Book of Abstracts

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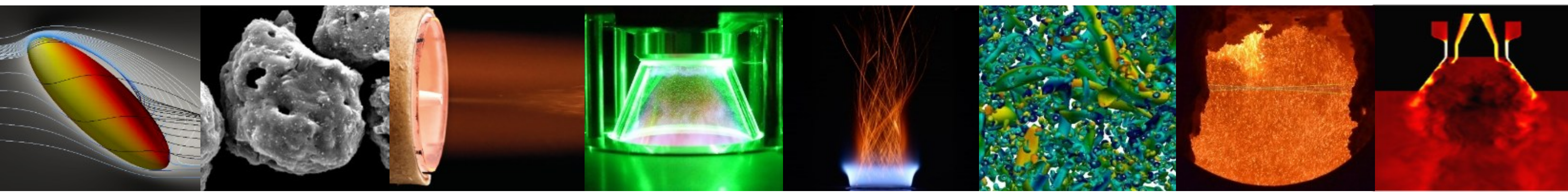

5th International Workshop on Oxy-Fuel Combustion

organized by the

Collaborative Research Center "Oxyflame"

March 19th –20th, 2025
WSA, RWTH Aachen University, Germany

Photos: Alexander Müller

SFB/TRR 129 Oxyflame

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5th International Workshop on Oxy-Fuel Combustion

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2025

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S. Pielsticker[1], A. Maßmeyer[1], V. Scherer[2], H. Pitsch[3],
A. Dreizler[4], and R. Kneer[1]

[1] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*
[2] *Department of Energy Plant Technology (LEAT), Ruhr-Universität Bochum, Universitätsstr. 150, 44780, Bochum, Germany*
[3] *Institute for Combustion Technology (ITV), RWTH Aachen University, Templergraben 64, 52056 Aachen, Germany*
[4] *Institute of Reactive Flow and Diagnostics (RSM), Technical University of Darmstadt, Germany*

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Preface

For the fifth time, the International Workshop on Oxy-Fuel Combustion has been organized by the Collaborative Research Center (CRC) Oxyflame (SFB/Transregio 129) – funded by the German national science organization (DFG). This time the workshop took place in Aachen.

Within Oxyflame, scientists of RWTH Aachen University, Ruhr-Universität Bochum, and the Technical University of Darmstadt are combining their expertise in the fields of homogenous gas combustion and heterogeneous particle combustion for the investigation of oxy-fuel combustion of solid fuels, such as coal and biomass. Oxy-fuel combustion involves burning fuels in an atmosphere consisting mainly of CO_2, H_2O, and O_2. By replacing nitrogen with CO_2 and H_2O, which are chemically active and have non-negligible spectral radiative characteristics, the combustion behavior changes. This can affect chemical conversion rates, flame stability, and ignition/extinction. The project investigates these effects from the atomistic scale to furnace dimensions. This includes experiments from laboratory scale to semi-industrial scale on the one hand and modeling approaches, including molecular dynamics simulations, resolving turbulence, as well as large eddy simulation (LES) on the other hand.

After four successful workshops in 2016, 2018, 2020, and 2023 this fifth edition has been organized by Prof. Reinhold Kneer and his group from WSA (Aachen). The 5th International Workshop on Oxy-Fuel Combustion took place from 19th to 20th of March 2025 in Aachen (Germany). To top off the good food during the conference, the social dinner on the evening of the first day took place at the restaurant La Fabrik. These workshop catalyzed fruitful discussions that launched new, and deepened existing, cooperation, and the poster session gave the young scientists a chance to get into direct contact with renowned colleagues. Scientifically, the workshop was subdivided into six different topics: “Biomass Pyrolysis” , “Char Combustion and Gasification”, “Modeling and Simulation”, “Optical Measurements”, “Oxy-fuel Processes”, with two keynote lectures, 17 oral presentations and 20 posters.

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List of Abstracts

Biomass Pyrolysis

Consideration of Interacting Biomass Components in Sophisticated Pyrolysis Network Models

S. Pielsticker[1*], **L. L. Berkel**[2], **P. Debiagi**[3], **O. Senneca**[4], **C. Hasse**[2], **and R. Kneer**[1]
*pielsticker@wsa.rwth-aachen.de

[1] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University,*
Augustinerbach 6, 52056 Aachen, Germany

[2] *Institute for Simulation of Reactive Thermo-Fluid Systems (STFS), Technische Universität Darmstadt,*
Otto-Berndt-Str. 2, 64287 Darmstadt, Germany

[3] *China Beacons Institute, University of Nottingham Ningbo China,*
No. 211, Xingguang Road, Yinzhou District, Ningbo, China

[4] *Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS),*
Consiglio Nazionale delle Ricerche (CNR), Place le Tecchio 80, 80125 Naples, Italy

Biomass is primarily composed of three main organic molecule types: cellulose, hemicellulose, and lignin, along with smaller amounts of extractives (e.g., oils, fats, and waxes) and inorganic minerals (ash). Cellulose is a linear polysaccharide made of glucose units, providing structural rigidity to plant cell walls. Cell wall flexibility is enabled by hemicellulose molecules that include branched polysaccharides composed of various sugar monomers like xylose, mannose, and arabinose. Lignin – showing an amorphous aromatic structure – is responsible for the strength and hydrophobicity of the biomass. Biomass plays a vital role in reducing greenhouse gas emissions caused by human activities, facilitating the shift from fossil fuels to renewable energy sources. Through biomass pyrolysis – processing solid biogenic materials in an oxygen-free environment – agricultural and organic waste can be converted into high-value products like biochar, bio-oil, and syngas. These products have diverse applications, such as soil enrichment, renewable energy generation, and chemical feedstocks. Mathematical modeling is essential for optimizing biomass conversion processes, understanding complex reactions, predicting outcomes, and scaling sustainable solutions efficiently.

The biochemical percolation devolatilization (Bio-CPD) model is a phenomenologically based model that attempts to take into account the chemical-physical processes during pyrolysis [1]. In the Bio-CPD model, the solid is assumed to be a network of macromolecular clusters that are linked together by various chemical bonds. The bonds between the clusters – also known as bridges – have different stabilities and are divided into labile and stable bridges. Labile bridges can be converted into stable bridges during the pyrolysis process or break apart to form side chains. For each biomass component, parameters to describe the molecular structure and reaction kinetics for the bridge-breaking behavior are available in the literature and have been compared in detail [2]. Based on the bridge population, the Bio-CPD model provides yields divided into light gas, tars of different molecular sizes, and solid residual char.

A lot of previous studies applying the Bio-CPD model to natural biomass have relied on a linear superposition of its three individual components, assuming no interactions between them. However, interactions between the components are expected in natural biomass. The Bio-CPD model consists of different submodels – the particle model, the bridge-breaking model, the percolation theory, the vapor-liquid-equilibrium calculation, and the release characteristics – that allow interactions on different levels. Figure 1a) illustrates two modeling approaches: the traditional linear superposition approach and a mixed approach. In the mixed version, energy and mass balances are

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solved simultaneously for all three components. The joint particle model (PM) ensures that all reactions occur concurrently under the same particle temperature. Additionally, all generated fragments are processed within a joint vapor-liquid equilibrium. The general effects of the two approaches are investigated for an artificial biomass particle with equal fractions of the components reacting under different boundary conditions, e.g., in a thermogravimetric analyzer or a fluidized bed reactor (FBR) [3]. For the FBR conditions, where heat-up and reaction have similar time scales, the mixed approach leads to higher volatile release rates and higher total volatile yields compared to the superposition approach. Likewise, the molecular composition of the tar fraction changes.

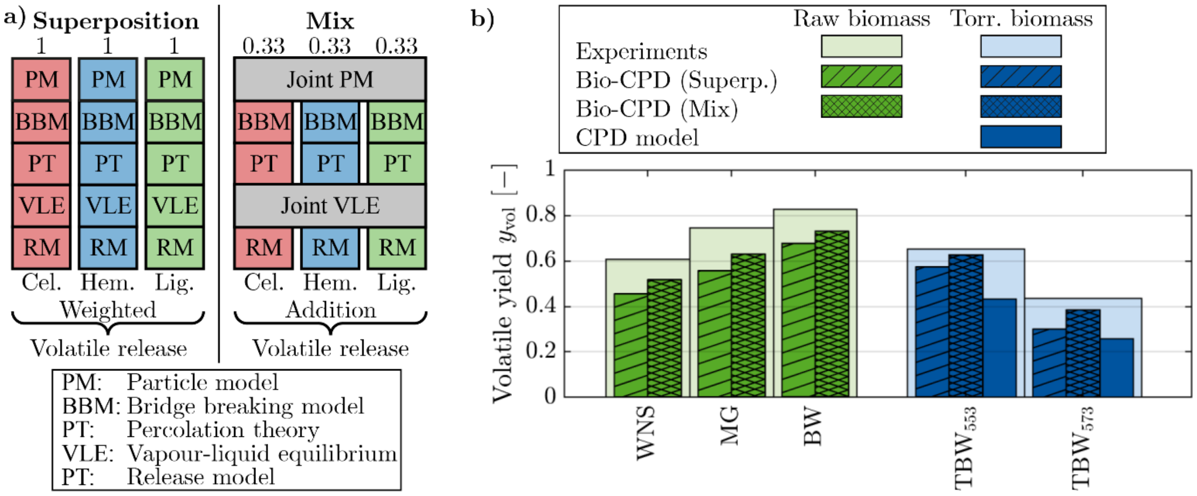

Figure 1. Differences between the linear superposition and mixed approaches for modeling biomass pyrolysis in the Bio-CPD model **a):** Illustration of interactions in the submodels **b):** Volatile yields obtained for different natural biomass in the fluidized bed reactor at 973 K.

The application of the mixed approach on different natural biomass (walnut shells (WNS), miscanthus giganteus (MG), and beech wood (BW)) with different fractions of the basic components shows a better agreement with the experimental results as illustrated in Figure 1b). Also, for torrefied beech wood (TBW), the mixed approach yields significantly better predictions than the linear superposition or the original CPD model.

Acknowledgments

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Pyrolysis of Hydrochars Derived from Co-Hydrothermal Carbonization of PVC and Biomass

J. Böttger[1], F.Cerciello[2], and M. Muhler[1*]
*martin.muhler@ruhr-uni-bochum.de

[1] *Laboratory of Industrial Chemistry, Ruhr University Bochum, 44801 Bochum, Germany*
[2] *Istituto di Scienze e Tecnologia per l'Energia e la Mobilità Sostenibili (STEMS)-CNR, 80125 Napoli, Italy*

The disposal of plastic wastes represents one of the major environmental challenges of the future, with polyvinyl chloride (PVC) being one of the most widely used plastics. Mechanical recycling is a well-established method for recovering PVC in the form of recycled flakes, which can be reused in various applications. However, this technique has its limitations, particularly when dealing with contaminants such as other plastics, additives and mixed materials, which can significantly degrade the quality of the recycled PVC. For certain types of PVC waste, landfill disposal or energy recovery through incineration remain the only viable options. However, the incineration of PVC involves serious environmental and technical challenges, including the emission of hazardous dioxins, the high-temperature corrosion of incineration equipment, heavy metals in the fly ash and the contamination of soil and water. Consequently, the removal of chlorine prior to incineration is crucial to improve the safety and efficiency of energy recovery from PVC waste. Hydrothermal carbonization (HTC) offers a promising pathway to convert PVC wastes with complex and mixed materials into Cl-poor hydrochar. This study investigates the co-HTC of PVC with walnut shells (WS). While there are some studies in literature that investigate co-HTC of PVC with biomass components and biomass, this work provides a detailed characterization of the obtained hydrochar and focuses on the hydrochar properties as fuel. Furthermore, the residence time of the autoclave in the oven was varied to investigate the influence of time on the co-HTC process and the characteristics of the resulting hydrochar. To distinguish between the effect of the HTC on PVC and the potential synergistic effects of the added biomass, HTC was performed using pure PVC and WS. The pure hydrochars and their mixtures were compared to identify the interactions between PVC and WS during the hydrothermal treatment. A special focus was on the dechlorination efficiency and, therefore, the ability to produce a Cl-poor fuel. The influence on the chemical structure was analyzed using ATR-IR spectroscopy. To determine how the PVC-biomass interactions influence the fuel properties, conversion tests were performed including TG analysis and conversion in high-temperature setups with heating rates that are industrially relevant.

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Walnut Shell Pyrolysis: Feedstock Characterization and Kinetics Considering Hemicellulose-Lignin Interactions

L.L. Berkel[1*], P. Debiagi[2], H. Nicolai[1], F. Cerciello[3], S. Pielsticker[4], O. Senneca[3], R. Kneer[4], T. Faravelli[5], and C. Hasse[1]
*berkel@stfs.tu-darmstadt.de

[1] *Institute for Simulation of Reactive Thermo-Fluid Systems (STFS), Technische Universität Darmstadt, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany*

[2] *China Beacons Institute, University of Nottingham Ningbo China, No. 211, Xingguang Road, Yinzhou District, Ningbo, China*

[3] *Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS), Consiglio Nazionale delle Ricerche (CNR), Place le Tecchio 80, 80125 Naples, Italy*

[4] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*

[5] *CRECK Modeling Lab, Department of Chemistry, Materials and Chemical Engineering "G. Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, Milano 20133, Italy*

Biomass is a promising energy resource for fulfilling the increasing clean energy demand. It shares similarities with coal, and hence, is suitable for retrofitting existing infrastructure. Nevertheless, predictive simulations of biomass are still a challenging task, mainly because of the complex kinetics involved. Lignocellulosic biomass is composed of structural fibers that are long polymer chains – cellulose, hemicellulose, and lignin – and additional extractive species. When heated, the long chains of polymers breakdown in a process called pyrolysis and smaller molecules are released into the gas phase. All biochemical components inside the biomass have different reaction pathways, as a result, they breakdown with different rates and a broad spectrum of molecules are released to the gas phase.

Several models have been proposed for simulating biomasses with varying complexities and predictive capabilities [1]. On one end, phenomenological models such as Bio-CPD and Bio-FLASHCHAIN® provide accurate results with high computational costs. On the other hand, fully empirical models such as the competing 2-step model (C2SM) are very fast but lack predictivity unless they are calibrated with experimental measurements for individual biomass samples. The recently developed CRECK-S-B model [2] provides a reasonable balance of predictivity and complexity, and is selected as the basis of this work. The CRECK-S-B model seamlessly incorporates both pyrolysis and char conversion reactions and can be effortlessly coupled with a detailed gas-phase mechanism thanks to its CHEMKIN-compatible format. Most approaches for modelling biomass pyrolysis, including the CRECK-S-B model, assume that the individual decomposition paths of cellulose, hemicellulose and lignin do not affect each other. On the other hand, several experimental works [3] conclude that decomposition rates in native biomass are different compared to the weighted decomposition rates of its individual components. Additionally, multiple studies have shown that there are covalent linkages present between the polysaccharides (cellulose and hemicellulose) and lignin in native biomass [4].

The CRECK-S-B model represents the biomass with 7 reference species. Their mass fractions can be obtained based on the elemental composition of the biomass and splitting parameters describing the commonly observed ratios of biochemical molecules [2]. In this work, walnut shells are used as the biomass sample. The average biochemical composition measurements from the literature suggest that walnut shells are rich in lignin. Using the default characterization method of the CRECK-S-B model, a similar result can be obtained (C1). The splitting parameters can also be further adjusted to match the average literature values (C2). The characterization results are shown in Figure 1a. The performance of the model is assessed by comparison to thermogravimetric analysis (TGA) measurements. An exemplary TGA result from the model and the measurements are shown in Figure 1b.

The objective of this study is to investigate the discrepancies in model and measurement dTG curves. Figure 1b shows that the first dTG peak (~280°C) is underpredicted with the original model while the third one (~400°C) is overpredicted. Based on evidence suggesting interactions between polysaccharides and lignin, the model is modified to include an additional reaction representing accelerated lignin decomposition in the presence of hemicellulose. Simulating the same conditions with the modified mechanism (C1-int and C2-int) aims to achieve improved agreement with the experimental data, as demonstrated in Figure 1b.

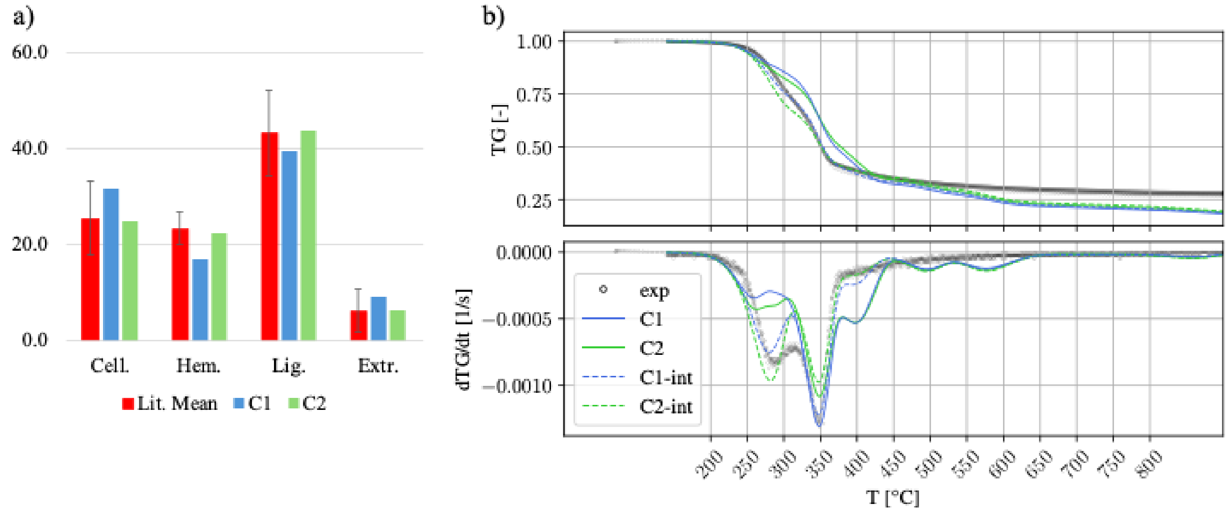

Figure 1. Composition and TGA of walnut shells. a): Literature-averaged and simulated characterizations. Error bars show standard deviation. b): Measured and simulated TGA (10 K/min) for walnut shell pyrolysis in N_2. Simulations are done both with the original model and with the addition of lignin-hemicellulose interaction reaction (C1-int and C2-int).

