler, M. "Catalytic Influence of Mineral Compounds on the Reactivity of Cellulose-Derived Char in O₂-, CO₂-, and H₂O-Containing Atmospheres". *Fuel* 287 (2021), 119584. 




- [20] Pielsticker, S., **Debiagi, P.**, Cerciello, F., **Hasse, C.** and Kneer, R. "Comparative Analysis of Pyrolysis Models Including SFOR, CRECK, and Bio-CPD to Predict Reaction Kinetics and Products from Extracted Biomass Components". *Fuel* 371 (2024), 131867. [doi](#) [a](#)
- [21] Shamooni, A., **Debiagi, P.**, Wang, B., Luu, T. D., Stein, O. T., Kronenburg, A., Bagheri, G., Stagni, A., Frassoldati, A., Faravelli, T., Kempf, A. M., Wen, X. and **Hasse, C.** "Carrier-Phase DNS of Detailed NO_x Formation in Early-Stage Pulverized Coal Combustion with Fuel-Bound Nitrogen". *Fuel* 291 (2021). [doi](#)
- [22] Shamooni, A., Stein, O. T., Kronenburg, A., Kempf, A. M., **Debiagi, P.**, Li, T., Dreizler, A., Böhm, B. and **Hasse, C.** "Fully-Resolved Simulations of Volatile Combustion and NO_x Formation from Single Coal Particles in Recycled Flue Gas Environments". *Proceedings of the Combustion Institute* 39.4 (2023), 4529–4539. [doi](#)
- [23] Steffens, P., **Berkel, L.**, Gierth, S., **Debiagi, P.**, Özer, B., Maßmeyer, A., Nicolai, H. and **Hasse, C.** "LES of a Swirl-Stabilized 40 kW_{th} Biomass Flame and Comparison to a Coal Flame". *Fuel* 372 (2024), 132098. [doi](#) [a](#)
- [24] Trespi, S., Nicolai, H., **Debiagi, P.**, Janicka, J., Dreizler, A., **Hasse, C.** and Faravelli, T. "Development and Application of an Efficient Chemical Reactor Network Model for Oxy-Fuel Combustion". *Energy & Fuels* 35.9 (2021). [doi](#)
- [25] Wang, B., Shamooni, A., Stein, O. T., Kronenburg, A., Kempf, A. M., **Debiagi, P.** and **Hasse, C.** "Investigation of Turbulent Pulverized Solid Fuel Combustion with Detailed Homogeneous and Heterogeneous Kinetics". *Energy & Fuels* 35.9 (2021). [doi](#)
- [26] Wen, X., **Debiagi, P.** and **Hasse, C.** "Flamelet Tabulation Methods for SO_x Formation in Pulverized Solid Fuel Combustion". *Combustion and Flame* 218 (2020), 150–167. [doi](#)
- [27] Wen, X., **Debiagi, P.**, Stein, O. T., Kronenburg, A., Kempf, A. M. and **Hasse, C.** "Flamelet Tabulation Methods for Solid Fuel Combustion with Fuel-Bound Nitrogen". *Combustion and Flame* 209 (2019), 155–166. [doi](#)
- [28] Wen, X., Nicolai, H., **Debiagi, P.**, Zabrodiec, D., Maßmeyer, A., Kneer, R. and **Hasse, C.** "Flamelet LES of a 40 kW_{th} Pulverized Torrefied Biomass Furnace in Air and Oxy-Fuel Atmospheres". *Proceedings of the Combustion Institute* 39.4 (2023), 4563–4572. [doi](#)
- [29] Wen, X., Stein, O. T., **Debiagi, P.**, Scholtissek, A., Kronenburg, A., Kempf, A. M. and **Hasse, C.** "Detailed Simulations for Flamelet Modelling of SO_x Formation from Coal". *PAMM* 19.1 (2019). [doi](#) [a](#)
- [30] Wen, X., Stein, O. T., Tufano, G. L., Kronenburg, A., Scholtissek, A. and **Hasse, C.** "Multi-Dimensional and Transient Effects on Flamelet Modeling for Turbulent Pulverized Coal Combustion". *Fuel* 255 (2019), 115772. [doi](#)
- [31] Yönder, Ö., Schmitz, G., Hättig, C., Schmid, R., **Debiagi, P.**, **Hasse, C.**, Locaspi, A. and Faravelli, T. "Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics". *The Journal of Physical Chemistry A* 124.46 (2020), 9626–9637. [doi](#)
- [32] Zou, X., **Debiagi, P.**, Amjed, M. A., Zhai, M. and Faravelli, T. "Impact of High-Temperature Biomass Pyrolysis on Biochar Formation and Composition". *Journal of Analytical and Applied Pyrolysis* 179 (2024), 106463. [doi](#) [a](#)

Conference papers

- [33] Nicolai, H., **Debiagi, P.**, Janicka, J. and **Hasse, C.** "Flamelet LES of Oxy-Coal Swirling Flames with Different O₂/CO₂ Ratios Using Directly Coupled Seamless Multistep Kinetics for Homogeneous and Heterogeneous Solid Fuel Kinetics". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.

b) Other publications (non peer-review)





Book chapters

- [56] **Berkel, L., Debiagi, P.**, Pielsticker, S., Tarlinski, D., Senneca, O., Faravelli, T., Scherer, V., Kneer, R. and **Hasse, C.** "Kinetic Modelling of Thermochemical Conversion of Solid Fuels". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  
- [57] **Debiagi, P.**, Faravelli, T., **Hasse, C.** and Ranzi, E. "Kinetic Modeling of Solid, Liquid and Gas Biofuel Formation from Biomass Pyrolysis". *Production of Biofuels and Chemicals*. Ed. by Fang, Z., Smith, R. L. and Xu, L. Singapore: Springer, 2020, pp. 31–76. 





Conference papers

















- [34] **Debiagi, P.**, Nicolai, H., Han, W., Janicka, J. and **Hasse, C.** "Towards Predictive CFD Simulations of Coal Combustion – Using Machine Learning for Efficient Representation of Solid Fuel Kinetics". *9th International Symposium on Coal Combustion*. Qingdao, China, 2019.
- [35] **Debiagi, P.**, Ontyd, C., Heuer, S., Pielsticker, S., Schiemann, M., Faravelli, T., Kneer, R., Scherer, V. and **Hasse, C.** "Solid Fuel Kinetics for Oxy-Fuel Conditions". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [36] **Debiagi, P.**, Ranzi, E., Faravelli, T. and **Hasse, C.** "Coal Combustion: Integrating Nitrogen and Sulfur Fraction in a Single Kinetic Mechanism". *1st International Conference on Smart Energy Carriers*. Naples, Italy, 2019.
- [37] **Debiagi, P.**, Yildiz, C., Ströhle, J., Epple, B., Faravelli, T. and **Hasse, C.** "Validation of a Comprehensive Kinetic Mechanism for Sulfur Release During Pyrolysis of Solid Fuels". *9th International Symposium on Coal Combustion*. Qingdao, China, 2019.

Data sets

- [38] Pielsticker, S., **Debiagi, P.**, Cerciello, F., **Hasse, C.** and Kneer, R. *Comparative Analysis of Pyrolysis Models Including SFOR, CRECK, and Bio-CPD to Predict Reaction Kinetics and Products from Extracted Biomass Components – Supplementary Dataset*. 2024.  
- [39] Schnieder, B., **Debiagi, P.**, Pelucchi, M., Schmid, R. and Hättig, C. *Raw Data to "Computational Study on the Pyrolysis of 2,5-Diketopiperazine: From Electronic Structure Calculations to Kinetic Modeling"*. 2025.  

Presentations and Posters

- [40] **Berkel, L., Debiagi, P.**, Nicolai, H., Cerciello, F., Pielsticker, S., Senneca, O., Kneer, R., Faravelli, T. and **Hasse, C.** "Walnut Shell Pyrolysis: Feedstock Characterization and Kinetics Considering Hemicellulose-Lignin Interactions (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 10–11.  
- [41] **Berkel, L., Debiagi, P.**, Stagni, A., Nicolai, H., **Hasse, C.** and Faravelli, T. "Fluidized Bed Reactor Modelling Using Multiphase Reactor Networks (Presentation)". *44th Meeting of The Italian Section of The Combustion Institute*. Naples, Italy, 2022.
- [42] **Berkel, L.**, Steffens, P., Nicolai, H., Gierth, S., **Debiagi, P.**, Schneider, H., Dreizler, A. and **Hasse, C.** "Comprehensive Analysis of the Effect of Oxyfuel Atmospheres on Solid Fuel Combustion Using Large Eddy Simulations (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

- [43] **Debiagi, P.** and Farmand, P. "Single Hydrocarbon Particle and Particle Group Combustion in Laminar Flows (Presentation)". *4th Workshop on Clean Solids Conversion*. Kyoto, Japan, 2024.
- [44] **Debiagi, P.**, Locaspi, A., **Hasse, C.** and Faravelli, T. "A Fundamental Model of Char Oxidation (Presentation)". *Fuels, Processes, and Combustion Physics in the Energy Transformation*. Bad Honnef, Germany, 2020.
- [45] **Debiagi, P.**, Pielsticker, S., Cerciello, F., Scherer, V., Kneer, R., Faravelli, T. and **Hasse, C.** "Development of a Comprehensive Kinetic Model of Biomass Conversion in Inert, Air and Oxy-Fuel Conditions (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [46] **Debiagi, P.**, Yildiz, C., Ströhle, J., Epple, B., Faravelli, T. and **Hasse, C.** "Systematic Evaluation and Kinetic Modeling of Low Heating Rate Sulfur Release in Pyrolysis and Oxidation in Various Atmospheres (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [47] Dübal, S., **Berkel, L.**, **Debiagi, P.**, Nicolai, H., Faravelli, T., **Hasse, C.** and Hartl, S. "Chemical Reactor Network Modeling of a Self-Sustained Solid Fuel Combustion Chamber Under Oxy-Fuel Atmospheres (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [48] Farmand, P., Boehme, C., Nicolai, H., Loffredo, F., **Debiagi, P.**, Gauding, M., **Hasse, C.** and Pitsch, H. "Modeling of NO_x Emissions in Laminar Solid Pulverized Biomass Fuels Flames (Presentation)". *19th International Conference on Numerical Combustion*. Kyoto, Japan, 2024.
- [49] Pielsticker, S., **Berkel, L.**, **Debiagi, P.**, Senneca, O., **Hasse, C.** and Kneer, R. "Consideration of Interacting Biomass Components in Sophisticated Pyrolysis Network Models (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 7–8.  
- [50] Pielsticker, S., **Debiagi, P.**, Cerciello, F., Coppola, A., **Hasse, C.** and Kneer, R. "Prediction of Pyrolysis Kinetics with Models of Different Complexity for Isolated Biomass Components (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [51] Shamooni, A., **Debiagi, P.**, Wang, B., Stein, O. T., Kronenburg, A., Stagni, A., Frassoldati, A., Faravelli, T., Kempf, A. M. and **Hasse, C.** "Carrier-Phase DNS of NO_x Formation in Pulverized Coal Flames with Fuel-Bound Nitrogen (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [52] Steffens, P., **Berkel, L.**, Gierth, S., **Debiagi, P.**, Özer, B., Maßmeyer, A., Nicolai, H. and **Hasse, C.** "Large Eddy Simulation of a 40 kW Self-Sustained Pulverized Biomass Combustion Chamber Using Tabulated Chemistry (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [53] Steffens, P., **Berkel, L.**, Vahl, A., Steinhausen, M., Nicolai, H. and **Hasse, C.** "From Single-Particle Studies to MW_{th} Reactor Simulations: OxySim129 – A High-Fidelity CFD Framework for Carbonaceous Solid Fuel Combustion (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 24–25.  
- [54] Suleiman, M. Y., Benedetto, E., Piazza, V., Lietti, L., Beretta, A., **Berkel, L.**, Musyoka, N., Faravelli, T. and **Debiagi, P.** "Effect of Compositional Differences in Hemicellulose Pyrolysis Products (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 12–13.  
- [55] Vahl, A., Steffens, P., **Berkel, L.**, **Hasse, C.** and Nicolai, H. "Large Eddy Simulation of a Gas-Assisted Pulverized Biomass Combustion Chamber Under Varying Oxygen Concentrations Using the OxySim-129 Framework (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 31–32.  

4.8 B1 – Theoretical and experimental investigation on the devolatilisation and oxidation of solid-fuel particles in a counterflow burner under oxy-fuel conditions

4.8.1 Project members

a) Project leader(s)

- Pitsch, Heinz

b) Scientific project workers

- Baroncelli, Martina
- Beeckmann, Joachim
- Cai, Liming
- Chen, Bingjie
- Faller, Sebastian
- Felsmann, Daniel
- Kruse, Stefan
- Langer, Raymond
- Meraviglia, Anita

4.8.2 Project summary









Project **B1** investigated and modeled gas-phase kinetics of volatile biomass components under oxy-fuel conditions through coordinated experimental and numerical studies. Molecular-beam mass spectrometry (MBMS) at ITV and the Advanced Light Source (ALS), complemented by GC-MS, yielded high-resolution speciation in counterflow diffusion flames, a jet-stirred reactor, a flat-flame setup, and compressed pulverised biomass plates in stagnation-point flows. Light volatiles (methane, acetylene, 1-butene, cyclopentene) and selected tar surrogates (anisole, furfural, pyrrole, pyridine, piperazine) were examined, including tailored mixtures to isolate cyclic formation pathways and isomer-resolved detection. An oxy-fuel chemical mechanism was established, extensively validated against literature and in-house data, and substantially improved. Reduced versions enabled simulations in **B3**, **B8**, and **C2**. Pollutant chemistry received particular attention: pathways for oxygen-containing polycyclic aromatic hydrocarbons (OPAH) and fuel-nitrogen NO_x were identified and incorporated, supported by measurements and quantum-chemical input from **A7**. Information on volatile nitrogen from **A1** and **A3** refined the treatment of NH₃, HCN, and NO. Biomass-specific surrogate formulations for gas-phase kinetics were developed with **A8** and Prof. Tiziano Faravelli and integrated into the CRECK-S-B framework in **A8**.

4.8.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **Baroncelli, M., Felsmann, D.,** Hansen, N. and **Pitsch, H.** "Investigating the Effect of Oxy-Fuel Combustion and Light Coal Volatiles Interaction: A Mass Spectrometric Study". *Combustion and Flame* 204 (2019), 320–330. [doi](#)
- [2] **Baroncelli, M.,** Mao, Q., Galle, S., Hansen, N. and **Pitsch, H.** "Role of Ring-Enlargement Reactions in the Formation of Aromatic Hydrocarbons". *Physical Chemistry Chemical Physics* 22.8 (2020), 4699–4714. [doi](#)
- [3] **Baroncelli, M.,** Mao, Q., **Pitsch, H.** and Hansen, N. "Effects of C₁–C₃ Hydrocarbon Blending on Aromatics Formation in 1-Butene Counterflow Flames". *Combustion and Flame* 230 (2021), 111427. [doi](#)
- [4] **Cai, L.,** Kruse, S., **Felsmann, D.** and **Pitsch, H.** "A Methane Mechanism for Oxy-Fuel Combustion: Extinction Experiments, Model Validation, and Kinetic Analysis". *Flow, Turbulence and Combustion* 34 (2020), 6970. [doi](#)
- [5] **Cai, L.,** Kruse, S., **Felsmann, D.,** Thies, C., Yalamanchi, K. K. and **Pitsch, H.** "Experimental Design for Discrimination of Chemical Kinetic Models for Oxy-Methane Combustion". *Energy & Fuels* 31.5 (2017), 5533–5542. [doi](#)
- [6] **Chen, B., Faller, S.,** Pratali Maffei, L., Nobili, A., Pelucchi, M., Lu, X. and **Pitsch, H.** "N-Containing Pollutant Formation in Pyrrole Counterflow Diffusion Flames". *Combustion and Flame* 276 (2025), 114136. [doi](#) [orcid](#)
- [7] **Chen, B.,** Hellmuth, M., **Faller, S.,** May, L., Liu, P., **Cai, L.,** Roberts, W. L. and **Pitsch, H.** "Exploring the Combustion Chemistry of Anisole in Laminar Counterflow Diffusion-Flames Under Oxy-Fuel Conditions". *Combustion and Flame* 243 (2022), 111929. [doi](#)
- [8] **Chen, B.,** Ilies, B. D., Chen, W., Xu, Q., Li, Y., Xing, L., Yang, J., Wei, L., Hansen, N., **Pitsch, H.,** Sarathy, S. M. and Wang, Z. "Exploring Low Temperature Oxidation of 1-Butene in Jet-Stirred Reactors". *Combustion and Flame* 222 (2020), 259–271. [doi](#)
- [9] **Chen, B.,** Kruse, S., Schmid, R., **Cai, L.,** Hansen, N. and **Pitsch, H.** "Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach". *Energy & Fuels* 35.2 (2021). [doi](#)
- [10] **Chen, B.,** Liu, P., Pelucchi, M., Guidici, C., Maffei, L. P., **Faller, S.,** Xu, Q., Huang, J., Zhang, F., Huang, C., Leonhard, K., Wang, Z., Mehl, M., Roberts, W. L., Faravelli, T. and **Pitsch, H.** "New Insights into the Oxidation Chemistry of Pyrrole, an N-Containing Biomass Tar Component". *Proceedings of the Combustion Institute* 39.1 (2023), 73–84. [doi](#)
- [11] **Chen, B.,** Lyu, H., Liu, P., Samaras, V. G., Lu, X., Gao, X., Roberts, W. L. and **Pitsch, H.** "On the Formation of Pyridine, the First Nitrogen Heterocyclic Ring in NPAHs". *Proceedings of the Combustion Institute* 40.1-4 (2024), 105675. [doi](#)
- [12] Emmert, J., **Baroncelli, M.,** van der Kley, S., **Pitsch, H.** and Wagner, S. "Axisymmetric Linear Hyperspectral Absorption Spectroscopy and Residuum-Based Parameter Selection on a Counter Flow Burner". *Energies* 12.14 (2019), 2786. [doi](#) [orcid](#)
- [13] **Felsmann, D., Baroncelli, M.,** **Beeckmann, J.** and **Pitsch, H.** "Molecular-Beam Mass Spectrometry Study of Oxy-Combustion in a Novel Coal-Plate Experiment". *Proceedings of the Combustion Institute* 37.3 (2019), 2801–2808. [doi](#)



- [14] Hellmuth, M., Cameron, F., **Faller, S.**, Schmückert, L., **Chen, B.**, Ren, Y. and **Pitsch, H.** "Synergistic Effect on PAH and Soot Formation in Ethylene Counterflow Diffusion Flames by the Addition of 1,3-Dioxolane – a Bio-Hybrid Fuel". *Proceedings of the Combustion Institute* 39.1 (2023), 899–908. 
- [15] Hellmuth, M., **Chen, B.**, Bariki, C., **Cai, L.**, Cameron, F., Wildenberg, A., Huang, C., **Faller, S.**, Ren, Y., **Beeckmann, J.**, Leonhard, K., Heufer, K. A., Hansen, N. and **Pitsch, H.** "A Comparative Study on the Combustion Chemistry of Two Bio-Hybrid Fuels: 1,3-Dioxane and 1,3-Dioxolane". *The Journal of Physical Chemistry. A* 127.1 (2023), 286–299. 
- [16] Hellmuth, M., **Langer, R.**, **Meraviglia, A.**, **Beeckmann, J.** and **Pitsch, H.** "The Role of C₃ and C₄ Species in Forming Naphthalene in Counterflow Diffusion Flames". *Proceedings of the Combustion Institute* 40.1-4 (2024), 105620.  
- [17] Liu, P., **Chen, B.**, Bennett, A., **Pitsch, H.** and Roberts, W. L. "Probing the Influence of Hydrogen Cyanide on PAH Chemistry". *Proceedings of the Combustion Institute* 39.1 (2023), 1139–1146. 
- [18] Liu, P., **Chen, B.**, Li, Z., Bennett, A., Sioud, S., **Pitsch, H.**, Sarathy, S. M. and Roberts, W. L. "Experimental and Theoretical Evidence for the Temperature-Determined Evolution of PAH Functional Groups". *Proceedings of the Combustion Institute* 38.1 (2021), 1467–1475. 
- [19] Wen, X., Nicolai, H., Schneider, H., **Cai, L.**, Janicka, J., **Pitsch, H.** and Hasse, C. "Flamelet LES of a Swirl-Stabilized Multi-Stream Pulverized Coal Burner in Air and Oxy-Fuel Atmospheres with Pollutant Formation". *Proceedings of the Combustion Institute* 38.3 (2021), 4141–4149. 
- [20] Wen, X., Shamooni, A., Stein, O. T., **Cai, L.**, Kronenburg, A., **Pitsch, H.**, Kempf, A. M. and Hasse, C. "Detailed Analysis of Early-Stage NO_x Formation in Turbulent Pulverized Coal Combustion with Fuel-Bound Nitrogen". *Proceedings of the Combustion Institute* 38.3 (2021), 4111–4119. 
- [21] Xu, K., Zhang, H., Wu, Y., **Baroncelli, M.** and **Pitsch, H.** "Transient Model for Soot Formation During the Combustion of Single Coal Particles". *Proceedings of the Combustion Institute* 36.2 (2017), 2131–2138. 

