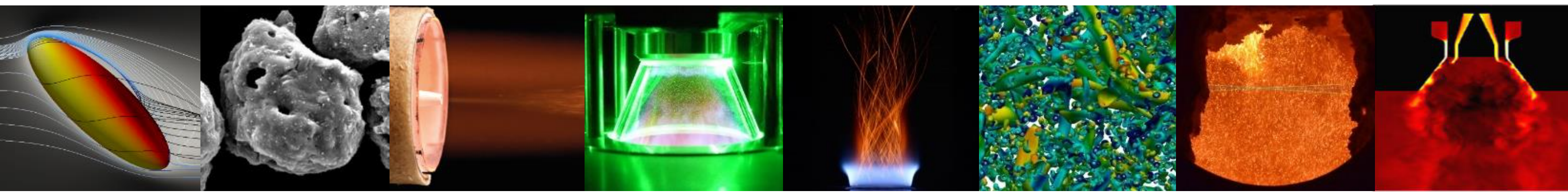
Book of Abstracts

edited by
S. Pielsticker, A. Maßmeyer, V. Scherer, H. Pitsch,
A. Dreizler, O. Senneca, R. Kneer



4th International Workshop on Oxy-Fuel Combustion

organized by the

Collaborative Research Center “Oxyflame”

in cooperation with

STEMS-CNR Naples

March 22nd–23rd, 2023
STEMS-CNR in Naples, Italy

SFB/TRR 129 Oxyflame STEMS

doi 10.18154/RWTH-2023-06259

4th International Workshop on Oxy-Fuel Combustion

Book of Abstracts

2023

edited by

S. Pielsticker[1], A. Maßmeyer[1], V. Scherer[2], H. Pitsch[3],
A. Dreizler[4], O. Senneca[5] 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] Simulation of reactive Thermo-Fluid Systems (STFS), TU Darmstadt, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany
[5] Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS), Piazzale Vincenzo Tecchio 80, 80125 Napoli, Italy

Available via the institutional repository of RWTH Aachen University:

DOI: 10.18154/RWTH-2023-06259

Preface

For the 4th 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 in cooperation with the Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS) of the Italian National Research Council (CNR).

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 three successful workshops in 2016, 2018, and 2020, this fourth edition has been organized by Prof. Viktor Scherer and his group from LEAT (Bochum) with the help of the local organizing committee led by Prof. Osvalda Senneca (Naples) at the Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS) of the National Research Council (CNR). The 4th International Workshop on Oxy-Fuel Combustion took place from 22nd to 23rd of March 2023 in Naples (Italy), where everyone could benefit from the mild Neapolitan spring temperatures, that even permitted an outdoor poster session. To top off the good food during the conference, the social dinner on the evening of the first day took place at the seaside restaurant La Bersagliera. These fortunate circumstances 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: “Oxy-fuel Processes”, “Biomass Pyrolysis”, “Modeling and Simulation”, “Gasification, Pyrolysis & Heat Transfer”, “Optical Measurements”, and “Combustion Fundamentals”, with one keynote lecture, 36 oral presentations and 23 posters.

Abstracts

Oxy-fuel Processes

Biomass Pyrolysis

Modeling and Simulation

Gasification, Pyrolysis & Heat Transfer

Optical Measurements

Combustion Fundamentals

NH_3 oxidation and NH_3-NO interaction in air and oxy-fuel combustion conditions

M. U. Alzueta[1*], V. Mercader[1] and J. Giménez-López[1]

*uxue@unizar.es

[1] Aragón Institute of Engineering Research (I3A), Dept. of Chemical and Environmental Engineering. Río Ebro Campus, University of Zaragoza. 50018 Zaragoza, Spain

Ammonia conversion has become a major topic of research, mainly because of its interest as a carbon free fuel [1, 10, 11, 17, 18, 19]. Ammonia can also be generated as an intermediate product in conversion of coal, biomass and other fuels containing nitrogen [7]. While, ideally, ammonia combustion will generate molecular nitrogen and water vapor as reaction products, practical devices may run far from ideality and thus contribute to the generation of nitrogen oxides, mainly NO, depending on the operating conditions [1, 3, 16].

Additionally, the use of different combustion strategies, such as oxy-fuel combustion, may affect the oxidation regimes of ammonia and the formation of pollutant species. The presence of high amounts of CO_2, as found in oxy-fuel combustion, can lead to significant differences in the oxidation behavior of species. Studies dealing with oxidation of HCN [4], HCN-NO [5], NH_3 [2] or NH_3-CH_4 [12, 13] under oxy-fuel combustion conditions have shown an important influence of the presence of CO_2 for the conversion of nitrogen species. The presence of CO_2 has been reported to affect the concentration and speciation of the O/H radical pool [6, 13, 4], since CO_2 competes with O_2 for atomic hydrogen through the $CO_2+H=CO+OH$ reaction (r1). Reaction r1 reduces the formation of chain carriers by the $O_2+H=O+OH$ reaction (r2), thus affecting the conversion of reactants.

NO can be produced from ammonia oxidation, and thus the interaction of NH_3 and NO is of interest. Selective non-catalytic reduction (SNCR) of NO by NH_3 is a well-known process [8, 9, 14,15], but the impact of a high CO_2 concentration such as that occurring in oxy-fuel combustion may affect the interaction of the nitrogen species (NO and NH_3).