Acknowledgments

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Effect of Compositional Differences in Hemicellulose Pyrolysis Products

M. Y. Suleiman[1], **E. Benedetto**[2], **V. Piazza**[2], **L. Lietti**[2], **A. Beretta**[2], **L. L. Berkel**[3],
N. Musyoka[1], **T. Faravelli**[4], **and P. Debiagi**[1,*]
*paulo.debiagi@nottingham.edu.cn

[1] *Nottingham Ningbo China Beacons of Excellence, Research and Innovation Institute,*
University of Nottingham Ningbo China, Ningbo, China

[2] *Laboratory of Catalysis and Catalytic Processes, Dipartimento di Energia, Politecnico di Milano, 20156 Milano, Italy*

[3] *Institute for Simulation of reactive Thermo-Fluid Systems, Technische Universität Darmstadt,*
Otto-Berndt-Str. 2, Darmstadt, 64287, Germany

[4] *CRECK Modeling group, Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano, 20133 Milano, Italy*

Lignocellulosic biomass wastes are abundant sources of renewable energy that can be thermochemically converted (i.e. pyrolysis, gasification, combustion) into sustainable energy, chemicals and fuel products. Among these processes, pyrolysis consists the initial step of conversion, and is the basis for understanding biomass devolatilization. Lignocellulosic biomass is a complex material containing several components including cellulose, hemicellulose, lignin, proteins and other extractive compounds. Hemicellulose is among the major components in lignocellulosic biomass, and its composition and concentration vary among biomass types. The hemicellulose fractions from softwood mainly consists of hexose-based polysaccharides while the fractions from hardwood is mainly built by pentose-based polysaccharides. Generally, xylan is used as a model compound to represent hardwood hemicellulose and glucomannan to represent softwoodwood hemicellulose. A number of investigations into hemicellulose pyrolysis has extensively been carried out to characterize the distribution of pyrolysis products leading to the development of reaction mechanisms of the biomass devolatilization. The CRECK-S-B model developed by the CRECK Modeling group in Politecnico di Milano consists of a detailed multi-step kinetic mechanism specifically designed for simulating the pyrolysis of biomass [1]. The model captures the thermal degradation pathways of key biomass components like cellulose, hemicellulose and lignin, and provide real time information for the rate of products formation during the biomass pyrolysis. The previous CRECK S-B model simplifies the representation of all hemicellulose types with a pentose-based polysaccharide, which form shorter chain units of hemicelluloses that further decompose to form gases, bio-oils, water and solid biochar. A thorough analysis of experimental findings [2] highlighted discrepancies with the model, particularly with overprediction of bio-oil and CO_2, and underprediction of water yields. It was found that the ultimate analysis of experimental samples (commercially available beechwood xylan (C/H/O = 40/6.67/53.3 wt.%) was not consistent with the definition of pseudo-species XYHW (i.e. xylan in hardwoods) containing the molecular formula $C_5H_8O_4$ (C/H/O = 45.45/6.06/48.48 wt.%), explaining some of the discrepancies. To this aim, we propose to modify the xylan pseudo-species molecular formula into $C_5H_{10}O_5$ (C/H/O = 40/6.67/53.3 wt.%) and its pyrolysis kinetic mechanism, leveraging the new experimental findings to accurately predict the biomass devolatilization trend and the detailed product distribution. Preliminary simulations incorporating the increased hydration of the hemicellulose structure support the assessment on the impact of modifying the definition of this pseudo-species on pyrolysis product distributions. Further modifications in stoichiometries were proposed to better agree with experimental measurements. Figure 1 (a-c) compares the experimental and predicted thermogravimetric analysis (TGA) at different heating rates, and (d) compares the pyrolysis products distribution obtained at 500°C in a fixed bed reactor after 8.5 min of pyrolysis. The comparisons highlight the discrepancies introduced by the previous model's simplified characterization and demonstrate the improved model performance as a result of the modifications proposed. In particular, significant decrease in bio-oil yields and increase in water yields was achieved, narrowing the gap between experimental results and model predictions. The modified model will be further improved and validated with large dataset collected from literature. Ongoing experimental and modelling activity are deepening the understanding of the pyrolysis kinetics of other hemicellulose types, with focus on detailed speciation of products; proposing an adequate characterization procedure for real hemicelluloses is then a major objective to close the gap between model and real biomass.

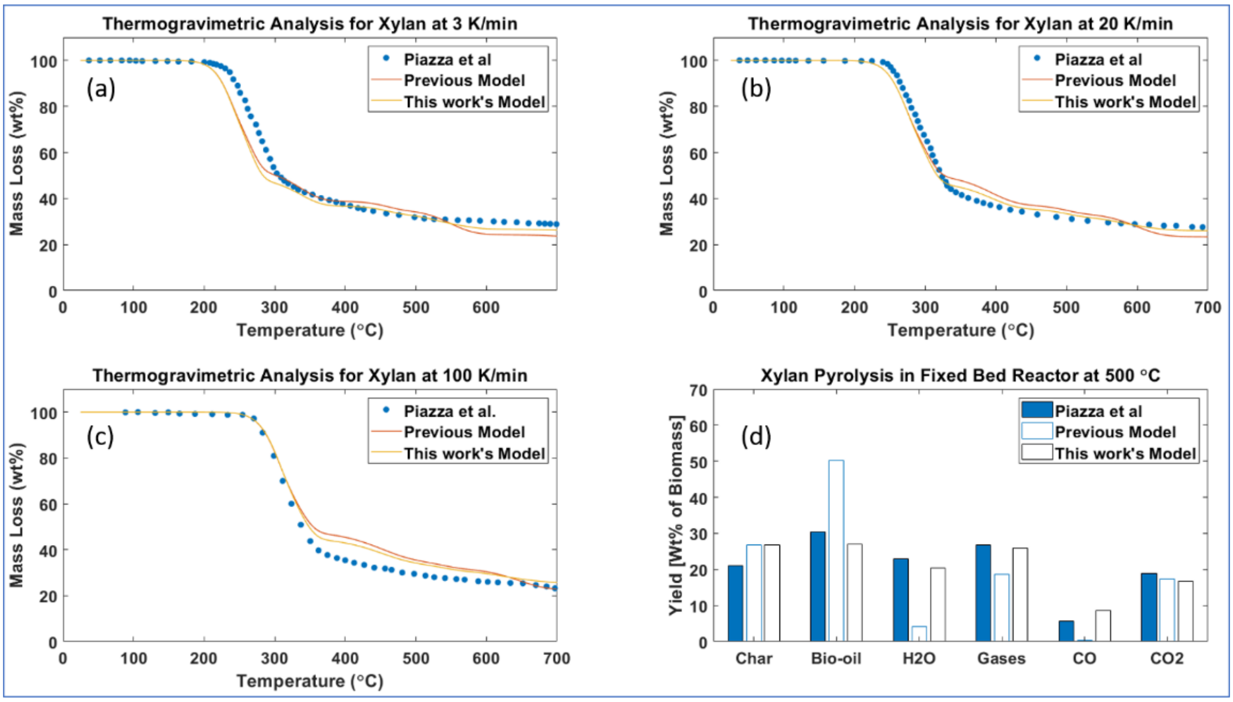

Figure 1. Comparison of experimental data [2] and CRECK-S-B model predictions for previous [1] and the modified model (This work) in TGA (a-c), and product distribution in fixed bed reactor at 500°C after 8.5 min of pyrolysis (d).

Acknowledgments

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Char Combustion and Gasification

Conversion of Suspension Fuel Droplets Under Entrained Flow Gasification Conditions Investigated Using a Reduced Modeling Approach

M. Haas[1*], S. Fleck[1], T. Kolb[1,2], and F. Scheiff[1,2]
*manuel.haas@kit.edu

[1] *Institute for Technical Chemistry, Karlsruhe Institute of Technologie,*
Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[2] *Engler-Bunte-Institute, Fuel Technology, Karlsruhe Institute of Technology, Engler-Bunte-Ring 1, 76131 Karlsruhe, Germany*

The High-pressure Entrained Flow Gasification (EFG) process can play an important role in future production chains with a closed carbon cycle because of its ability to generate a high-quality syngas from waste-based fuels, e.g. pyrolysis oils and suspensions derived from biomass and mixed plastic wastes. In EFG systems, the processes in the burner near field determine temperature field and fuel conversion and are thus critical for overall process efficiency. Typically, the fuel is fed to the reactor through a burner nozzle together with a gasification medium (oxygen and steam). A flame zone is stabilized in the burner near field, in which suspension droplets can experience oxidizing and reducing atmospheres under high temperature and pressure conditions. This results in a wide range of complex droplet conversion phenomena. The outcome of the processes in the flame zone is decisive for the morphology and composition of intermediate solid products that further react in an outer recirculation zone and a downstream gasification zone.

This work aims for improving the understanding of the fuel conversion processes in the EFG flame zone and their dependence on fuel specification by applying a model suspension fuel in a combined experimental and numerical approach. A 2-Phase Free Jet Model is used to numerically investigate the reacting fuel spray by performing sensitivity studies on process parameters and sub-process models. The model was developed based on Single-Phase Free Jet Theory using experimental data and theoretical considerations [1,2]. The model was previously applied to liquid single-component fuels using the d^2-law as evaporation model and is now extended to describe the conversion of suspension fuels, which is the focus of this conference contribution.

The model investigations are accompanied by experimental studies at an atmospheric EFG plant using a suspension of mono ethylene glycol and beech-wood char. OH-LIF is applied to characterize the main reaction zone for different solid mass fractions in the suspension fuel in order to validate the model predictions. The measured flame structures and their dependence on solid mass fraction show good agreement with the model calculations. In a sensitivity study, different suspension droplet evaporation models are compared, showing an impact of the modeling approach on the amount of fuel evaporation and char conversion within the flame zone. The insights serve as a valuable basis for further research elucidating the coupled transport and reaction phenomena in the EFG flame, in particular the formation and conversion of intermediate solid products [3].

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Molecular-Level Modeling of NO_x Precursor Release During the Oxy-Fuel Combustion of Biochar

B. Schnieder[*,1], **C. Hättig**[1], **and R. Schmid**[2]
*bastian.schnieder@rub.de

[1] *Lehrstuhl für Theoretische Chemie I, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[2] *Computational Materials Chemistry Group , Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

Atomistic models for the combustion of biochar molecules have been limited to direct pyrolysis reactions in recent decades. Molecular oxygen and hydroxyl radicals are essential in the combustion process but have frequently been overlooked in earlier studies. Here, we present an automated workflow [1] and techniques for combustion modeling, focusing on biochar compounds such as pyrrole and 2,5-piperazinediones to explore the evolution of fuel-nitrogen into environmentally harmful NO_x species. To investigate the reaction space of these char compounds in an oxy-fuel atmosphere, we employ reactive Molecular Dynamics simulations (ReaxFF, xTB). By applying our workflow, the user can automatically refine reaction events with Density Functional Theory (DFT) and Coupled Cluster (CC). Our approach and modeling strategies provide large-scale reaction networks for the formation of NO_x precursors from fuel-nitrogen, including mechanisms, reaction energies, barriers, and rate constants. We also compare our mechanisms to experimental data, demonstrating improved accuracy in modeling combustion at the atomistic level. In perspective, a detailed mechanistic network serves as the foundation for guiding emission control strategies during biochar combustion.

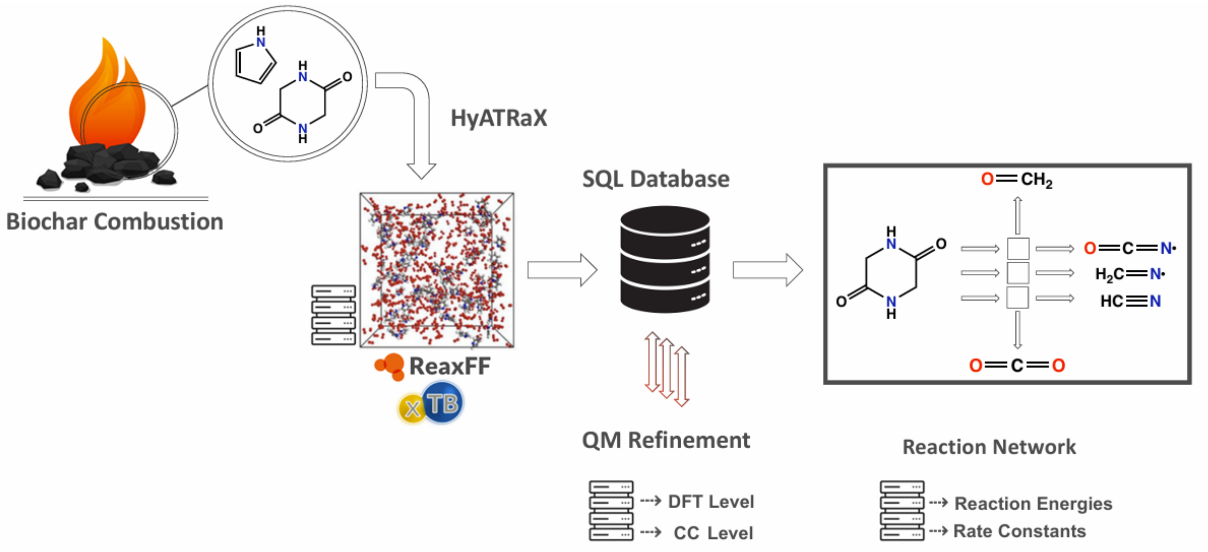

Figure 1. Schematic overview of the automated workflow.

Acknowledgments

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Role of Holocellulose on Thermal Annealing and Morphology of Biomass

E. Freisewinkel[1], **F. Cerciello**[2*], **D. Tarlinski**[1], **M. Schiemann**[1], **V. Scherer**[1], **and O. Senneca**[2]
*francesca.cerciello@stems.cnr.it

[1] *Institute of Energy Plant Technology, Ruhr University Bochum, 44801 Bochum, Germany*

[2] *Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS), Consiglio Nazionale delle Ricerche (CNR), Place le Tecchio 80, 80125 Naples, Italy*

Over the last years, under the driving force of low carbon technologies - particularly Bioenergy with Carbon Capture and Storage (BECUS) - a large number of studies focused on the fundamentals of pyrolysis and combustion of lignocellulosic biomass. These studies have also explored its potential as a sustainable substitute for coal and coke. Unlike coal samples, lignocellulosic materials are mixtures of bio-polymers, in particular cellulose (CEL), hemicellulose (HEM), lignin (LIG), plus extractives, minerals etc.

The way how CEL, HEM and LIG are distributed within a natural biomass is complex and can give rise to unpredictable behaviour upon pyrolysis and combustion. At the particles size scale, different behaviours have been observed. Sometimes, upon heat treatment in drop tube or flat flame burners, the biomass particles seem to keep memory of the original plant structure, remaining non isotropic, often elongated in shape. Sometimes, instead, drastic changes of particles shape and size are observed, for instance transforming initially elongated particles into rounded, even spherical, particles. From the point of view of biomass reactivity, a massive effort has been done over the last years to explore the role of bio-polymers in pyrolysis kinetics, both from the experimental and the modelling perspectives. Despite the important advances done in this field, the interference between biomass components are still poorly understood and accounted for.

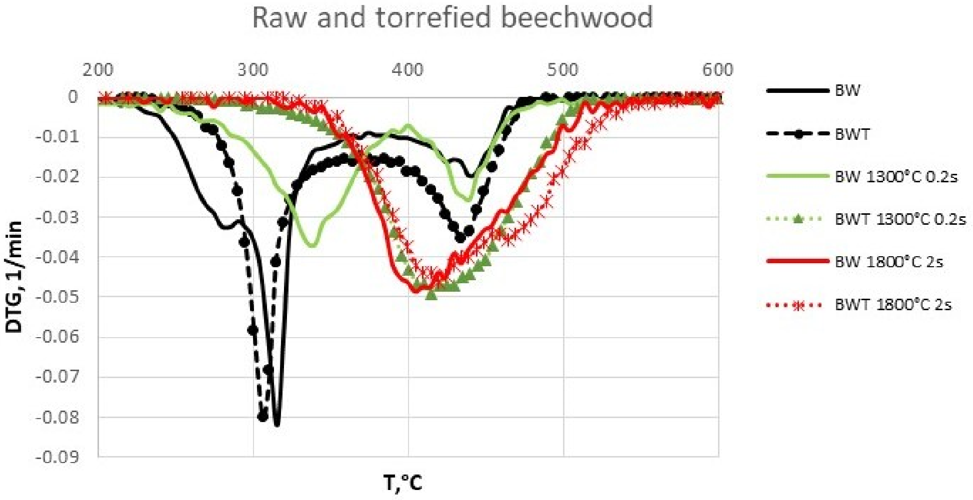

Figure 1. The combustion reactivity by TGA analyses of the raw (BW) and torrefied beech wood (BWT) particles in comparison with the pyrolysed particles from the DTR and HSR experiments in N_2 atmosphere.

A recent paper [1] suggested that in biomass chars formed upon different heat treatment, raw materials can coexist with newly formed (young) char, as well as with less reactive char fractions, as

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biopolymers vary in thermal stability and reactivity. On a parallel route it has been observed that Holocellulose, in particular Xylan, upon heat treatment is prone to melt and plasticize [2].

In the present work, in order to further highlight the effects of Holocellulose on structure and thermal annealing of biomass, the behavior upon pyrolysis of Beechwood (BW) and torrefied beech wood (BWT) has been compared, since torrefaction pre-treatment eliminates the more labile biopolymeric fractions.

Annealing experiments consisted in heat treatments in a drop tube reactor (DTR) and a heated strip reactor (HSR) with fast heating rates of 10^3 °C/s and maximum temperatures between 1300 and 1800°C. The extent of thermal annealing was assessed through the loss of combustion reactivity by standard TGA analysis. As illustrated in Figure 1, high temperature DTG peaks are more remarkable in the previously torrefied samples, indicating that removal of holocellulose makes the biomass more prone to undergo thermal annealing.

Morphological changes have been inferred by comparing SEM images and particles size distribution at different stages of heat treatment. Figure 2 shows the different behavior of raw and torrefied Beechwood at temperatures of 1300 °C in N_2 atmospheres, demonstrating remarkable spheroidization for the torrefied samples.

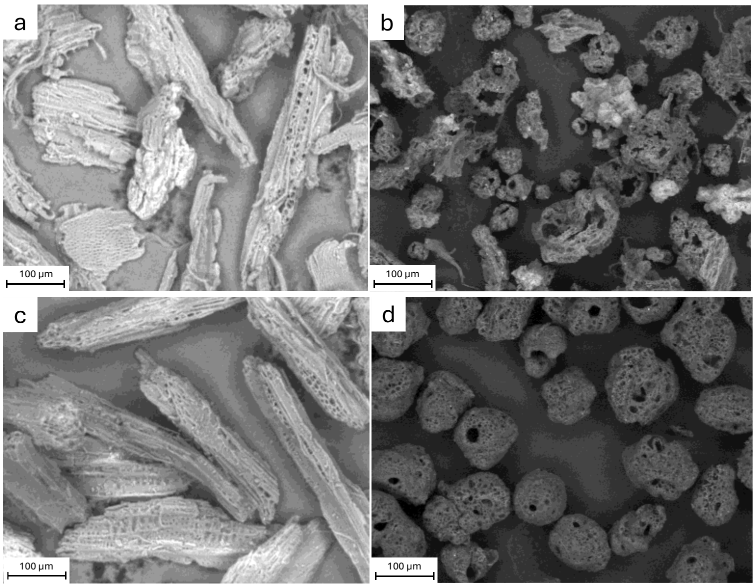

Figure 2. Particles morphology before and after pyrolysis in the DTR with a residence time of ~0.2 s in N_2 atmosphere: a) Raw BW; b) BW at 1300 °C (N_2); c) Raw BWT and d) BWT at 1300 °C (N_2).

Acknowledgements

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Modelling and Simulation

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Influence of Fly Ash on Flow and Temperature Fields in Numerical Simulations of Pulverised Fuel Swirl Flames

H. Askarizadeh[1*], **S. Pielsticker1**, **H. Nicolai**[2], **R. Kneer**[1],
C. Hasse[2], **and A. Maßmeyer**[1]
*askarizadeh@wsa.rwth-aachen.de

[1] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*
[2] *Institute for Simulation of Reactive Thermo-Fluid Systems (STFS), Technische Universität Darmstadt,*
Otto-Berndt-Str. 2, 64287 Darmstadt, Germany

Pulverised solid fuel (biogenic and fossil) combustion provides an important share of the world's energy supply and significantly contributes to anthropogenic CO_2 emissions [1]. Oxy-fuel combustion coupled with carbon capture and storage (CCS) can significantly reduce CO_2 emissions. Understanding the behaviour of pulverised fuel flames in oxy-fuel environments, through both experimental and numerical analysis, is crucial for advancing CCS technologies. Numerical studies are subject to high computational costs if all aspects are modelled with a high level of detail, e.g., coupling schemes for mass and energy between the continuous and the discrete phases or complex kinetic mechanisms with multiple reactions taking place. Therefore, knowing the required level of detail for modelling different processes that occur during combustion can significantly speed up simulations and thus lower the corresponding computational costs.

One of the important aspects in the simulation of pulverised fuel flames is the presence of fly ash particles in the chamber. Ash particles resulting from the combustion of pulverised fuels can be nearly considered massless and inertia-free. Therefore, from the hydrodynamics point of view, the reciprocal influence between the ash particles and the continuous phase can be considered negligible. However, from the heat transfer point of view, the presence of ash particles can significantly affect radiation interaction between the particles and consequently, the net heat flux from/to a computational cell, despite their low mass. This hypothesis is followed in this study to show to which extent the removal of ash particles during simulations can, on the one hand, affect the flame and, on the other hand, facilitate the simulations, which has not yet been investigated in the literature. The removal of ash particles is carried out when two conditions are fulfilled: (1) a particle is tracked until only its ash content remains, and (2) the temperature difference between the tracked particle and the continuous phase is sufficiently small. As a reference case, an experimentally characterised 60 kW_{th} Rhenish lignite flame [2,3] is studied.