Conference papers

- [22] **Baroncelli, M.**, **Felsmann, D.**, Kruse, S., Falkenstein, T., **Beeckmann, J.** and **Pitsch, H.** "Extinction Strain Rates for Coal Light Volatiles Under Oxy-Fuel Conditions". *China National Symposium on Combustion*. Ma'anshan, Anhui, China, 2016.
- [23] **Cai, L.**, **Baroncelli, M.**, Kruse, S., **Felsmann, D.**, Thies, C. and **Pitsch, H.** "Extinction Characteristics of Methane Counterflow Flames Under Oxy-Fuel and Air Conditions". *China National Symposium on Combustion*. Ma'anshan, Anhui, China, 2016.

b) Other publications (non peer-review)

Book chapters



- [29] Loffredo, F., **Langer, R.**, Hellmuth, M., Girhe, S., **Meraviglia, A.**, **Chen, B.** and **Pitsch, H.** "Gas-Phase Chemistry of Solid-Fuel Particle Combustion". *Clean Energy Conversion*. Ed. by Kneer, R., **Pitsch, H.**, Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers

- [24] **Baroncelli, M.**, Kruse, S. and **Pitsch, H.** "Experimental and Numerical Investigation of Extinction Strain Rates of Coal Devolatilization Products Under Oxy-Fuel Conditions". *Proceedings of the European Combustion Meeting*. Budapest, Hungary, 2015.

- [25] Hellmuth, M., **Chen, B.**, Bariki, C., **Cai, L.**, Cameron, F., Wildenberg, A., Huang, C., **Faller, S.**, Ren, Y., **Beeckmann, J.**, Leonhard, K., Heufer, K. A., Hansen, N. and **Pitsch, H.** "A Comprehensive Study on the Combustion Chemistry of Two Bio-Hybrid Fuels: 1,3-Dioxane and 1,3-Dioxolane". *12th Mediterranean Combustion Symposium*. Luxor, Egypt, 2023.
- [26] Vorobiev, N., Kruse, S., **Pitsch, H.** and Schiemann, M. "Demonstration of Laser-Induced Incandescence in Single Coal Particle Enveloping Flames". *9th European Combustion Meeting*. Lisbon, Portugal, 2019.

Presentations and Posters

- [27] **Chen, B.**, **Faller, S.**, Nobili, A., Pelucchi, M. and **Pitsch, H.** "Exploring Formation of N-Containing Pollutants in Pyrrole Counterflow Diffusion Flame (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [28] **Chen, B.**, Kruse, S., Schmid, R., **Cai, L.**, Hansen, N. and **Pitsch, H.** "Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.

4.9 B2 – Development of modelling approaches for fluid-particle interactions in turbulent flow by direct particle-fluid simulations

4.9.1 Project members

a) Project leader(s)

- Meinke, Matthias
- Schröder, Wolfgang

b) Scientific project workers

- André, Laurent
- Fröhlich, Konstantin
- Schneiders, Lennart






4.9.2 Project summary







Project **B2** employed highly resolved direct particle-fluid simulations to resolve turbulent scales, particle boundary layers, and wakes, and used the results to develop Lagrangian models for ellipsoidal particles in turbulent carrier flows relevant to large-eddy simulations of combustion chambers. A high-performance computing framework generated a large database in isotropic turbulence with up to tens of thousands of fully resolved ellipsoids, from which turbulence-modulation behavior and deficiencies of existing two-way coupling strategies were identified. New drag correlations across particle Reynolds numbers and orientation-dependent dynamics were derived and integrated into improved Lagrangian formulations. The investigation then generalized to turbulent round jets with hot co-flow, using a setup designed for validation against **B7** measurements. Isothermal and non-isothermal cases were simulated, and deviations between ideal ellipsoids and realistic biomass particles were assessed with **B8**. Hydrodynamic interaction models were combined with particle-chemistry models from **B3**. The final, carefully validated Lagrangian model for ellipsoidal particle dynamics, turbulence modulation, and heat exchange incorporated finite-size and shear-flow corrections and was provided to the OxySim-129 framework via **C2**, thereby enhancing predictive accuracy for CRC/TRR 129 simulations.

4.9.3 Published project results



a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Brito Gadeschi, G., **Schneiders, L., Meinke, M.** and **Schröder, W.** "A Numerical Method for Multiphysics Simulations Based on Hierarchical Cartesian Grids". *Journal of Fluid Science and Technology* 10.1 (2015), JFST0002.  
- [2] **Fröhlich, K.**, Farmand, P., Pitsch, H., **Meinke, M.** and **Schröder, W.** "Particle Reynolds Number Effects on Settling Ellipsoids in Isotropic Turbulence". *International Journal of Multiphase Flow* 139 (2021). 
- [3] **Fröhlich, K., Meinke, M.** and **Schröder, W.** "Correlations for Inclined Prolates Based on Highly Resolved Simulations". *Journal of Fluid Mechanics* 901 (2020), A5. 
- [4] **Fröhlich, K., Schneiders, L., Meinke, M.** and **Schröder, W.** "Validation of Lagrangian Two-Way Coupled Point-Particle Models in Large-Eddy Simulations". *Flow, Turbulence and Combustion* 101.2 (2018), 317–341. 



- [5] Gronarz, T., Schnell, M., Siewert, C., **Schneiders, L., Schröder, W.** and Kneer, R. "Comparison of Scattering Behaviour for Spherical and Non-Spherical Particles in Pulverized Coal Combustion". *International Journal of Thermal Sciences* 111 (2017), 116–128. 
- [6] Kiwitt, T., **Fröhlich, K., Meinke, M.** and **Schröder, W.** "Nusselt Correlation for Ellipsoidal Particles". *International Journal of Multiphase Flow* 149 (2022), 103941. 
- [7] **Schneiders, L., Fröhlich, K., Meinke, M.** and **Schröder, W.** "The Decay of Isotropic Turbulence Carrying Non-Spherical Finite-Size Particles". *Journal of Fluid Mechanics* 875 (2019), 520–542. 
- [8] **Schneiders, L., Günther, C., Meinke, M.** and **Schröder, W.** "An Efficient Conservative Cut-Cell Method for Rigid Bodies Interacting with Viscous Compressible Flows". *Journal of Computational Physics* 311 (2016), 62–86. 
- [9] **Schneiders, L., Meinke, M.** and **Schröder, W.** "Direct Particle-Fluid Simulation of Kolmogorov-Length-Scale Size Particles in Decaying Isotropic Turbulence". *Journal of Fluid Mechanics* 819 (2017), 188–227. 
- [10] **Schneiders, L., Meinke, M.** and **Schröder, W.** "On the Accuracy of Lagrangian Point-Mass Models for Heavy Non-Spherical Particles in Isotropic Turbulence". *Fuel* 201 (2017), 2–14. 

Conference papers


- [11] Geschwindner, C., Werner, M., **André, L., Nicolas, A., Peterson, B., Meinke, M., Schröder, W., Dreizler, A.** and Böhm, B. "High-Resolution Two-Phase Velocimetry of Aspherical Particles Using Wavelet-Based Optical Flow Velocimetry (wofv) Benchmarked with Fully Resolved Direct Numerical Simulations". *21st International Symposium on Applications of Laser and Imaging Techniques to Fluid Mechanics*. Lisbon, Portugal, 2024.
- [12] Vorspohl, J., **André, L., Rüttgers, M.** and **Schröder, W.** "Drag Correlations for Multiphase Flows Using Artificial Neural Networks". *35th International Conference on Parallel Computational Fluid Dynamics*. Bonn, Germany, 2024.  




b) Other publications (non peer-review)

Book chapters





- [29] **André, L., Fröhlich, K., Meinke, M.** and **Schröder, W.** "Modelling and Analysis of Fluid-Particle Interactions". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers



- [13] **Fröhlich, K., Schneiders, L., Meinke, M.** and **Schröder, W.** "Assessment of Non-Spherical Point-Particle Models in LES Using Direct Particle-Fluid Simulations". *AIAA Paper 2018-3714* (2018). 
- [14] **Fröhlich, K., Schneiders, L., Meinke, M.** and **Schröder, W.** "Direct Particle-Fluid Simulation of Kolmogorov-Length-Scale Size Ellipsoidal Particles in Isotropic Decaying Turbulence". *11th International Symposium on Turbulence and Shear Flow Phenomena*. Southampton, United Kingdom, 2019.
- [15] **Fröhlich, K., Schneiders, L., Meinke, M.** and **Schröder, W.** "Ambient Flow Properties of Kolmogorov-Length-Scale Size Non-Spherical Particles in Isotropic Turbulence". *ERCOfTAC Workshop Direct and Large Eddy Simulation XII*. Springer Nature, 2020, pp. 175–181.

- [16] **Schneiders, L.**, Grimm, J. H., **Meinke, M.** and **Schröder, W.** "An Efficient Numerical Method for Fully-Resolved Particle Simulations on High-Performance Computers". *PAMM* 15.1 (2015), 495–496.  
- [17] **Schneiders, L.**, Günther, C., Grimm, J. H., **Meinke, M.** and **Schröder, W.** "Sharp Resolution of Complex Moving Geometries Using a Multi-Cut-Cell Viscous Flow Solver". *AIAA Paper 2015-3427* (2015), 507. 

Data sets

- [18] Kiwitt, T., **Fröhlich, K.**, **Meinke, M.** and **Schröder, W.** *Dataset for Nusselt Correlation for Ellipsoidal Particles*. 2025.  
- [19] Vorspohl, J., **André, L.**, Rüttgers, M. and **Schröder, W.** *Dataset for "Drag Correlations for Multiphase Flows Using Artificial Neural Networks"*. 2025.  

Presentations and Posters

- [20] **André, L.**, Kiwitt, T., **Meinke, M.** and **Schröder, W.** "Direct Particle-Fluid Simulations of Pipe Flow (Presentation)". *EUROMECH Colloquium 625*. Udine, Italy, 2022.
- [21] **André, L.**, Kiwitt, T., **Meinke, M.** and **Schröder, W.** "Assessment of Point-Particle Models for Non-Spherical Particles in Turbulent Flow (Presentation)". *11th International Conference on Multiphase Flow*. Kobe, Japan, 2023.
- [22] **André, L.**, Kiwitt, T., **Meinke, M.** and **Schröder, W.** "Lagrangian Point-Particle Models for Non-Spherical Particles in Turbulent Flow (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [23] **André, L.**, **Meinke, M.**, Krug, D. and **Schröder, W.** "Accuracy of Non-Spherical Point-Particle Models in Turbulent Shear Flows (Presentation)". *12th International Conference on Multiphase Flow*. Toulouse, France, 2025.
- [24] **André, L.**, **Meinke, M.**, Krug, D. and **Schröder, W.** "Assessment of Non-Spherical Point-Particle Dynamics in Turbulent Pipe and Jet Flows (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 26–27.  
- [25] **Fröhlich, K.**, **Schneiders, L.**, **Meinke, M.** and **Schröder, W.** "Analysis of the Interphase Coupling Using Direct Particle-Fluid Simulations for Finite-Size Particles (Presentation)". *16th European Turbulence Conference*. Stockholm, Sweden, 2017.
- [26] **Fröhlich, K.**, **Schneiders, L.**, **Meinke, M.** and **Schröder, W.** "Assessment of Lagrangian Two-Way Coupled Point-Particle Models Using Direct Particle-Fluid Simulations (Presentation)". *18. STAB-Workshop*. Göttingen, Germany, 2017.
- [27] **Fröhlich, K.**, **Schneiders, L.**, **Meinke, M.** and **Schröder, W.** "Improved Lagrangian Two-Way Coupled Point-Particle Models Using Direct Particle-Fluid Simulations (Presentation)". *11th workshop on Direct and Large Eddy Simulation*. Pisa, Italy, 2017.
- [28] **Fröhlich, K.** and **Schröder, W.** "B2 – Development of Fluid-Particle Interaction Models in Turbulent Flows (Poster)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.

4.10 B3 – Direct numerical simulation and modelling of oxy-fuel combustion processes

4.10.1 Project members

a) Project leader(s)

- Pitsch, Heinz

b) Scientific project workers

- Attili, Antonio
- Farazi, Sima
- Farmand, Pooria
- Gauding, Michael
- Xu, Wen

4.10.2 Project summary



In project **B3**, high-fidelity direct numerical simulations were developed to examine ignition and combustion of pulverised solid fuels in laminar and turbulent flows under air and oxy-fuel atmospheres. An Euler-Lagrange framework captured devolatilisation and ignition for single particles and particle groups, and a pulverised-coal combustion model was validated against literature ignition delays and the laminar flat-flame burner of **B7**. Channel and jet configurations quantified group-combustion effects, while isotropic-turbulence cases revealed strong particle-interaction impacts on local ignition. The resulting benchmark datasets supported a comprehensive assessment of **C2** combustion models and improved the Euler-Lagrange description used in large-eddy simulations.















Subsequent work targeted lignocellulosic biomass and aimed to develop reduced-order models for heat and mass transfer of non-spherical particles and leveraged non-reactive formulations from **B2**. Simulations of biomass-plate experiments from **B1** validated and refined PAH and NO_x chemistry manifolds for LES. Direct numerical simulations designed to emulate **B7** turbulent conditions supported model development and a priori/a posteriori validation of **C2** within the CRC/TRR 129. Biomass combustion in a realistic swirl-stabilised burner (**B4**) extended earlier simulations and enabled validation of soot and fuel- and gas-phase NO_x models. Radiation effects on particle heat-up and flame stabilisation were analysed using the **C4** radiation model.

4.10.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **Attili, A., Farmand, P.,** Schumann, C., **Farazi, S.,** Böhm, B., Li, T., Geschwindner, C., Köser, J., Dreizler, A. and **Pitsch, H.** "Numerical Simulations and Experiments of Ignition of Solid Particles in a Laminar Burner: Effects of Slip Velocity and Particle Swelling". *Flow, Turbulence and Combustion* 106 (2020), 515–531.  [DOI](#)
- [2] **Farazi, S., Attili, A.,** Kang, S. and **Pitsch, H.** "Numerical Study of Coal Particle Ignition in Air and Oxy-Atmosphere". *Proceedings of the Combustion Institute* 37.3 (2019), 2867–2874.  [DOI](#)



- [3] **Farazi, S.**, Hinrichs, J., Davidovic, M., Falkenstein, T., Bode, M., Kang, S., **Attili, A.** and **Pitsch, H.** "Numerical Investigation of Coal Particle Stream Ignition in Oxy-Atmosphere". *Fuel* 241 (2019), 477–487. 
- [4] **Farazi, S.**, Sadr, M., Kang, S., Schiemann, M., Vorobiev, N., Scherer, V. and **Pitsch, H.** "Resolved Simulations of Single Char Particle Combustion in a Laminar Flow Field". *Fuel* 201 (2017), 15–28. 
- [5] **Farmand, P.**, Boehme, C., Steffens, P., Nicolai, H., Loffredo, F., Debiagi, P., Girhe, S., Chu, H., **Gauding, M.**, Hasse, C. and **Pitsch, H.** "Numerical Investigation and Modeling of NO_x Formation in Pulverized Biomass Flames Under Air and Oxyfuel Conditions". *Combustion and Flame* 279 (2025).  
- [6] **Farmand, P.**, Nicolai, H., Schumann, C., **Attili, A.**, Berger, L., Li, T., Geschwindner, C., di Mare, F., Hasse, C., Böhm, B., Janicka, J. and **Pitsch, H.** "Numerical Investigation and Assessment of Flamelet-Based Models for the Prediction of Pulverized Solid Fuel Homogeneous Ignition and Combustion". *Combustion and Flame* 235 (2022), 111693. 
- [7] **Farmand, P.**, Nicolai, H., Usman, M., Berger, L., **Attili, A.**, **Gauding, M.**, Hasse, C. and **Pitsch, H.** "Modeling Homogeneous Ignition Processes of Clustering Solid Particle Clouds in Isotropic Turbulence". *Fuel* 371 (2024), 132054.  
- [8] Fröhlich, K., **Farmand, P.**, **Pitsch, H.**, Meinke, M. and Schröder, W. "Particle Reynolds Number Effects on Settling Ellipsoids in Isotropic Turbulence". *International Journal of Multiphase Flow* 139 (2021). 
- [9] Li, T., **Farmand, P.**, Chen, H., Boehme, C., Nicolai, H., Hasse, C., **Pitsch, H.** and Böhm, B. "Homogeneous Ignition and Volatile Flame Structure of Single Bituminous Coal and Walnut Shell Particles: Effects of Particle Size and Gas Atmosphere". *Fuel* 371 (2024), 131955.  
- [10] Li, T., **Farmand, P.**, Geschwindner, C., Greifenstein, M., Köser, J., Schumann, C., **Attili, A.**, **Pitsch, H.**, Dreizler, A. and Böhm, B. "Homogeneous Ignition and Volatile Combustion of Single Solid Fuel Particles in Air and Oxy-Fuel Conditions". *Fuel* 291 (2021). 
- [11] Li, T., Li, B., **Farmand, P.**, Dreizler, A., **Pitsch, H.** and Böhm, B. "Motion and Swelling of Single Coal Particles During Volatile Combustion in a Laminar Flow Reactor". *Proceedings of the Combustion Institute* 39.3 (2023), 3333–3341. 
- [12] Sayadi, T., **Farazi, S.**, Kang, S. and **Pitsch, H.** "Transient Multiple Particle Simulations of Char Particle Combustion". *Fuel* 199 (2017), 289–298. 
- [13] Xing, J., Luo, K., **Pitsch, H.**, Wang, H., Bai, Y., Zhao, C. and Fan, J. "Predicting Kinetic Parameters for Coal Devolatilization by Means of Artificial Neural Networks". *Proceedings of the Combustion Institute* 37.3 (2019), 2943–2950. 