In this context, the present work addresses the effect of a CO_2 environment, representative of oxy-fuel combustion conditions, compared to an O_2/N_2 environment, representative of conventional combustion, on the conversion of ammonia. Furthermore, the impact of the presence of NO, both related to conversion of ammonia and to the minimization of this pollutant, in a CO_2 atmosphere is compared to the conventional combustion scenario.

Acknowledgement

Grant Ref. PID2021-124032OB-I00 funded by MCIN/AEI/ 10.13039/501100011033 and by ERDF A way of making Europe.

References

[1] M. Abián, M. Benés, A. de Goñi, B. Muñoz, M. U. Alzueta, Study of the Oxidation of Ammonia in a flow reactor. Experiments and kinetic modeling simulation, Fuel 300 (2021) 120979.

[2] M.U. Alzueta, J. Giménez-López, V.D. Mercader, R. Bilbao. Conversion of NH_3 and NH_3-NO in a CO_2 atmosphere. A parametric study, Fuel 327 (2022) 125133.

[3] M. Barbas, M. Costa. S. Vranckx, R.X. Fernandes, Experimental and chemical kinetic study of CO and NO formation in oxy-methane premixed laminar flames doped with NH_3, Combust. Flame 162 (2015) 1294–1303.

[4] J. Giménez-López, A. Millera, R. Bilbao, M.U. Alzueta. HCN oxidation in an O_2/CO_2 atmosphere: An experimental and kinetic modeling study. Combust. Flame, 157 (2010) 267-276.

[5] J. Giménez-López, A. Millera, R. Bilbao, M.U. Alzueta. Interactions of HCN with NO in a CO_2 atmosphere representative of oxy-fuel combustion conditions. Energy Fuels, 29 (2015) 6593-6597.

[6] P. Glarborg, L.L.B. Bentzen. Chemical effects of a high CO_2 concentration in oxy-fuel combustion of methane. Energy Fuels, 22 (2008) 291-296.

[7] P. Glarborg, A.D. Jensen, J.E. Johnson. Fuel nitrogen conversion in solid fuel fired systems. Prog. Energy Combust. Sci., 29 (2003) 89-113.

[8] P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Modeling nitrogen chemistry in combustion, Prog. Energy Combust. Sci. 57 (2018) 31-68.

[9] S.J. Klippenstein, P. Glarborg. Theoretical kinetics predictions for NH_2+HO_2. Combust. Flame 236 (2022) 111787.

[10] H. Kobayashi, A. Hayakawa, K.D.K.A. Somarathne. E.C. Okafor, C. Ekenechukwu, Science and technology of ammonia combustion, Proc. Combust. Inst. 37 (2019) 109-133.

[11] M.V. Manna, P. Sabia, R. Ragucci, M. de Joannon, Oxidation and pyrolysis of ammonia mixtures in model reactors, Fuel 264 (2020) 116768.

[12] T. Mendiara, P. Glarborg, Ammonia chemistry in oxy-fuel combustion of methane, Combust. Flame 156 (2009a) 1937-1949.

[13] T. Mendiara, P. Glarborg, NO reduction in oxy-fuel combustion of methane, Energy Fuel 23 (2009b) 3565-3572.

[14] J.A. Miller, C.T. Bowman. Mechanism and modeling of nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 15, 287-338, 1989.

[15] J.A. Miller, M.C. Branch, R.J. Kee, "A chemical kinetic model for the selective reduction of nitric oxide by ammonia." Combust. Flame 43 (1981) 81–98.

[16] J.A: Miller, M. D. Smooke, R. M. Green, R. J. Kee. "Kinetic modeling of the oxidation of ammonia in flames." Combust. Sci. Technol. 34 (1983) 149-176.

[17] Y. Song, H. Hashemi, J.M. Christensen, C. Zhou, P. Marshall, P. Glarborg, Ammonia oxidation at high pressure and intermediate temperatures, Fuel 181 (2016) 358-365.

[18] A. Stagni, C. Cavalloti, S. Arunthanayothin, Y. Song, O. Herbinet, F. Battin-Leclerc, T. Faravelli, An experimental, theoretical and kinetic-modeling study of the gas-phase oxidation of ammonia, React. Chem. Eng. 5 (2020) 696-711.

[19] A. Valera-Medina, H. Xiao, M. Owen-Jones, W.I.F. David, P.J. Bowen PJ. Ammonia for power, Prog. Energy Combust. Sci. 69 (2018) 63-102.

Development of a comprehensive kinetic model of biomass conversion in inert, air and oxy-fuel conditions

P. Debiagi[1*], S. Pielsticker[2], F. Cerciello[3], V. Scherer[4],
R. Kneer[2], T. Faravelli[5] and C. Hasse[1]

*debiagi@stfs.tu-darmstadt.de

[1] *Institute for Simulation of reactive Thermo-Fluid Systems, TU Darmstadt, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany*
[2] *Institute of Heat and Mass Transfer (WSA), RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*
[3] *Laboratory of Industrial Chemistry, Ruhr-University Bochum, Universitätsstr. 150, 44780 Bochum, Germany*
[4] *Institute of Energy Plant Technology (LEAT), Ruhr-University Bochum, Universitätsstr. 150, 44780, Bochum, Germany*
[5] *Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milan, Italy*

The thermochemical conversion of biomass is a complex process that comprehends a pyrolysis step when chemical bonds break and different products are formed, including gases, tars, and a carbon-rich solid char. These products further react with the surrounding atmosphere in homogeneous gas-phase reactions and heterogeneous gas-solid reactions. As the pyrolysis rate and product distribution strongly influence the subsequent thermochemical conversion processes, an adequate mathematical modeling is required for simulations of combustion furnaces.