The simulation results are compared for two cases: (1) with and (2) without ash removal. The comparison includes the gas and the mean axial and tangential particle velocities and the gas and the mean particle temperatures in the near-burner and downstream regions. Figure 1 presents comparisons of the gas velocities and temperatures for these simulations. Velocity comparisons follow the hypothesis explained above concerning the negligible reciprocal influence between the ash particles and the continuous phase. In addition, the hypothesis regarding a possible significant influence of the ash particles on the temperature field is also observed. These results will also be compared with the experimental [2,3] and LES [4] data. Further comparisons will show whether the conditions chosen for removing ash particles are correct to find other necessary constraints such as consideration of the size of the ash particles for removing them to correctly facilitate the numerical simulations. After having the ash removing conditions verified for the reference case (Rhenish lignite flame), a biomass (walnut shell) flame with the same thermal output of 60 kW_{th}, recently investigated experimentally at the RWTH Aachen University, Institute of Heat and Mass Transfer (WSA), is also simulated to explore the influence of the ash content of the particles on the conditions for removing ash particles without influencing the flame.

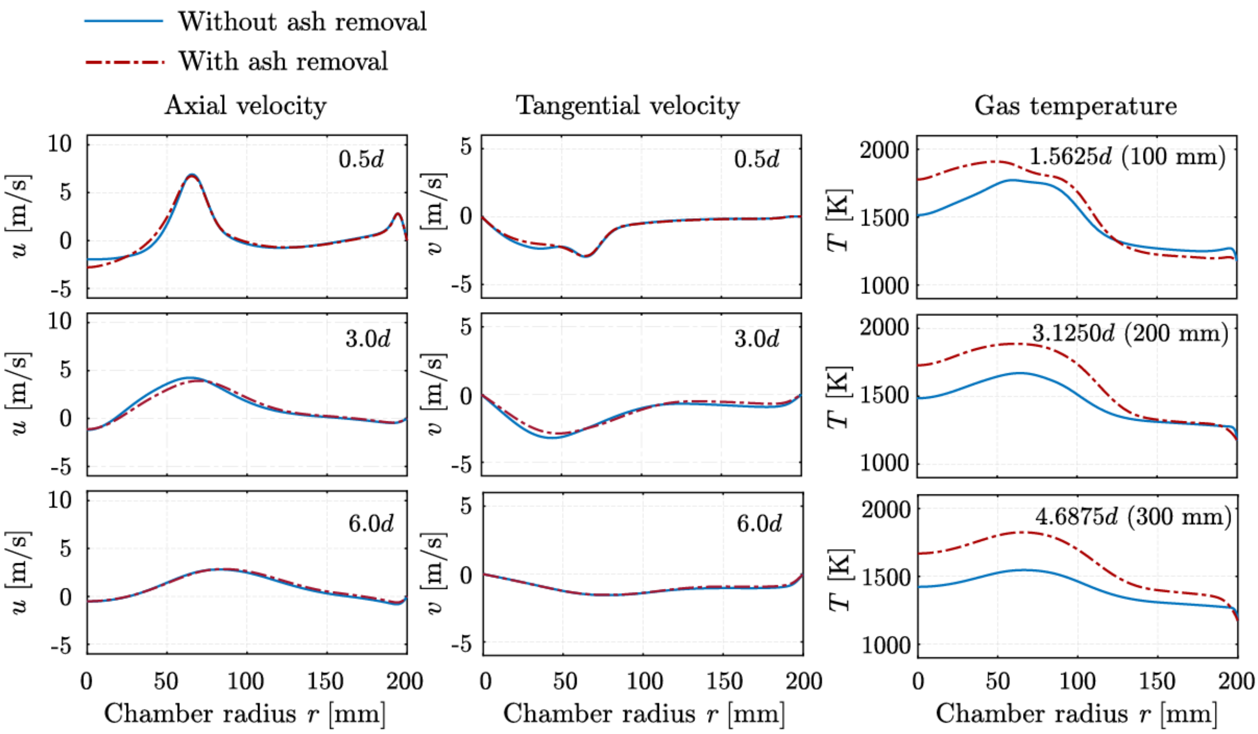

Figure 1. Comparison of the gas axial (left column) and tangential (middle column) velocity components as well as gas temperature (right column) obtained in two simulations: (1) without ash removal (solid blue line) and (2) with ash removal (dashed-dotted red line). The ash removal criterion is when only ash is left from fuel particles.

Acknowledgements

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Efficient Modelling of Radiative Properties for Non-Spherical Particles

M. Koch[1*], **S. Pielsticker**[1], **and R. Kneer**[1]
*koch@wsa.rwth-aachen.de

[1] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*

In pulverized fuel combustion systems, thermal radiation is the primary heat transfer mechanism [1]. Thereby, particle radiation dominates, in most cases, gas radiation [2]. Thus, adequate modeling of particle-radiation interactions in full-scale simulations of combustion chambers may primarily affect the overall accuracy. The radiation behavior depends strongly on the shape of the interacting particles. While it is sufficient to approximate the shape of coal particles by spheres, biomass like pine, poplar, or beech wood are distinctly more non-spherical, and thus, rotational ellipsoids are more fitting as a shape approximation. These types of biomasses retain the non-spherical shape during the conversion up to a burnout of 50 % [3]. However, modeling the radiation interaction with non-spherical particles is computationally demanding, so typically, volume-equivalent spheres are used to approximate biomass particles. Then, the Mie theory is applied, which provides an analytical solution for radiation interaction with spheres. Koch et al. highlighted in [4] that approximating the non-spherical particle by a volume-equivalent sphere leads to relative deviations of up to 50 % for the radiation properties – the absorption and scattering efficiency Q_i, and the phase function Φ. Therefore, this study aims to develop an efficient and precise non-spherical particle model. Here, the non-spherical particles are approximated by prolate ellipsoids (see Figure 1), whereas the diameter of the base area D_B and the aspect ratio $\zeta = H/D_\mathrm{B}$ define the shape. Due to the non-sphericity, the orientation angle β is additionally required to describe the angle between orientation of the particle and the direction of radiation propagation. The index of refraction m defines the material properties. First, the discrete dipole approximation (DDA), a numerical exact but demanding method, is applied to calculate the radiative properties of non-spherical particles. The base diameter D_B is varied between 10 and 50 µm, the axis ratio between 1 and 15, and the orientation angle between 0° and 90°. The direction of propagation of the radiation is kept constant, as well as the wavelength $\lambda = 3$ µm and the index of refraction $m = 1.4 + 0.1\mathrm{i}$. From this exact data, the following function is derived,

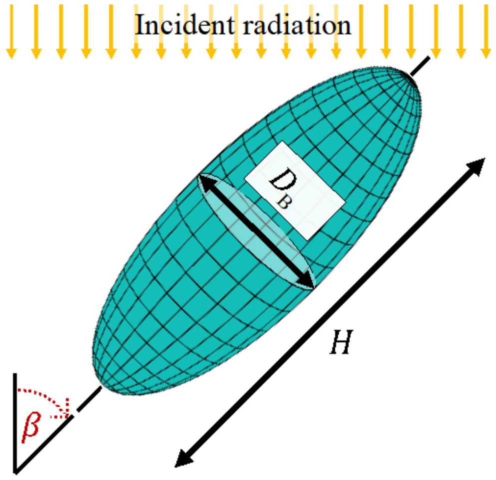

Figure 1. General representation of the non-spherical particle. The orientation of the particle is defined by β and its shape by the base diameter D_B and the height H.

$$Q_\mathrm{i}(\zeta, \beta, m, \lambda, D_\mathrm{B}) = Q_\mathrm{i,Mie}(m, \lambda, D_\mathrm{B}) + C_Q(\zeta, \beta)$$
$$\Phi(\zeta, \beta, m, \lambda, D_\mathrm{B}) = \Phi_\mathrm{Mie}(m, \lambda, D_\mathrm{B}) + C_\Phi(\zeta, \beta)$$

where $Q_\mathrm{i,Mie}$ and Φ_Mie represent the Mie-solution for a sphere with diameter D_B and C is a correction function considering the non-sphericity.

Afterward, the DDA is applied to verify the accuracy of this function and to compare its accuracy to the one of the volume-equivalent model. The new model outperforms the volume equivalent model for $D_\mathrm{B} > 10\ \mu\mathrm{m}$. For $D_\mathrm{B} < 10\ \mu\mathrm{m}$, the volume equivalent model's accuracy is better but still indicates relative deviations to the DDA of 10 – 50 %.

Acknowledgments

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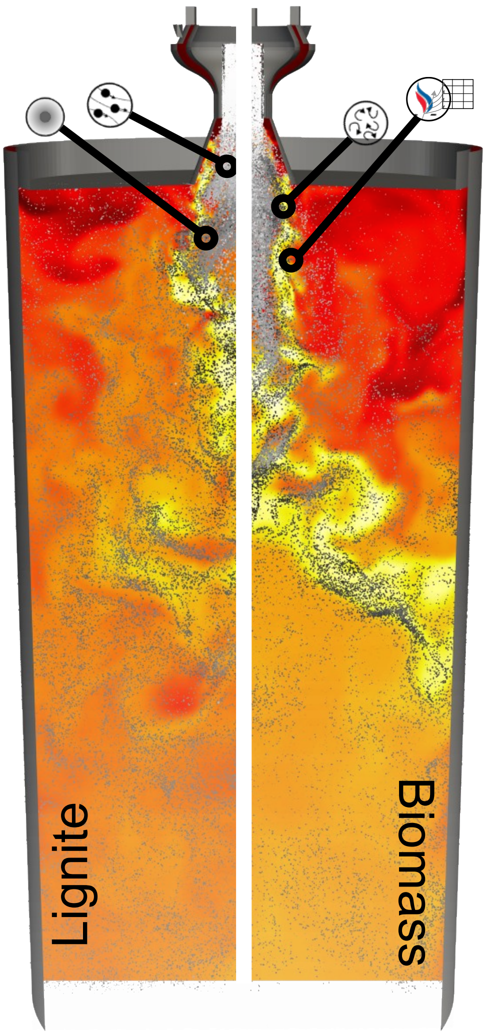
From Single-Particle Studies to MW$_{th}$ Reactor Simulations: OxySim129 – A High-Fidelity CFD Framework for Carbonaceous Solid Fuel Combustion

P. Steffens[1*], **L. L. Berkel**[1], **A. Vahl**[1], **M. Steinhausen**[1], **H. Nicolai**[1], **and C. Hasse**[1]
*steffens@stfs.tu-darmstadt.de

[1] *Institute for Simulation of reactive Thermo-Fluid Systems, Technical University Darmstadt,*
Otto-Berndt-Straße 3, 64287 Darmstadt, Germany



To fight climate change, a drastic cut of CO_2 emissions is needed. The *Intergovernmental Panel on Climate Change* even suggests that carbon capturing technologies may be required to avoid catastrophic warming. One promising method to permanently remove CO_2 from the atmosphere, while at the same time supplying dispatchable electricity, is called *bioenergy carbon capture and storage* (BECCS). Energy crops pull CO_2 from the atmosphere while they grow. When burnt in a BECCS process, they release heat for energy production, and the carbon stored in the plants is captured. This approach can be further improved by burning biomass in a CO_2/O_2 atmosphere (oxy-fuel atmosphere) that facilitates carbon capture. To encourage large-scale adoption of such technologies, power plant operators and energy companies need to be given the right tools for the design of new combustion systems and retrofitting existing ones.

OxySim129 is a computational fluid dynamics (CFD) framework for pulverized solid fuel combustion that is based on the popular OpenFOAM® library. Three main modelling domains have to be addressed for high-fidelity simulations of carbonaceous solid fuels like biomass: (a) Turbulent flow, mixing, and heat transfer, (b) turbulence / chemistry interaction, and (c) particle treatment and solid fuel kinetics. In OxySim129, turbulence and mixing are modelled with Large Eddy Simulation (LES) allowing for the resolution of the large turbulent structures. Multiple models are available from the base-OpenFOAM®. The heat transfer includes radiation, modelled with a discrete ordinates method (DOM). The second aspect – turbulence / chemistry interaction – is tackled with a tabulated flamelet manifold method. Tabulated flamelet methods have been extensively used in scientific studies of carbonaceous solid fuel combustion. By pre-calculating a range of one-dimensional flamelets for conditions that are present in the burner, the thermo-chemical state can be represented with high accuracy using only a minimal number of controlling variables. Finally, particles are treated as Lagrangian point particles. Solid kinetics are crucial for accurate volatile composition and release rates. In OxySim129, a reduced-order model based on detailed kinetics from the CRECK-S(B) model is utilized. The detailed model provides the volatile composition based on the raw solid fuel and devolatilization rates dependent on the heating rate.

OxySim129 has been demonstrated for cases ranging from small-scale laboratory burners to a 1 MW_{th} burner, for coal and for biomass, and for air and oxy-fuel conditions. The laminar flow reactor (LFR) is a small burner configuration featuring a flat pilot flame. Particles are injected in the centre and react in the hot exhaust gases of the pilot flame. This setup allows the detailed study of single particle combustion and group combustion phenomena. The Darmstadt and Aachen burners are turbulent lab-scale burners featuring swirl-induced recirculation. The Darmstadt solid fuel combustor offers optical access and ample experimental validation data running on a methane-assisted solid fuel flame. The Aachen burner is very similar, but its heated walls allow for self-sustained combustion and more realistic conditions. Finally, the 1 MW_{th} burner bridges the gap between lab-scale burners and industrial combustors.

OxySim129 will be made available on Github as open-source framework after the conclusion of the Oxyflame project with test and tutorial cases. The test cases validate the code on a small scale. The tutorial cases demonstrate the capabilities of the code in the above-mentioned scenarios and give users step-by-step instructions. Further reference data will be provided on the Clean Solids Conversion Flame Database.

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Assessment of Non-Spherical Point-Particle Dynamics in Turbulent Pipe and Jet Flows

L. André[1*], M. Meinke[1], D. Krug[1], and W. Schröder[1]
*l.andre@aia.rwth-aachen.de

[1] *Chair of Fluid Mechanics and Institute of Aerodynamics,RWTH Aachen University, Wüllnerstr. 5a, 52062 Aachen, Germany*

Introduction

Particle-laden flows play a crucial role in a wide range of natural and industrial processes, ranging from pollutant transport over biomedical applications and biomass combustion. An accurate modelling of the particle phase is essential for reliable predictions, especially when considering non-spherical particles. Fully resolving the particle phase, however, is computationally expensive and often infeasible. This drives the interest in Lagrangian point-particle models capable of accurately modelling the particle dynamics at a reduced computational cost. Traditional point-particle models often assume spherical particles with negligible particle size, assumptions that may be insufficient for practical applications, where particle shape and size strongly influence flow behaviour and turbulence modulation. This contribution evaluates spherical (SLM) and ellipsoidal (ELM) Lagrangian point-particle models under anisotropic turbulent conditions.

Numerical Methods

The simulations are conducted using a finite-volume solver with hierarchical Cartesian meshes, allowing the use of solution adaptive mesh refinements. Lagrangian point-particle models are used for the simulation of the particle phase. The SLM models the translation motion using a simplified form of the Maxey–Riley–Gatignol equation while neglecting the rotational motion. The ELM in contrast incorporates particle shape and rotational dynamics. Initially derived under creeping flow assumptions, the ELM has been extended to include orientation-dependent correlations for drag, lift, and torque for prolate particles with aspect ratios $1 \leq \beta \leq 8$ and particle Reynolds numbers $1 \leq Re_p \leq 100$ [1].

Results and Discussion

The behaviour of prolate particles with aspect ratios $2 \leq \beta \leq 8$ and equivalent spherical diameters on the order of the smallest scales is studied in anisotropic turbulent flows. Simulations of particle-laden pipe flows with a Reynolds number of $Re_D = 7500$ based on the pipe diameter D, which also serve as inflow condition for axisymmetric round jet simulations, are conducted. The different Lagrangian point-particle models are compared, focusing on preferential particle distribution, orientation, and alignment with the turbulent flow structures. The findings of this study provide valuable insights for the development of robust and accurate point-particle models suitable for large-scale turbulent flow simulations. Figure 1 shows a particle-laden round jet.

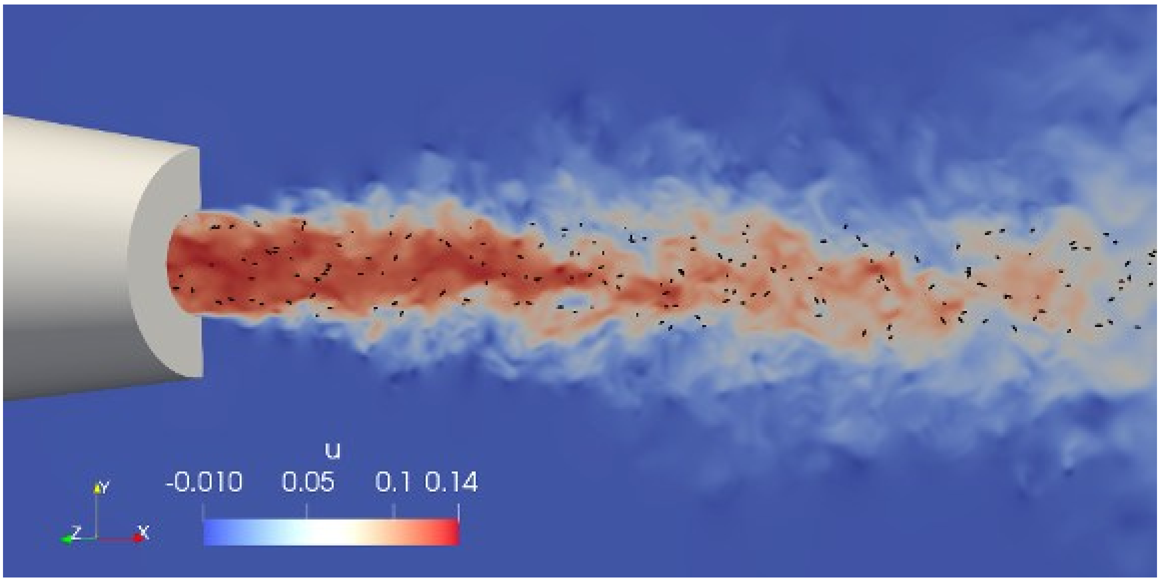

Figure 1. Turbulent round jet laden with prolate particles with an aspect ratio of $\beta = 3$ and an equivalent spherical diameter of $d_{eq}/D = 0.036$. The colour scale represents the non-dimensional streamwise velocity.

Acknowledgments

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Effects of Carbon Dioxide Dissociation on Heat Distribution, Heat Transfer and High-Temperature Chemistry in Thermal Plasmas for Rotary Kiln Application

E. Ehlmé[1*], A. Gunnarsson[1], F. Normann[1], and K. Andersson[1]
[*]ehlme@chalmers.se
[1]*Division of Energy Technology, Chalmers University of Technology, Göteborg, Sweden*

Industrial users of rotary kilns for heat treatment of solid materials are seeking low-carbon alternatives by transitioning from fossil fuel-based heating to applying thermal plasma systems. Rotary kilns used in cement clinkerization processes are such high-temperature applications.

This work examines thermal plasmas specifically using CO_2 as a working gas, as CO_2 from the calcination reaction is inherent in the cement process. Radiative heat transfer is the dominant heat transfer mechanism in cement kilns, influenced by the participating gases and particles in the kiln. In the absence of particles, scattering effects are negligible, making accurate modelling of high-temperature gas radiation critical. Furthermore, the temperature distribution within the kiln can be divided into two zones; zones of peak temperatures, affected by CO_2 dissociation; and colder zones where the temperature is affected by the oxidation of CO. This introduces additional complexities in characterizing the heat transfer conditions within such kilns.

The aim of this work is, therefore, to investigate the effects of dissociation/formation of CO_2 to/from CO on heat distribution and heat transfer within the temperature zones of a pilot-scale CO_2-plasma-heated kiln. The flow field is solved by a computational fluid dynamics (CFD) model, generating temperature and gas profiles. From the CFD model, a high-temperature zone within the kiln is identified. In a separate Chemkin model, the chemistry of the thermal plasma working gas in the high-temperature zone is analyzed. The results from the Chemkin model are used as inputs to a radiation model, which uses a statistical narrow-band model to estimate the gas emissions from the CO_2 and CO species within the high-temperature zone. This work concludes that CO_2 dominates the gas emissions compared to CO, which is observed to be a weak emitter of radiation relative to CO_2 in the high-temperature zone within the kiln. As such, the gas emissions from CO can effectively be treated as a clear gas for future calculations on CO_2-plasma heated systems, thus reducing the computational demand of the models.