Conference papers

- [14] **Farazi, S.**, Sayadi, T. and **Pitsch, H.** "Numerical Analysis of the Drag Force Acting on the Reactive Single Char Particle Under Oxy-Fuel Condition". *China National Symposium on Combustion*. Ma'anshan, Anhui, China, 2016.

b) Other publications (non peer-review)







Book chapters

- [27] **Farmand, P.** and **Pitsch, H.** "Modelling Ignition, Combustion, and Pollutant Emissions". *Clean Energy Conversion*. Ed. by Kneer, R., **Pitsch, H.**, Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers

- [15] **Farazi, S.**, Schiemann, M., Vorobiev, N., Scherer, V., Kang, S. and **Pitsch, H.** "A New Variable Transport Coefficient Single-Film Model for Char Combustion". *8th European Combustion Meeting*. Dubrovnik, Croatia, 2017.

Data sets

- [16] **Farmand, P.**, **Gauding, M.** and **Pitsch, H.** *DNS Dataset for Modelling Homogeneous Ignition Processes of Clustering Solid Particle Clouds in Isotropic Turbulence*. 2024.  
- [17] **Farmand, P.**, **Gauding, M.** and **Pitsch, H.** *Dataset for Modeling NO_x Formation in Pulverized Biomass Flames Under Air and Oxyfuel Conditions*. 2025.  
- [18] **Farmand, P.**, **Gauding, M.** and **Pitsch, H.** *Dataset for Modeling of Homogeneous Ignition and Volatile Flame Structure of Single Biomass Particles in Comparison with Coal Particles*. 2025.  

Presentations and Posters

- [19] Debiagi, P. and **Farmand, P.** "Single Hydrocarbon Particle and Particle Group Combustion in Laminar Flows (Presentation)". *4th Workshop on Clean Solids Conversion*. Kyoto, Japan, 2024.
- [20] **Farazi, S.**, **Attili, A.**, Heuer, S., Schiemann, M., Scherer, V. and **Pitsch, H.** "Modeling and Simulation of Coal Ignition and Combustion Under Oxy-Fuel Condition (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [21] **Farazi, S.** and **Pitsch, H.** "Fully Resolved Simulation of Single and Group Particle Combustion in an Oxy-Fuel Atmosphere (Presentation)". *1st International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2016.
- [22] **Farmand, P.**, Boehme, C., Niazmehr, A., **Gauding, M.** and **Pitsch, H.** "Numerical Study of Ignition, Combustion, and Pollutant Formation of Biomass Compared to Coal (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 33–34.  
- [23] **Farmand, P.**, Boehme, C., Nicolai, H., Loffredo, F., Debiagi, P., **Gauding, M.**, Hasse, C. and **Pitsch, H.** "Modeling of NO_x Emissions in Laminar Solid Pulverized Biomass Fuels Flames (Presentation)". *19th International Conference on Numerical Combustion*. Kyoto, Japan, 2024.
- [24] **Farmand, P.**, Nicolai, H., Berger, L., **Attili, A.**, Hasse, C. and **Pitsch, H.** "Modeling Homogeneous Ignition Processes of Clustering Solid Particle Clouds in Isotropic Turbulence (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [25] **Farmand, P.**, Schumann, C., **Attili, A.** and **Pitsch, H.** "Direct Numerical Simulation of Solid Fuel Ignition and Combustion in Laminar and Turbulent Conditions (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [26] Li, T., **Farmand, P.**, **Pitsch, H.**, Dreizler, A. and Böhm, B. "Ignition and Flame Structures of Single Coal and Walnut Shell Particles in N₂/O₂ and CO₂/O₂ Atmospheres – Particle Size Effect (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.11 B4 – Detailed experimental investigation and characterisation of oxy-fuel biomass burners via laser-optical methods

4.11.1 Project members

a) Project leader(s)

- Dreizler, Andreas
- Kneer, Reinhold

b) Scientific project workers

- Hebel, Janik
- Johchi, Lukas Georg (born Becker)
- Schneider, Henrik
- Weinkauff, Johannes



4.11.2 Project summary

Project **B4** advanced understanding of fluid-mechanical, particle-dynamical, and chemical processes governing pulverised solid-fuel combustion under oxy-fuel conditions in the near-nozzle region using an optically accessible combustor with a nozzle identical to **C1** and **C7**. Parametric campaigns across Reynolds numbers, fuel/oxidiser compositions, and increasing flow complexity (single-phase/non-reacting to two-phase/reacting) were conducted. Full optical access enabled particle-based velocimetry (PIV/PTV), laser-induced phosphor thermometry, CARS, and pyrometry in cooperation with **A2**. Absorption spectroscopy with **B5** provided residence times, gas temperatures, and species. Measurements of flow fields, particle dynamics, slip velocities, particle trajectories, and wall/gas/particle temperatures established a benchmark case for gas-assisted pulverised flames up to 60 kW_{th}, bridged to larger scales in **C1** and **C7**, and supported validation and model development in **C2**. The program transitioned to pulverised biomass under oxy-fuel atmospheres, where thermochemical states were characterised by local gas temperatures and CO₂/O₂ concentrations. Pollutant formation was quantified via LII and LIF of aromatics. Methods were adapted for the semi-technical, water-cooled chamber (**C7**), employing chemiluminescence imaging, PIV/PTV, and CARS on O₂ and N₂ to analyse upscaling effects on flame stabilisation and thermochemical states. The resulting high-fidelity datasets provided robust validation data and improved physics-based models for the CRC/TRR 129.







4.11.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers



- [1] **Becker, L.**, Kosaka, H., Böhm, B., Doost, S., Knappstein, R., Habermehl, M., **Kneer, R.**, Janicka, J. and **Dreizler, A.** "Experimental Investigation of Flame Stabilization Inside the Quarl of an Oxyfuel Swirl Burner". *Fuel* 201 (2017), 124–135. 
- [2] **Becker, L.**, Langenthal, T. von, Pielsticker, S., Böhm, B., **Kneer, R.** and **Dreizler, A.** "Experimental Investigation of Particle-Laden Flows in an Oxy-Coal Combustion Chamber for Non-Reacting Conditions". *Fuel* 235 (2019), 753–762. 

- [3] **Becker, L.**, Pielsticker, S., Böhm, B., **Kneer, R.** and **Dreizler, A.** "Particle Dynamics in a Gas Assisted Coal Combustion Chamber Using Advanced Laser Diagnostics". *Fuel* 269 (2020), 117188. [doi](#)
- [4] Berkel, L., Steffens, P., Nicolai, H., Gierth, S., Debiagi, P., **Schneider, H.**, **Dreizler, A.** and Hasse, C. "Comprehensive Analysis of the Effect of Oxyfuel Atmospheres on Solid Fuel Combustion Using Large Eddy Simulations". *Fuel* 380 (2025), 133449. [doi](#) [orcid](#)
- [5] Bürkle, S., **Becker, L.**, Agizza, M. A., **Dreizler, A.**, Ebert, V. and Wagner, S. "In-Situ Measurement of Residence Time Distributions in a Turbulent Oxy-Fuel Gas-Flame Combustor". *Experiments in Fluids* 58.7 (2017), 647. [doi](#)
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- [17] Nicolai, H., Künne, G., Knappstein, R., **Schneider, H.**, **Becker, L.**, Hasse, C., di Mare, F., **Dreizler, A.** and Janicka, J. "Large Eddy Simulation of a Laboratory-Scale Gas-Assisted Pulverized Coal Combustion Chamber Under Oxy-Fuel Atmospheres Using Tabulated Chemistry". *Fuel* 272 (2020), 117683. [doi](#)




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- [19] **Schneider, H.**, **Hebel, J.**, Böhm, B., **Kneer, R.** and **Dreizler, A.** "Rotational-Vibrational O₂-CO₂ Coherent Anti-Stokes Raman Spectroscopy for Determination of Thermochemical States in Oxy-Fuel Biomass Combustion". *Proceedings of the Combustion Institute* 40.1-4 (2024), 105457.  
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b) Other publications (non peer-review)

Book chapters



- [36] **Hebel, J.**, **Schneider, H.**, **Becker, L.**, Böhm, B. and **Dreizler, A.** "Laboratory Scale Pulverised Solid Fuel Combustion Experiments". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., **Dreizler, A.**, Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers







- [23] Agizza, M. A., Bürkle, S., **Becker, L.**, Greifenstein, M., Bagheri, G., Doost, S., Faravelli, T., Janicka, J., Wagner, S. and **Dreizler, A.** "Reactor Network Modelling of a Close to Reality Combustor Using Residence Time Measurements". *10th Mediterranean Combustion Symposium*. Naples, Italy, 2017.  
- [24] Bürkle, S., Ebert, V., Rauen, D., **Dreizler, A.**, Möller, G. H., Hees, J., Zabrodiec, D., Maßmeyer, A., **Kneer, R.**, Ebert, V. and Wagner, S. "Laserbasierte Messung von Temperatur und Spezieskonzentrationen bei der Verbrennung von torrefizierter Biomasse in einer 100 kW_{th}-Staubfeuerungsversuchsanlage". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017. 
- [25] Köser, J., Knappstein, R., Goßmann, A.-K., **Becker, L.**, Böhm, B., Janicka, J. and **Dreizler, A.** "An Experimental and Numerical Study of Volatile Combustion of Single Coal Particles in an Oxygen Enriched Atmosphere". *32nd Annual International Pittsburgh Coal Conference*. Pittsburgh, Pennsylvania, USA, 2015.
- [26] Richter, M., **Schneider, H.**, Özer, B., Maßmeyer, A., Ströhle, J. and Epple, B. "Untersuchung der Flammenstabilität und thermischen Strahlung in einer 1 MW_{th}-Brennkammer unter Oxyfuel-Bedingungen". *31. Deutscher Flammentag*. Berlin, Germany, 2023.
- [27] **Schneider, H.**, **Becker, L.**, **Kneer, R.** and **Dreizler, A.** "Visualisierung und Analyse von Gasphasengeschwindigkeit und Partikeltrajektorien in einem gasassistierten Oxyfuel-Staubbrenner". *29. Deutscher Flammentag*. Bochum, Germany, 2019.

- [28] **Schneider, H., Becker, L.,** Pielsticker, S., Böhm, B., **Kneer, R. and Dreizler, A.** "Experimental Investigation and Comparison of Particle-Laden Flows in a Gas-Assisted Oxycoal Combustion Chamber for Reacting and Non-Reacting Conditions". *9th European Combustion Meeting*. Lisbon, Portugal, 2019.

Data sets

- [29] Emmert, J., **Schneider, H.,** Meißner, C., Sidiropoulos, E., Hölzer, J. I., Seeger, T., Böhm, B., **Dreizler, A.** and Wagner, S. *Data for "Characterization of Temperature Distributions in a Swirled Oxy-Fuel Coal Combustor Using Tomographic Absorption Spectroscopy with Fluctuation Modelling"*. 2020.  

Presentations and Posters

- [30] **Becker, L. and Dreizler, A.** "B4 – Detailed Experimental Investigation and Characterization of Oxycoal Burners via Laser Optical Methods (Poster)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [31] Berkel, L., Steffens, P., Nicolai, H., Gierth, S., Debiagi, P., **Schneider, H., Dreizler, A.** and Hasse, C. "Comprehensive Analysis of the Effect of Oxyfuel Atmospheres on Solid Fuel Combustion Using Large Eddy Simulations (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [32] **Hebel, J.,** Bonarens, M., König, D., Münzenberger, J., Böhm, B., Wagner, S., Epple, B. and **Dreizler, A.** "Particle Dynamics and Gas Phase Investigation in Semi-Industrial Oxy-Fuel Biomass Combustion (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, p. 53.  
- [33] Hees, J., Bürkle, S., **Becker, L.,** Zabrodiec, D., Wagner, S., **Dreizler, A.** and **Kneer, R.** "A Complementary Approach for the Experimental Investigation of Solid Oxy-Fuel Combustion Using Optical Diagnostics (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [34] **Schneider, H.,** Böhm, B., **Kneer, R.** and **Dreizler, A.** "B4 – Visualization and Analysis of Solid Fuel Particle Trajectories in a Gas-Assisted Oxy-Fuel Combustion Chamber (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [35] **Schneider, H.,** Hamel, H., **Hebel, J.,** Emmert, J., Böhm, B., Wagner, S., **Kneer, R.** and **Dreizler, A.** "Combined Flow, Temperature and Soot Investigation in Oxy-Fuel Biomass Combustion Under Varying Oxygen Concentrations Using Laser-Optical Diagnostics (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.12 B5 – Robust absorption-spectroscopic diagnostics for biomass combustion: measurement methods for gas species, gas temperatures and particle loading

4.12.1 Project members

a) Project leader(s)

- Dreizler, Andreas
- Ebert, Volker
- Wagner, Steven

b) Scientific project workers

- Blume, Niels Göran
- Bonarens, Matthias
- Bürkle, Sebastian
- Emmert, Johannes
- Köser, Jan























4.12.2 Project summary





Project **B5** developed robust in-situ absorption-spectroscopic diagnostics to quantify gas-species mole fractions, temperature, pressure, residence times, and particle load in turbulent pulverised-fuel combustion under oxy-fuel conditions from laboratory to semi-industrial scales. Broadband super-continuum laser absorption spectroscopy (SCLAS) and mid-IR interband cascade lasers, together with calibration-free retrieval algorithms and refined spectroscopic models for oxy-fuel mixtures, enabled multi-parameter, simultaneous measurements with turbulence-relevant temporal resolution and tomographic reconstructions of 2D fields in optically accessible systems, while extending effective resolution in optically restricted setups to millisecond and faster scales. The methods were applied across two-phase reacting and non-reacting configurations in **A3**, **B1**, **B4**, **B7**, and **C1**, and were scaled to **C7**, delivering quantitative fields of CO₂, O₂, and NO_x alongside temperature and residence-time distributions. Using a common instrument suite across platforms ensured comparability of operating conditions and accelerated transfer of reduced-order models to larger systems. The resulting multi-scale reference datasets supported validation and improvement of combustion and large-eddy simulation models in **C2** and enabled online process monitoring under harsh oxy-fuel environments. Transitioning from sequential to simultaneous SCLAS measurements reduced instrumentation needs, uncertainty, and experimental effort while increasing temporal fidelity, thereby advancing diagnostics for pollutant formation and thermochemical state characterisation in pulverised biomass and coal combustion.

4.12.3 Published project results

a) Publications with scientific quality assurance (peer-review)



Journal papers

- [1] Agizza, M. A., Bagheri, G., **Bürkle, S.**, Faravelli, T., **Wagner, S.** and **Dreizler, A.** "Investigation of Oxy-Fuel Combustion Through Reactor Network and Residence Time Data". *Energies* 15.1 (2022), 252.  
- [2] **Blume, N. G.**, **Ebert, V.**, **Dreizler, A.** and **Wagner, S.** "Broadband Fitting Approach for the Application of Supercontinuum Broadband Laser Absorption Spectroscopy to Combustion Environments". *Measurement Science and Technology* 27.1 (2016), 015501. 
- [3] **Bürkle, S.**, Becker, L., Agizza, M. A., **Dreizler, A.**, **Ebert, V.** and **Wagner, S.** "In-Situ Measurement of Residence Time Distributions in a Turbulent Oxy-Fuel Gas-Flame Combustor". *Experiments in Fluids* 58.7 (2017), 647. 
- [4] **Bürkle, S.**, Becker, L., Agizza, M. A., **Dreizler, A.** and **Wagner, S.** "Comparison of Two Measurement Strategies to Obtain the Residence Time Distribution in Combustion Chambers Using Tunable Diode Laser Absorption Spectroscopy". *Applied Optics* 58.10 (2019), C36. 
- [5] **Bürkle, S.**, Becker, L., **Dreizler, A.** and **Wagner, S.** "Experimental Investigation of the Flue Gas Thermochemical Composition of an Oxy-Fuel Swirl Burner". *Fuel* 231 (2018), 61–72. 
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- [9] **Emmert, J.**, **Blume, N. G.**, **Dreizler, A.** and **Wagner, S.** "PolySpec: Polynomial Spectrum Models for Fast and Light-Weight Spectroscopic Evaluation". *Applied Optics* 57.34 (2018), 9907. 
- [10] **Emmert, J.**, Grauer, S. J., **Wagner, S.** and Daun, K. J. "Efficient Bayesian Inference of Absorbance Spectra from Transmitted Intensity Spectra". *Optics Express* 27.19 (2019), 26893–26909.  
- [11] **Emmert, J.**, Schneider, H., Böhm, B., **Dreizler, A.** and **Wagner, S.** "Phase-Locked Absorption Tomography for Retrieving 5 kHz Time-Resolved Tracer Profiles in Solid Fuel Combustion". *Applications in Energy and Combustion Science* 12 (2022), 100093.  
- [12] **Emmert, J.**, Schneider, H., Meißner, C., Sidiropoulos, E., Hölzer, J. I., Seeger, T., Böhm, B., **Dreizler, A.** and **Wagner, S.** "Characterization of Temperature Distributions in a Swirled Oxy-Fuel Coal Combustor Using Tomographic Absorption Spectroscopy with Fluctuation Modelling". *Applications in Energy and Combustion Science* 6 (2021), 100025.  
- [13] **Emmert, J.**, **Wagner, S.** and Daun, K. J. "Quantifying the Spatial Resolution of the Maximum a Posteriori Estimate in Linear, Rank-Deficient, Bayesian Hard Field Tomography". *Measurement Science and Technology* 32 (2021), 025403.  
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- [16] **Köser, J.**, Becker, L., Goßmann, A.-K., Böhm, B. and **Dreizler, A.** "Investigation of Ignition and Volatile Combustion of Single Coal Particles within Oxygen-Enriched Atmospheres Using High-Speed OH-PLIF". *Proceedings of the Combustion Institute* 36.2 (2017), 2103–2111. 
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- [18] Li, G., Serdyukov, A., Gisi, M., Werhahn, O. and **Ebert, V.** "FTIR-Based Measurements of Self-Broadening and Self-Shift Coefficients as Well as Line Strength in the First Overtone Band of HCl at 1.76 μm ". *Journal of Quantitative Spectroscopy and Radiative Transfer* 165 (2015), 76–87. 
- [19] Schneider, H., **Bonarens, M.**, Hebel, J., Hamel, H., **Emmert, J.**, Böhm, B., **Wagner, S.**, Kneer, R. and **Dreizler, A.** "Combined Flow, Temperature and Soot Investigation in Oxy-Fuel Biomass Combustion Under Varying Oxygen Concentrations Using Laser-Optical Diagnostics". *Fuel* 362 (2024), 130771. 

b) Other publications (non peer-review)





Book chapters

- [30] **Bonarens, M.**, **Emmert, J.** and **Wagner, S.** "Robust Laser Diagnostics for Quantitative Process Characterisation". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., **Dreizler, A.**, Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  








Conference papers

- [20] Agizza, M. A., **Bürkle, S.**, Becker, L., Greifenstein, M., Bagheri, G., Doost, S., Faravelli, T., Janicka, J., **Wagner, S.** and **Dreizler, A.** "Reactor Network Modelling of a Close to Reality Combustor Using Residence Time Measurements". *10th Mediterranean Combustion Symposium*. Naples, Italy, 2017.  
- [21] **Bürkle, S.**, **Ebert, V.**, Rauen, D., **Dreizler, A.**, Möller, G. H., Hees, J., Zabrodiec, D., Maßmeyer, A., Kneer, R., **Ebert, V.** and **Wagner, S.** "Laserbasierte Messung von Temperatur und Spezieskonzentrationen bei der Verbrennung von torrefizierter Biomasse in einer 100 kW_{th}-Staubfeuerungsversuchsanlage". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017. 
- [22] **Köser, J.**, Knappstein, R., Goßmann, A.-K., Becker, L., Böhm, B., Janicka, J. and **Dreizler, A.** "An Experimental and Numerical Study of Volatile Combustion of Single Coal Particles in an Oxygen Enriched Atmosphere". *32nd Annual International Pittsburgh Coal Conference*. Pittsburgh, Pennsylvania, USA, 2015.