In this work, a comprehensive multi-step kinetic model is proposed, developed to seamlessly describe the pyrolysis of biomass including a detailed gas and tar product distribution, and the subsequent char conversion in oxy-fuel environments. The model considers the decomposition of biomass as a linear combination of its main constituents: cellulose, hemicellulose, lignin, and extractives, which are modeled using a set of reference species: CELL represents the cellulose polymer; GM_{SW}, XY_{HW}, and XY_{GR} represent hemicellulose from softwoods, hardwoods and grass/cereal biomasses; LIG_C, LIG_H, and LIG_O represent lignin with varying elemental composition; TGL and TANN represent extractive species (see Fig. 1). Since the thermal decomposition of these species widely differ in terms of rates and products, for each reference species a dedicated multi-step kinetic mechanism is proposed, which contains competing reactions for low- and high-temperature decomposition. By combining the pyrolysis behavior of the reference species, the decomposition of real biomass feedstocks can be described. Within this study, pulverized walnut shells serve as a representative biomass.

Walnut shells have been analyzed with proximate (76.7 % volatiles, 20.9 % fixed carbon, and 0.53 % ash) and ultimate (52.1 % C, 5.8 % H, and 41.8 % O) analysis. Different analytical methods were used to quantify the main constituents: An innovative approach combining analysis and TGA experiments supported the quantification of hemicellulose (31 %), cellulose (17 %), lignin (38.5 %), and extracts (8.5 %) on a dry basis. The extractive fraction, mainly phenolic compounds, was not accurately represented by the existing TANN species, so a new species, $TANN_H$, was proposed. The organic fraction of walnut shells was characterized as a mixture of 17 % CELL, 31 % XY_{HW}, 17 % LIG_C, 17 % LIG_H, 4.5 % LIG_O, and 8.5 % $TANN_H$.

In the first step of the development phase of the model, the CRECK-S-B [1] model was initially used to benchmark the rate of decomposition and product distribution for the biomass components from walnut shells. Using the abovementioned characterization, the model predicted pyrolysis products obtained at 1073 K in an inert thermogravimetric analysis (TGA) at a low heating rate

(10 K/min) resulted in 21.8 % of char, in comparison to 21.4 % obtained experimentally. This indicates an adequate characterization of the sample as well as the model's suitability to describe the pyrolysis of this biomass. The comparison of the mass loss rate (Fig. 1), showed agreement in the presence of two main mass loss peaks (550 and 630 K), corresponding to hemicellulose and cellulose decomposition, respectively. The model, however, predicts slower decomposition to hemicellulose, resulting in a less intense peak when compared to the experiment. The cellulose instead shows nearly identical peak height but predicted the peak at about 10–20 K later than in the experiments. These discrepancies can be directly related to the particularities of the walnut shell components, which could be caused by the degree of acetylation in the hemicellulose polymer, the crystallinity of the cellulose polymer, and the catalytic effects of minerals in the ashes. These characteristics lead to divergences from the general behavior described by the CRECK-S-B, which is not fuel-specific. Such particularities need to be considered when developing a fuel-specific model.

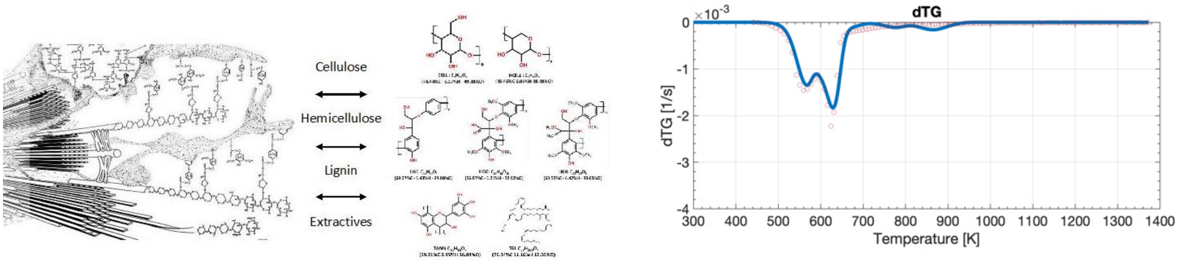


Figure 1. Depiction of the biomass main components, translation into the model's reference species, and the comparison of walnut shell mass loss rate in a TGA under inert conditions.

The development and validation of the fuel-specific model are then performed using the large experimental data set obtained for the walnut shell feedstock [2], including TGA, fixed bed reactor, heated strip reactor (HSR), drop-tube reactor (DTR), fluidized bed reactor (FBR) and flat-flame burner (FFB). The TGA provides kinetically controlled data at very low heating rates, supporting the necessary calibration of the model's rate of decomposition and overall phase product distribution for such conditions. The drop-tube reactor experiments provide high heating rate data on volatile products and solid residue yields. The effect of the particle temperature history along the reactor was thoroughly evaluated, highlighting the need for considering heat transfer effects and reliable data for accurate predictions of mass loss and yields. In future works, the proposed kinetic mechanism must be further validated for the additional experimental data available for these samples, allowing to complete the kinetic modeling of all steps of the thermochemical conversion.