Analysis of the Overlap of Devolatilisation and Char Conversion During Single Coal Particle Burning Using a Detailed Multi-Step Kinetic Approach

T. D. Luu[1*], **Y. Zhou**[2], **A. Shamooni**[2], **A. Kronenburg**[2], **and O. T. Stein**[1]
*tien.luu@kit.edu

[1] *Engler-Bunte-Insitute (EBI), Simulation of Reacting Thermo-Fluid Systems (TFS),*
Karlsruhe Institute of Technology, Engler-Bunte-Ring 7, 76131 Karlsruhe, Germany

[2] *Institute of Reactive Flows (IRST), University of Stuttgart, Pfaffenwaldring 31, 70569 Stuttgart, Germany*

To guarantee a secure energy supply in the next few decades, reliability and efficiency have highest priority. Solid fuel conversion of conventional fossil fuels like coal is a proven technology and has been a reliable energy source for decades. However, the inherent pollution caused by solid fuels drives significant research efforts to gain a deeper understanding of its ignition and combustion behaviour to mitigate pollution and climate change.

Previous experimental studies [1-3] have reported that solid fuel particles can undergo various ignition modes, namely homogeneous, heterogeneous and hetero-homogenous ignition. The stages of particle conversion determine the mode of ignition. These stages are (i) particle heat-up, (ii) drying, (iii) devolatilisation, (iv) homogeneous gas combustion, and (v) heterogeneous char conversion. Homogenous/Heterogeneous ignition mode can be attributed to the isolated processes (iv) and (v), whereas hetero-homogeneous ignition is associated with simultaneous processes (iv) and (v). Various modelling strategies have been applied [2-4] to quantify the hetero-homogeneous ignition mode for a range of conditions, typically based on simplified devolatilisation and char conversion models.

Instead, in the present work we focus on the quantification of the potential overlap of processes (iii, devolatilisation) and (v, char conversion) using a detailed multi-step kinetic description of the coal particle [5]. The work is motivated by a limitation of standard modelling approaches for solid fuel conversion, e.g. flamelets. In the flamelet approach processes (iii, iv) and (v) are pre-calculated independently and superimposed in the final flamelet table [6]. However, this superimposition neglects possible interference effects of processes (iii, iv) and (v) at the particle surface, e.g. when devolatilisation displaces oxygen that would otherwise be available for char conversion. Neglecting this interference induces an error in the particle near-field and affects the overall burning behaviour.

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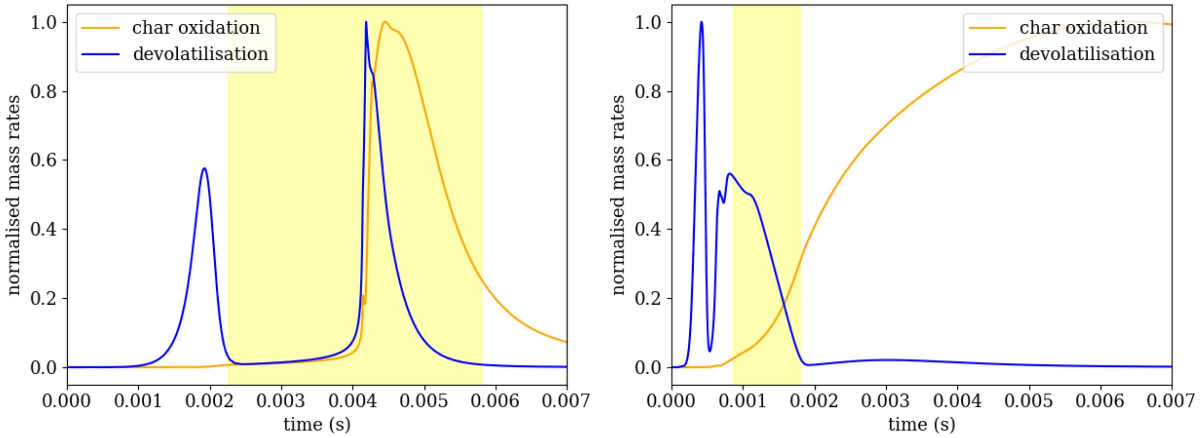

Figure 1. Normalised mass release rates of devolatilisation and char oxidation with the overlap region marked in yellow for $T_g = 1000$ K (left) and $T_g = 1800$ K (right).

This work investigates the conversion of a single solid coal particle using a fully-resolved (FR) simulation approach. The simulation resolves the mass and heat transfer inside the solid and across the particle boundary layer. The gas phase is described with detailed homogeneous kinetics (76 species/973 reactions), while the solid phase is treated as a porous medium with a multi-step kinetic approach (devolatilisation: 32 species/36 reactions, char oxidation: 8 species/14 reactions) [7]. The overlap analysis is based on the reaction rates for processes (iii) and (v), and the period of overlap is identified as the time range where the two process rates r_{dev} and r_{char} do not significantly differ, i.e. when $\log(r_{char}/r_{dev}) < 1$. The overlap analysis is performed for various conditions and gas environments (d_p, T_{gas}, $Y_{gas,O2}$, …). Figure 1 shows the normalised mass release rates of devolatilisation (blue) and char oxidation (orange) for a single coal particle ($d_p = 25\mu m$, $T_{p,0} = 600$ K, $Y_{gas,O2} = 0.233$) at intermediate ($T_g = 1000$ K) and high ($T_g = 1800$ K) ambient gas temperature vs. time. The two peaks in the blue lines indicate the two-stage devolatilisation process predicted by the multi-step kinetics, with the first peak corresponding to the release of light volatile gases and the second peak to heavier tars. The lower gas temperature $T_g = 1000$ K in Fig. 1 (left) exhibits a comparatively long time of overlap with limited char oxidation at late time times, whereas the higher $T_g = 1800$ K leads to a shorter overlap time and increasingly more char conversion at late times.

Acknowledgements

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Large Eddy Simulation of a Gas-Assisted Pulverized Biomass Combustion Chamber Under Varying Oxygen Concentrations Using the OxySim-129 Framework

A. Vahl[1*], **P. Steffens**[1], **L. Berkel**[1], **C. Hasse**[1], **and H. Nicolai**[1]
*vahl@stfs.tu-darmstadt.de

[1] *Institute for Simulation of reactive Thermo-Fluid Systems, Technical University of Darmstadt,*
Otto-Berndt-Straße 2, 64287 Darmstadt, Germany

The global climate crisis is underscoring the need to reduce greenhouse gas emissions. One promising strategy to significantly reduce CO_2 emissions is carbon capture and storage (CCS) in combustion processes. Oxy-fuel combustion, where fuel is burned in oxygen-enriched recycled flue gas, offers a key advantage by producing flue gas with high concentrations of CO_2, thereby increasing the efficiency of CCS. When combined with biomass as a renewable fuel, this approach can achieve negative CO_2 emissions. As the amount of added oxygen to the oxidiser stream can be controlled, the flame can be adjusted by changing the oxygen concentration and thus the reactivity of the mixture. Understanding the influence of oxidiser composition, together with the complex interactions between fluid mechanics, particle dynamics and chemical processes in pulverised biomass combustion, is crucial to unlock its full potential and meet the challenges of large-scale deployment. An important step in gaining this understanding is the simulation of pulverised biomass flames, which allows detailed analysis of key factors such as combustion efficiency, particle trajectories and flame stabilisation, particularly under oxy-fuel conditions. These simulations provide valuable insights that can help optimise combustion processes and improve overall performance.

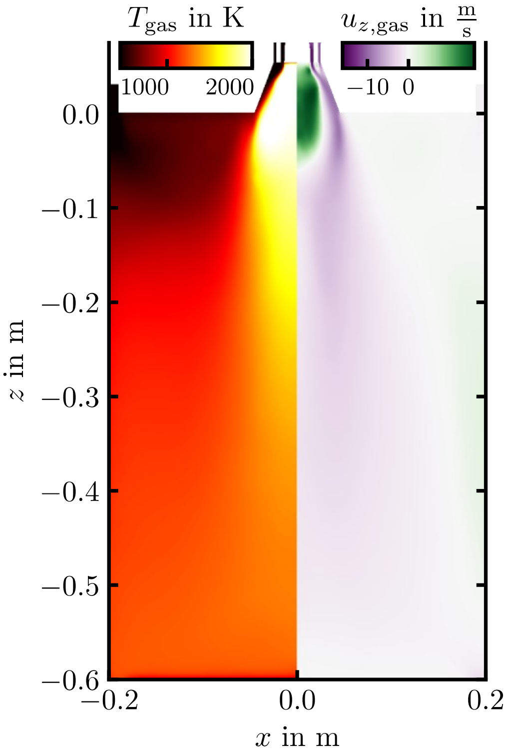

Figure 1. Laboratory scale swirl burner mean temperature (left) and axial velocity (right) of the single-phase methane flame in an oxy-fuel atmosphere, consisting of 27 vol% O_2 and 73 vol% CO_2.

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The combustion of pulverised biomass involves a wide range of multi-scale physical phenomena, which pose a significant challenge to its numerical modelling and simulation. As these phenomena are complex and strongly coupled, the development of appropriate models is crucial for accurate CFD simulations. The increased availability of computational resources enables scale-resolving simulation techniques such as Large Eddy Simulation (LES). In OxySim-129 LES is coupled with a Lagrangian description of the solid particle dynamics for the simulation of large-scale systems. Given the large number of reactions required to describe the gas-phase combustion of both methane and volatile and gaseous char products from biomass particles, a tabulated chemistry approach is developed to capture finite-rate chemistry effects in the simulation using a six-dimensional flamelet table.

In this work, a fully coupled model implemented in OxySim-129 is used to simulate a methane-assisted pulverised walnut shell combustor designed to generate flames up to 70 kW_{th} under varying oxygen concentrations. The simulations are validated against a unique experimental dataset that includes flow and particle velocities, as well as gas temperature distributions for the respective operation conditions. The validation process ensures that the developed tabulated chemistry model accurately captures the complex chemical reactions occurring during combustion. To distinguish between particle-driven and atmosphere-driven changes, single-phase and multi-phase operation conditions are analysed and compared. Preliminary results of the single-phase flame are shown in Figure 1. The numerical results for varying oxygen concentrations are further analysed and compared to provide key insights into their effect on flame structure, operational stability, local oxidation behaviour, and particle conversion which are critical factors in determining overall combustion efficiency.

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Numerical Study of Ignition, Combustion, and Pollutant Formation of Biomass Compared to Coal

P. Farmand[1*], **C. Boehme**[1], **A. Niazmehr**[1], **M. Gauding**[1], **and H. Pitsch**[1]
*p.farmand@itv.rwth-aachen.de

[1] *Institute for Combustion Technology (ITV), RWTH Aachen University, Templergraben 64, 52056 Aachen, Germany*

This work aims to numerically investigate ignition, combustion, and pollutant formation of single coal and biomass particles. Coal and biomass combustion processes are modeled in an Eulerian-Lagrangian framework using the point-particle approximation of the dispersed solid phase. Solid kinetics are modeled in the context of the film model, and it is fully coupled with the gas phase, which is described with finite rate chemistry using a specially designed chemical mechanism for solid fuel combustion. Due to the different characteristics of biomass compared to coal, such as non-sphericity, high volatile content, different internal structures, and elemental composition, the reactive behavior of biomass particles is different compared to coal and different sensitivities to the operating parameters during ignition, combustion, and pollutant formation processes are expected.

In the point-particle modeling approach, particles are usually assumed to be spherical with no rotational motion, which is not the case for biomass particles. The hydrodynamic drag on biomass particles is different due to the non-sphericity and orientation of the particles, which can affect the ignition process. Therefore, the coal point-particle model is extended to be consistent with biomass-specific characteristics to investigate these effects. Also, due to the different internal structure and elemental composition in solid biomass fuels compared to coal, the solid kinetics and the released volatile composition during biomass devolatilization are different, which changes the ignition, combustion, and pollutant formation compared to coal. Therefore, reactive coal and biomass single-particle simulations are conducted using a hot co-flow configuration in laminar conditions. Particles are injected in the mid-section of the inlet using a carrier gas with an initial temperature equal to the hot ambient co-flow.

Based on these simulations, the effects of different parameters, such as fuel composition, particle diameter, shape, and orientation, on devolatilization, ignition, combustion, and pollutant formation for biomass particles compared to coal are investigated. The numerical results are validated against experimentally measured ignition delay times. These validated results can provide data inaccessible in experiments, such as the history and distribution of intermediate species and local temperature changes, enabling a more profound analysis of the combustion behavior of biomass particles.

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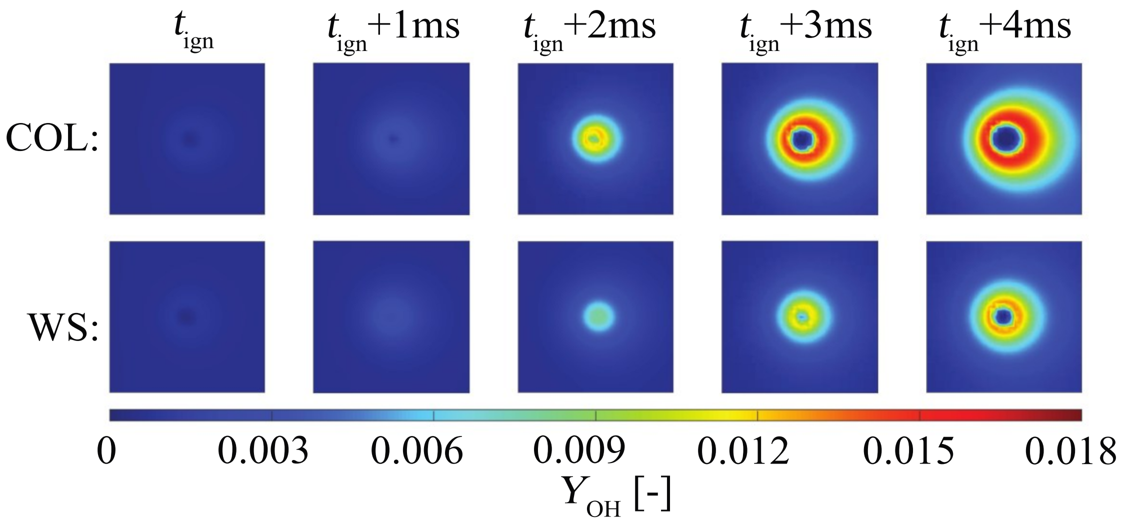

Figure 1. Diffusion flame around single biomass particle (WS) compared to coal (COL).

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Atomistic Simulations of Volatile Diffusion in Char – Quantifying the Effect of the Pore Size Regime

B. Farhadi Jahromi[1*], M. U. Khan[1], and R. Schmid[1]
*Babak.Farhadi-Jahromi@ruhr-uni-bochum.de

[1] *Computational Materials Chemistry Group, Chair of Inorganic Chemistry II, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

Recently, a rigorous yet flexible methodology was developed to generate realistic molecular char models that take experimental data on char geometry and elemental composition into account parametrically[1]. Such models can yield important atomistic insights on the structural and dynamical properties of char. Here, these models were employed to investigate the mobility of some important volatile compounds typically present in oxy-fuel atmospheres confined in char nanopores. To this end, non-reactive molecular dynamics simulations were performed for several nanoseconds, using a modified formulation of the generic Universal Force Field[2]. The applied modifications were made to tailor the force field towards a physically meaningful and computationally stable molecular description of functionalized polycyclic aromatic hydrocarbons including radical sites, not considered in the original force field parameterization. The studied combinations of char systems and volatiles were investigated systematically with respect to volatile load and char pore size regime in order to resolve the dependence of the diffusion dynamics of the confined volatile compounds on these two parameters. Their interplay was quantified by computing self-diffusion coefficients for the confined volatile compounds by averaging their mean squared displacement during the simulations. The obtained self-diffusion coefficients may be used to derive corrections to frequently used general diffusion equations that take the pore size regime into account and that can be used to supplement future experimental studies on volatile diffusion in char. Furthermore, the employed computational workflow can be used to characterize char beyond experimental capabilities by exploring the model systems and therein confined volatiles in experimentally inaccessible conditions.

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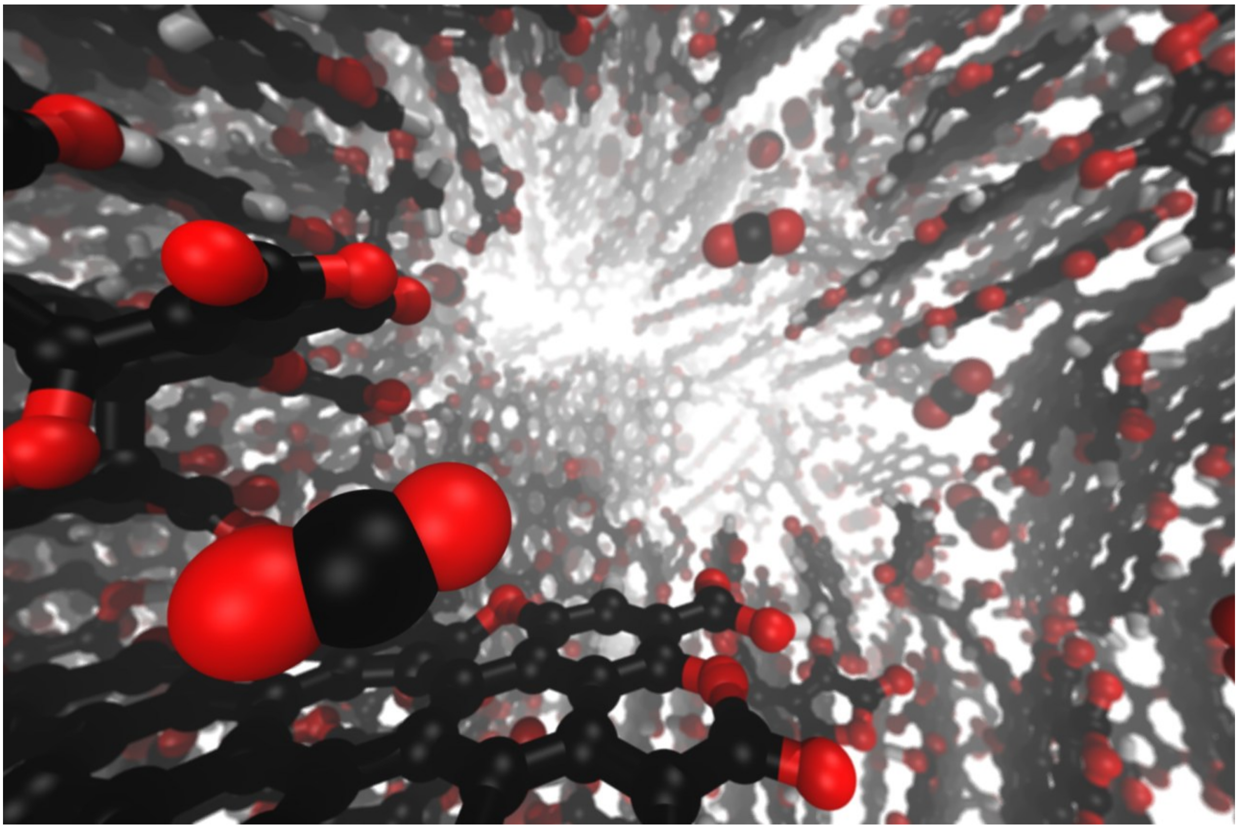

Figure 1. Snapshot from a molecular dynamics simulation of carbon dioxide molecules in a char nanopore

Acknowledgments

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Modeling Mass Transport Properties of Oxyfuel Species in Solid Biomass Fuel Particles

T. Eisenbach[1] **and** **R. Span**[1*]
*roland.span@thermo.rub.de

[1] *Thermodynamics, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany*

A promising method to reduce CO_2 emissions in solid fuel conversion is the substitution of fossil fuels by biomass in an oxyfuel combustion atmosphere. This way, capturing CO_2 from the produced flue gas, which is primarily composed of CO_2 and H_2O, in Carbon Capturing and Storage (CCS) units is much more efficient. The varying properties of solid biomass fuels of different origin (e.g., high mineral and volatile content) and the reactive oxyfuel environment result in changed combustion characteristics. A considerable impairment of the reaction kinetics in biomass conversion can be ascribed to the limiting effect of gas transport within the porous structure of particles, preceding the actual chemical reaction at the inner surface [1]. CO_2, as the major component of the oxyfuel atmosphere, exhibits pronounced diffusion behaviour in small pores of the micro- and ultra micropore regime [2]. Biomass chars tend to develop high porosities due to the release of moisture and volatiles during pyrolysis [3], highlighting the importance of a close investigation of mass transport of CO_2 in the intraparticle pore structure of biomass particles. The time-, temperature- and pressure-dependent mass transport of gaseous species can be approached by adsorption kinetic measurements using suitable samples of biomass char particles. In this presentation, the development of a relative-pressure (RP) and pore structure-dependent sorption kinetic (PSK) model is presented using a comprehensive sorption kinetic data basis for CO_2 and two representative biomass chars. The RP-PSK model provides time- and pore-structure resolved mass transport properties and, thus, claims for a physically sound description of diffusion processes in the established char conversion kinetic (CCK) models, which use fitted or calculated diffusion coefficients.