Data sets

- [23] **Emmert, J.**, Schneider, H., Meißner, C., Sidiropoulos, E., Hölzer, J. I., Seeger, T., Böhm, B., **Dreizler, A.** and **Wagner, S.** *Data for "Characterization of Temperature Distributions in a Swirled Oxy-Fuel Coal Combustor Using Tomographic Absorption Spectroscopy with Fluctuation Modeling"*. 2020.  
- [24] Hansemann, C., **Bonarens, M.**, **Emmert, J.**, Daun, K. J. and **Wagner, S.** *Data for "Towards a Spatially Resolved, Single-Ended TDLAS System for Characterizing the Distribution of Gaseous Species"*. 2024.  

Presentations and Posters

- [25] **Bonarens, M.**, König, D., Linke, P., Goet, G., Hansemann, C., Ströhle, J., Epple, B. and **Wagner, S.** "Simultaneous Measurement of Temperatures at Various Distances from the Burner of a Semi-Industrial-Scale Biomass Combustion Chamber (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 47–48.  
- [26] Hansemann, C., **Bonarens, M.**, Daun, K. J., **Emmert, J.** and **Wagner, S.** "Towards Spatially Resolved, Single-Ended Tunable Diode Laser Absorption Spectroscopy in Particle-Laden Flows (Presentation)". *Conference on Lasers and Electro-Optics*. Charlotte, North Carolina, USA, 2024. 
- [27] Hebel, J., **Bonarens, M.**, König, D., Münzenberger, J., Böhm, B., **Wagner, S.**, Epple, B. and **Dreizler, A.** "Particle Dynamics and Gas Phase Investigation in Semi-Industrial Oxy-Fuel Biomass Combustion (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, p. 53.  
- [28] Hees, J., **Bürkle, S.**, Becker, L., Zabrodiec, D., **Wagner, S.**, **Dreizler, A.** and Kneer, R. "A Complementary Approach for the Experimental Investigation of Solid Oxy-Fuel Combustion Using Optical Diagnostics (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [29] Schneider, H., Hamel, H., Hebel, J., **Emmert, J.**, Böhm, B., **Wagner, S.**, Kneer, R. and **Dreizler, A.** "Combined Flow, Temperature and Soot Investigation in Oxy-Fuel Biomass Combustion Under Varying Oxygen Concentrations Using Laser-Optical Diagnostics (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.13 B6 – Modeling of particle-turbulence-chemistry interaction for oxy-fuel processes

4.13.1 Project members

a) Project leader(s)

- Janicka, Johannes
- Sadiki, Amsini

b) Scientific project workers

- Knappstein, Robert
- Ries, Florian



4.13.2 Project summary

The project **B6** addressed the core task of modeling unsteady turbulence-chemistry interaction for solid-fuel combustion under oxy-fuel conditions. It developed a cross-regime flamelet-generated-manifold description, captured finite-rate chemistry based on detailed mechanisms, and employed oxy-fuel-specific reaction kinetics. Particle-turbulence-chemistry interaction was described consistently, including an Euler-Lagrange formulation with two-way coupling, and the CFD code Fastest was adapted to the requirements of oxy-fuel combustion. Submodels describing subprocesses of coal combustion were integrated and validated against experimental data. For this, results from **A1**, **A2**, and **B3** as well as measurements from **B4** and **B5** were used. Further couplings and integration were carried out in **C2**. Overall, a consistent model emerged that accounted for the fluctuating nature of turbulent flows, detailed chemistry, and feedback from the particle phase on flow and reaction, laying the groundwork for robust predictions in oxy-fuel flames.

4.13.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **Knappstein, R.**, Künne, G., Ketelheun, A., Köser, J., Becker, L., Heuer, S., Schiemann, M., Scherer, V., Dreizler, A., **Sadiki, A.** and **Janicka, J.** "Devolatilization and Volatiles Reaction of Individual Coal Particles in the Context of FGM Tabulated Chemistry". *Combustion and Flame* 169 (2016), 72–84. 
- [2] **Knappstein, R.**, Künne, G., Meier, T., **Sadiki, A.** and **Janicka, J.** "Evaluation of Coal Particle Volatiles Reaction by Using Detailed Kinetics and FGM Tabulated Chemistry". *Fuel* 201 (2017), 39–52. 

b) Other publications (non peer-review)

Conference papers

- [3] Ketelheun, A., Mehdizadeh, A., **Knappstein, R.**, **Sadiki, A.** and **Janicka, J.** "Investigation of Unsteady Simulation Methods in an Oxyfuel Configuration". 27. *Deutscher Flammentag*. Clausthal-Zellerfeld, Germany, 2015.

- [4] Köser, J., **Knappstein, R.**, Goßmann, A.-K., Becker, L., Böhm, B., **Janicka, J.** and Dreizler, A. "An Experimental and Numerical Study of Volatile Combustion of Single Coal Particles in an Oxygen Enriched Atmosphere". *32nd Annual International Pittsburgh Coal Conference*. Pittsburgh, Pennsylvania, USA, 2015.

4.14 B7 – Investigation of ignition and combustion processes of solid fuel particles under oxy-fuel conditions

4.14.1 Project members

a) Project leader(s)

- Böhm, Benjamin
- Schiemann, Martin

b) Scientific project workers

- Geschwindner, Christopher
- Köser, Jan
- Li, Tao
- Tarlinski, David
- Valentiner, Sarah
- Vorobiev, Nikita



4.14.2 Project summary


















Project **B7** experimentally characterised particle-turbulence-chemistry interactions governing ignition and combustion of pulverised solid fuels at the scale of individual particles. A stepwise program – from single particles in laminar flat-flame conditions to particle clouds in a plasma-heated turbulent hot-gas co-flow rig – combined time-resolved, multi-parameter laser diagnostics developed with **A2**, **B4**, and **B5**. Pyrolysis, ignition, volatile combustion, and the onset of char were tracked using volumetric tomographic and scanning OH-LIF for 3D flame topology. Methodological advances included volumetric CH₂O-LIF with an acousto-optic deflector and simultaneous tomographic PIV. The campaigns were extended to biomass fuels, where gas-phase fields near individual particles were resolved, particle shape/composition effects and particle-particle interactions were quantified via number-density variations, and atmosphere effects were assessed by switching between air and oxy-fuel at different O₂ levels. The resulting datasets supported validation of highly resolved simulations in **B2**, **B3**, and **C2**, uncertainty analyses in **B8**, and provided benchmark cases for model development inside and outside the CRC/TRR 129, improving understanding of particle heating, flame stabilisation, soot, and NO_x formation in particle-laden turbulent flows.












4.14.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Attili, A., Farmand, P., Schumann, C., Farazi, S., **Böhm, B.**, **Li, T.**, **Geschwindner, C.**, **Köser, J.**, Dreizler, A. and Pitsch, H. "Numerical Simulations and Experiments of Ignition of Solid Particles in a Laminar Burner: Effects of Slip Velocity and Particle Swelling". *Flow, Turbulence and Combustion* 106 (2020), 515–531.  [DOI](#)
- [2] Chen, H., Abdallah, M., Dreizler, A., **Böhm, B.** and **Li, T.** "Simultaneous LII, PAH-LIF, OH-LIF, and Mie Scattering Measurements in Solid Fuel Particle Combustion". *Proceedings of the Combustion Institute* 40.1-4 (2024), 105711.  [DOI](#)

- [3] Farmand, P., Nicolai, H., Schumann, C., Attili, A., Berger, L., **Li, T., Geschwindner, C.**, di Mare, F., Hasse, C., **Böhm, B.**, Janicka, J. and Pitsch, H. "Numerical Investigation and Assessment of Flamelet-Based Models for the Prediction of Pulverized Solid Fuel Homogeneous Ignition and Combustion". *Combustion and Flame* 235 (2022), 111693. 
- [4] **Geschwindner, C.**, Nicolas, A., Westrup, K., Dreizler, A., Peterson, B. and **Böhm, B.** "Resolving Biomass-Turbulence Interactions at the Particle Scale Using Ultra-High-Speed Wavelet-Based Optical Flow Velocimetry (wofv)". *Proceedings of the Combustion Institute* 40.1-4 (2024), 105461.  
- [5] **Geschwindner, C.**, Westrup, K., Dreizler, A. and **Böhm, B.** "Pulse Picking of a Fiber Laser Enables Velocimetry of Biomass-Laden Jets at Low and Ultra-High Repetition Rates". *Proceedings of the Combustion Institute* 39.1 (2023), 1325–1335. 
- [6] Johchi, A., Pareja, J., **Böhm, B.** and Dreizler, A. "Quantitative Mixture Fraction Imaging of a Synthetic Biogas Turbulent Jet Propagating into a NO-Vitiated Air Co-Flow Using Planar Laser-Induced Fluorescence (PLIF)". *Experiments in Fluids* 60.5 (2019), 60. 
- [7] **Köser, J., Li, T., Vorobiev, N.**, Dreizler, A., **Schiemann, M.** and **Böhm, B.** "Multi-Parameter Diagnostics for High-Resolution In-Situ Measurements of Single Coal Particle Combustion". *Proceedings of the Combustion Institute* 37.3 (2019), 2893–2900. 
- [8] **Li, T.**, Farmand, P., Chen, H., Boehme, C., Nicolai, H., Hasse, C., Pitsch, H. and **Böhm, B.** "Homogeneous Ignition and Volatile Flame Structure of Single Bituminous Coal and Walnut Shell Particles: Effects of Particle Size and Gas Atmosphere". *Fuel* 371 (2024), 131955.  
- [9] **Li, T.**, Farmand, P., **Geschwindner, C.**, Greifenstein, M., **Köser, J.**, Schumann, C., Attili, A., Pitsch, H., Dreizler, A. and **Böhm, B.** "Homogeneous Ignition and Volatile Combustion of Single Solid Fuel Particles in Air and Oxy-Fuel Conditions". *Fuel* 291 (2021). 
- [10] **Li, T., Geschwindner, C.**, Dreizler, A. and **Böhm, B.** "An Experimental Study of Coal Particle Group Combustion in Conventional and Oxy-Fuel Atmospheres Using Multi-Parameter Optical Diagnostics". *Proceedings of the Combustion Institute* 39 (2023), 3259–3269. 
- [11] **Li, T., Geschwindner, C.**, Dreizler, A. and **Böhm, B.** "Particle-Resolved Optical Diagnostics of Solid Fuel Combustion for Clean Power Generation: A Review". *Measurement Science and Technology* 34.12 (2023), 122001.  
- [12] **Li, T., Geschwindner, C., Köser, J., Schiemann, M.**, Dreizler, A. and **Böhm, B.** "Investigation of the Transition from Single to Group Coal Particle Combustion Using High-Speed Scanning OH-LIF and Diffuse Backlight-Illumination". *Proceedings of the Combustion Institute* 38 (2021), 4101–4109. 
- [13] **Li, T.**, Li, B., Farmand, P., Dreizler, A., Pitsch, H. and **Böhm, B.** "Motion and Swelling of Single Coal Particles During Volatile Combustion in a Laminar Flow Reactor". *Proceedings of the Combustion Institute* 39.3 (2023), 3333–3341. 
- [14] **Li, T.**, Pareja, J., Fuest, F., Schütte, M., Zhou, Y., Dreizler, A. and **Böhm, B.** "Tomographic Imaging of OH Laser-Induced Fluorescence in Laminar and Turbulent Jet Flames". *Measurement Science and Technology* 29.1 (2018), 015206. 
- [15] **Li, T., Schiemann, M., Köser, J.**, Dreizler, A. and **Böhm, B.** "Experimental Investigations of Single Particle and Particle Group Combustion in a Laminar Flow Reactor Using Simultaneous Volumetric OH-LIF Imaging and Diffuse Backlight-Illumination". *Renewable and Sustainable Energy Reviews* 136 (2021), 110377. 
- [16] **Li, T.**, Zhou, B., Frank, J. H., Dreizler, A. and **Böhm, B.** "High-Speed Volumetric Imaging of Formaldehyde in a Lifted Turbulent Jet Flame Using an Acousto-Optic Deflector". *Experiments in Fluids* 61.4 (2020), 2903. 



- [17] Nicolai, H., **Li, T.**, **Geschwindner, C.**, di Mare, F., Hasse, C., **Böhm, B.** and Janicka, J. "Numerical Investigation of Pulverized Coal Particle Group Combustion Using Tabulated Chemistry". *Proceedings of the Combustion Institute* 38.3 (2021), 4033–4041. 
- [18] Panahi, A., **Vorobiev, N.**, **Schiemann, M.**, Tarakcioglu, M., Delichatsios, M. A. and Levendis, Y. A. "Combustion Details of Raw and Torrefied Biomass Fuel Particles with Individually-Observed Size, Shape and Mass". *Combustion and Flame* 207 (2019), 327–341. 
- [19] Pareja, J., Johchi, A., **Li, T.**, Dreizler, A. and **Böhm, B.** "A Study of the Spatial and Temporal Evolution of Auto-Ignition Kernels Using Time-Resolved Tomographic OH-LIF". *Proceedings of the Combustion Institute* 37.2 (2019), 1321–1328. 
- [20] Schneider, H., **Valentiner, S.**, **Vorobiev, N.**, **Böhm, B.**, **Schiemann, M.**, Scherer, V., Kneer, R. and Dreizler, A. "Investigation on Flow Dynamics and Temperatures of Solid Fuel Particles in a Gas-Assisted Oxy-Fuel Combustion Chamber". *Fuel* 286 (2021), 119424. 
- [21] Shamooni, A., Stein, O. T., Kronenburg, A., Kempf, A. M., Debiagi, P., **Li, T.**, Dreizler, A., **Böhm, B.** and Hasse, C. "Fully-Resolved Simulations of Volatile Combustion and NO_x Formation from Single Coal Particles in Recycled Flue Gas Environments". *Proceedings of the Combustion Institute* 39.4 (2023), 4529–4539. 
- [22] **Tarlinski, D.**, Freisewinkel, E., Eisenbach, T., Span, R., **Schiemann, M.** and Scherer, V. "Combustion of Single Walnut Shell Particles in a Laminar Flow Reactor Under Oxy-Fuel Conditions: Optical Measurements and Particle Sampling". *Fuel* 369 (2024), 131613.  
- [23] **Tarlinski, D.**, **Geschwindner, C.**, **Li, T.**, **Böhm, B.** and **Schiemann, M.** "Particle Temperature and Composition Measurements in the Ignition Phase of Single Coal Particles and Particle Groups Under Conventional and Oxy-Fuel Atmospheres". *Fuel* 332 (2023), 125894. 
- [24] **Tarlinski, D.**, Yao, Y., Chang, D., Levendis, Y., **Schiemann, M.** and Scherer, V. "Optical Measurements of Emissivity, Flame and Char Temperatures of Pulverized Pine Needles in a Drop Tube Furnace". *International Journal of Energy for a Clean Environment* (2025). 
- [25] **Vorobiev, N.**, **Valentiner, S.**, **Schiemann, M.** and Scherer, V. "Comprehensive Data Set of Single Particle Combustion Under Oxy-Fuel Conditions, Part I: Measurement Technique". *Combustion Science and Technology* 56.2 (2020), 1–22. 
- [26] Zhou, B., **Li, T.**, Frank, J. H., Dreizler, A. and **Böhm, B.** "Simultaneous 10 kHz Three-Dimensional CH₂O and Tomographic PIV Measurements in a Lifted Partially-Premixed Jet Flame". *Proceedings of the Combustion Institute* 38.1 (2021), 1675–1683. 

Conference papers

- [27] Chen, H., Li, Y., **Böhm, B.** and **Li, T.** "Tracking Solid Fuel Particles via Multi-Object Detection with Machine Learning". *13th Mediterranean Combustion Symposium*. Corfu, Greece, 2025.
- [28] **Geschwindner, C.**, Werner, M., André, L., Nicolas, A., Peterson, B., Meinke, M., Schröder, W., Dreizler, A. and **Böhm, B.** "High-Resolution Two-Phase Velocimetry of Aspherical Particles Using Wavelet-Based Optical Flow Velocimetry (wofv) Benchmarked with Fully Resolved Direct Numerical Simulations". *21st International Symposium on Applications of Laser and Imaging Techniques to Fluid Mechanics*. Lisbon, Portugal, 2024.
- [29] **Li, T.**, Chen, H. and **Böhm, B.** "Assessing the Gas Composition Effects on Volatile Flames of Solid Fuels Using Multi-Parameter Optical Diagnostics". *13th Mediterranean Combustion Symposium*. Corfu, Greece, 2025.

b) Other publications (non peer-review)





Book chapters





- [45] **Geschwindner, C., Tarlinski, D., Li, T., Köser, J., Schiemann, M.**, Dreizler, A. and **Böhm, B.** "Experimental Investigation of Particle-Flow-Chemistry Interactions". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Conference papers

- [30] Eckhard, T., Lotz, K., Pflieger, C., **Vorobiev, N., Valentiner, S.**, Scherer, V. and Muhler, M. "Hydrothermal carbonisierte mikrokristalline Cellulose als aschefreier Modellbrennstoff für Flachflammenbrenner". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [31] **Geschwindner, C.**, Westrup, K., **Li, T.**, Dreizler, A. and **Böhm, B.** "Experimentelle Untersuchung der Interaktion von Biomasse mit einem turbulenten plasmabeheizten Oxidatorgasstrom". *30. Deutscher Flammentag*. Hannover, Germany, 2021.
- [32] **Li, T., Köser, J.**, Dreizler, A., **Schiemann, M.** and **Böhm, B.** "Time-Resolved Volumetric Measurement of OH Radicals on Single Particle and Particle Group Combustion". *14th International Conference on Sustainable Development of Energy, Water and Environment Systems*. Dubrovnik, Croatia, 2019.
- [33] **Li, T., Köser, J., Schiemann, M.**, Dreizler, A. and **Böhm, B.** "Untersuchungen der Verbrennung von Einzelpartikeln und Partikelgruppen mit zeitaufgelöster volumetrischer Messung des OH-Radikals". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [34] **Tarlinski, D., Geschwindner, C., Li, T., Böhm, B.** and **Schiemann, M.** "Optische Charakterisierung der volatilen Flamme in Partikelstrahlen in Abhängigkeit von der Partikelanzahldichte". *30. Deutscher Flammentag*. Hannover, Germany, 2021.
- [35] **Tarlinski, D.** and **Schiemann, M.** "Messung der laserinduzierten Inkandeszenz zu der Charakterisierung von Rußbildung um einzelne Kohle- und Biomassepartikel". *31. Deutscher Flammentag*. Berlin, Germany, 2023.
- [36] **Tarlinski, D.**, Yao, D., Chang, Y., Levensis, Y. A., **Schiemann, M.** and Scherer, V. "Optical Measurements of Pulverized Pine Needles Burning in a Drop Tube Furnace". *48th International Conference on Clean Energy*. Clearwater, USA, 2024.
- [37] **Vorobiev, N.**, Kruse, S., Pitsch, H. and **Schiemann, M.** "Demonstration of Laser-Induced Incandescence in Single Coal Particle Enveloping Flames". *9th European Combustion Meeting*. Lisbon, Portugal, 2019.
- [38] Werner, M., **Geschwindner, C.**, Nicolas, A., Peterson, B., Dreizler, A. and **Böhm, B.** "Wavelet-Based Optical Flow Velocimetry (wofv) for Tracking the Rotational Motion of Aspherical Particles in Two-Phase Flows". *32. Fachtagung "Experimentelle Strömungsmechanik"*. Darmstadt, Germany, 2025.