Acknowledgements

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

References

[1] Debiagi, P., Faravelli, T., Hasse, C. and Ranzi, E., 2020. Kinetic Modeling of Solid, Liquid and Gas Biofuel Formation from Biomass Pyrolysis. In *Production of Biofuels and Chemicals with Pyrolysis* (pp. 31-76). Springer, Singapore.

[2] Senneca, O., Cerciello, F., Cortese, L., Heuer, S., Schiemann, M. and Scherer, V., 2018. Effects of CO_2 enriched atmosphere on chars from walnut shells pyrolysis in a drop tube reactor. *Fuel*, *229*, pp.235-240.

Oxy-co-firing coal and agro-waste biomass under O_2/CO_2 and $O_2/CO_2/H_2O$ atmospheres

L. I. Díez[1*], A. García-Mariaca[1], E. Llera[1] and P. Canalís[1]

*luisig@unizar.es

[1] Department of Mechanical Engineering, University of Zaragoza, María de Luna s/n, 50018 Zaragoza, Spain

Oxy-fuel combustion is one of the CO_2 capture techniques that can be implemented in large-scale power plants and some heat-intensive industrial processes. A lot of research has been done in the last 15–20 years addressing fossil fuels combustion (conversion, fluid dynamics, heat transfer and pollutants formation) under O_2/CO_2 atmospheres, from lab-scale facilities to singular demo-scale plants. Nevertheless, the available experiences related to oxy-fuel combustion of biomass are much more limited. The integration of bio-fuels with CO_2 capture and storage techniques (Bio-CCS) leads to the concept of negative emissions energy systems.

In this paper, an experimental investigation concerning oxy-fuel combustion of blends of coal and biomass is described and discussed. Three different types of biomass were selected to proceed with the experimental campaigns, two of them obtained from agro-wastes (vineyard, corn) and the third one from forestry residues (pine). O_2-enriched atmospheres could offer a good chance for low-to-mid grade biomasses, whit a very restricted use so far in conventional combustion.

The experimental campaigns were carried out in an entrained flow reactor (see Figure 1), able to operate under O_2/N_2, O_2/CO_2 and $O_2/CO_2/H_2O$ atmospheres. The shares of the biomass in the blends were 20 % and 50 % (mass basis) in order to not only seek the effect of the biomass type but also the coal-to-biomass ratio. O_2 concentration was 21 % and 35 %, covering a typical range used in oxy-fired units. Two H_2O concentrations were initially used (replacing CO_2) to resemble dry-recycle oxy-combustion (0% H_2O) and wet-recycle oxy-combustion (10 % H_2O). Two additional larger H_2O concentrations were also tested, 25 % and 40 %, aiming to provide further knowledge about the effect of steam, towards the so-called oxy-steam combustion. This concept has recently received some attention, proposing H_2O recycling – instead of CO_2 – to dilute oxygen concentration and moderate flame temperature.

Three variables were obtained after each experiment and related to the fuel fired and the test conditions: burnout (solid-to-gas conversion), C-fuel conversion to CO and N-fuel conversion to NO. Fuel conversion is logically the largest when co-firing 50 % coal and 50 % pine wood, but the differences with agro-biomasses are significantly reduced when O_2 concentration is raised from 21 % to 35 %. As concerns the effect of CO_2 replacement by H_2O, maximum burnout rates are obtained for 25 % H_2O in most cases. Steam increases flame temperature, O_2 diffusivity and char gasification, but a reduction of char specific surface is also detected for the experiments conducted under the largest steam concentrations.

Nitrogen bound in the fuel and O_2 concentration largely determine NO formation rates. Since nitrogen content in the selected agro-waste biomasses is about 8 times the nitrogen content in forestry biomass, maximum NO levels are obtained when co-firing 50 % agro-biomass under 35 % O_2 atmosphere. As concerns the effect of CO_2 replacement by H_2O, significant reductions in N-fuel to NO formation are observed, but not proportional to the steam concentrations. The volatile-to-fixed carbon ratio in the blends is also influencing the results: the higher the ratio, the lower the reducing effect of the added H_2O in comparison to the dry atmospheres.