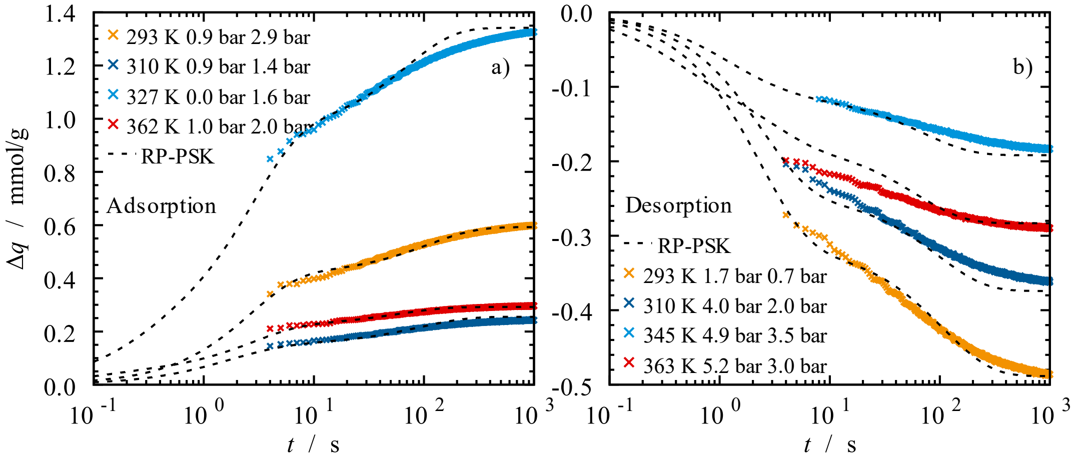

Figure 1. Experimental relative-pressure adsorption (a) and desorption (b) kinetics of CO_2 on TBW at different pressure and temperature conditions (T, p_1, p_2) along with the RP-PSK modelling.

Sorption kinetic measurements

The underlying sorption kinetic data basis consists of ad- and desorption kinetics measured in a gravimetric sorption system. Details regarding the experimental set up are explained elsewhere [4], as this study mainly focuses on the modelling. The pressure dependence of the sorption process is examined at a constant sorption temperature by setting different bulk-phase pressures along an ad-

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and desorption isotherm. A total of four isotherms between 293 and 373 K were measured for each of the two representative samples, which are walnut shell (WNS) char particles, pyrolyzed at 1,300 K in a N_2 atmosphere, and torrefied beechwood (TBW) char particles, gasified at 1,273 K in a CO_2 atmosphere. The measurement procedure follows a systematic investigation of the time-dependent sorption behaviour of CO_2 induced by a relative-pressure difference Δp between the pressure of the previous sorption equilibrium p_1 and the new bulk-phase pressure p_2. For example, looking at an adsorption process, the previous pressure p_1 represents the back pressure that is initially present in the pores before the adsorption process begins. This methodology can be seen as an analogy to a relative pressure difference-driven mass transport of gaseous species from the bulk-phase to the intraparticle surface partially occupied by CO_2.

Modeling

In accordance with the experimental data basis, the RP-PSK model describes the ad- and desorption kinetics between two sorption equilibrium loadings $\Delta q = q_2 - q_1$:

$$\Delta q(T, p_1, \Delta p, t) = \sum_{i=1}^{3} \rho_{\mathrm{m}} \cdot A_i \cdot c_i \left(\frac{(p_1 + \Delta p) \cdot k_i \cdot e^{\frac{H_i}{RT}}}{1 + (p_1 + \Delta p) \cdot k_i \cdot e^{\frac{H_i}{RT}}} - \frac{p_1 \cdot k_i \cdot e^{\frac{H_i}{RT}}}{1 + p_1 \cdot k_i \cdot e^{\frac{H_i}{RT}}} \right) \cdot \left(1 - \exp\left(\frac{-t}{a_i \cdot \left(\frac{T}{T_{\mathrm{Ref}}}\right)^{-n_i} \left(1 + \left(\frac{\min(p_1,\, p_1 + \Delta p)}{p_{\mathrm{Ref}}}\right)^{m_i}\right)^{l_i}} \right) \right)$$

The model incorporates a Langmuir isotherm-based equilibrium part, which predicts the temperature and pressure dependent sorption equilibria. The time-dependent sorption kinetic is modelled by a simple fractional uptake function incorporating temperature- and pressure-dependent time constants a_i. The RP-PSK modelling distinguishes between three pre-defined pore regimes i as the adsorption process takes place at different speeds in different pore regimes. Each adsorption process is characterized by its own time-constant a_i, while the contribution to the overall adsorption loading is summarized for all three considered pore regimes. The RP-PSK model contains a total of 21 adjustable parameters with a direct physical meaning to the sorption process. Furthermore, each pore regime is characterized by its specific pore surface area as introduced by the structural parameters A_i. Figure 1 shows the sufficient representation of the experimental data along different temperature and pressure conditions.

Its physically reasonable structure enables the RP-PSK model to extrapolate to higher temperatures relevant for char conversion processes. Given a sufficient representation of the experimental data and a physically reasonable range for the fitted parameters, a reliable derivation of mass transport properties, like a time- and pore-structure-dependent mass transfer coefficient k or an adsorption flow rate $\dot{q}$ is possible.

Acknowledgments

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Optical Measurements

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Single Fuel Particle Emissivity Evolution of Biomass, Coal and Coal Char

L. Pörtner[1*] **and M. Schiemann**[1]
*poertner@leat.rub.de

[1] *Institute of Energy Plant Technology, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

As the properties of individual particles in combustion systems change during burnout, a precise knowledge of these properties evolutions is mandatory for a valid reaction description. In fields of radiation heat transfer, the single fuel particle emissivity is a parameter of major interest, as it describes the particle's ability to emit radiation of a certain wavelength. Thereby various publication showed the influence of the particle type, temperature and composition on the emissivity. Consequently, the evolution of the single particle emissivity is assumed to vary during particle burnout.

A further developed version of the laser induced single particle reactor setup (see Figure 1), initially presented in [1], was applied to determine the reaction time and wavelength resolved emissivity of individual fuel particles during burnout.

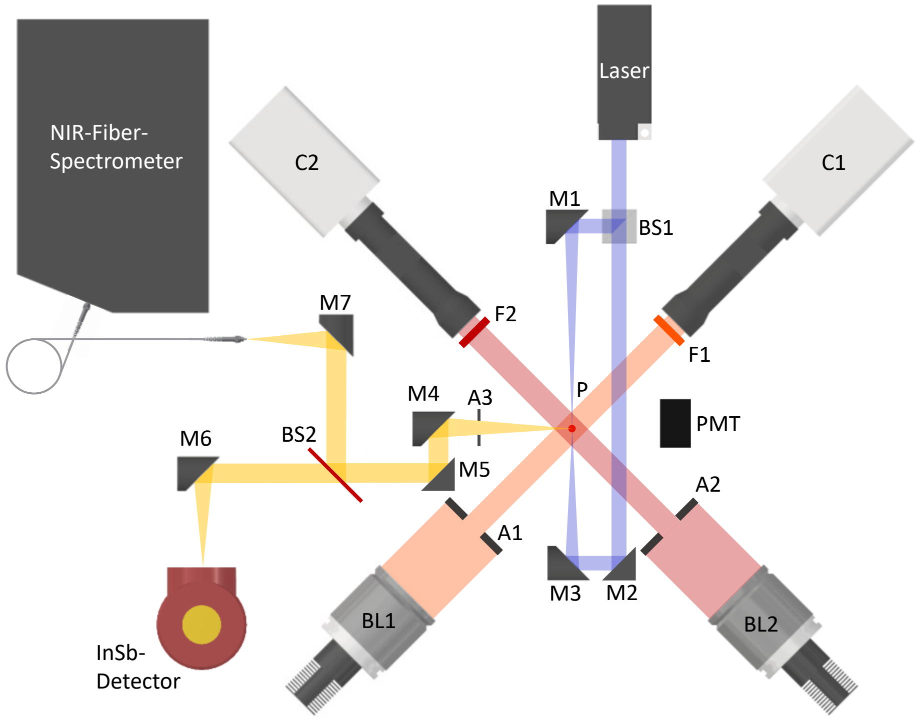

Figure 1. Principal of the reaction setup for single particle emissivity measurements.

Therefore, the particle temperature is measured by a multiple two-colour-pyrometry approach in the near infrared wavelength region (NIR), the particle representative diameter via bidirectional high-speed imaging and the total emitted radiation intensity in two different wavelength ranges (wavelength resolved from 0.85-2.4µm (NIR) and integrated from 2.4-5.5µm (MIR). Following, the respective individual results allow the determination of the single particle emissivity.

Besides the modified reactor setup, the individual setup component calibrations are presented, including the temperature, diameter and total emitted radiation referencing procedures. Furthermore, single fuel particles of different fuels were investigated, covering a range of typical fuels applied in pulverized fuel combustion. The investigated fuel samples include raw Colombian bituminous coal, Colombian bituminous coal char produced by a drop tube reactor presented in [2] and raw walnut shells. Thereby, the size fractions of the coal and char samples were 160-200µm while the walnut shells had a size of 200-250µm. Measurement results of an exemplary particle are displayed in Figure 2.

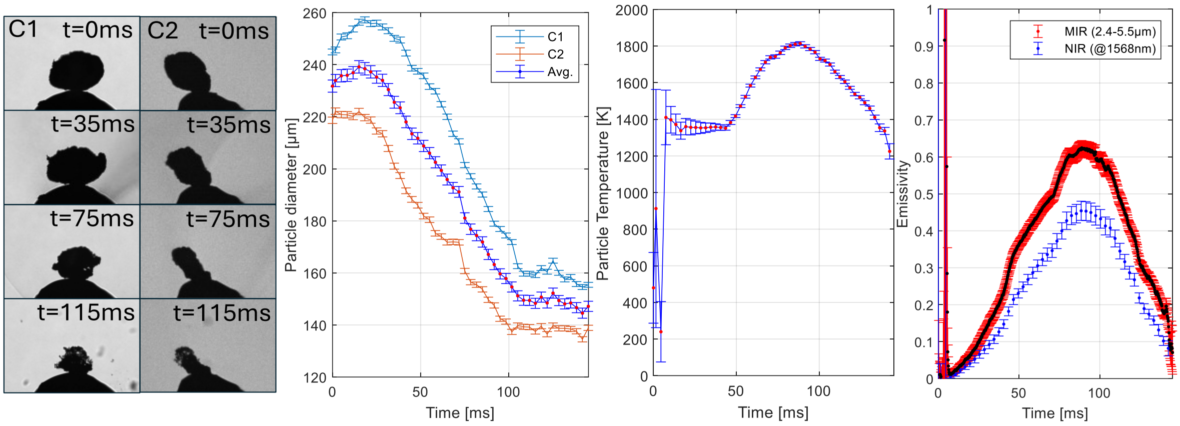

Figure 2. Exemplary single walnut shell particle results including individual images, and diameter, temperature and emissivity evolutions.

In studies of multiple fuel particles, global trends were found, showing a directly decreasing representative diameter of the char and walnut shell particles with particle ignition, while the raw coal sample showed swelling effects in the beginning of the reaction. Furthermore, the maximum average temperatures of the fuels differ significantly. As the char samples reached the highest average temperature (~1958K) followed by the raw coal (~1796K) and the walnut shells (~1643K). The same behaviour was also found in the emissivity. The maximum average emissivity in the mid infrared region (MIR) (2.4-5.5µm) is highest for char (0,97), followed by raw coal (0,8) and walnut shells (0,74). In the near infrared region (NIR) (0.85-2.4µm) the emissivity of all investigated fuels was found constantly lower than in the MIR. Thereby, walnut shells show a grey body like emission behaviour, while the raw coal and coal char emissivity is significantly higher for smaller wavelengths over the whole reaction progress.

Acknowledgements

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Hemispherical Radiometer Measurements of the Spectral Resolved Radiative Heat Flux in a Combustion Chamber

L. Pörtner[1*], B. Özer[2], D. König[3], M. Schiemann[1],
A. Maßmeyer[2], J. Ströhle[3], and B. Epple[3]
*poertner@leat.rub.de

[1] *Institute of Energy Plant Technology (LEAT), Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[2] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*
[3] *Institute for Energy Systems & Technology (EST), TU Darmstadt, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany*

In combustion systems, the total radiative heat flux is a parameter of major interest, as it contributes significantly to total heat transfer. Therefore, a detailed knowledge is mandatory for a valid system description. Several approaches of different studies, mostly based on a thermopile measurement technique, enable the determination of the total radiative heat flux with the application of integrating single channel detectors [1–4]. However, the preservation of individual wavelength dependent radiation intensity information has the potential of inner system mechanism investigations, which remains unutilised in an application of these detector types. Unfortunately, the needed detectors for the respective spectral resolved radiation analysis are typically unapplicable in the harsh combustion environment. Therefore, Tree et al. [5] and Adams et al. [6] extracted radiation from the combustion chamber via guiding optical fibers and coupled it to a specifically designed wavelength sensitive detector setup.

Combining the individual setup properties of some of the previously mentioned studies, a radiometer was developed, which enables total radiative heat flux measurements inside a combustion chamber with chamber external and spectral resolved radiation analysis setup application. A conceptional illustration is presented in Figure 1.

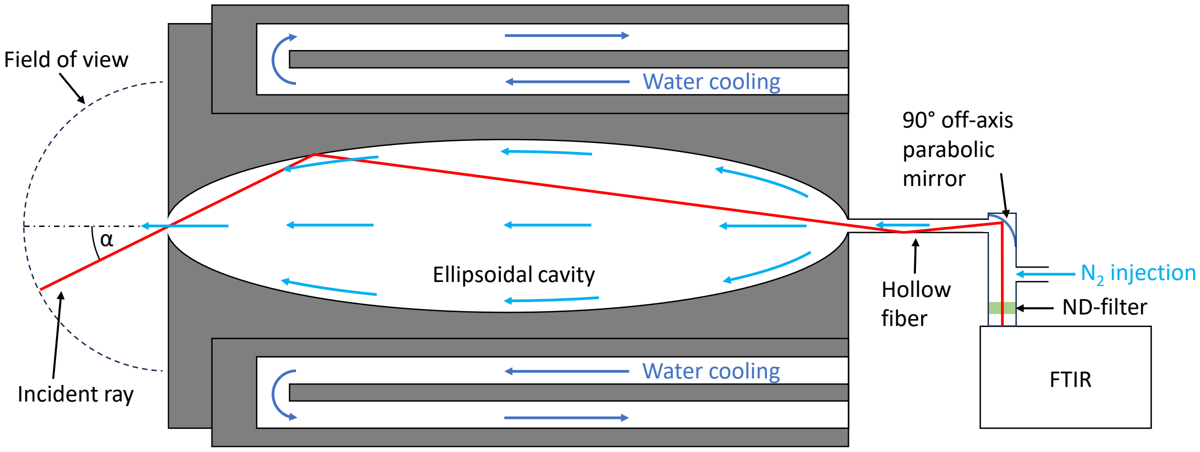

Figure 1. Principle of the radiometer concept for hemispherical wavelength resolved total radiative heat flux measurements inside a combustion chamber.

Therefore, the known concept of elliptical hemispheric radiometer cavities has been extended by the radiation guiding technique of hollow optical fibers. This combination enables the application of chamber external radiation analysis devices, such as a FTIR-spectrometer. Via calibration measurements, the angular dependent response of the radiometer was determined, and a wavelength resolved intensity calibration performed. This enables a valid interpretation of the received radiation signals from the inside of a combustion chamber.

Furthermore, the radiometer was applied at a 1MW test facility investigating three different pulverized-walnut shell flames including one air and two oxyfuel atmospheres. The received results enable the identification of various gas species as water vaper, CO_2, CH_4 via their characteristic emission lines (see Figure 2), as well as total radiative heat flux distributions within different measurement positions inside the combustion chamber.

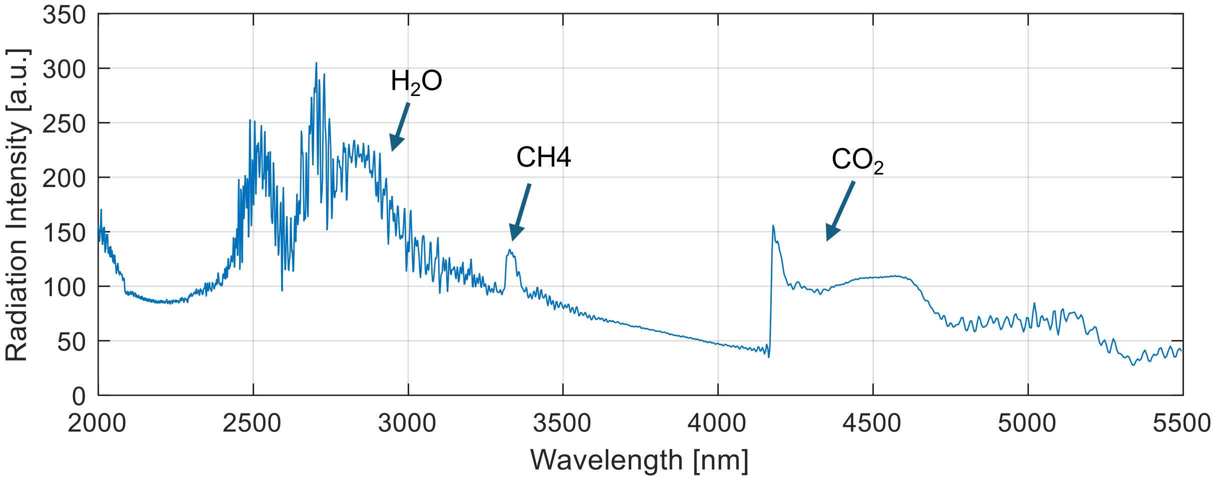

Figure 2. Exemplary received spectral resolved radiation intensity distribution from a pulverized walnut shell driven air flame.

Acknowledgements

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Structural Features of Flames in Plasma-Assisted Hybrid Combustion Systems

S. Mishra[1*], **I. Qasim**[1], **A. Gunnarsson**[1], **Nerijus Striūgas**[2],
A. Tamošiūnas[2], **and K. Andersson**[1]
*mishrasa@chalmers.se

[1] *Department of Space, Earth and Environment, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*
[2] *Lietuvos energetikos instituta, Breslaujos g. 3, LT-44403 Kaunas, Lietuva*

Conventional combustion processes in industrial and transportation sectors are significant contributors to environmental pollution and global warming. These systems often exhibit incomplete combustion, resulting in the emission of harmful pollutants such as carbon monoxide (CO), nitrogen oxides (NO_X), and particulate matter (PM). Thermal plasma emerges as a viable alternative by offering highly uniform, elevated-temperature environments conducive to complete combustion, thereby mitigating pollutant emissions. Its capacity to function under extreme conditions establishes plasma technology as an environmentally sustainable substitute for traditional combustion methodologies.