Presentations and Posters

- [39] **Geschwindner, C.**, Westrup, K., Dreizler, A. and **Böhm, B.** "Particle Dynamics within a High-Velocity Biomass-Laden Jet Investigated by Two-Phase Velocimetry at Low to Ultra-High Repetition Rates (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [40] **Li, T.**, Farmand, P., Pitsch, H., Dreizler, A. and **Böhm, B.** "Ignition and Flame Structures of Single Coal and Walnut Shell Particles in N₂/O₂ and CO₂/O₂ Atmospheres – Particle Size Effect (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

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- [41] Nicolai, H. and **Geschwindner, C.** "Swirling Coal and Biomass Flames (Presentation)". *4th Workshop on Clean Solids Conversion*. Kyoto, Japan, 2024.
- [42] **Tarlinski, D.**, Freisewinkel, E., Scherer, V. and **Schiemann, M.** "Metal Fuels Reacting in Oxy-Fuel Flue Gas Mixtures (Poster)". *Renewable Metal Fuels Symposium*. Rapperswil, Switzerland, 2025.
- [43] **Tarlinski, D.**, Freisewinkel, E., **Schiemann, M.** and Scherer, V. "Combustion and Pyrolysis of Aluminum and Magnesium Particles in Oxy-Fuel Atmosphere (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 57–58.  
- [44] Werner, M., **Geschwindner, C.**, Nicolas, A., Peterson, B., Dreizler, A. and **Böhm, B.** "Shape-Dependent Motion Estimation of Solid Fuel Particles in Two-Phase Flows Using Wavelet-Based Optical Flow Velocimetry (wofv) (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 54–55.  

4.15 B8 – Sensitivity analysis and uncertainty quantification of pulverised solid fuel combustion

4.15.1 Project members

a) Project leader(s)

- Sayadi, Taraneh

b) Scientific project workers

- Hassan, Ahmed
- Maës, Pierre-Antoine

4.15.2 Project summary


Project **B8** quantified sensitivities and uncertainties in models for pulverised solid-fuel combustion to enable predictive large-scale simulations under air and oxy-fuel atmospheres. An adjoint-based framework was developed to extract gradients of key quantities (e.g. burning rate, surface temperature, drag) with respect to many parameters at once. Sensitivities were obtained for single solid particles during steady and unsteady char conversion using surface-kinetic models from **A2** and gas-phase kinetics from **B1**, and were extended to inert and reactive particle groups to capture clustering effects and turbulence influences. Local drag sensitivities to particle shape and orientation were derived in two- and three-dimensional configurations aligned with the experiments of **B7** and simulations of **B2**. The methodology was prepared for application to mechanisms from **A8**. Sensitivity information supported uncertainty quantification for group-combustion setups and for particle size and orientation, yielding error estimates consistent with experimental practice. The results identified dominant kinetic and hydrodynamic parameters controlling ignition and char conversion, clarified the impact of particle interactions on model responses, and constrained drag and kinetic closures. The findings were integrated into reactor-network and reduced-order workflows in **C2**, where they propagated parametric uncertainties to real-scale predictions and improved the credibility of simulations for biomass combustion under oxy-fuel conditions.

4.15.3 Published project results

a) Publications with scientific quality assurance (peer-review)



Journal papers

- [1] Fikl, A., Le Chenadec, V. and **Sayadi, T.** "Control and Optimization of Interfacial Flows Using Adjoint-Based Techniques". *Fluids* 5.3 (2020), 156. [doi](#) [a](#)
- [2] **Hassan, A.**, Sabry, M., Le Chenadec, V. and **Sayadi, T.** "Uncertainty Quantification of Kinetic Models Using Adjoint-Driven Active Subspace Algorithms". *Proceedings of the Combustion Institute* 39.4 (2023), 5209–5218. [doi](#)
- [3] **Hassan, A.**, **Sayadi, T.**, Le Chenadec, V. and Attili, A. "Sensitivity Analysis of an Unsteady Char Particle Combustion". *Fuel* 287 (2021). [doi](#)
- [4] **Hassan, A.**, **Sayadi, T.**, Le Chenadec, V., Pitsch, H. and Attili, A. "Adjoint-Based Sensitivity Analysis of Steady Char Burnout". *Combustion Theory and Modelling* 25.1 (2021), 96–120. [doi](#)
- [5] **Hassan, A.**, **Sayadi, T.**, Schiemann, M. and Scherer, V. "Adjoint-Based Sensitivity Analysis of Char Combustion Surface Reaction Kinetics". *Fuel* 287 (2021). [doi](#)



- [6] **Hassan, A.**, Schumacher, L., Sabry, M., Le Chenadec, V. and **Sayadi, T.** "Uncertainty Quantification and Sensitivity Analysis of an Unsteady Axisymmetric Reacting Solid Particle". *Combustion and Flame* 262 (2024), 113365. 

b) Other publications (non peer-review)

Book chapters

- [8] **Hassan, A.** and **Sayadi, T.** "Sensitivity Analysis and Uncertainty Quantification of a Single Combusting Particle". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

Presentations and Posters

- [7] **Hassan, A.**, Schumacher, L., Le Chenadec, V. and **Sayadi, T.** "Sensitivity Analysis and Uncertainty Quantification of an Axisymmetric Reacting Particle (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.16 C1 – Experimental investigation of pulverised biomass combustion for validation of numerical models

4.16.1 Project members

a) Project leader(s)

- Dreizler, Andreas
- Kneer, Reinhold
- Maßmeyer, Anna

b) Scientific project workers

- Askarizadeh, Hossein
- Hatzfeld, Oliver
- Hees, Johannes
- Zabrodiec, Diego
- Özer, Burak



4.16.2 Project summary

Project **C1** investigated self-sustained pulverised biomass combustion in air and oxy-fuel atmospheres across a broad thermal-load range, providing high-fidelity datasets of local velocity fields, major species concentrations, flame temperatures, flame structure, and radiative heat flux. Operating conditions and advanced diagnostics were established and then used for parametric studies comparing fuels (lignite, bituminous coal, torrefied biomass), oxidiser O₂ content, and inflow conditions. Using geometrically similar burners as **B4** revealed strong sensitivities to chamber geometry, wall temperatures, and pilot-methane flames. Results validated numerical models in **C2**. **C1** bridged scales between optically accessible gas-assisted flames in **B4** and the semi-industrial **C7** facility, characterised the transition from gas-assisted to self-sustained biomass combustion, and analysed low-frequency oscillations and their impact on averaged quantities. By extending thermal loads up to 100 kW_{th} and complementing measurements at **C7** (1 MW_{th}) **C1** played a major role in assessing dominant physico-chemical processes across laboratory, pilot, and semi-industrial scales.





4.16.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **Askarizadeh, H.**, Pielsticker, S., Nicolai, H., **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** "Investigation of the Coupling Schemes Between the Discrete and the Continuous Phase in the Numerical Simulation of a 60 kW_{th} Swirling Pulverised Solid Fuel Flame Under Oxyfuel Conditions". *Fire* 7.6 (2024), 185.  [a](#)
- [2] **Askarizadeh, H.**, Pielsticker, S., Nicolai, H., Koch, M., **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** "Radiation Modelling Considering Burnout-Dependent Properties and Cellwise Non-Uniform Particle Distributions in the Numerical Simulation of Pulverised Solid Fuel Combustion". *Fuel* 381 (2025), 133338.  [a](#)

- [3] **Askarizadeh, H.**, Pielsticker, S., Nicolai, H., **Özer, B.**, **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** "Influence of the Devolatilisation Kinetics on the Numerical Simulation of Pulverised Fuel Swirl Flames Under Oxyfuel Conditions". *Fuel* 393 (2025), 135177. [doi](#) [a](#)
- [4] Becker, L., Kosaka, H., Böhm, B., Doost, S., Knappstein, R., Habermehl, M., **Kneer, R.**, Janicka, J. and **Dreizler, A.** "Experimental Investigation of Flame Stabilization Inside the Quarl of an Oxyfuel Swirl Burner". *Fuel* 201 (2017), 124–135. [doi](#)
- [5] Habermehl, M., **Hees, J.**, **Maßmeyer, A.**, **Zabrodiec, D.**, **Hatzfeld, O.** and **Kneer, R.** "Comparison of Flame Stability Under Air and Oxy-Fuel Conditions for an Aerodynamically Stabilized Pulverized Coal Swirl Flame". *Journal of Energy Resources Technology* 138.4 (2016), 042209. [doi](#)
- [6] **Hees, J.**, **Zabrodiec, D.**, **Maßmeyer, A.**, Habermehl, M. and **Kneer, R.** "Experimental Investigation and Comparison of Pulverized Coal Combustion in CO₂/O₂- and N₂/O₂-Atmospheres". *Flow, Turbulence and Combustion* 96.2 (2016), 417–431. [doi](#)
- [7] **Hees, J.**, **Zabrodiec, D.**, **Maßmeyer, A.**, **Hatzfeld, O.** and **Kneer, R.** "Experimental Investigation into the Influence of the Oxygen Concentration on a Pulverized Coal Swirl Flame in Oxy-Fuel Atmosphere". *Fuel* 240 (2019), 64–74. [doi](#)
- [8] **Hees, J.**, **Zabrodiec, D.**, **Maßmeyer, A.**, Pielsticker, S., Gövert, B., Habermehl, M., **Hatzfeld, O.** and **Kneer, R.** "Detailed Analyzes of Pulverized Coal Swirl Flames in Oxy-Fuel Atmospheres". *Combustion and Flame* 172 (2016), 289–301. [doi](#)
- [9] **Maßmeyer, A.**, **Zabrodiec, D.**, **Hees, J.**, Kreitzberg, T., **Hatzfeld, O.** and **Kneer, R.** "Flame Pattern Analysis for 60 kW_{th} Flames Under Conventional Air-Fired and Oxy-Fuel Conditions for Two Different Types of Coal". *Fuel* 271 (2020), 117457. [doi](#)
- [10] Nicolai, H., Debiagi, P., Wen, X., Dressler, L., **Maßmeyer, A.**, Janicka, J. and Hasse, C. "Flamelet LES of Swirl-Stabilized Oxy-Fuel Flames Using Directly Coupled Multi-Step Solid Fuel Kinetics". *Combustion and Flame* 241 (2022), 112062. [doi](#)
- [11] Nicolai, H., Wen, X., Miranda, F., **Zabrodiec, D.**, **Maßmeyer, A.**, di Mare, F., **Dreizler, A.**, Hasse, C., **Kneer, R.** and Janicka, J. "Numerical Investigation of Swirl-Stabilized Pulverized Coal Flames in Air and Oxy-Fuel Atmospheres by Means of Large Eddy Simulation Coupled with Tabulated Chemistry". *Fuel* 287 (2021), 119429. [doi](#)
- [12] **Özer, B.**, **Kneer, R.** and **Maßmeyer, A.** "Experimental Assessment of Velocity and Narrow-Band Measurements in Oxy-Fuel Combustion of Pulverized Walnut Shells". *Experimental Thermal and Fluid Science* 172 (2026). [doi](#)
- [13] **Özer, B.**, **Zabrodiec, D.**, **Kneer, R.** and **Maßmeyer, A.** "Experimental Investigation of 40 kW_{th} Methane-Assisted and Self-Sustained Pulverized Biomass Flames". *Proceedings of the Combustion Institute* 39.3 (2023), 3343–3351. [doi](#)
- [14] Sadiki, A., Agrebi, S., Chrigui, M., Doost, S., Knappstein, R., di Mare, F., Janicka, J., **Maßmeyer, A.**, **Zabrodiec, D.**, **Hees, J.** and **Kneer, R.** "Analyzing the Effects of Turbulence and Multiphase Treatments on Oxy-Coal Combustion Process Predictions Using LES and RANS". *Chemical Engineering Science* 166 (2017), 283–302. [doi](#)
- [15] Steffens, P., Berkel, L., Gierth, S., Debiagi, P., **Özer, B.**, **Maßmeyer, A.**, Nicolai, H. and Hasse, C. "LES of a Swirl-Stabilized 40 kW_{th} Biomass Flame and Comparison to a Coal Flame". *Fuel* 372 (2024), 132098. [doi](#) [a](#)
- [16] Wen, X., Nicolai, H., Debiagi, P., **Zabrodiec, D.**, **Maßmeyer, A.**, **Kneer, R.** and Hasse, C. "Flamelet LES of a 40 kW_{th} Pulverized Torrefied Biomass Furnace in Air and Oxy-Fuel Atmospheres". *Proceedings of the Combustion Institute* 39.4 (2023), 4563–4572. [doi](#)



- [17] **Zabrodiec, D.**, Becker, L., **Hees, J.**, **Maßmeyer, A.**, Habermehl, M., **Hatzfeld, O.**, **Dreizler, A.** and **Kneer, R.** "Detailed Analysis of the Velocity Fields from 60 kW Swirl-Stabilized Coal Flames in CO₂/O₂- and N₂/O₂-Atmospheres by Means of Laser Doppler Velocimetry and Particle Image Velocimetry". *Combustion Science and Technology* 189.10 (2017), 1751–1775. 
- [18] **Zabrodiec, D.**, **Hees, J.**, **Maßmeyer, A.**, Lehn, F. vom, Habermehl, M., **Hatzfeld, O.** and **Kneer, R.** "Experimental Investigation of Pulverized Coal Flames in CO₂/O₂- and N₂/O₂-Atmospheres: Comparison of Solid Particle Radiative Characteristics". *Fuel* 201 (2017), 136–147. 
- [19] **Zabrodiec, D.**, **Hees, J.**, Möller, G. H., **Hatzfeld, O.** and **Kneer, R.** "Pulverized Coal Swirl Flames in Oxy-Fuel Conditions: Effects of Oxidizer O₂ Concentration on Flow Field and Local Gas Composition". *Proceedings of the Combustion Institute* 37.4 (2019), 4471–4478. 
- [20] **Zabrodiec, D.**, **Maßmeyer, A.**, **Hees, J.**, **Hatzfeld, O.** and **Kneer, R.** "Flow Pattern and Behavior of 40 kW_{th} Pulverized Torrefied Biomass Flames Under Atmospheric and Oxy-Fuel Conditions". *Renewable and Sustainable Energy Reviews* 138 (2021), 110493. 

Conference papers




- [21] **Askarizadeh, H.**, Pielsticker, S., Nicolai, H., **Kneer, R.**, Hasse, C., **Özer, B.** and **Maßmeyer, A.** "Numerical Study on the Influence of Devolatilisation Kinetics on Pulverised Solid Fuel Turbulent Swirling Flames Under Oxyfuel Conditions". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.
- [22] **Özer, B.**, **Kneer, R.** and **Maßmeyer, A.** "Experimental Assessment of Velocity and Narrow-Band Measurements in Oxy-Fuel Combustion of Pulverized Walnut Shells". *13th Mediterranean Combustion Symposium*. Corfu, Greece, 2025.
- [23] Pörtner, L., **Özer, B.**, Richter, M., König, D., Schiemann, M., **Maßmeyer, A.**, Ströhle, J. and Epple, B. "Spectral Resolved Radiative Heat Flux Measurements in a Combustion Chamber". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.






b) Other publications (non peer-review)

Book chapters



- [59] **Özer, B.**, **Kneer, R.** and **Maßmeyer, A.** "Pilot Scale Pulverised Solid Fuel Combustion Experiments". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., **Dreizler, A.**, Scherer, V., **Maßmeyer, A.** and Pielsticker, S. Springer, 2025.  















Conference papers

- [24] **Askarizadeh, H.**, Koch, M., Nicolai, H., Pielsticker, S., **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** "Influence of Gas Radiation, Particle Radiation Interactions, and Conversion-Dependent Particle Radiative Properties on Pulverized Solid Fuel Combustion". *31. Deutscher Flammentag*. Berlin, Germany, 2023.
- [25] **Askarizadeh, H.**, Nicolai, H., **Zabrodiec, D.**, Pielsticker, S., Hasse, C., **Kneer, R.** and **Maßmeyer, A.** "Numerische Untersuchung zur Relevanz von Teilmodellen für Pyrolyse und Koksabbrand in turbulenten drallbehafteten Flammen unter Oxyfuel-Bedingungen". *30. Deutscher Flammentag*. Hannover, Germany, 2021.  
- [26] Bürkle, S., Ebert, V., Rauen, D., **Dreizler, A.**, Möller, G. H., **Hees, J.**, **Zabrodiec, D.**, **Maßmeyer, A.**, **Kneer, R.**, Ebert, V. and Wagner, S. "Laserbasierte Messung von Temperatur und Spezieskonzentrationen bei der Verbrennung von torrefizierter Biomasse in einer 100 kW_{th}-Staubfeuerungsversuchsanlage". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017. 





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- [28] Habermehl, M., Hees, J., Zabrodiec, D. and Kneer, R. "Comparison of Flame Stability Under Air and Oxy-Fuel Conditions for an Aerodynamically Stabilized Pulverized Coal Swirl Flame". *40th International Technical Conference on Clean Coal & Fuel Systems*. Clearwater, Florida, USA, 2015.
- [29] Hees, J., Zabrodiec, D., Maßmeyer, A., Hatzfeld, O., Habermehl, M. and Kneer, R. "Kohlenstaubverbrennung in Oxyfuel-Atmosphäre: Einfluss der Oxidatorzusammensetzung auf den Verbrennungsprozess". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017.  
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- [36] Zabrodiec, D., Hees, J., Maßmeyer, A. and Kneer, R. "Progress and Challenges in Flow Field Studies of 40–60 kW_{th} Pulverized Coal Flames". *Joint Meeting the German and Italian Sections of the Combustion Institute*. Sorrento, Italy, 2018.  
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- [41] **Askarizadeh, H.**, Pielsticker, S., Nicolai, H., Koch, M., **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** *Radiation Modelling Considering Burnout-Dependent Properties and Cellwise Non-Uniform Particle Distributions in the Numerical Simulation of Pulverised Solid Fuel Combustion – Dataset*. RWTH Aachen University. 2024.  
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- [45] **Zabrodiec, D.**, **Hees, J.**, **Maßmeyer, A.** and **Kneer, R.** *Experimental Dataset: Pulverized Coal Swirl Flames in Oxy-Fuel Conditions: Effects of Oxidizer O₂ Concentration on Flow Field and Local Gas Composition*. 2020.  
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- [47] **Askarizadeh, H.**, Nicolai, H., Koch, M., Pielsticker, S., Hasse, C., **Kneer, R.** and **Maßmeyer, A.** "Numerical Study on the Influence of Conversion- and Temperature-Dependent Particle Radiative Properties on Pulverised Solid Fuel Flames (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [48] **Askarizadeh, H.**, Nicolai, H., Pielsticker, S., **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** "Assessment of Turbulence Modulation for the Simulation of a 60 kW_{th} Swirling Flame of Pulverized Solid Fuel Under Oxy-Fuel Conditions (Presentation)". *14th International Conference on Computational Heat and Mass Transfer*. Düsseldorf, Germany, 2023.
- [49] **Askarizadeh, H.**, Pielsticker, S., Nicolai, H., **Kneer, R.**, Hasse, C. and **Maßmeyer, A.** "Influence of Fly Ash on Flow and Temperature Fields in Numerical Simulations of Pulverised Fuel Swirl Flames (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 20–21.  
- [50] **Askarizadeh, H.**, **Zabrodiec, D.**, **Maßmeyer, A.**, Kreitzberg, T. and **Kneer, R.** "Numerical Simulation of Swirl Oxy-Coal Combustion in a 60 kW Test Facility Using the SST k- ω Turbulence Model (Poster)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.
- [51] **Hees, J.**, Bürkle, S., Becker, L., **Zabrodiec, D.**, Wagner, S., **Dreizler, A.** and **Kneer, R.** "A Complementary Approach for the Experimental Investigation of Solid Oxy-Fuel Combustion Using Optical Diagnostics (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.
- [52] **Maßmeyer, A.**, **Zabrodiec, D.**, **Dreizler, A.** and **Kneer, R.** "Stability Analysis of 60 kW_{th} Coal Flames Under Air and Oxyfuel Conditions (Presentation)". *3rd International Workshop on Oxy-Fuel Combustion*. Montabaur, Germany, 2020.