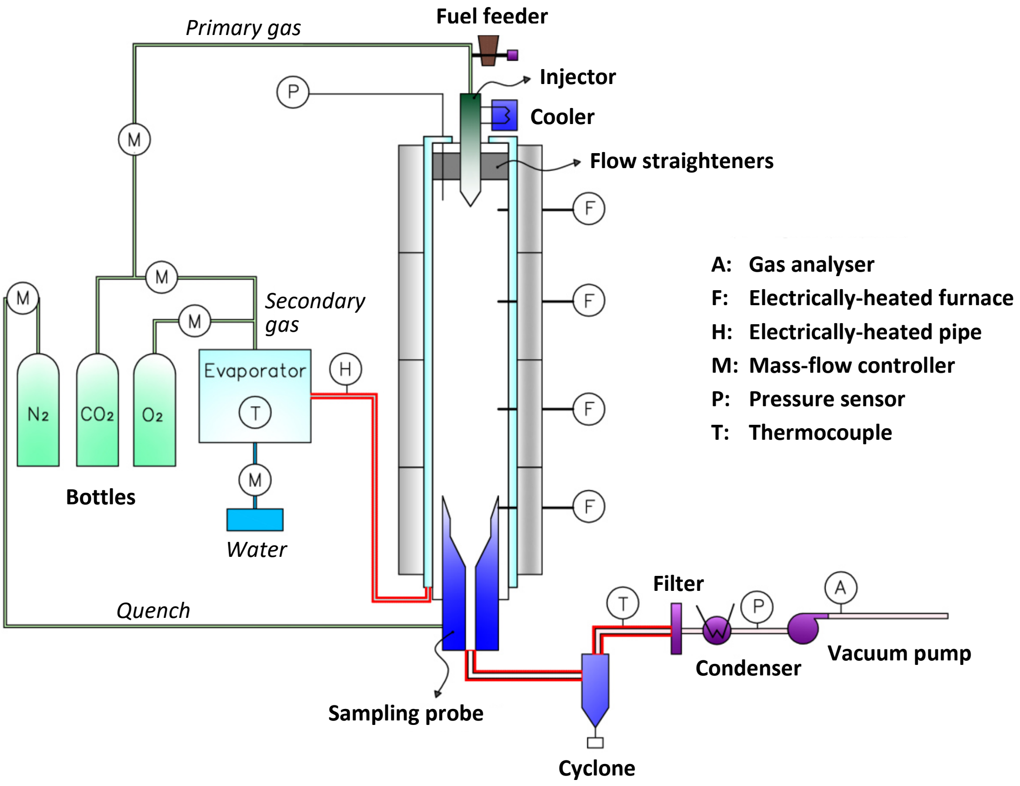


Figure 1. Lab-scale entrained flow reactor.

10.18154/RWTH-2023-06259

On the inaccuracies of particle models for char conversion

T. R. Jayawickrama[1], N. E. L. Haugen[1,2] and K. Umeki[1*]

*kentaro.umeki@ltu.se

[1] *Division of Energy Science, Luleå University of Technology, Universitetsområdet Porsön, 971 87 Luleå, Sweden*

[2] *Department of Thermal Energy, SINTEF Energy Research, Kolbjørn Hejes vei 1 A, 7491 Trondheim, Norway*

Introduction

Char conversion is a complex phenomenon that involves not only heterogeneous reactions but also external and internal heat and mass transfer. Reactor-scale simulation often uses a point-particle approach (PP) as sub-models for char conversion because of its low computational cost. Despite a number of simplifications involved in the PP, there are very few studies that systematically investigate the inaccuracies of the PP.

This study aims to compare and identify the origins of inaccuracies in the point-particle approach for char gasification modelling. We simulated a char particle undergoing CO_2 gasification under zone II conditions (*i.e.,* pore diffusion control) using both point particle approaches and particle resolved (RP) approaches. Both the exterior and interior of the particle are resolved simultaneously to study the interaction of heat and mass transfer between the particle interior and the boundary layer. A non-equimolar gasification reaction is considered to create a Stefan flow. We try to identify the differences between the two approaches and the reasons behind the differences. Suggestions for improvements of the point-particle approaches are also made.

Major results

Analyses showed that existing models underestimate external heat transfer and overestimate external mass transfer rates. The overall effects of external heat and mass transfer are dominated by the low particle temperature prediction, mainly due to the strong temperature dependence of reaction rates. None of the heat transfer terms, including conduction through the boundary layer, advective heat transfer due to Stefan flow, or Dufour effects in the boundary layer could explain this deviation.

The dominant source of inaccuracies for the intra-particle heat and mass transfer is the effect of non-uniform temperature distribution, *i.e.,* lower particle temperature due to endothermic reactions. Since the effectiveness factor commonly applied in char conversion models does not consider the effects of non-uniform temperature, it always overestimates the effectiveness factor. The inaccuracy in predicting the effectiveness factor also results in the inability to predict the particle size changes.

When the inaccuracies of both external and internal heat and mass transfer are accounted for, the outcome is dependent on the effectiveness factor because of the shift in their relative importance. When the effectiveness factor is relatively large (close to zone I conditions), the errors in external heat transfer dominate the overall conversion rates. When the effectiveness factor is smaller (near zone III conditions), the inaccuracy of assuming a uniform particle temperature becomes more important, and the results from the point particle approach tend to overestimate the conversion rates.

Interestingly, this study sheds light on many occasions when one or more parameters from the results agreed very well with the RP results, solely by the coincidence of two or more errors canceling each other. It strongly suggests that the accuracy of the point particle approach should be examined thoroughly by comparing several parameters, preferably at a wide range of reaction conditions.

Other potential sources of errors, such as the 2D/3D asymmetry and intra-particle convective flows, were also identified. Future studies should include comprehensive comparisons of several different modeling approaches, such as the point particle approach, one-dimensional particle model, and multi-dimensional resolved-particle model with and without the direct solution of external flows.

Numerical study of the flame instability in oxy-fuel combustion with differential diffusion effect

X. Jiang[1], J. Guo[2*], Hong G. Im[2] and Z. Liu[1]

*junjun.guo@kaust.edu.sa

[1] *State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan 430074, China*

[2] *Clean Combustion Research Center, Physical Sciences and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia*

In oxy-fuel combustion, the high CO_2 concentration leads to changes in the flow structure and combustion characteristics, which significantly affect the flame stability. The experiments in the 35 MW_{th} oxy-fuel combustion facilities found that the fluctuations of temperature and radiant energy of the oxy-fuel flame were significantly different from those of the air-fuel flame. Numerical studies of flame instability in turbulent conditions are challenged by the need to fully describe the complex interaction of molecular diffusion, turbulence, and chemical reactions. Many exiting combustion sub-models commonly employ the unity Lewis number assumption. However, the low molecular diffusion of CO_2 results in strong differential diffusion effects in turbulent oxy-fuel flames, and the both effects of molecular diffusion and turbulent diffusion on flame instability cannot be ignored. To the end, the purpose of this study is to numerically study the effects of the thermal, chemical, and transport properties of CO_2 on the flame instability in oxy-fuel conditions by considering differential diffusion effects.