A profound understanding of flame structure is pivotal for optimizing thermal transfer mechanisms, predicting flame dimensions, and assessing potential interactions. The current work examines the structural dynamics of flames in an experimental hybrid plasma combustion system utilizing methane (CH_4) and hydrogen (H_2), with and without plasma assistance. High-resolution visual imaging captured flame characteristics from a 50 kW_{el} plasma generator and a 100 kW_{th} combustion burner, insights used to advance the characterization of plasma-enhanced combustion systems.

A high-performance visual camera, a FORGE 5GigE, was utilised for recording the flames. The camera is equipped with a 5-megapixel CMOS sensor, offering a resolution of 2448 x 2048 pixels, with a pixel size of 2.74 micrometres, and a frame rate ranging from 122 to 997 frames per second, enabling precise and high-speed visual capture. The captured flame videos were processed in MATLAB to extract structural parameters of length and diameter for which the analysis involved converting colour images to binary for easier quantification. Flame length was measured as axial distance from the burner exit to the tip, while flame diameters were calculated by averaging multiple measurements at different axial positions and then taking temporal average across all frames. Flame volume was estimated by approximating the flame as a series of cylindrical segments, each having a length corresponding to a single pixel, and the sum of these volumes estimates the total reaction zone volume. The procedure for image analysis is illustrated in Figure 1.

The structural characteristics of methane flames without plasma assistance were analysed initially, and while the flame length showed no consistent trend with supplied burner power, the flame diameter decreased linearly as power was increased, likely due to enhanced inlet turbulence at a constant equivalence ratio of 1. Flame volume is theoretically more dependent on flame diameter than on length, and therefore, its trend aligns more closely with the diameter.

For the burner, employing plasma-assisted combustion with hydrogen and methane, flame characteristics were assessed across varying plasma powers and fuel inlets. Results for constant hydrogen with varying plasma powers showed an increase in both flame length and diameter, with minor variations. A similar pattern was noted for constant methane with varying plasma, where both length and diameter increased with power.

When plasma power was instead kept constant, and hydrogen or methane feed varied, flame length remained relatively stable, slightly increasing with power, while the diameter decreased, reducing flame volume and projected area. Compared to pure combustion, plasma-assisted combustion exhibited reduced variations in structural properties, particularly in volume. Plasma power notably influenced flame length, while fuel inlet changes impacted diameter and volume.

This study provides foundational insights into flame structure properties in hybrid plasma combustion systems, paving the way for optimizing fuel flexibility, combustion efficiency, and sustainable glass production in future pilot-scale applications.

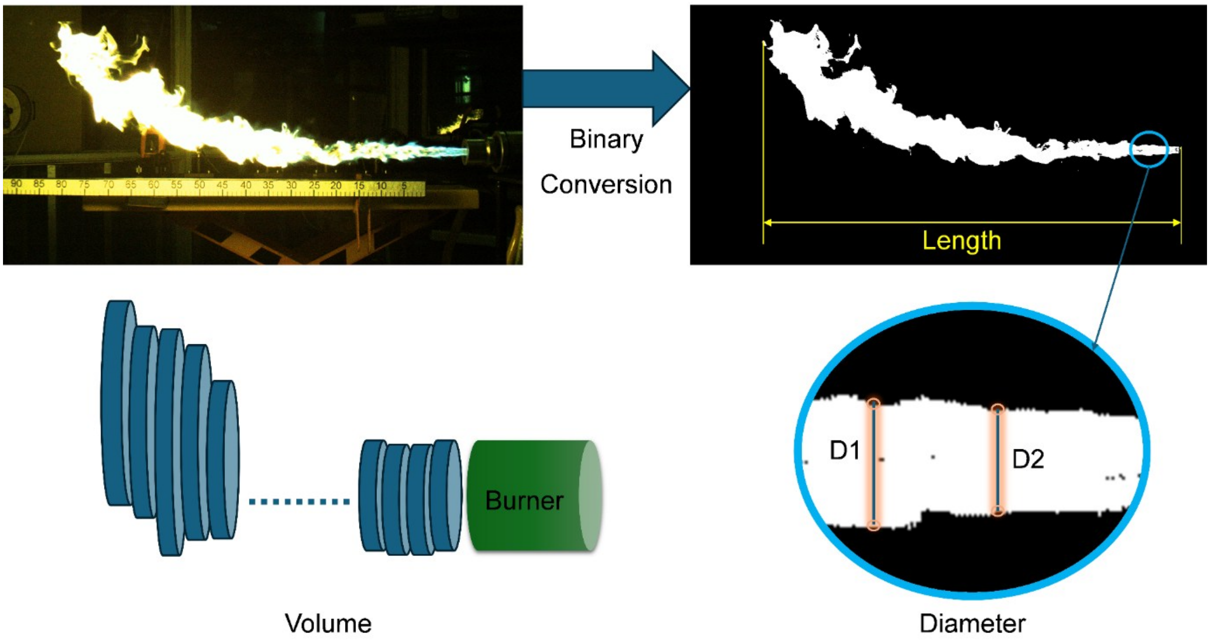

Figure 1. Procedure of image analysis.

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Particle Temperature and Dynamics in Turbulent Iron Dust Flames: A Combined Pyrometry and PIV Study

J. Hebel[1*], İ. Alp[1], M. P. Groß[1], A. Dreizler[1], and B. Böhm[1]
*hebel@rsm.tu-darmstadt.de

[1] *Institute of Reactive Flow and Diagnostics (RSM), Technical University of Darmstadt, Germany*

Metal dust combustion has gained attention as one step in a redox cycle for storing and transporting renewable energy. Iron, in particular, is well suited for this purpose due to its non-toxic nature and the minimal nanoparticle formation observed during its oxidation compared to metals oxidizing in the gas phase. Nanoparticle formation is still a major concern in the context of iron dust combustion because it results in material losses within the redox cycle and potentially high flue gas treatment costs. Consequently, mitigation of nanoparticle formation is a key objective in the research of iron dust flames.

In this study, simultaneous three-color pyrometry and particle image velocimetry (PIV) measurements are performed to investigate particle temperatures and dynamics in a 50 kW_{th} methane-assisted swirl-stabilized iron dust flame. The experimental setup consists of a top-fired burner coupled to a combustion chamber. Previous experimental and numerical investigations have shown that particle temperature, which is a driving factor for nanoparticle formation, is mainly influenced by oxygen availability. To investigate this in more detail experimentally, the oxygen volume fraction is systematically varied with a focus on its effects on particle temperature and dynamics.

For the first time, three-color pyrometry is applied to study turbulent iron dust flames using a low-speed, high-resolution color camera equipped with a triple bandpass filter (TBPF). This method uses the three color channels of a Bayer sensor calibrated to account for spectral overlap. By determining the ratio between the spectral bands of the TBPF and using a calibrated tungsten lamp as a reference, the particle temperature is determined. Compared to classical two-color pyrometry, which typically requires multiple cameras, three-color pyrometry simplifies the experimental setup, providing greater flexibility and a simplified calibration process.

This study combines particle temperature measurements from three-color pyrometry with velocity data from PIV and introduces an expanded set of operating conditions compared to previous studies. By varying oxygen volume fractions, it fills knowledge gaps from previous experimental and numerical studies and provides new insights into iron dust flame dynamics and nanoparticle formation.

Simultaneous Measurement of Temperatures at Various Distances from the Burner of a Semi-Industrial-Scale Biomass Combustion Chamber

M. Bonarens[1], D. König[2], P. Linke[1], G. Goet[1], C. Hansemann[1], J. Ströhle[2], B. Epple[2], and S. Wagner[1*]
*wagner@rsm.tu-darmstadt.de

[1] *Institute of Reactive Flows and Diagnostics (RSM), Technical University of Darmstadt, Otto-Berndt-Str. 3, 64287 Darmstadt, Germany*

[2] *Institute for Energy Systems and Technology (EST), Technical University of Darmstadt, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany*

In order to optimize the combustion of biomass in future power plants, it is essential to understand the fundamental processes and transfer this knowledge to industrial-scale systems. However, not only the combustion chambers must be upscaled, but also the measurement technologies needed to characterize the thermochemical system must be adapted accordingly.

Therefore, a novel laser spectrometer that has been applied to a water-cooled top-fired pulverized fuel furnace with a capacity of 1 MW_{th} in full operation is presented herein. Due to the size of the chamber and the cooled walls, the combustion process shows highly transient behavior and poses a challenging experimental environment.

The single-ended spectrometer is therefore designed to facilitate robust measurements of the gas temperature within the combustion chamber with a high temporal resolution. Hence, it provides insights that contribute to an increased understanding of the process, which is valuable for designing both experimental and numerical upscaling of such processes.

The laser spectrometer, which is based on tunable diode laser absorption spectroscopy, uses a new fiber coupled stand-off-detection setup to distribute the light emitted by a diode laser to the four sensor systems mounted at the combustion chamber. The four channels are arranged in a vertical direction at different distances from the burner quarl.

On each position, the laser light was introduced into the chamber via flanges equipped with integrated wedged windows. The light passes the volume of interest to the opposite wall and is reflected by an integrated retro-reflecting optic. After passing the volume twice, the light is detected in the transceiver unit. The spectrometer was scanning the molecular transitions of water vapor with a repetition rate of 1000 Hz to determine the integrated temperature.

The spectrometer will be presented in detail, together with initial outcomes of the quantitative temperature evaluation. The advantages and drawbacks of the approach, as well as the uncertainties of the line-of-sight approach, will be discussed.

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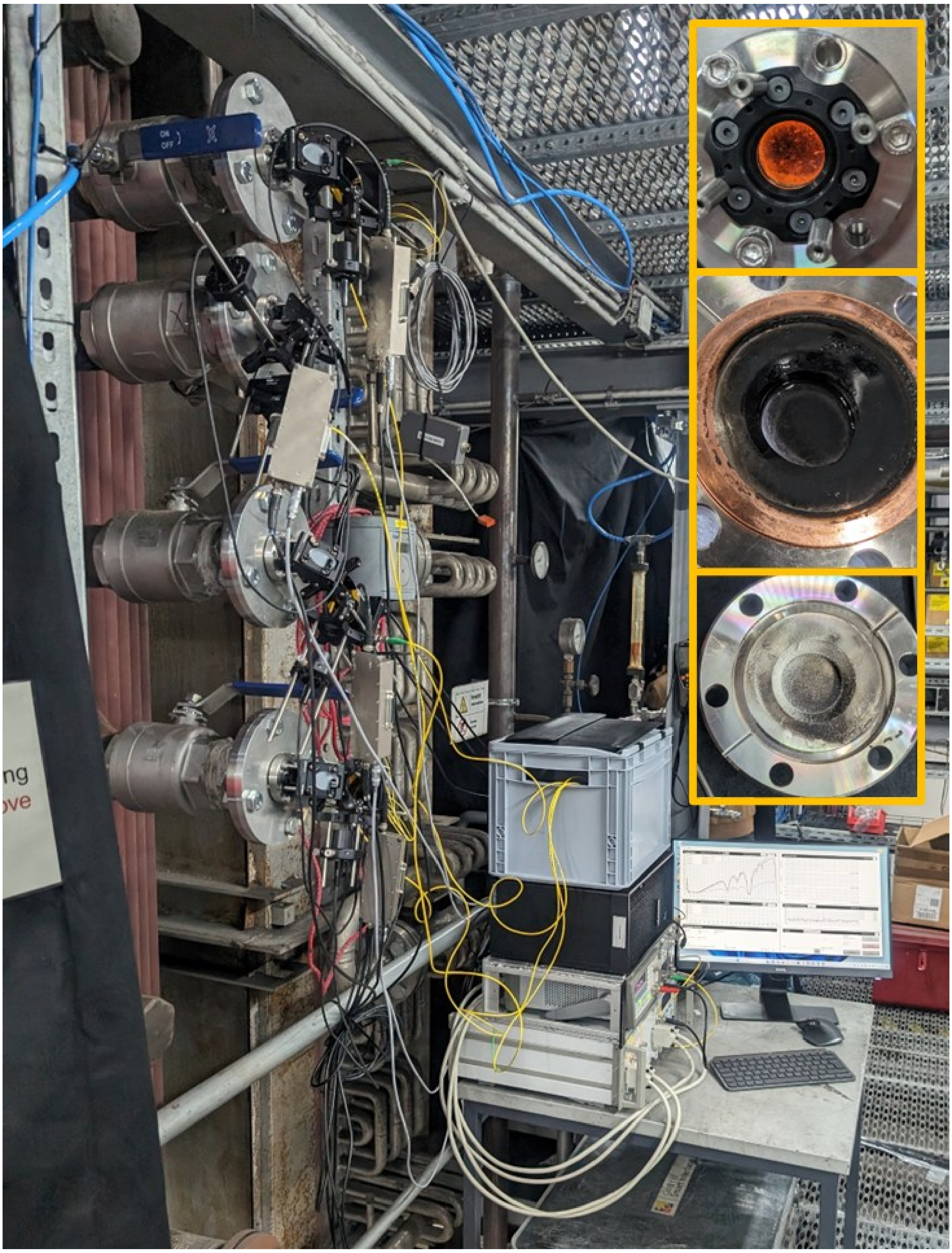

Figure 1. The configuration of the four optical channels (left) at the chamber flanges of the furnace. The insets on the right depict the optical window during (top) and after the measurement campaign (middle, below). Despite plenty of deposits on the optics, measurement was possible over the entire campaign.

Spectral Analysis of Methane-Assisted Pulverized Solid Fuel Flame

B. Özer[1*], P. Augustin[1], M. A. Reddemann[1], R. Kneer[1], and A. Maßmeyer[1]
*oezer@wsa.rwth-aachen.de

[1] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*

The spectral information of a flame provides valuable data about the flame characteristics, i.e. gas-phase species in the flame. Employing line-of-sight spectroscopic measurements and following a whisk broom recording procedure, the spectral information can be extended from single pixel pointwise measurement to a 2D mapping. Thus, a detailed analysis of the flame operating conditions and their effect on the local radiative emissions at different flame sections can be performed.

In this study, hyperspectral mapping is meant to be used on methane-assisted solid fuel (walnut shell) oxyfuel combustion set in well-described swirl burner [1]. As a control experiment the well-characterized SpraySyn [2] burner is used to generate spray flames as reference for spectral analysis and enable comparison to other existing methods.

In spray burners, liquid fuels are atomized into fine droplets, mixed with oxidizer, and combusted, enabling efficient energy conversion with a wide variety of fuels, including traditional hydrocarbons, biofuels, and even carbon-free fuels such as liquid ammonia (NH_3). Beyond energy applications, spray flames find use in advanced material synthesis such as flame-spray-pyrolysis (FSP), a process for synthesizing nanoparticles. In FSP, precursor solutions are atomized and combusted, enabling the formation of high-purity materials with tailored nanostructures, making spray flames integral to both energy and material science advancements.

The hyperspectral mapping of the flame is completed for the spectral ranges of 2000 - 5995 nm to map distribution of selected gaseous species in the flame. The optical setup is built with off-axis-parabolic protected silver-coated mirrors to avoid chromatic aberration and minimize light absorption of the optical path. The findings of the hyperspectral mapping are combined with high-speed Schlieren measurements, and spectrally narrow -band imaging of CH*, OH*, and C_2* radicals to investigate the effects of the varying inlet flow rates of O_2 (as a dispersion gas for the atomization of the liquid fuel) on the formation of the resulting reaction zones in the studied flames: 1) Ethanol 2) solvent mixture (35% Ethanol + 65% Ethylhexanoic acid + 0.1 mol/l iron nitrate).

Figure 1 shows that in lean ethanol flames, an increase in the oxidizer flow rate leads to a decrease in the overall heat release rate (OH* emission emission). This behavior is consistent with the expected reduction in flame temperature due to increased dilution and reduced fuel-oxygen ratio per unit volume. Additionally, the flame front (CH* emission images) becomes visibly elongated as the fuel velocity increases, indicating the influence of flow field on flame shape. Schlieren images and hyperspectral images reveal that unburned methane at the boundary between the methane pilot flame and secondary air flow, highlighting a decrease in gas phase temperature and so reaction activity.

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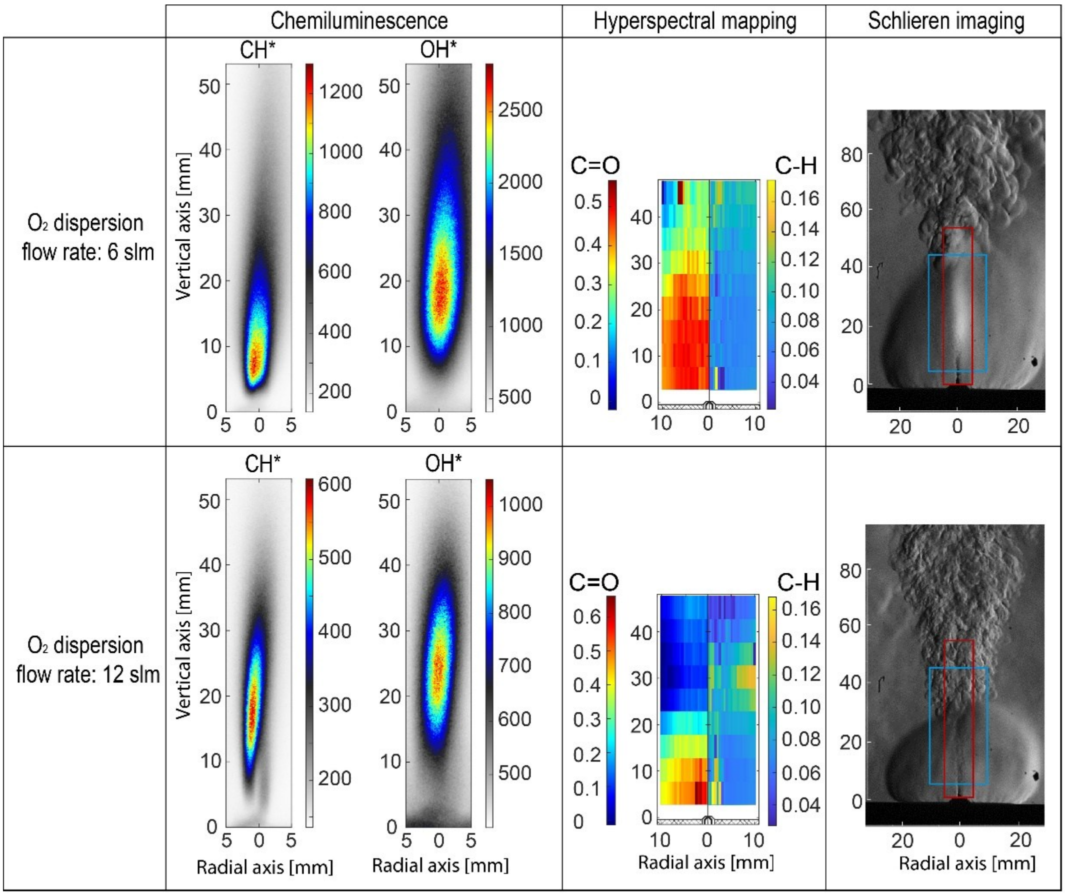

Figure 1. Images of ethanol flames with two different O_2 dispersion flow rates measured by three optical methods: Chemiluminescence, hyperspectral mapping, and Schlieren imaging. Red and blue rectangles on the Schlieren images represent the optical boundaries of the Chemiluminescence hyperspectral mapping, respectively.

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Aluminium Droplet Combustion in Hot H_2O/N_2 Flows

C. Ruan[1], **S. Shi**[1*], **D. Ning**[1], **T. Krenn**[1], **T. Li**[1], **and A. Dreizler**[1]
*shi@rsm.tu-darmstadt.de

[1] *Institute of Reactive Flows and Diagnostics, Technical University of Darmstadt, Otto-Berndt-Straße 3, 64287, Germany*

Significance statement

This paper presents the dynamic combustion process and burning time of aluminium (Al) droplets in high-temperature H_2O/N_2 mixtures using high-resolution optical diagnostics. The burning time and stand-off distance of the flame envelope with varied H_2O contents and temperatures are characterized. These unprecedented datasets are useful for model development and contribute to a deeper understanding of the combustion of Al in hot steam-dominated atmospheres.