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- [54] **Özer, B.**, **Kneer, R.** and **Maßmeyer, A.** "An Experimental Study on Oscillating Behaviour of the Radiation Spectrum of Self-Sustained Biomass Flames at Different Thermal Loads (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [55] Pörtner, L., **Özer, B.**, König, D., Schiemann, M., **Maßmeyer, A.**, Ströhle, J. and Epple, B. "Hemispherical Radiometer Measurements of the Spectral Resolved Radiative Heat Flux in a Combustion Chamber (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 42–43.  
- [56] Richter, M., **Maßmeyer, A.**, **Askarizadeh, H.**, Ströhle, J. and Epple, B. "Up-Scaling of a Lab-Scale Oxyfuel Burner to a 1 MW_{th} Semi-Industrial Oxyfuel Combustion Chamber (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
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4.17 C2 – Unsteady modelling and simulation of oxy-fuel combustion chambers

4.17.1 Project members

a) Project leader(s)

- Hasse, Christian
- Janicka, Johannes
- Sadiki, Amsini
- di Mare, Francesca

b) Scientific project workers

- Avdic, Amer
- Berkel, Leon
- Doost, Samim
- Ketelheun, Anja
- Miranda, Flavia Cavalcanti
- Nicolai, Hendrik
- Ries, Florian
- Steffens, Pascal
- Vahl, Antje
- Vance, Faizan
- Xu, Wen




















4.17.2 Project summary

Project **C2** developed OxySim-129, a comprehensive 3D CFD framework in OpenFOAM for pulverised solid-fuel combustion under air and oxy-fuel atmospheres across laboratory, pilot, and semi-industrial scales. The model coupled LES with flamelet-based chemistry, integrated radiation advances from **C3** and **C4**, and incorporated non-spherical particle drag/heat-transfer updates from **B2** alongside kinetic mechanisms from **A8** and **B1**. Validation against **B7**, **B4**, and **C1** established accuracy for increasing chamber sizes and complexities. The framework analysed ignition, soot and NO_x formation, and turbulence-particle-radiation interactions in biomass particle clouds, and quantified steady and transient flame behaviour, including extrinsic and intrinsic fluctuations, in collaboration with **C1**. Chemical reactor networks complemented LES for semi-industrial systems, enabling sensitivity studies and efficient scale-up. High-performance computing developments and collaboration with **C7** demonstrated predictive capability at 1 MW_{th} load. As the central integration hub, **C2** transferred and reduced submodels, performed validated simulations for laboratory and pilot systems, and delivered a versatile tool for analysing and predicting biomass combustion, pollutant formation, and radiation-turbulence-particle interactions in oxy-fuel chambers.








4.17.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Kneer, R., **Hasse, C.** and Maßmeyer, A. "Investigation of the Coupling Schemes Between the Discrete and the Continuous Phase in the Numerical Simulation of a 60 kW_{th} Swirling Pulverised Solid Fuel Flame Under Oxyfuel Conditions". *Fire* 7.6 (2024), 185.  
- [2] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Koch, M., Kneer, R., **Hasse, C.** and Maßmeyer, A. "Radiation Modelling Considering Burnout-Dependent Properties and Cellwise Non-Uniform Particle Distributions in the Numerical Simulation of Pulverised Solid Fuel Combustion". *Fuel* 381 (2025), 133338.  
- [3] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Özer, B., Kneer, R., **Hasse, C.** and Maßmeyer, A. "Influence of the Devolatilisation Kinetics on the Numerical Simulation of Pulverised Fuel Swirl Flames Under Oxyfuel Conditions". *Fuel* 393 (2025), 135177.  
- [4] Avdić, A., Künne, G., **di Mare, F.** and **Janicka, J.** "LES Combustion Modeling Using the Eulerian Stochastic Field Method Coupled with Tabulated Chemistry". *Combustion and Flame* 175 (2017), 201–219. 
- [5] Avdić, A., Künne, G. and **Janicka, J.** "Flow Physics of a Bluff-Body Swirl Stabilized Flame and Their Prediction by Means of a Joint Eulerian Stochastic Field and Tabulated Chemistry Approach". *Flow, Turbulence and Combustion* 97.4 (2016), 1185–1210. 
- [6] **Berkel, L.**, Debiagi, P., **Nicolai, H.**, Amjed, M. A., Stagni, A., **Hasse, C.** and Faravelli, T. "Development of a Multiphase Chemical Reactor Network Method as a Tool for Simulating Biomass Gasification in Fluidized Beds". *Fuel* 357 (2024), 129731. 
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- [9] **Doost, S.**, **Ries, F.**, Becker, L., Bürkle, S., Wagner, S., Ebert, V., Dreizler, A., **di Mare, F.**, **Sadiki, A.** and **Janicka, J.** "Residence Time Calculations for Complex Swirling Flow in a Combustion Chamber Using Large-Eddy Simulations". *Chemical Engineering Science* 156 (2016), 97–114. 
- [10] Farmand, P., Boehme, C., **Steffens, P.**, **Nicolai, H.**, Loffredo, F., Debiagi, P., Girhe, S., Chu, H., Gauding, M., **Hasse, C.** and Pitsch, H. "Numerical Investigation and Modeling of NO_x Formation in Pulverized Biomass Flames Under Air and Oxyfuel Conditions". *Combustion and Flame* 279 (2025).  
- [11] Farmand, P., **Nicolai, H.**, Schumann, C., Attili, A., Berger, L., Li, T., Geschwindner, C., **di Mare, F.**, **Hasse, C.**, Böhm, B., **Janicka, J.** and Pitsch, H. "Numerical Investigation and Assessment of Flamelet-Based Models for the Prediction of Pulverized Solid Fuel Homogeneous Ignition and Combustion". *Combustion and Flame* 235 (2022), 111693. 
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- [15] Hidouri, A., Chrigui, M., Boushaki, T., **Sadiki, A.** and **Janicka, J.** "Large Eddy Simulation of Two Isothermal and Reacting Turbulent Separated Oxy-Fuel Jets". *Fuel* 192 (2017), 108–120. [doi](#)
- [16] Knappstein, R., Künne, G., Becker, L., **di Mare, F.**, **Sadiki, A.**, Dreizler, A. and **Janicka, J.** "Large Eddy Simulation of a Novel Gas-Assisted Coal Combustion Chamber". *Flow, Turbulence and Combustion* 101.3 (2018), 895–926. [doi](#)
- [17] Knappstein, R., Künne, G., **Nicolai, H.**, **di Mare, F.**, **Sadiki, A.** and **Janicka, J.** "Description of the Char Conversion Process in Coal Combustion Based on Premixed FGM Chemistry". *Fuel* 236 (2019), 124–134. [doi](#)
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- [19] Mehdizadeh, A., **Doost, S.**, **Sadiki, A.**, **Janicka, J.** and Karimi, N. "Assessment of Predictive Capability of Hybrid URANS/LES Methods in Residence Time Calculation". *Chemical Engineering Science* 183 (2018), 47–59. [doi](#)
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- [22] **Miranda, F.**, **di Mare, F.**, **Sadiki, A.** and **Janicka, J.** "Performance Analysis of Different Solvers for Computing the Radiative Transfer Equation in Complex Geometries Using Finite Volume Method and Block Structured Grids". *Computational Thermal Sciences: An International Journal* 9.3 (2017), 269–282. [doi](#)
- [23] **Nicolai, H.**, Debiagi, P., **Janicka, J.** and **Hasse, C.** "Flamelet LES of Oxy-Fuel Swirling Flames with Different O₂/CO₂ Ratios Using Directly Coupled Seamless Multi-Step Solid Fuel Kinetics". *Fuel* 344 (2023), 128089. [doi](#)
- [24] **Nicolai, H.**, Debiagi, P., Wen, X., Dressler, L., Maßmeyer, A., **Janicka, J.** and **Hasse, C.** "Flamelet LES of Swirl-Stabilized Oxy-Fuel Flames Using Directly Coupled Multi-Step Solid Fuel Kinetics". *Combustion and Flame* 241 (2022), 112062. [doi](#)
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- [27] **Nicolai, H.**, Wen, X., **Miranda, F.**, Zabrodiec, D., Maßmeyer, A., **di Mare, F.**, Dreizler, A., **Hasse, C.**, Kneer, R. and **Janicka, J.** "Numerical Investigation of Swirl-Stabilized Pulverized Coal Flames in Air and Oxy-Fuel Atmospheres by Means of Large Eddy Simulation Coupled with Tabulated Chemistry". *Fuel* 287 (2021), 119429. [doi](#)
- [28] **Sadiki, A.**, Agrebi, S., Chrigui, M., **Doost, S.**, Knappstein, R., **di Mare, F.**, **Janicka, J.**, Maßmeyer, A., Zabrodiec, D., Hees, J. and Kneer, R. "Analyzing the Effects of Turbulence and Multiphase Treatments on Oxy-Coal Combustion Process Predictions Using LES and RANS". *Chemical Engineering Science* 166 (2017), 283–302. [doi](#)



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- [30] Trespi, S., **Nicolai, H.**, Debiagi, P., **Janicka, J.**, Dreizler, A., **Hasse, C.** and Faravelli, T. "Development and Application of an Efficient Chemical Reactor Network Model for Oxy-Fuel Combustion". *Energy & Fuels* 35.9 (2021). 
- [31] Wen, X., **Nicolai, H.**, Debiagi, P., Zabrodiec, D., Maßmeyer, A., Kneer, R. and **Hasse, C.** "Flamelet LES of a 40 kW_{th} Pulverized Torrefied Biomass Furnace in Air and Oxy-Fuel Atmospheres". *Proceedings of the Combustion Institute* 39.4 (2023), 4563–4572. 
- [32] Wen, X., **Nicolai, H.**, Schneider, H., Cai, L., **Janicka, J.**, Pitsch, H. and **Hasse, C.** "Flamelet LES of a Swirl-Stabilized Multi-Stream Pulverized Coal Burner in Air and Oxy-Fuel Atmospheres with Pollutant Formation". *Proceedings of the Combustion Institute* 38.3 (2021), 4141–4149. 
- [33] Wen, X., **Nicolai, H.**, Stein, O. T., **Janicka, J.**, Kronenburg, A. and **Hasse, C.** "Effects of Air and Oxy-Fuel Atmospheres on Flamelet Modeling of Pollutant Formation in Laminar Counterflow Solid Fuel Flames". *Fuel* 285 (2021), 119079. 
- [34] Wen, X., Shamooni, A., Stein, O. T., Cai, L., Kronenburg, A., Pitsch, H., Kempf, A. M. and **Hasse, C.** "Detailed Analysis of Early-Stage NO_x Formation in Turbulent Pulverized Coal Combustion with Fuel-Bound Nitrogen". *Proceedings of the Combustion Institute* 38.3 (2021), 4111–4119. 

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- [35] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Kneer, R., **Hasse, C.**, Özer, B. and Maßmeyer, A. "Numerical Study on the Influence of Devolatilisation Kinetics on Pulverised Solid Fuel Turbulent Swirling Flames Under Oxyfuel Conditions". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.
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- [37] **Nicolai, H.**, Debiagi, P., **Janicka, J.** and **Hasse, C.** "Flamelet LES of Oxy-Coal Swirling Flames with Different O₂/CO₂ Ratios Using Directly Coupled Seamless Multistep Kinetics for Homogeneous and Heterogeneous Solid Fuel Kinetics". *13th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2022.





b) Other publications (non peer-review)

Book chapters









- [60] **Steffens, P., Vahl, A., Berkel, L., Nicolai, H.** and **Hasse, C.** "OxySim-129 Simulation Framework". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  

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- [38] Askarizadeh, H., Koch, M., **Nicolai, H.**, Pielsticker, S., Kneer, R., **Hasse, C.** and Maßmeyer, A. "Influence of Gas Radiation, Particle Radiation Interactions, and Conversion-Dependent Particle Radiative Properties on Pulverized Solid Fuel Combustion". *31. Deutscher Flammentag*. Berlin, Germany, 2023.













- [39] Askarizadeh, H., **Nicolai, H.**, Zabrodiec, D., Pielsticker, S., **Hasse, C.**, Kneer, R. and Maßmeyer, A. "Numerische Untersuchung zur Relevanz von Teilmodellen für Pyrolyse und Koksabbrand in turbulenten drallbehafteten Flammen unter Oxyfuel-Bedingungen". *30. Deutscher Flammentag*. Hannover, Germany, 2021.  
- [40] **Ketelheun, A.**, Mehdizadeh, A., Knappstein, R., **Sadiki, A.** and **Janicka, J.** "Investigation of Unsteady Simulation Methods in an Oxyfuel Configuration". *27. Deutscher Flammentag*. Clausthal-Zellerfeld, Germany, 2015.
- [41] Knappstein, R., Künne, G., **Sadiki, A.** and **Janicka, J.** "Flamelet-Tabellierung im Kontext der Simulation von Kohlestaubverbrennung". *28. Deutscher Flammentag*. Darmstadt, Germany, 2017.  
- [42] **Nicolai, H.**, **Doost, S.**, **di Mare, F.**, **Hasse, C.** and **Janicka, J.** "Large Eddy Simulation of Pulverized Coal Combustion Under Oxy Atmospheres Using Tabulated Chemistry". *12th European Conference on Industrial Furnaces and Boilers : INFUB 12*. online, 2020.
- [43] **Nicolai, H.**, Künne, G., Knappstein, R., **di Mare, F.** and **Janicka, J.** "Entwicklung einer Simulationsmethode zur Beschreibung der Feststoffverbrennung in Oxy-Atmosphären auf Basis tabellierten Chemie". *29. Deutscher Flammentag*. Bochum, Germany, 2019.

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- [44] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Kneer, R., **Hasse, C.** and Maßmeyer, A. *Investigation of the Coupling Schemes Between the Discrete and the Continuous Phase in the Numerical Simulation of a 60 kW_{th} Swirling Pulverised Solid Fuel Flame Under Oxyfuel Conditions – Supplementary Dataset*. 2024.  
- [45] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Kneer, R., **Hasse, C.**, Sauerland, H., Tschunko, S., Toporov, D., Gronarz, T. and Maßmeyer, A. *Development of a Numerical Simulation Tool in Ansys Fluent for Pulverised Fuel Combustion Under Oxyfuel Conditions: Oxy-RANS 129*. RWTH Aachen University. 2025.  
- [46] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Koch, M., Kneer, R., **Hasse, C.** and Maßmeyer, A. *Radiation Modelling Considering Burnout-Dependent Properties and Cellwise Non-Uniform Particle Distributions in the Numerical Simulation of Pulverised Solid Fuel Combustion – Dataset*. RWTH Aachen University. 2024.  
- [47] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Özer, B., Kneer, R., **Hasse, C.** and Maßmeyer, A. *Influence of the Devolatilisation Kinetics on the Numerical Simulation of Pulverised Fuel Swirl Flames Under Oxyfuel Conditions – Supplementary Dataset*. 2025.  

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- [48] Askarizadeh, H., **Nicolai, H.**, Koch, M., Pielsticker, S., **Hasse, C.**, Kneer, R. and Maßmeyer, A. "Numerical Study on the Influence of Conversion- and Temperature-Dependent Particle Radiative Properties on Pulverised Solid Fuel Flames (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [49] Askarizadeh, H., **Nicolai, H.**, Pielsticker, S., Kneer, R., **Hasse, C.** and Maßmeyer, A. "Assessment of Turbulence Modulation for the Simulation of a 60 kW_{th} Swirling Flame of Pulverized Solid Fuel Under Oxy-Fuel Conditions (Presentation)". *14th International Conference on Computational Heat and Mass Transfer*. Düsseldorf, Germany, 2023.
- [50] Askarizadeh, H., Pielsticker, S., **Nicolai, H.**, Kneer, R., **Hasse, C.** and Maßmeyer, A. "Influence of Fly Ash on Flow and Temperature Fields in Numerical Simulations of Pulverised Fuel Swirl Flames (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 20–21.  

- [51] **Berkel, L.**, Debiagi, P., Stagni, A., **Nicolai, H.**, **Hasse, C.** and Faravelli, T. "Fluidized Bed Reactor Modelling Using Multiphase Reactor Networks (Presentation)". *44th Meeting of The Italian Section of The Combustion Institute*. Naples, Italy, 2022.
- [52] **Berkel, L.**, **Steffens, P.**, **Nicolai, H.**, Gierth, S., Debiagi, P., Schneider, H., Dreizler, A. and **Hasse, C.** "Comprehensive Analysis of the Effect of Oxyfuel Atmospheres on Solid Fuel Combustion Using Large Eddy Simulations (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [53] Dübal, S., **Berkel, L.**, Debiagi, P., **Nicolai, H.**, Faravelli, T., **Hasse, C.** and Hartl, S. "Chemical Reactor Network Modeling of a Self-Sustained Solid Fuel Combustion Chamber Under Oxy-Fuel Atmospheres (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [54] Farmand, P., Boehme, C., **Nicolai, H.**, Loffredo, F., Debiagi, P., Gauding, M., **Hasse, C.** and Pitsch, H. "Modeling of NO_x Emissions in Laminar Solid Pulverized Biomass Fuels Flames (Presentation)". *19th International Conference on Numerical Combustion*. Kyoto, Japan, 2024.
- [55] Farmand, P., **Nicolai, H.**, Berger, L., Attili, A., **Hasse, C.** and Pitsch, H. "Modeling Homogeneous Ignition Processes of Clustering Solid Particle Clouds in Isotropic Turbulence (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [56] **Nicolai, H.** and Geschwindner, C. "Swirling Coal and Biomass Flames (Presentation)". *4th Workshop on Clean Solids Conversion*. Kyoto, Japan, 2024.
- [57] **Steffens, P.**, **Berkel, L.**, Gierth, S., Debiagi, P., Özer, B., Maßmeyer, A., **Nicolai, H.** and **Hasse, C.** "Large Eddy Simulation of a 40 kW Self-Sustained Pulverized Biomass Combustion Chamber Using Tabulated Chemistry (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [58] **Steffens, P.**, **Berkel, L.**, **Vahl, A.**, Steinhausen, M., **Nicolai, H.** and **Hasse, C.** "From Single-Particle Studies to MW_{th} Reactor Simulations: OxySim129 – A High-Fidelity CFD Framework for Carbonaceous Solid Fuel Combustion (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 24–25.  
- [59] **Vahl, A.**, **Steffens, P.**, **Berkel, L.**, **Hasse, C.** and **Nicolai, H.** "Large Eddy Simulation of a Gas-Assisted Pulverized Biomass Combustion Chamber Under Varying Oxygen Concentrations Using the OxySim-129 Framework (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 31–32.  