The target flame is a turbulent CH_4/H_2 oxy-fuel flame experimentally studied by Sevault et al. [1]. The fuel nozzle has an inner diameter of 5 mm, surrounded by co-flow. The bulk velocity of the fuel jet is 117.8 m/s with the Reynolds number of 18,000. The fuel is a mixture of 45 % CH_4 and 55 % H_2 by volume, and the co-flow is 32 % O_2 and 68 % CO_2 by volume. To isolate the effects of the thermal, chemical, and transport properties of CO_2, two fictitious species (FN_2 and FCO_2) are introduced to replace CO_2 in the oxidant, as shown in Table 1. FN_2 has the same chemical and transport properties of N_2, while its thermal properties are the same with CO_2. FCO_2 has the same thermal and transport properties of CO_2, but is not allowed to participate in any chemical reactions.

Table 1. Simulated cases

Cases	Oxidizer components [vol. %]				
	O_2	N_2	FN_2	FCO_2	CO_2
B3N2	32	68	--	--	--
B3FN2	32	--	68	--	--
B3FCO2	32	--	--	68	--
B3	32	--	--	--	68

Large eddy simulations are performed. Under the framework of progress/variable model (FPV), a species-weighted flamelet (SWF) model proposed in our previous study [*Jiang et al. CNF 2022 (under review)*] is used to consider the differential diffusion effects on turbulent flame modelling. The GRI-Mech 3.0 mechanism is used for fuel pyrolysis and oxidation.

Figure 1 shows the instantaneous scatters of temperature and conditional mean temperature profiles in the mixture fraction space. The transport properties of CO_2 provide the greatest effect on the flame instability in oxy-fuel conditions, followed by the chemical properties of CO_2. In contrast, the thermal properties have the weakest effect. Moreover, further analysis shows that the transport properties of CO_2 significantly increase the magnitude and frequency of local extinction, while the chemical properties of CO_2 increase the local extinction time. The chemical and transport properties of CO_2 enhance the thermo-diffusive instability of the flame.

References

[1] Alexis Sevault, Matthew Dunn, Robert S. Barlow, Mario Ditaranto, On the structure of the near field of oxy-fuel jet flames using Raman/Rayleigh laser diagnostics, Combustion and Flame159 (11), 2012, 3342–3352