Introduction

The combustion of Al particles in steam is emerging as an innovative approach to generate heat and hydrogen without the emissions of CO_2. While the combustion mechanisms of Al in oxygen-dominated atmospheres have been widely investigated due to its wide application as energetic additive in solid prepollents [1], very limited studies are currently available concerning its combustion characters in steam [2,3]. However, these studies were conducted at relatively low temperature, i.e., 410 K in Ref. [2] and below 523 K in Ref. [3]. As a result, detailed studies on Al combustion in high-temperature steam are rather rare. In this work, a unique Al foil test platform was developed to study the combustion process, burning time and flame envelope stand-off distance using direct and diffuse back-light illumination imaging techniques with high spatial resolution.

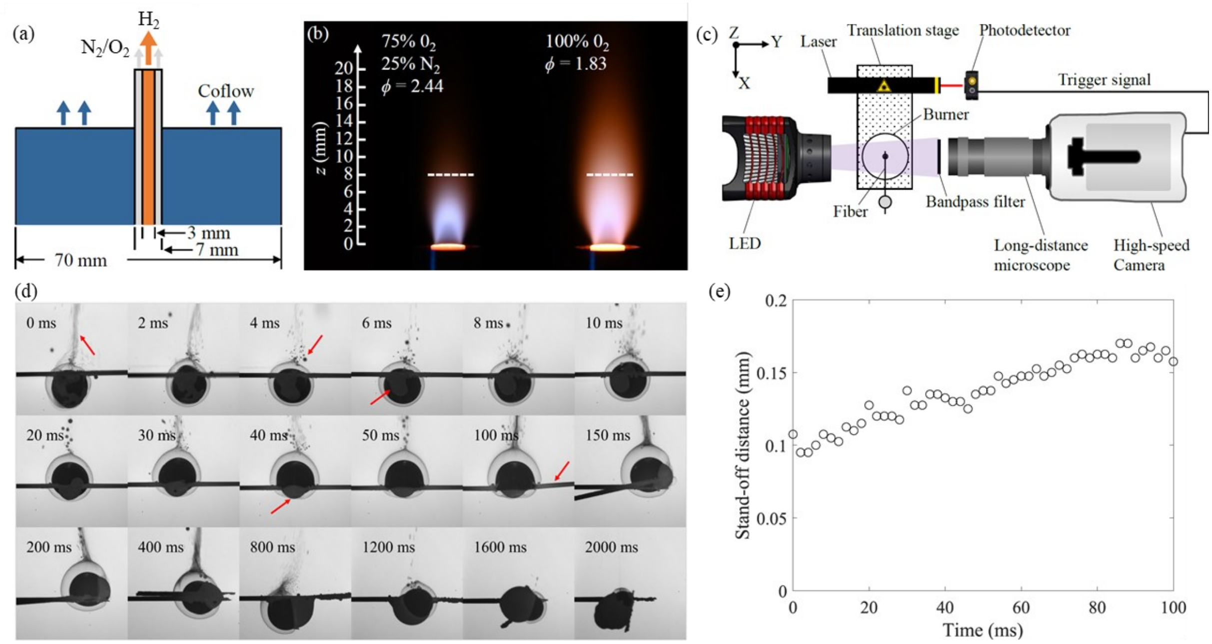

Figure 1. (a) Schematic of the H_2-O_2 diffusion flame burner; (b) Images of the diffusion flame. The dotted lines indicate the position of the Al foil; (c) Optical setup; (d) Representative snapshots of the DBI measurement; (e) Evolution of the stand-off distance of the flame envelope.

Experimental setup and representative results

The experimental setup along with several typical results are shown in Fig. 1. As illustrated in Figs. 1(a) and (b), a H_2-O_2 diffusion flame is used to generate the high-temperature H_2O/N_2 atmosphere, and, after melting, an Al foil (thickness of 8 µm, diameters of 3 mm and 6 mm) is combusted at a height above the burner of 8 mm. The combustion process of the Al foil is visualized using a joint direct and diffuse back-light illumination (DBI) system (Fig. 1(c)). The latter employs an ultraviolet LED (centred at 385 nm), and a high-speed camera (v711, Phantom) equipped with a long-distance microscope (Model K2/SC, Infinity) and a bandpass filter (385 nm±10, Thorlabs). Typical DBI images are shown in Fig. 1(d). These images clearly demonstrate the formation of Al_2O_3 condensation layer (termed as 'flame envelope'), the interplay between the molten Al droplet and the alumina cap, and the shrinking of the Al droplet. The evolution of the stand-off distance of the flame envelope is depicted in Fig. 1(e). It is evident that the flame moves away from the Al droplet as it develops during the initial 100 ms period. This might be caused by the gradual increase of the Al droplet temperature and the resultant higher evaporation rate of Al vapor, which pushes the flame envelope away from the droplet surface as it is formed in regions under stoichiometric conditions.

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Particle Dynamics and Gas Phase Investigation in Semi-Industrial Oxy-Fuel Biomass Combustion

J. Hebel[1*], **M. Bonarens**[1], **D. König**[2], **J. Münzenberger**[1], **B. Böhm**[1], **S. Wagner**[1],
B. Epple[2], **and A. Dreizler**[1]
*hebel@rsm.tu-darmstadt.de

[1] *Institute of Reactive Flow and Diagnostics (RSM), Technical University of Darmstadt, Germany*
[2] *Institute of Energy Systems and Technology (EST), Technical University of Darmstadt, Germany*

Understanding the complex interaction between fluid mechanics, particle dynamics, and chemical processes in oxy-fuel combustion is key to its commercial application. Previous research in this field has focused on the investigation of an optically accessible, swirl-stabilized combustion chamber supporting a methane-assisted biomass flame of ground walnut shells at thermal powers up to 70 kWth. Findings from this laboratory-scale setup were used to upscale the burner to a semi-industrial scale, allowing the study of a system that closely represents industrial oxy-fuel combustion applications.

This work presents the first application of Particle Tracking Velocimetry (PTV) to measure fuel particle velocities and Tunable Diode Laser Absorption Spectroscopy (TDLAS) to measure gas phase temperatures and species concentrations in a 1 MWth semi-industrial oxy-fuel combustion chamber. Pulverized walnut shells were used as biomass fuel under various operating conditions, including air and oxy-fuel atmospheres with oxygen volume fractions ranging from 27% to 33%. The effects of swirl intensity and oxygen volume fraction on particle dynamics and flame characteristics, i.e., gas phase temperature, were systematically analyzed.

The results revealed significant variations in velocity fields and gas phase temperature influenced by combustion atmosphere and swirl configurations, providing valuable insights for optimizing oxy-fuel combustion processes for carbon capture and utilization. Despite limited optical access and harsh conditions, advanced laser diagnostics were successfully implemented, demonstrating their ability to improve understanding in complex semi-industrial environments.

Acknowledgments

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Shape-Dependent Motion Estimation of Solid Fuel Particles in Two-Phase Flows Using Wavelet-Based Optical Flow Velocimetry (wOFV)

M. Werner[1*], C. Geschwindner[1], A. Nicolas[2], B. Peterson[2], A. Dreizler[1], and B. Böhm[1]
*werner@rsm.tu-darmstadt.de

[1] *Technical University of Darmstadt, Department of Mechanical Engineering, Reactive Flows and Diagnostics, Otto-Berndt-Str. 3, 64287 Darmstadt, Germany*

[2] *University of Edinburgh, School of Engineering, Institute for Multiscale Thermofluids, The King's Buildings, Edinburgh EH9 3FD, United Kingdom*

A better understanding of physical phenomena in two-phase flows, including particle-turbulence interactions, particle heat transfer mechanisms, and particle clustering dynamics is critical for the advancement of sustainable combustion science. In two-phase flow experiments, the objective is typically to capture both fluid and particle motion simultaneously. For fluid flows, Particle Image Velocimetry (PIV) is the state-of-the-art post-processing method for velocity field measurements (Raffel et al. 2018). However, recent findings indicate that wavelet-based Optical Flow Velocimetry (wOFV) can surpass PIV in terms of spatial resolution and accuracy of the velocity measurement, which was demonstrated in a variety of flows such as homogeneous isotropic turbulence flows (Schmidt and Sutton 2019), boundary layer flows (Nicolas et al. 2023), and jet flames (Schmidt et al. 2021).

For the solid phase, the motion of fuel particles such as biomass or coal is characterized by a translational and a rotational velocity component. The estimation of the translational velocity can be achieved in a robust and accurate manner by applying intensity-weighted centroid tracking algorithms. For predicting the angular velocity of solid fuel particles, tracking of the orientation of an ellipse fit is frequently employed (Li et al. 2023; Geschwindner et al. 2023). However, ellipse fit tracking struggles to resolve the rotational motion of nearly spherical particles with low aspect ratios (Köser et al. 2019), such as ground walnut shells, which is a well-researched biomass and climate-neutral substitute of bituminous coal.

This study explores the feasibility of using wOFV to track the rotational motion of nearly spherical particles. The proposed methodology leverages the capability of wOFV to resolve small-scale surface features which manifest themselves as varied directional intensity gradients of the imaged particle and aims to establish a unified methodological approach that can complement ellipse fit tracking and is expected to enhance the overall accuracy of rotational motion estimation.

The applied methodology involves three key steps: (1) the extraction of particle outlines from experimental data, (2) the generation of synthetic ground truth data consisting of two consecutive images with user-defined translational and rotational particle displacements, and (3) the application of wOFV and ellipse fit tracking to predict the angular velocity.

The results reveal two distinct regimes based on the two quantified shape characteristics, aspect ratio and ellipticity. As illustrated in Figure 1, it was found that wOFV computations outperform ellipse fit tracking in terms of accuracy for particles with low aspect ratio and low ellipticity. wOFV is advantageous in this regard because it resolves the movement of rugged surface features, which ellipse tracking does not resolve in equal detail. However, the ellipse fit tracking algorithm yields more accurate results for particles exhibiting high aspect ratio and high ellipticity, as such shapes are well approximated by an ellipse. Building upon these findings, a Support Vector Machine (SVM) classifier is trained on the proposed particle shape characteristics to distinguish between the two regimes. This leads to an adaptive tracking approach that dynamically selects the most suitable method for each particle.

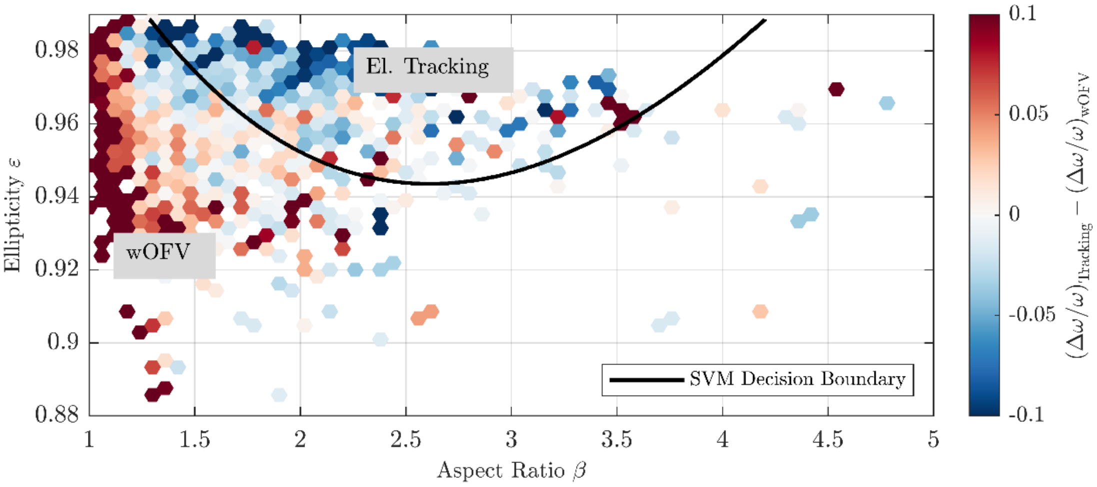

Figure 1. Difference in the predicted relative error of the angular velocity $\Delta\omega/\omega$ between ellipse fit tracking and wOFV. In total the results of 2000 different walnut shell fragments moving with velocities of $[u_x, u_y] = \pm 5$ pixels per frame and $\omega_p = \pm 0 - 20$ degrees per frame are included. Blue and red areas indicate a higher prediction accuracy of ellipse fit tracking and wOFV, respectively. The decision boundary differentiating between the two regimes is shown as a solid line.

Acknowledgments

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”.

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Oxy-Fuel Processes

Combustion and Pyrolysis of Aluminum and Magnesium Particles in Oxy-Fuel Atmosphere

D. Tarlinski[1*], **E. Freisewinkel**[1], **M. Schiemann**[1], **and V. Scherer**[1]
*tarlinski@leat.rub.de

[1] *Institute of Energy Plant Technology, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

Recycling carbon from CO_2 has been suggested for CCUS, shifting away from traditional terminal storage to a more dynamic and integrated approach. In an oxy-fuel combustion process, the resulting process gas contains CO_2, H_2O, and O_2. Metal fuels (abbreviated as M in equations 1 and 2), due to their high energy density and solid-state stability, offer a compelling option for energy storage via exothermic oxidation reactions with gases like CO_2 and H_2O as follows:

$$M + CO_2 \rightarrow MO + CO \qquad (1)$$
$$M + H_2O \rightarrow MO + H_2 \qquad (2)$$

Previous research and studies [1,2] have explored the potential of iron as a metal fuel in power plants for combustion with H_2O and O_2. This study shifts the focus to magnesium and aluminum as potential alternatives to iron. The exothermic reactions of these metals with CO_2 and H_2O, producing metal oxides along with CO and H_2, are investigated for their potential to support carbon-neutral energy storage and conversion in an oxy-fuel context.

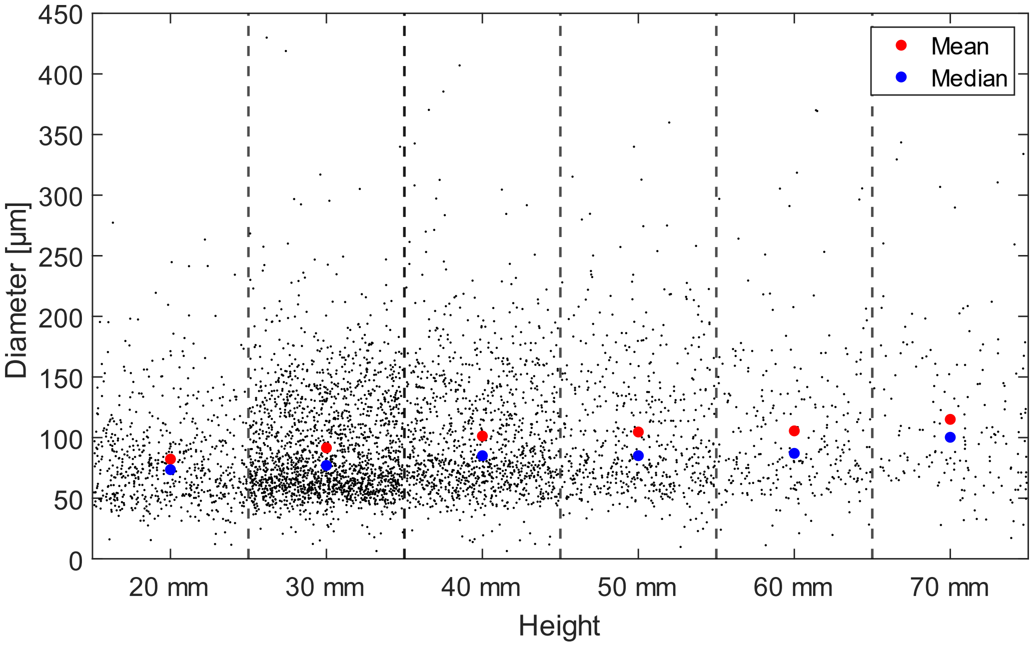

Figure 2. Evolution of aluminium particle diameter as a function of height above the particle inlet into the burner with an atmosphere of 5 %Vol O_2, 20 %Vol H_2O and 75 %Vol CO_2 (captured using the ICCD camera).

Experimental setup and results

In this study, the experimental setup based on a flat flame burner as reactor from previous work [3,4] has been modified to obtain more detailed information in order to characterize the combustion in oxy-fuel atmosphere of aluminum and magnesium particles. In addition to SCOT (Stereoscopic

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Camera system for Optical Thermography), three additional optical measurement methods were applied. First, two different cameras were used: one for high-speed recordings of the particle streak, capturing frame rates of up to 1000 frames per second. Second, a SLR (single-lens reflex) camera was used to capture images of the combustion process. By overlaying these individual images of the SLR camera, it is possible to visualize the entire particle streak in a single image. Third, a spectrometer with a detection range from 200 nm to 1000 nm was employed to identify preliminary trends in intensity and spectrum during the combustion of the investigated metal powders, which may later on be important for temperature measurements.

Figure 2 illustrates the development of the aluminium particle diameter in an atmosphere consisting of O_2, H_2O and CO_2. It is evident that the particle diameter increases along the height of the reactor due to the formation of an oxide layer on the particles.

Measurements on magnesium and aluminum in oxy-fuel atmospheres with 1 $\%_{\mathrm{Vol}}$ and 5 $\%_{\mathrm{Vol}}$ oxygen. The focus is on the development of particle size during combustion, the explosion behaviour of individual magnesium particles, and the optical analysis of the SLR images, the high-speed camera recordings and images from the Stereoscopic Camera system for Optical Thermography (SCOT). The spectrometer results are intended to provide insight into which phase of the combustion of magnesium and aluminium particles exhibits the highest radiation, allowing initial conclusions to be drawn.

In addition to the flat flame burner, a drop tube reactor (DTR) is employed for flash pyrolysis experiments extracting solid samples and perform gas analysis. The data from solid sampling deliver information on the transformation of aluminium and magnesium particles in an H2O and CO_2 atmosphere. The focus of the gas analysis is on the formation of CO and H2 in different atmospheric compositions. The DTR reactor has been previously described in earlier studies [5].

Acknowledgements

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Research on Oxyfuel Combustion of Waste

I. Kaphahn[1*], **K. Stark**[1], **and P. Quicker**[1]
*kaphahn@teer.rwth-aachen.de

[1] *Teaching and Research Unit Thermoprocesses and Emission Control in Waste Management and Recycling, RWTH Aachen University, Wüllnerstr. 2, 52062 Aachen, Germany*

In order to achieve Germany's goal of climate neutrality by 2045, it is necessary to consider CO_2 point sources that are either difficult or impossible to avoid. The climatic impact of municipal solid waste incineration (MSWI) plants is largely determined by the quantity of CO_2 released. The thermal utilisation of one Mg of waste releases, on average, 1.1 Mg of CO_2, approximately half of which is attributed to biogenic sources. Assuming a CO_2 capture rate of 90 %, approximately 13 million Mg/a of fossil CO_2 could be avoided in German MSWI plants [1,2]. It is anticipated that in the future, MSWI plants will assume a central role in a decarbonised, CO_2-neutral hydrogen economy. The capture of CO_2 will become an important source of carbon for the chemical industry, facilitating the closure of the carbon cycles of our society. [3]

The implementation of the oxyfuel process in MSWI plants offers significant advantages with regard to CO_2 capture. In the oxyfuel process, pure oxygen and recirculated exhaust gas are fed into the combustion chamber instead of air. This allows the N_2 content in the exhaust gas stream to be minimised, thereby producing a CO_2-rich exhaust gas stream. Following the separation of impurities, a carbon dioxide-water vapour mixture is produced, from which a CO_2-rich gas stream is obtained by condensing the water. It is expected that the oxyfuel process will result in an enhanced heat transfer within the boiler of the waste incineration plant. [4, 5] In the future, the use of oxygen as a by-product from the electrolysis of water for the production of hydrogen will be a viable option. Further synergies may be realised if the hydrogen is employed in the synthesis of basic chemicals or fuels as part of a CCU route, ideally at the same site. [3, 4]

The combustion of coal in an oxyfuel process has been the subject of extensive research. Using waste as a fuel, the heterogeneous composition results in significant differences in combustion behavior. [6] Individual studies on the oxyfuel process on a pilot scale have been conducted in fluidized bed plants (refuse derived fuels (RDF)/sewage sludge) and in grate furnaces (wood pellets/RDF). Experimental investigations using different gas compositions have demonstrated that an oxyfuel atmosphere comprising 30 vol.% O_2 and 70 vol.% CO_2 resulted in combustion parameters that were comparable to those observed in combustion with air. To date, there has been little consideration of the impact on the composition of the ashes and emissions generated by oxyfuel-combustion of waste. Furthermore, there is currently no definitive analysis of whether the altered pollutant emissions can be safely reduced with the existing flue gas cleaning systems in the context of large-scale implementation in MSWI plants, in order to ensure continued compliance with legal limits. [6, 7, 8, 9, 10]

The objective of our research is to gain a deeper understanding of oxyfuel incineration of waste, with a particular focus on the impact of varying parameters, including gas and waste composition, on emissions and ash composition. The aim is to identify potential technical challenges at a large scale, with a view to enabling the implementation of large-scale tests at two industrial plants in the longer term.