4.18 C3 – Spectral modelling of thermal radiation in oxy-fuel pulverised fuel combustion

4.18.1 Project members

a) Project leader(s)

- Epple, Bernd
- Ströhle, Jochen

b) Scientific project workers

- Alobaid, Falah
- Kez, Vitali
- Richter, Marcel
- von Bohnstein, Maximilian

4.18.2 Project summary








Project **C3** developed efficient, precise models for radiative heat transfer in industrial oxy-fuel combustion chambers, where elevated CO₂ and H₂O concentrations and higher temperatures strengthened radiative effects and demanded accurate wall heat-flux prediction. Spectral discretisations and radiative transfer equation solvers were implemented and evaluated in a 3D virtual furnace using line-by-line calculations as the benchmark. The narrowband correlated-*k* (NBCK) model achieved near-benchmark accuracy with far fewer solves. The full-spectrum correlated-*k* (FSCK) model delivered fidelity close to NBCK with computational cost comparable to weighted-sum-of-grey-gases (WSGG), while WSGG offered fast, simple implementation. A real industrial oxy-fuel boiler was simulated, models and strategies were adapted to furnace conditions, and validation with experimental data was initiated. Turbulence-radiation interaction at small scales was analysed with **C2** and found negligible, and wavelength-dependent particle properties were incorporated with **C4**. A non-commercial CFD code was used to implement NBCK for reference solutions and FSCK for CFD coupling, and radiation measurements from **C1** were prepared for validation. The resulting methodologies and datasets supported integration into the comprehensive oxy-fuel modelling framework of **C2**, advancing predictive simulations of biomass and coal combustion with reliable gas- and particle-radiation treatment.

4.18.3 Published project results



a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Debiagi, P., Yildiz, C., **Richter, M.**, **Ströhle, J.**, **Epple, B.**, Faravelli, T. and Hasse, C. "Experimental and Modeling Assessment of Sulfur Release from Coal Under Low and High Heating Rates". *Proceedings of the Combustion Institute* 38.3 (2021), 4053–4061. [doi](#)
- [2] Gronarz, T., Schulze, J., Laemmerhold, M., Graeser, P., Gorewoda, J., **Kez, V.**, Habermehl, M., Schiemann, M., **Ströhle, J.**, **Epple, B.**, Scherer, V. and Kneer, R. "Quantification of the Influence of Parameters Determining Radiative Heat Transfer in an Oxy-Fuel Operated Boiler". *Fuel Processing Technology* 157 (2017), 76–89. [doi](#)

- [3] **Kez, V.**, Consalvi, J.-L., Liu, F., Gronarz, T., **Ströhle, J.**, Kneer, R. and **Epple, B.** "Investigation of Gas and Particle Radiation Modelling in Wet Oxy-Coal Combustion Atmospheres". *International Journal of Heat and Mass Transfer* 133 (2019), 1026–1040. 
- [4] **Kez, V.**, Consalvi, J.-L., Liu, F., **Ströhle, J.** and **Epple, B.** "Assessment of Several Gas Radiation Models for Radiative Heat Transfer Calculations in a Three-Dimensional Oxy-Fuel Furnace Under Coal-Fired Conditions". *International Journal of Thermal Sciences* 120 (2017), 289–302. 
- [5] **Kez, V.**, Liu, F., Consalvi, J.-L., **Ströhle, J.** and **Epple, B.** "A Comprehensive Evaluation of Different Radiation Models in a Gas Turbine Combustor Under Conditions of Oxy-Fuel Combustion with Dry Recycle". *Journal of Quantitative Spectroscopy and Radiative Transfer* 172 (2016), 121–133. 
- [6] Miranda, F., Coelho, P. J., **Ströhle, J.** and Janicka, J. "Large-Eddy Simulation of a Bluff-Body Stabilised Nonpremixed Flame with Radiation Heat Transfer". *Combustion Theory and Modelling* 133 (2020), 1–18. 
- [7] **von Bohnstein, M.**, **Richter, M.**, Graeser, P., Schiemann, M., **Ströhle, J.** and **Epple, B.** "3D CFD Simulation of a 250 MW_{el} Oxy-Fuel Boiler with Evaluation of Heat Radiation Calculation". *Renewable and Sustainable Energy Reviews* 137 (2021). 
- [8] **von Bohnstein, M.**, Yildiz, C., Frigge, L., **Ströhle, J.** and **Epple, B.** "Simulation Study of the Formation of Corrosive Gases in Coal Combustion in an Entrained Flow Reactor". *Energies* 13.17 (2020), 4523.  

Conference papers

- [9] **von Bohnstein, M.**, **Ströhle, J.** and **Epple, B.** "CFD Simulation of an Oxy-Fuel Demonstration Power Plant with Application of a WSGG Radiation Model". *Energy Procedia* 158 (2019), 1993–1998.  

b) Other publications (non peer-review)

Conference papers

- [10] **Kez, V.**, Consalvi, J.-L., Liu, F., Koch, M., **von Bohnstein, M.**, **Ströhle, J.**, Hatzfeld, O. and Kneer, R. "Entwicklung eines Weighted-Sum-of-Gray-Gases Modells zur Berücksichtigung nicht-grauer Strahlungseigenschaften von Partikeln in Feststoffverbrennungen". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [11] **von Bohnstein, M.**, Graeser, P., Schiemann, M., **Ströhle, J.** and **Epple, B.** "3D CFD Simulation of a 250 MW_{el} Oxy-Fuel Boiler with Evaluation of Heat Radiation Calculation". *14th International Conference on Sustainable Development of Energy, Water and Environment Systems*. Dubrovnik, Croatia, 2019.
- [12] **von Bohnstein, M.**, Graeser, P., Schiemann, M., **Ströhle, J.** and **Epple, B.** "3D CFD Simulation of a 250 MW_{el} Oxy-Fuel Boiler with Evaluation of Heat Radiation Calculation". *29. Deutscher Flammentag*. Bochum, Germany, 2019.

Presentations and Posters

- [13] **Ströhle, J.**, **Kez, V.** and **von Bohnstein, M.** "Evaluation of Gas Radiation Models Regarding Their Applicability to 3D Simulations of Oxyfuel Combustion Systems (Presentation)". *2nd International Workshop on Oxy-Fuel Combustion*. Bochum, Germany, 2018.

4.19 C4 – Modelling of radiative properties of pulverised biomass particles during oxy-fuel combustion

4.19.1 Project members

a) Project leader(s)

- Kneer, Reinhold
- Ströhle, Jochen

b) Scientific project workers

- Figuereido, Patric
- Gronarz, Tim
- Habermehl, Martin
- Hatzfeld, Oliver
- Jörg, Johannes
- Kez, Vitali
- Koch, Matthias


4.19.2 Project summary

C4 investigated thermal-radiation interaction with solid fuel particles and developed computationally efficient models for coupled radiation/CFD simulations of pulverised-fuel flames. Single-particle scattering was measured using acoustic levitation, and Maxwell's equations were solved to obtain absorption, scattering, and phase functions. An inverse analysis with **C5** determined the complex index of refraction. Mie theory was validated for combusting coal particles, and a modified Henyey-Greenstein approximation enabled fast phase-function evaluation. Discrete dipole approximation for ellipsoids showed negligible deviation from Mie at axis ratios near two, with increasing discrepancies for more non-spherical shapes, highlighting the importance of biomass morphology. Spectral dependencies and particle-cloud effects were incorporated, and gas-radiation advances from **C3** were integrated. The resulting particle-radiation model, including soot contributions, was transferred to the LES framework of **C2** (OxySim-129) and validated against measurements from **B4**, **C1**, **C5**, and **C7**. These developments improved predictions of local source terms and wall heat fluxes in oxy-fuel combustion, enabling reliable treatment of particle radiation for coal and biomass within the CRC/TRR 129.

4.19.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Askarizadeh, H., Pielsticker, S., Nicolai, H., **Koch, M.**, **Kneer, R.**, Hasse, C. and Maßmeyer, A. "Radiation Modelling Considering Burnout-Dependent Properties and Cellwise Non-Uniform Particle Distributions in the Numerical Simulation of Pulverised Solid Fuel Combustion". *Fuel* 381 (2025), 133338.  doi.org/10.1016/j.fuel.2025.133338





- [2] **Gronarz, T., Habermehl, M. and Kneer, R.** "Modeling of Particle Radiation Interaction in Solid Fuel Combustion with Artificial Neural Networks". *Journal of Power Technologies* 96.3 (2016), 206–211. [DOI](#)
- [3] **Gronarz, T., Habermehl, M. and Kneer, R.** "Modeling of Particle Radiative Properties in Coal Combustion Depending on Burnout". *Heat and Mass Transfer* 53.4 (2017), 1225–1235. [DOI](#)
- [4] **Gronarz, T., Höges, C., Kez, V., Habermehl, M. and Kneer, R.** "Comparison of Scattering Behaviour for Inhomogeneous Particles in Pulverized Coal Combustion". *International Journal of Thermal Sciences* 140 (2019), 1–7. [DOI](#)
- [5] **Gronarz, T., Johansson, R. and Kneer, R.** "Modeling of Anisotropic Scattering of Thermal Radiation in Pulverized Coal Combustion". *Journal of Heat Transfer* 140.6 (2018), 062701. [DOI](#)
- [6] **Gronarz, T., Schnell, M., Siewert, C., Schneiders, L., Schröder, W. and Kneer, R.** "Comparison of Scattering Behaviour for Spherical and Non-Spherical Particles in Pulverized Coal Combustion". *International Journal of Thermal Sciences* 111 (2017), 116–128. [DOI](#)
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- [8] Johansson, R., **Gronarz, T. and Kneer, R.** "Influence of Index of Refraction and Particle Size Distribution on Radiative Heat Transfer in a Pulverized Coal Combustion Furnace". *Journal of Heat Transfer* 139.4 (2017), 042702. [DOI](#)
- [9] **Kez, V., Consalvi, J.-L., Liu, F., Gronarz, T., Ströhle, J., Kneer, R. and Epple, B.** "Investigation of Gas and Particle Radiation Modelling in Wet Oxy-Coal Combustion Atmospheres". *International Journal of Heat and Mass Transfer* 133 (2019), 1026–1040. [DOI](#)
- [10] **Koch, M., Pielsticker, S. and Kneer, R.** "Numerical Investigation of the Radiative Properties of a Fully Resolved Particle Cloud". *International Journal of Thermal Sciences* 185 (2023), 108102. [DOI](#)
- [11] **Koch, M., Pielsticker, S. and Kneer, R.** "Biomass Particle-Radiation-Interaction and the Effect of Shape and Structure Simplifications". *Fuel* 361 (2024). [DOI](#)
- [12] **Koch, M., Pielsticker, S., Ströhle, J. and Kneer, R.** "Experimental Determination of the Optical Properties of Walnut Shell Particles". *Journal of Quantitative Spectroscopy and Radiative Transfer* 329 (2024), 109202. [DOI](#) [ORCID](#)
- [13] **Koch, M., Pielsticker, S., Tarlinski, D., Scherer, V. and Kneer, R.** "Coupling Radiative Properties with Detailed Char Conversion Kinetics". *Fuel* 363 (2024), 130973. [DOI](#) [ORCID](#)
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- [16] **Koch, M., Pielsticker, S., Ströhle, J. and Kneer, R.** "Numerical Investigation of the Radiative Properties of Fully Resolved Polydisperse Particle Clouds". *17. International Heat Transfer Conference*. Cape Town, South Africa, 2023. [DOI](#)

b) Other publications (non peer-review)

Book chapters

- [40] **Koch, M.**, Askarizadeh, H., Pielsticker, S., Pörtner, L. and **Kneer, R.** "Radiation Modelling". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  
- [41] Pörtner, L., Graeser, P., Gorewoda, J., **Koch, M.**, Schiemann, M., Scherer, V. and **Kneer, R.** "Experimental Radiation Investigations". *Clean Energy Conversion*. Ed. by **Kneer, R.**, Pitsch, H., Dreizler, A., Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  









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- [17] Askarizadeh, H., **Koch, M.**, Nicolai, H., Pielsticker, S., **Kneer, R.**, Hasse, C. and Maßmeyer, A. "Influence of Gas Radiation, Particle Radiation Interactions, and Conversion-Dependent Particle Radiative Properties on Pulverized Solid Fuel Combustion". *31. Deutscher Flammentag*. Berlin, Germany, 2023.
- [18] **Gronarz, T.**, **Habermehl, M.** and **Kneer, R.** "Approximations for Particle Scattering Phase Functions in Solid Fuel Combustion". *41st International Technical Conference on Clean Coal & Fuel Systems*. Clearwater, Florida, USA, 2016.
- [19] **Gronarz, T.**, **Habermehl, M.** and **Kneer, R.** "Influence of Approximations for Particle Scattering Phase Functions on Heat Transfer". *10th Mediterranean Combustion Symposium*. Naples, Italy, 2017.
- [20] **Gronarz, T.**, **Hatzfeld, O.**, **Habermehl, M.** and **Kneer, R.** "On the Importance of Particle Radiation Interaction in the Numerical Simulation of Pulverized Coal Combustion". *10th European Conference on Industrial Furnaces and Boilers : INFUB 10*. Porto, Portugal, 2015.
- [21] **Gronarz, T.**, Schiemann, M. and **Kneer, R.** "Sensitivity Analysis for Parameters for Radiative Heat Transfer in a 3-D Pulverized Coal Combustion Scenario". *Eurotherm Seminar 110 – Computational Thermal Radiation in Participating Media – VI*. Cascais, Portugal, 2018.
- [22] **Kez, V.**, Consalvi, J.-L., Liu, F., **Koch, M.**, **Hatzfeld, O.** and **Kneer, R.** "Development of a Weighted-Sum-of-Gray-Gases Model for Modeling Radiative Heat Transfer in Coal-Fired Oxy-Fuel Boilers". *9th International Symposium on Radiative Transfer*. Athens, Greece, 2019.  
- [23] **Kez, V.**, Consalvi, J.-L., Liu, F., **Koch, M.**, von Bohnstein, M., **Ströhle, J.**, **Hatzfeld, O.** and **Kneer, R.** "Entwicklung eines Weighted-Sum-of-Gray-Gases Modells zur Berücksichtigung nicht-grauer Strahlungseigenschaften von Partikeln in Feststoffverbrennungen". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [24] **Koch, M.**, **Jörg, J.**, Zabrodiec, D., Schnell, M., **Hatzfeld, O.** and **Kneer, R.** "Entwicklung eines Experimentes zur Messung der Streuung von Wärmestrahlung an akustisch levitierenden Partikeln". *29. Deutscher Flammentag*. Bochum, Germany, 2019.
- [25] **Koch, M.**, Pielsticker, S. and **Kneer, R.** "Einfluss inhomogener Partikelverteilungen innerhalb dichter Partikelwolken auf die Wärmestrahlung bei der Feststoffverbrennung". *30. Deutscher Flammentag*. Hannover, Germany, 2021. 
- [26] **Koch, M.**, Pielsticker, S. and **Kneer, R.** "Biomass Particle Radiation Interaction and the Effect of Shape and Structure Simplifications". *12th Mediterranean Combustion Symposium*. Luxor, Egypt, 2023.
- [27] **Koch, M.**, Pielsticker, S., **Ströhle, J.** and **Kneer, R.** "Experimentelle Untersuchung der Streu- und Absorptionseigenschaften von Biomassepartikeln". *31. Deutscher Flammentag*. Berlin, Germany, 2023.

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- [28] Askarizadeh, H., Pielsticker, S., Nicolai, H., **Koch, M., Kneer, R.**, Hasse, C. and Maßmeyer, A. *Radiation Modelling Considering Burnout-Dependent Properties and Cellwise Non-Uniform Particle Distributions in the Numerical Simulation of Pulverised Solid Fuel Combustion – Dataset*. RWTH Aachen University. 2024.  
- [29] **Koch, M.**, Pielsticker, S. and **Kneer, R.** *Dataset to "Biomass Particle-Radiation-Interaction and the Effect of Shape and Structure Simplifications"*. 2025.  
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- [31] **Koch, M.**, Pielsticker, S., **Ströhle, J.** and **Kneer, R.** *Dataset to "Experimental Determination of the Optical Properties of Walnut Shell Particles"*. 2024.  
- [32] **Koch, M.**, Pörtner, L., Gu, Y., Schiemann, M., Rohlf, W. and **Kneer, R.** *Dataset to "Comparison of Scattering Phase Functions of Reacting and Non-Reacting Pulverised Fuel Particles"*. RWTH Aachen University. 2024.  
- [33] **Koch, M.**, Tarlinski, D., Pielsticker, S., Scherer, V. and **Kneer, R.** *Dataset to "Coupling Radiative Properties with Detailed Char Conversion Kinetics"*. 2024.  

Presentations and Posters

- [34] Askarizadeh, H., Nicolai, H., **Koch, M.**, Pielsticker, S., Hasse, C., **Kneer, R.** and Maßmeyer, A. "Numerical Study on the Influence of Conversion- and Temperature-Dependent Particle Radiative Properties on Pulverised Solid Fuel Flames (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [35] **Gronarz, T.**, **Habermehl, M.**, **Hatzfeld, O.** and **Kneer, R.** "Investigation of Modelling Approaches for Scattering and Absorption Properties of Particles in Pulverized Coal Combustion". *Industrial Combustion* (2016), 201602.
- [36] **Gronarz, T.** and **Kneer, R.** "Modellierung der Streuung und Absorption von Wärmestrahlung an Partikeln bei der Verbrennung von Kohlenstaub (Presentation)". *Jahrestreffen der Fachgruppe Wärme- und Stoffübertragung*. Kassel, Germany, 2016.
- [37] **Koch, M.**, Pielsticker, S. and **Kneer, R.** "Efficient Modelling of Radiative Properties for Non-Spherical Particles (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 22–23.  
- [38] **Koch, M.**, Pielsticker, S., Tarlinski, D., Scherer, V. and **Kneer, R.** "Coupling Radiative Properties with Detailed Char Conversion Kinetics (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [39] Pörtner, L., **Koch, M.**, Freiswinkel, E., Pielsticker, S., Schiemann, M., **Kneer, R.** and Scherer, V. "Investigations on Solid Fuel Particle Porosities and Their Influence on the Particle Radiation Interaction (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  

4.20 C5 – Measurement of the radiative properties of solid fuel particles in oxy-fuel atmospheres

4.20.1 Project members

a) Project leader(s)

- Schiemann, Martin

b) Scientific project workers

- Graeser, Philipp
- Gu, Ying
- Pörtner, Lukas
- Scherer, Viktor

4.20.2 Project summary

Project **C5** developed and applied experimental techniques to determine optical properties of burning particles under oxy-fuel conditions, enabling efficient modelling of particle radiation in pulverised flames. An in-flight emissivity method quantified dependencies on particle temperature, mineral composition (notably Fe_2O_3), conversion, and fuel rank, and was extended to levitated particles. A complementary setup measured in-flight scattering intensities. Complex refractive indices were obtained via an inverse Mie-theory approach, supported by an analysis code developed with **C4**. Scattering of cold and burning particles was characterised, and a fuel-specific radiation property database was expanded. Directional scattering and extinction of selected biomass fuels were measured, and radiation probes were adapted for spectrally and directionally resolved gas, particle, and wall radiation. Methods were applied across scales from **B4** over **C1** to **C7**. The resulting measurements provided key inputs for **C4** to complete a comprehensive particle-radiation model and facilitated its incorporation into the full-scale combustion framework of **C2**, improving understanding and prediction of radiative heat transfer in biomass oxy-fuel flames.