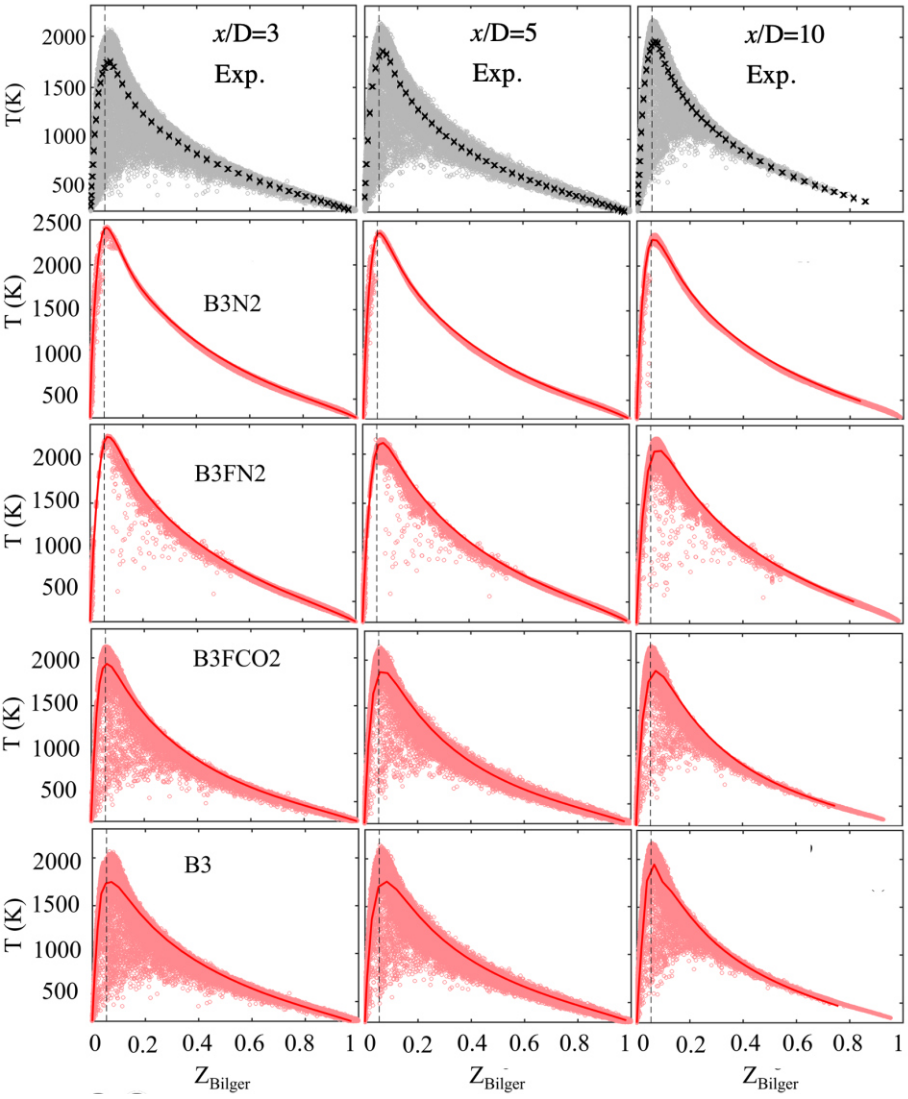


Figure 1. Comparison of instantaneous scatters of temperature in mixture fraction space. The black dash line is the Z_{st}.

Oxy-fuel combustion of hydrogen for the decarbonization of high-temperature process heat

J. Leicher[1*], T. Nowakowski[1], A. Giese[1] and K. Görner[1]

*joerg.leicher@gwi-essen.de

[1] *Gas- und Wärme-Institut Essen e.V (GWI)., Hafenstrasse 101, 45356 Essen, Germany*

While the combustion of solid or gaseous fuels with an O_2/CO_2 oxidizer is being discussed as measure to enable CCS and thus reduce greenhouse gas emissions from power generation, the combustion of natural gas (or other combustible gas blends) with almost pure oxygen has long been industrial practice for high-temperature process heating, e. g. in the metals or glass industries. Here, oxy-fuel combustion offers benefits in process efficiency, excellent heat transfer, better heating rates and reduced pollutant emissions.

Process heat plays a significant role in the global energy demand. Given the need for decarbonizing energy-intensive manufacturing processes, there is a growing interest in the oxy-fuel combustion of carbon-free fuels such as hydrogen, especially for high-temperature applications. The very different combustion characteristics of hydrogen (or natural gas/hydrogen blends) compared to natural gas require, however, a good understanding of how the fuel switch will affect sensitive industrial manufacturing processes in terms of product quality, heat transfer, efficiency or pollutant emissions, particularly nitrogen oxides emissions (NO_X)

Both computational fluid simulations (CFD) and experimental investigations on a semi-industrial scale are important tools to gain a better understanding of these new fuels and their impact on oxy-fuel combustion processes in energy-intensive industries. This contribution focuses on the differences in the oxy-fuel combustion of hydrogen in comparison to natural gas in high-temperature gas-fired industrial manufacturing processes, based on both detailed investigations in semi-industrial combustion test rigs and RANS simulations, carried out at GWI. Corresponding investigations with natural gas are used as a baseline of common industrial practice today.

One additional aspect to consider when using hydrogen-rich fuels in combustion applications is the question of how to quantify and assess pollutant emissions, especially compared to conventional fuels such as natural gas. This is particularly relevant in the context of oxy-fuel combustion of hydrogen, where the flue gas primarily consists of water vapor. This issue and its consequences for the deployment on hydrogen-rich fuels will also be discussed.

Up-scaling of a lab-scale oxyfuel burner to a 1 MW$_{th}$ semi-industrial oxyfuel combustion chamber

M. Richter[1*], A. Maßmeyer[2], H. Askarizadeh[2], J. Ströhle[1] and B. Epple[1]

*marcel.richter@est.tu-darmstadt.de

[1] Institute of Energy Systems and Technology, TU Darmstadt, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany

[2] Institute of Heat and Mass Transfer, RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany

A major challenge in engineering is the transfer of findings from laboratory-scale experiments and simulations to a large-scale industrial application.

In this study, a detailed flow analysis is used to scale-up a 60 kW$_{th}$ pulverised solid fuel burner working under oxyfuel conditions to a semi-industrial scale with 1 MW thermal power. One way to scale the burner is to use the same velocities at the burner outlet. For this purpose, the inlets of the semi-industrial burner have to be adjusted in order to imply similar flow conditions entering the combustion chamber as in the lab-scale chamber. Unfortunately, this approach is not always feasible, since semi-industrial systems have a higher pulverised fuel loading in the metering system, in the pipes of the facility and in the burner channels themselves. Excessive pulverised fuel loading, due to insufficient velocities of the carrier medium, can cause blockages in the piping and in the burner channels. The present approach focuses on similarities for the scaling of an oxyfuel pulverised fuel fired chamber. Especially, the flow field of the laboratory combustion chamber is used as the reference with focus on recirculation zones. These zones are important for the transport of hot combustion gases, unburned particles and radicals back into the reaction zone of the flame. Recirculation zones in the flame lead to stabilization of the flame and offer an aerodynamic alternative to flame stabilisation under oxyfuel conditions with higher oxygen concentrations. For the investigated oxyfuel combustion chamber of 60 kW$_{th}$, which will be scaled up to 1 MW$_{th}$, CFD simulations (RANS) showed that the geometry of the burner diffuser and the velocity ratio of primary and secondary oxidiser stream of approx. 1:2 are decisive. Another important parameter for the recirculation in the flame is the swirl number, which is kept identical for the lab-scale and the semi-industrial burner.