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The first step will be to conduct a comprehensive literature review, with the aim to present the current state of the art of the oxyfuel combustion of waste materials. Furthermore, the oxyfuel combustion of coal in fluidized bed reactors will be considered and investigated with regard to its potential transferability to the oxyfuel combustion of waste in grate furnaces.

A reactor is being designed on a lab scale to investigate the oxyfuel combustion of waste materials in relation to the waste material, oxygen ratio, gas composition and temperature. The effects on the combustion parameters and the flue gas composition will be evaluated. The aim is to achieve similar combustion parameters as observed with air, which is essential to guarantee the operational integrity of the boiler and steam cycle when adapting an existing MSWI facility. The tests are to be conducted with various waste materials with the aim of analyzing the impact of gas and fuel composition on emissions and ash. Moreover, the impact of water vapor in the atmosphere will be examined to evaluate the feasibility of wet or dry recirculation during large-scale implementation.

Concurrently, a theoretical model will be constructed based on the fundamental principles of combustion to calculate the emissions produced by oxyfuel combustion. This will enable the comparison of these calculated values with the experimental results. Additionally, the impact of varying recirculation pathways and rates on the formation of an equilibrium within the combustion atmosphere will be investigated. Finally, the question of the applicability of common exhaust gas cleaning processes in a large-scale implementation of the oxyfuel process will be addressed on the basis of the determined exhaust gas composition and quantity.

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Comparative Analysis of Oxy-Fuel Flames Using Either Carbon Dioxide or Recycled Flue Gas as Diluent with an Air Flame

D. König[*1], **D. Hülsbruch**[1], **J. Ströhle**[1], **and B. Epple**[1]
*dominik.koenig@est.tu-darmstadt.de

[1] *Institute of Energy Systems and Technology, Technical University Darmstadt, Otto Berndt Str. 2, 64287 Darmstadt, Germany*

When changing existing systems from classical air to oxy-fuel combustion, the air is replaced by a mixture of oxygen and recycled flue gas. Here, a similarity between oxy-fuel combustion and air combustion processes is beneficial to avoid significant changes in the existing infrastructure. However, recent scientific research has primarily focused on oxy-fuel combustion using mixtures of pure O_2 and CO_2. In contrast, flue gas recirculation introduces differences in the composition of the oxidizer due to water vapor and impurities such SO_x and NO_x. To effectively evaluate to what extend results obtained with CO_2 as diluent are relevant for industrial-scale applications, it is crucial to conduct comparative measurements under these different oxy-fuel conditions.

This study presents comparative measurements for a reference air case, an oxy-fuel operating condition with flue gas recirculation, and an oxy-fuel condition using a mixture of CO_2 and O_2 that have been carried out in a semi-industrial combustion chamber. All operating conditions maintain a constant thermal power of 420 kW_{th}, along with a consistent momentum flux into the combustion chamber. Under the oxy-fuel conditions, the oxygen content in the flue gas is 33%. As a result, the air-to-fuel ratio differs between the air case and the oxy-fuel conditions. Milled walnut shells are used as fuel in all cases.

To gain a deeper understanding of the flame characteristics, gas samples are extracted from the flame using a suction probe connected to a FTIR gas analyzer. Measurements are taken at four different heights within the combustion chamber, where radial profiles of the gas composition are recorded and analyzed. The primary focus of the analysis is on unburned hydrocarbons (UHC), and CO. These two groups of compounds provide valuable insights into the flame structure and highlight differences between the three operating conditions. Specifically, they reveal variations in temperature profiles and oxygen distribution throughout the flame. For easier interpretation, the experimental data collected are compared with results from other diagnostic techniques, such as flame imaging, under the same operating conditions.

The evaluations suggest that the distribution and peak concentration of UHC change when the combustion atmosphere is switched from N_2 to CO_2. In the upper part of the flame, a higher concentration of hydrocarbons is observed. Moreover, the maximum radial spread of these hydrocarbons shifts to a greater distance from the burner plane. This behavior is consistent for both flue gas recirculation and a synthetic mixture of O_2 and CO_2, though the synthetic flue gas case shows a slightly lower concentration of UHC compared to the recirculation case. It is hypothesized that the higher temperature in the upper part of the flame leads to increased pyrolysis of the fuel, and thus an increased release of hydrocarbons.

In contrast, the concentration of CO exhibits an opposite trend. The maximum radial spread of CO moves to a lower distance from the burner plane for both oxy-fuel operating conditions. However,

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the synthetic oxy-fuel case shows a higher radial spread of CO compared to the flue gas recirculation case. This suggests that changes in the combustion atmosphere influence the combustion chemistry, which in turn affects the distribution of both UHC and CO. The presence of CO in the oxidizer line in the flue gas recirculation appears to have no significant effect on the distribution or occurrence of CO in the flame.

A detailed analysis of various combustion species allows for a direct comparison between similar combustion conditions in air and oxy-fuel atmospheres. The differing properties of the gases involved alter the combustion chemistry, which is reflected in changes in the resulting gas composition. It can be demonstrated that oxy-fuel combustion leads to a higher concentration of UHC in the flame. However, this also results in changes to fuel-rich regions in the flame. With reduced water content in the flame, CO experiences a reduced conversion rate, leading to an increased occurrence of CO in certain areas of the flame.

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Deployment of the Oxyfuel Clinker Burning Process in Cement Industry

J. Lemke[1*], **T. Deck**[1], **I. Veckenstedt**[1], **A. Vogel**[1], **and T. Beisheim**[1]
*jost.lemke@thyssenkrupp.com

[1] *thyssenkrupp Polysius GmbH, Graf-Galen-Str. 17, 59269 Beckum, Germany*

General Situation

The current development of industrial projects for applying the oxyfuel process to Portland clinker production consists of three different approaches. Convertible kiln lines, dedicated oxyfuel kiln lines and hybrid systems with oxyfuel calcination. First industrial pilots have been finished in 2024. First commercial operation with CO_2 sequestration is expected for 2028. In parallel, further development is carried out regarding the combustion of alternative fuels under oxyfuel operating conditions.

Concept Overview

First, kiln lines are built as convertible plants which can operate under conventional and oxyfuel conditions. This is especially relevant for kiln lines which are going to be commissioned way before 2028. Second, kiln lines are being planned for only oxyfuel operation. This is relevant for plants which will step into operation 2028/29 or later. Third, hybrid concepts are being developed, including the oxyfuel operation of the calciner only and eventual post-combustion CO_2 capture of the residual flue gas. This approach is mostly based on project and technology de-risking, lower investment cost and the continued use of rather new equipment which is not subject to replacement.

Ongoing Development

Together with the Collaborative Research Center CRC/TRR 129 Oxyflame, the transfer project "Oxy-fuel combustion of Refuse Derived Fuels (RDF) under cement kiln conditions" supports and improves the engineering of oxyfuel kiln lines which can be operated with various alternative fuels. Lab tests and improved CFD models are employed to predict the alternative fuel combustion as well as the heat transfer inside the kiln.

Industrial Demonstration Projects

Two oxyfuel calciner projects adjacent to existing kiln lines at Zhonglian (Qingzhou, CN) and Heidelberg Materials (Devnya, BG) have been completed. A third project at Taiwan Cement (Hoping, TW) has been announced. The oxyfuel calciner installations consist of an oxyfuel fired hot gas generator, a calciner with cyclone preheater and the necessary oxygen supply. Some of them already include a CO_2 purification and compression, others are built only for demonstrating the calciner operation.

Different from those three projects, the catch4climate project at the Cement Innovation for Climate (CI4C) site (Heidenheim, DE) covers a full oxyfuel kiln line including rotary kiln and clinker cooler to be operated under oxyfuel conditions. This kiln line has been designed as a so-called second generation oxyfuel kiln line, a process patented by the thyssenkrupp Polysius GmbH.

Commercial Projects

While the industrial demonstration projects being commissioned, many commercial projects are already in the planning phase.

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First, convertible kiln lines are under construction. The projects are called Lumbres K6 (Lumbres, FR) and Go4Zero (Oubourg, BE), they are supposed to start conventional operation from 2026 on. Subsequently, the construction of necessary equipment for carbon capture is planned to allow a carbon capture operation from 2028 on.

At the same time, multiple dedicated oxyfuel kiln lines for commercial operation are planned in Croatia (Nexe CO_2NTESSA), Greece (Titan IFESTOS) as well as in Germany (Holcim Carbon2Business and Heidelberg Materials GEZERO). These industrial projects cover the kiln line and necessary equipment like air separation, CO_2 purification, transport, and storage concepts.

Finally, hybrid oxyfuel installations are also in the planning phase. Namely the projects Anthemis (Antoing, BE) and ANRAV (Devnya, BG), both belonging to Heidelberg Materials.

Oxyfuel Combustion of Waste Streams with Oxygen from Electrolysis and Analysis of Utilization Paths of Captured CO_2 with H_2 (WOxyfuel)

V. Nuredin*[1], H-J. Gehrmann[1], S. Grathwohl[2], J. Maier[2],
T. Glorius[3], and Dieter Stapf[1]
* vanessa.nuredin@kit.edu

[1] Institute of Technical Chemistry (ITC), Karslruhe Institute of Technology (KIT),
Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[2] Institute of Combustion and Power Plant Technology (IFK)), University Stuttgart,
Pfaffenwaldring 23, 70569 Stuttgart, Germany
[3] REMONDIS GmbH & Co. KG, Tonstraße 1, 50374 Erftstadt, Germany

Introduction

The utilisation of oxyfuel technology in waste incineration represents a potential path for enhanced CO_2 capture efficiency. The objective of "WOxyfuel" project is to evaluate possible routes to generate oxygen for the combustion process and supply experimental and theoretical data for a MSWI operating under oxyfuel conditions. Experiments are planned at batch and pilot scale. Initially, experiments are conducted at the laboratory fixed-bed reactor KLEAA at ITC. This is followed by experiments at the pilot plant with moving grate ROFEA at IFK. Based on the experimental data also from measurements at a MSWI and process simulations, different scenarios for a MSWI with oxyfuel combustion are calculated including an economic analysis. The study presented here shows preliminary experimental work in the fixed bed reactor.

Lab scale Fixed Bed Reactor

Experiments conducted at "Karlsruher Laboranlage zur Ermittlung des Abbrandverhaltens von Abfällen" (Karlsruhe laboratory facility for determining the combustion behaviour of waste, KLEAA) provide a straightforward method for evaluating the performance of diverse CO_2/O_2 mixtures in waste incineration. The scheme of the reactor is illustrated in Figure 1.

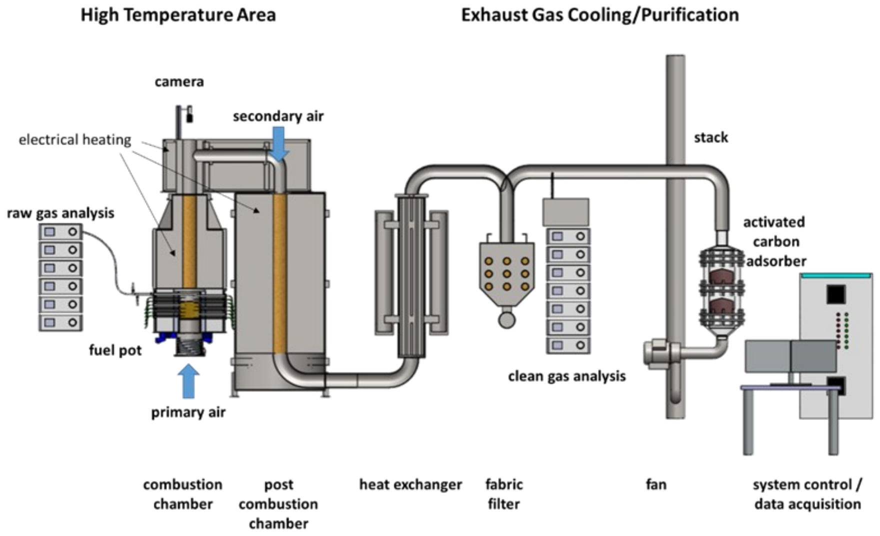

Figure 1. Scheme of the fixed bed reactor KLEAA

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KLEAA is an electrically heated fixed bed reactor with a post combustion chamber. The isothermal reactor has a thermal power of 40 kW. There is a fixed bed volume of 10 liters for the fuels. The reactor operates in a manner comparable to a waste incinerator, utilizing both primary and secondary air. Both pathways are capable of functioning as a mixture of CO_2 and O_2 instead of air. The post combustion chamber is followed by a dry flue gas treatment process with steam boiler, baghouse filter and activated coke filter. KLEAA offers a variety of measurement techniques that enable the analysis of gas in both the flue gas and the cleaned gas.

First results with the quality assured Solid Recovered Fuel SBS1® (RAL-GZ 724 and compliance with ISO 21640) produced from high calorific fractions of MSW and bulky waste by REMONDIS in Erftstadt show a significant influence of the oxygen in the mixture with carbon dioxide on the combustion behavior. The combustion behavior is evaluated by characteristic numbers like the ignition rate, the mass conversion rate and the reaction front velocity, among others. Together with the characteristic numbers the behavior of contaminants in the flue gas is investigated as a function of the oxygen content in the primary and secondary gas.

Simulation of the Flight and Conversion Behaviour of RDF in a Cement Rotary Kiln Under Oxyfuel Conditions Using OpenFOAM

R. Streier[1*], **R. Solana Gómez**[2], **R. Kneer**[2], **I. Veckenstedt**[3], **A. Vogel**[3],
T. Deck[3], **K. Lampe**[3], **and V. Scherer**[1]
*streier@leat.rub.de

[1] *Institute of Energy Plant Technology, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[2] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*
[3] *Cement Process Technology, thyssenkrupp Polysius GmbH, Graf-Galen Straße 17, 59269 Beckum, Germany*

Super-stoichiometric oxy-fuel combustion combined with carbon capture and utilisation (CCSU) is an innovative approach to avoid CO_2 emissions from cement production. Compared to standard oxy-fuel processes, CO_2 recirculation is omitted and replaced by excess oxygen which serves as a diluent to control the temperature inside of the kiln. This results in smaller plant dimensions due to reduced total gas volume flow, leading to lower investment costs. Additionally, replacing coal with refuse-derived fuels (RDF) offers further economic and environmental benefits, as RDF is cost-effective and contains CO_2-neutral biogenic components.

The switch to super-stoichiometric oxy-fuel combustion significantly alters the gas atmosphere compared to a conventional air-fired plant, which affects the local temperature field. These changes in temperature and atmosphere influence the conversion behaviour of RDF, such as flame length and radiative flux, and have to be carefully considered in the process design.

Due to the heterogeneous nature of RDF, conventional CFD mass-point approaches are insufficient to accurately model the complex flight and conversion behaviour of RDF particles. Therefore, corresponding models based on conventional air-fired systems (not for oxyfuel applications) have been developed in the past. These models have been implemented as user defined functions into the commercial software Ansys Fluent.

The present work focuses on an extension (for the purpose of oxyfuel processes) and implementation of already existing RDF simulations models into the open-source software OpenFOAM. Intrinsic kinetic parameters for the individual RDF fractions are obtained using a fluidised bed reactor. A single particle reactor, where oxygen content and temperature can be varied, is used to measure conversion times of individual RDF particles of realistic size. As the size and shape of RDF fractions vary, multiple measurements must be taken for different particles to cover the statistics of conversion times. These data are used to validate the single-particle simulation model. Furthermore, for verifying the simulated flight behaviour, experiments in a drop shaft are conducted, where two high-speed cameras provide a stereo vision of the particles to determine time resolved positions and velocities. The experimentally validated models for simulating the flight and conversion behaviour of RDF under oxyfuel condition are presented and discussed in detail. In addition, first results of a simulation of a cement rotary kiln on an industrial scale are shown.

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Radiative Heat Transfer and Temperature Conditions in a Hybrid Combustion System

I. Qasim[1*], **S. Mishra**[1], **A. Gunnarsson**[1], **N. Striūgas**[2], **A. Tamošiūnas**[2], **and K. Andersson**[1]
*ibrahim.qasim@chalmers.se

[1] *Department of Space, Earth and Environment, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*
[2] *Lietuvos energetikos instituta, Breslaujos g. 3, LT-44403 Kaunas, Lietuva*

Greenhouse gas (GHG) emissions, especially CO_2, are a significant global concern in many industries, where fossil fuels drive the energy-intensive, high-temperature processes required for production. This reliance on conventional fuels impacts climate change and highlights the industry's need for more sustainable and flexible energy solutions. Here, thermal plasma technology offers a promising path forward. With its ability to reach extremely high temperatures and support the combustion process of alternative fuels, plasma-based systems can directly reduce GHG emissions and lessen dependency on traditional fuels. This study aims to characterize the heat transfer in an experimental hybrid plasma combustion system for fuel-flexible glass manufacturing, focusing on methane (CH_4) and hydrogen (H_2) combustion with and without plasma assistance as well as presenting temperature estimations of the same.

The study is based on experiments conducted using a 50 kW_{el} plasma generator and 100 kW_{th} combustion burner to study the combustion of CH_4 and H_2 with and without plasma assistance. The experimental setup included detailed measurements of radiative intensity, flame structure, and temperature distribution, using Narrow Angle Radiometers (NAR) and a FLIR infrared (IR) camera. Four NAR probes, each equipped with a thermopile detector sensitive to wavelengths between 1-100 µm, were positioned along the flame axis, measuring radiative intensity, and the IR camera, with a spectral range of 7.5-14 µm, were placed opposite to these probes to capture detailed flame radiance profiles and structural dynamics across the axial length (Figure 1).

Figure 1. Experimental setup showing (a) IR camera (b) Plasma jet (c) NAR probes (d) Burner

The NAR measurements show a distinct radiative intensity profile, peaking at the second downstream NAR probe placed at 17 cm from the burner, indicating a somewhat local hot zone along the flame axis for both pure combustion and plasma-assisted combustion cases. The hydrogen cases consistently showed on higher radiative intensity values than the methane cases for both combustion modes. In both plasma-assisted and non-plasma-assisted cases, the radiative intensity increased with increasing plasma power, highlighting plasma's role in enhancing combustion.

In contrast to the NAR measurements, the IR camera radiance profiles showed on a concentrated radiance near the plasma source, decreasing gradually along the flame's axial length for the plasma-assisted cases. Still, both methane and hydrogen cases displayed similar radiance patterns, with the highest radiance recorded at the probe position close to the plasma generator suggesting the majority of radiative energy being emitted close to the plasma source. However, combustion cases show lower values near the burner end and increase along the flame's axis. This difference between the two measurement techniques in terms of radiance profile can probably be attributed to different spectral ranges of the equipment and is partly examined within this work.

This work further aims to present estimations of reasonable temperature ranges for the various cases. Based on basic combustion and heat balances, gas composition at the NAR probe positions are estimated and a discrete transfer method using the Malkmus statistical narrow-band model for gases is applied to fit modelled and measured radiative intensities as a function of temperature.

This initial experimental campaign provides foundational insights into heat transfer in a hybrid plasma combustion system. The findings on radiative intensity offer a basis for optimizing fuel flexibility and combustion efficiency. Future work will build on these results to refine plasma-assisted combustion models and support pilot-scale applications.

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Viktor Scherer
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RWTH Aachen University
Institute of Heat and Mass Transfer (WSA)
Augustinerbach 6
52056 Aachen
Germany

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