4.20.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] Freisewinkel, E., Eisenbach, T., Weise, V., Tarlinski, D., **Pörtner, L.**, Cerciello, F., Wedler, C., **Schiemann, M.**, Span, R., Senneca, O. and **Scherer, V.** "Porosity Measurement of Biomass Char by a Novel Combination of Adsorption Measurements and an Optical Method". *International Journal of Energy for a Clean Environment* (2025). [doi](#)
- [2] **Graeser, P.**, **Pörtner, L.** and **Schiemann, M.** "Influence of the Mineral Content on the Emissivity of Hydrothermal Char". *Chemical Engineering & Technology* 43.5 (2020), 1016–1020. [doi](#)
- [3] **Graeser, P.** and **Schiemann, M.** "Char Particle Emissivity of Two Coal Chars in Oxy-Fuel Atmospheres". *Fuel* 183 (2016), 405–413. [doi](#)
- [4] **Graeser, P.** and **Schiemann, M.** "Emissivity of Burning Bituminous Coal Char Particles – Burnout Effects". *Fuel* 196 (2017), 336–343. [doi](#)

- [5] **Graeser, P.** and **Schiemann, M.** "Investigations on the Emissivity of Burning Coal Char Particles: Influence of Particle Temperature and Composition of Reaction Atmosphere". *Fuel* 263 (2020), 116714. [doi](#)
- [6] **Graeser, P.**, Wütscher, A., Cerciello, F., Muhler, M. and **Schiemann, M.** "Emissivity Comparison Between Chars and Demineralized Coal Chars Under Oxycombustion Conditions". *Chemical Engineering & Technology* 41.7 (2018), 1490–1496. [doi](#)
- [7] Gronarz, T., Schulze, J., Laemmerhold, M., **Graeser, P.**, Gorewoda, J., Kez, V., Habermehl, M., **Schiemann, M.**, Ströhle, J., Epple, B., **Scherer, V.** and Kneer, R. "Quantification of the Influence of Parameters Determining Radiative Heat Transfer in an Oxy-Fuel Operated Boiler". *Fuel Processing Technology* 157 (2017), 76–89. [doi](#)
- [8] Koch, M., **Pörtner, L.**, **Gu, Y.**, **Schiemann, M.**, Rohlf, W. and Kneer, R. "Comparison of Scattering Phase Functions of Reacting and Non-Reacting Pulverised Fuel Particles". *Fuel* 287 (2021), 119415. [doi](#)
- [9] **Pörtner, L.**, **Gu, Y.** and **Schiemann, M.** "Investigation of Pulverized Biomass and Coal Char Emissivity". *Energies* 13.18 (2020), 4620. [doi](#) [orcid](#)
- [10] **Schiemann, M.**, Gronarz, T., **Graeser, P.**, Gorewoda, J., Kneer, R. and **Scherer, V.** "A Correlation Between Char Emissivity and Temperature". *Fuel* 256 (2019), 115889. [doi](#)
- [11] von Bohnstein, M., Richter, M., **Graeser, P.**, **Schiemann, M.**, Ströhle, J. and Epple, B. "3D CFD Simulation of a 250 MW_{el} Oxy-Fuel Boiler with Evaluation of Heat Radiation Calculation". *Renewable and Sustainable Energy Reviews* 137 (2021). [doi](#)

Conference papers

- [12] **Pörtner, L.**, Özer, B., Richter, M., König, D., **Schiemann, M.**, Maßmeyer, A., Ströhle, J. and Epple, B. "Spectral Resolved Radiative Heat Flux Measurements in a Combustion Chamber". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.

b) Other publications (non peer-review)

Book chapters



- [26] Koch, M., Askarizadeh, H., Pielsticker, S., **Pörtner, L.** and Kneer, R. "Radiation Modelling". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., **Scherer, V.**, Maßmeyer, A. and Pielsticker, S. Springer, 2025. [doi](#) [orcid](#)
- [27] **Pörtner, L.**, **Graeser, P.**, Gorewoda, J., Koch, M., **Schiemann, M.**, **Scherer, V.** and Kneer, R. "Experimental Radiation Investigations". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., Dreizler, A., **Scherer, V.**, Maßmeyer, A. and Pielsticker, S. Springer, 2025. [doi](#) [orcid](#)

Conference papers







- [13] Freiswinkel, E., Eisenbach, T., Weise, V., Tarlinski, D., **Pörtner, L.**, Cerciello, F., **Schiemann, M.**, Span, R., Senneca, O. and **Scherer, V.** "Porosity of Biomass Char: A Novel Determination Method and Changes in Walnut Shell with Progressing Pyrolysis". *48th International Conference on Clean Energy*. Clearwater, USA, 2024.
- [14] **Graeser, P.** and **Schiemann, M.** "An Attempt to Measure the Emissivity of Burning Coal Particles in Oxy-Fuel Atmospheres: Test Rig Calibration and First Results". *40th International Technical Conference on Clean Coal & Fuel Systems*. Clearwater, Florida, USA, 2015.
- [15] Gronarz, T., **Schiemann, M.** and Kneer, R. "Sensitivity Analysis for Parameters for Radiative Heat Transfer in a 3-D Pulverized Coal Combustion Scenario". *Eurotherm Seminar 110 – Computational Thermal Radiation in Participating Media – VI*. Cascais, Portugal, 2018.

- [16] **Pörtner, L.**, Özer, B., **Schiemann, M.** and Maßmeyer, A. "Radiometer Concept for Spectral Resolved Radiation Heat Flux Measurements". *31. Deutscher Flammentag*. Berlin, Germany, 2023.
- [17] **Pörtner, L.** and **Schiemann, M.** "Optimization of a Setup to Investigate the Morphology and Emissivity of Coal and Biomass Particles During Burnout". *46th International Technical Conference on Clean Energy*. Clearwater (USA), 2022.
- [18] **Schiemann, M.**, **Graeser, P.**, Heuer, S., Vorobiev, N. and **Scherer, V.** "Combustion Investigations with Colombian Coal: Summary of Experiments and Numerical Interpretation". *42nd International Technical Conference on Clean Energy*. Clearwater, Florida, USA, 2017.
- [19] **Schiemann, M.**, **Graeser, P.** and **Pörtner, L.** "Char Emissivity Measurements for Coal Chars". *9th European Combustion Meeting*. Lisbon, Portugal, 2019.
- [20] von Bohnstein, M., **Graeser, P.**, **Schiemann, M.**, Ströhle, J. and Eppele, B. "3D CFD Simulation of a 250 MW_{el} Oxy-Fuel Boiler with Evaluation of Heat Radiation Calculation". *14th International Conference on Sustainable Development of Energy, Water and Environment Systems*. Dubrovnik, Croatia, 2019.
- [21] von Bohnstein, M., **Graeser, P.**, **Schiemann, M.**, Ströhle, J. and Eppele, B. "3D CFD Simulation of a 250 MW_{el} Oxy-Fuel Boiler with Evaluation of Heat Radiation Calculation". *29. Deutscher Flammentag*. Bochum, Germany, 2019.

Data sets

- [22] Koch, M., **Pörtner, L.**, **Gu, Y.**, **Schiemann, M.**, Rohlf, W. and Kneer, R. *Dataset to "Comparison of Scattering Phase Functions of Reacting and Non-Reacting Pulverised Fuel Particles"*. RWTH Aachen University. 2024.  

Presentations and Posters

- [23] **Pörtner, L.**, Koch, M., Freisewinkel, E., Pielsticker, S., **Schiemann, M.**, Kneer, R. and **Scherer, V.** "Investigations on Solid Fuel Particle Porosities and Their Influence on the Particle Radiation Interaction (Presentation)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023.  
- [24] **Pörtner, L.**, Özer, B., König, D., **Schiemann, M.**, Maßmeyer, A., Ströhle, J. and Eppele, B. "Hemispherical Radiometer Measurements of the Spectral Resolved Radiative Heat Flux in a Combustion Chamber (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 42–43.  
- [25] **Pörtner, L.** and **Schiemann, M.** "Single Fuel Particle Emissivity Evolution of Biomass, Coal and Coal Char (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 40–41.  

4.21 C6 – Measurement of the temperature-dependent spectral emissivities of ashes and deposits under oxy-fuel conditions

4.21.1 Project members

a) Project leader(s)

- Scherer, Viktor

b) Scientific project workers

- Gorewoda, Jeanette





4.21.2 Project summary

Project **C6** provided radiative and material boundary conditions for ash wall deposits to describe the heat balance of oxy-fuel furnaces. The influence of surface structure and chemo-mineralogical composition on spectral radiative properties was quantified, focusing on binary and ternary systems of typical ash constituents and on carbonates and sulfates observed more frequently under oxy-fuel conditions. Transferability to natural solid-fuel ashes was demonstrated. Measurements showed a generic spectral wavelength-dependence of the emissivity. Carbonates and sulfates exhibited characteristic emission bands that vanished after thermal decomposition to the corresponding oxides. Purely oxidic ashes showed smooth spectral trends without pronounced bands. Phase transformations in CaCO_3 and MgSO_4 reduced spectrally averaged emissivities, while Fe generally increased emissivity in mineral mixtures. Emissivity depended on surface structure: with increasing particle size emissivity increases. Surface sintering led to irreversible increases via particle growth, particularly for small particles. A dedicated test rig reliably determined spectral emissivities of real and synthetic ashes and captured the characteristics of relevant mineral groups (oxides, carbonates, sulfates).



4.21.3 Published project results


a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **Gorewoda, J.** and **Scherer, V.** "Influence of Carbonate Decomposition on Normal Spectral Radiative Emittance in the Context of Oxyfuel Combustion". *Energy & Fuels* 30.11 (2016), 9752–9760. 
- [2] **Gorewoda, J.** and **Scherer, V.** "Normal Radiative Emittance of Coal Ash Sulfates in the Context of Oxyfuel Combustion". *Energy & Fuels* 31.4 (2017), 4400–4406. 
- [3] Greffrath, F., **Gorewoda, J.**, Schiemann, M. and **Scherer, V.** "Influence of Chemical Composition and Physical Structure on Normal Radiant Emittance Characteristics of Ash Deposits". *Fuel* 134 (2014), 307–314. 
- [4] Gronarz, T., Schulze, J., Laemmerhold, M., Graeser, P., **Gorewoda, J.**, Kez, V., Habermehl, M., Schiemann, M., Ströhle, J., Epple, B., **Scherer, V.** and Kneer, R. "Quantification of the Influence of Parameters Determining Radiative Heat Transfer in an Oxy-Fuel Operated Boiler". *Fuel Processing Technology* 157 (2017), 76–89. 

Conference papers

- [5] **Gorewoda, J.**, Maas, P. and **Scherer, V.** "Emittance of Typical Ash Minerals: Influence of Particle Size and Mixtures of Carbonates and Sulfates". *Energy Procedia* 158 (2019), 1780–1785.  

- [6] **Gorewoda, J.** and **Scherer, V.** "Key Parameters for the Radiative Emittance of Ashes of Solid Fuels". *Energy Procedia* 120 (2017), 181–188. 

b) Other publications (non peer-review)

Conference papers

- [7] **Gorewoda, J.** and **Scherer, V.** "Comparison of Normal Spectral Emittance of Sulfates and Carbonates – Significant Mineral Classes of Ashes Under Oxy-Fuel Conditions". *Combura Symposium*. Soesterberg, Netherlands, 2016.
- [8] **Gorewoda, J.**, Schiemann, M., **Scherer, V.** and Neuroth, M. "An Examination on the Influence of the Oxidation State of Iron on the Spectral Radiative Emittance of Synthetic Ash Layers". *40th International Technical Conference on Clean Coal & Fuel Systems*. Clearwater, Florida, USA, 2015.

Presentations and Posters

- [9] Draper, T., **Gorewoda, J.**, Kolczynski, L., Fry, A., **Scherer, V.**, Ring, T. and Eddings, E. "The Influence of Temperature on the Spectral Emittance of Ash Deposits Taken from a 1.5 MW, Pulverized Coal Test Facility (Presentation)". *42nd International Technical Conference on Clean Energy*. Clearwater, Florida, USA, 2017.

4.22 C7 – Experimental investigation on the interaction of flame stability, radiation, burnout, and emissions in a semi-industrial-scale swirl-stabilised oxy-fuel furnace

4.22.1 Project members

a) Project leader(s)

- Dreizler, Andreas
- Epple, Bernd

b) Scientific project workers

- König, Dominik
- Richter, Marcel









4.22.2 Project summary


Project **C7** investigated scale effects on pulverised solid-fuel oxy-fuel combustion in a 1 MW_{th}, water-cooled, top-fired furnace, focusing on how turbulence, gas-phase and surface kinetics, and radiation interacted to control flame stability and pollutant formation. Complementary diagnostics deployed with **B4**, **B5**, **C1**, and **C5** quantified time-resolved velocity, temperature, gas composition, and radiative heat flux along the furnace axis. Pollutants and precursors were measured by mass spectrometry and FTIR. Campaigns progressed from cold-flow to natural-gas firing and then biomass flames, with selected conditions intentionally driven into instability to assess sensitivities of flow, radiation, char conversion, and emissions. Variations in fuel (coal to biomass), load, swirl, and oxidiser composition (CO₂ versus recycled flue gas, O₂ level) established how cooled walls amplified radiative heat loss, promoted local extinction, and affected CO, soot, and hydrocarbon formation. Results were compared to geometrically similar laboratory and pilot systems in **B4** and **C1** and were used to validate and scale the OxySim-129 framework of **C2**.

4.22.3 Published project results

a) Publications with scientific quality assurance (peer-review)

Journal papers

- [1] **König, D., Richter, M., Ströhle, J. and Epple, B.** "Stability and Flame Structure Analysis of a Semi-Industrial Swirl-Stabilized Oxy-Fuel Combustion Chamber System for Biomass". *Energies* 18.6 (2025), 1513.  
- [2] **König, D., Ströhle, J. and Epple, B.** "Analysis of Unburned Hydrocarbon Species for Air and Oxy-Fuel Flames in a Semi-Industrial Combustion Chamber Using Fourier Transform Infrared Spectroscopy". *Fuel Processing Technology* 276 (2025), 108283.  
- [3] **König, D., Ströhle, J. and Epple, B.** "Investigation on the Formation of Nitrogen, Sulfur and Chlorine Species in Air and Oxy-Fuel Combustion of Biomass in a Semi-Industrial Combustion Chamber". *Fuel Processing Technology* 277 (2025), 108303.  
- [4] **Richter, M., König, D., Ströhle, J. and Epple, B.** "Radiative Heat Flux Measurement in a Semi-Industrial Oxyfuel Combustion Chamber with Biomass and Coal". *Energies* 17.11 (2024), 2735.  





- [5] **Richter, M.**, Ströhle, J. and **Epple, B.** "Up-Scaling of a Laboratory-Scale Pulverised Oxyfuel Burner to Semi-Industrial-Scale Through a Flow Similarity Approach". *Fuel* 371 (2024), 131809. 

Conference papers

- [6] **König, D.**, Ströhle, J. and **Epple, B.** "Comparison of Air and Various Oxy-Fuel Approaches for Similarity in a Swirl-Stabilized Biomass Flame". *13th Mediterranean Combustion Symposium*. Corfu, Greece, 2025.
- [7] Pörtner, L., Özer, B., **Richter, M.**, **König, D.**, Schiemann, M., Maßmeyer, A., Ströhle, J. and **Epple, B.** "Spectral Resolved Radiative Heat Flux Measurements in a Combustion Chamber". *14th European Conference on Industrial Furnaces and Boilers*. Algarve, Portugal, 2024.

b) Other publications (non peer-review)



Book chapters

- [17] **König, D.**, Hebel, J., Ströhle, J., **Dreizler, A.** and **Epple, B.** "Semi-Industrial Scale Pulverised Solid Fuel Combustion Experiments". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., **Dreizler, A.**, Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  
- [18] Pielsticker, S., Freisewinkel, E., Böttger, J., Cerciello, F., Senneca, O., **König, D.**, Scherer, V., Muhler, M., **Epple, B.** and Kneer, R. "Pyrolysis Products and Kinetics". *Clean Energy Conversion*. Ed. by Kneer, R., Pitsch, H., **Dreizler, A.**, Scherer, V., Maßmeyer, A. and Pielsticker, S. Springer, 2025.  





Conference papers





- [8] **König, D.**, Ströhle, J. and **Epple, B.** "Pilot-Scale Investigation on the Formation of Minority Species in Air and Oxy-Fuel Combustion of Biomass". *32. Deutscher Flammentag*. Paderborn, Germany, 2025.
- [9] **Richter, M.**, Schneider, H., Özer, B., Maßmeyer, A., Ströhle, J. and **Epple, B.** "Untersuchung der Flammenstabilität und thermischen Strahlung in einer 1 MW_{th}-Brennkammer unter Oxyfuel-Bedingungen". *31. Deutscher Flammentag*. Berlin, Germany, 2023.

Data sets

- [10] **König, D.** *OxyflameC7-Campaign2_AS-FTIR-Data*. 2025. 
- [11] **König, D.** *OxyflameC7-Campaign2_AS-FTIR-MS-Data*. 2025. 

Presentations and Posters

- [12] Bonarens, M., **König, D.**, Linke, P., Goet, G., Hansemann, C., Ströhle, J., **Epple, B.** and Wagner, S. "Simultaneous Measurement of Temperatures at Various Distances from the Burner of a Semi-Industrial-Scale Biomass Combustion Chamber (Presentation)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 47–48.  
- [13] Hebel, J., Bonarens, M., **König, D.**, Münzenberger, J., Böhm, B., Wagner, S., **Epple, B.** and **Dreizler, A.** "Particle Dynamics and Gas Phase Investigation in Semi-Industrial Oxy-Fuel Biomass Combustion (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, p. 53.  

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- [14] **König, D.**, Hülsbruch, D., Ströhle, J. and **Epple, B.** "Comparative Analysis of Oxy-Fuel Flames Using Either Carbon Dioxide or Recycled Flue Gas as Diluent with an Air Flame (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 61–62.  
- [15] Pörtner, L., Özer, B., **König, D.**, Schiemann, M., Maßmeyer, A., Ströhle, J. and **Epple, B.** "Hemispherical Radiometer Measurements of the Spectral Resolved Radiative Heat Flux in a Combustion Chamber (Poster)". *5th International Workshop on Oxy-Fuel Combustion*. Aachen, Germany, 2025, pp. 42–43.  
- [16] **Richter, M.**, Maßmeyer, A., Askarizadeh, H., Ströhle, J. and **Epple, B.** "Up-Scaling of a Lab-Scale Oxyfuel Burner to a 1 MW_{th} Semi-Industrial Oxyfuel Combustion Chamber (Poster)". *4th International Workshop on Oxy-Fuel Combustion*. Naples, Italy, 2023. 