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

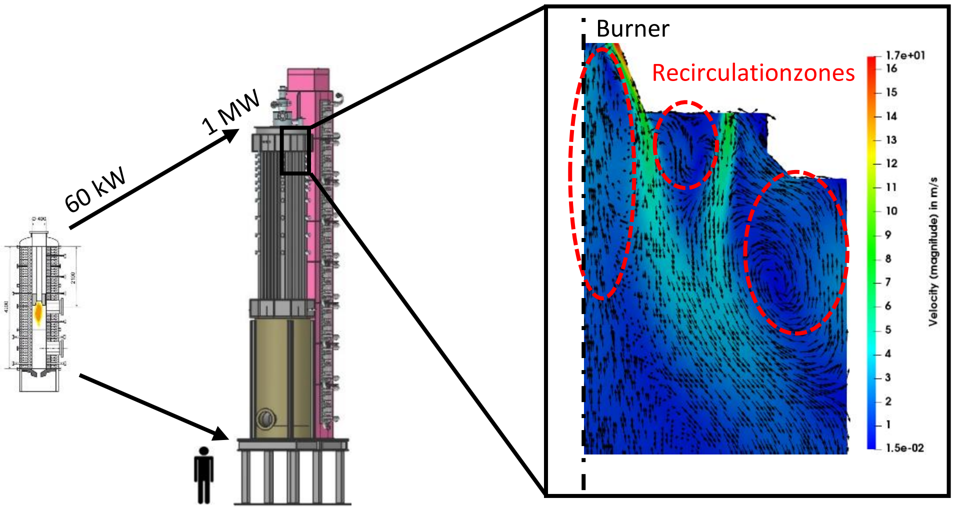


Figure 1. Scaling from a 60 kW$_{\text{th}}$ oxyfuel combustion chamber to a 1 MW$_{\text{th}}$ semi-industrial firing system with the simulation results of the velocity field.

Influence of minerals on the pyrolysis of hydrothermally carbonized biomass

J. Böttger[1], T. Eckhard[1], C. Pflieger[1], O. Senneca[2],
M. Muhler[1] and F. Cerciello[1]*

* francesca.cerciello@ruhr-uni-bochum.de

[1] *Laboratory of Industrial Chemistry, Ruhr University Bochum, Universitätsstraße 150, 44801 Bochum, Germany*
[2] *Istituto di Scienze e Tecnologia per l'Energia e la Mobilità Sostenibili (STEMS)-CNR, 80125 Napoli, Italy*

Biomass is a well-recognized renewable source of energy. Thermochemical conversion of biomass is one of the most common and convenient routes for the conversion into energy including combustion, gasification, liquefaction and carbonization processes. In all these processes, pyrolysis plays a key role concerning product distribution, composition and properties. In the last decades, extensive research has been conducted to understand the complexity of these processes in detail, which cannot exclude the influence of mineral matter. In fact, biomass contains alkali metals (K and Na) and alkaline earth metals (Ca and Mg) which have a notable influence on combustion and gasification processes.

To investigate the influence of a specific type of mineral, walnut shells as lignocellulosic biomass was first demineralized to subsequently perform a loading series of K and Ca. Hydrothermal carbonization (HTC) was used to remove the mineral matter in the biomass and at the same time to generate a hydrochar with higher carbon content than the raw biomass. This contribution reports on the effects of selected alkali and alkaline earth metals on fast pyrolysis products of doped biomass hydrochar generated in N_2 and CO_2 atmosphere using a heated strip reactor (HSR) (Figure 1). Thermogravimetric (TG) measurements were performed to investigate the effect of mineral doping on combustion and gasification char reactivity. While the devolatilization step was not influenced by mineral doping, K showed a significant influence on the combustion reaction, whereas the effect of Ca was more pronounced on gasification. Flash pyrolysis at 700 °C was performed in a pyrolysis-GC/MS-GC/TCD setup to gain insights on the effect of minerals on the formation of tars and gaseous products. Both K and Ca decreased the amounts of produced CO and CH_4, while CO_2 increased. Analyzing the produced tars showed a catalytic mineral effect on the decomposition of anhydrous sugar and a higher formation of one-ring aromatic compounds. Doping the biomass hydrochar with both K and Ca resulted in a synergic catalytic effect.

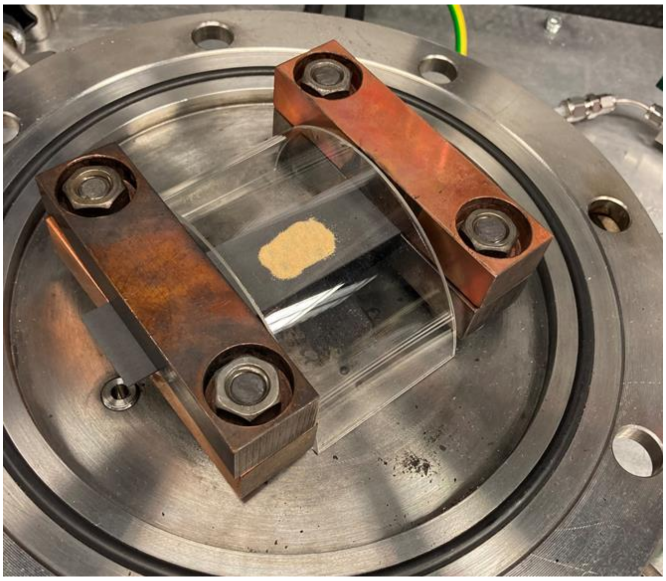


Figure 1. Image of the heated strip reactor.

Acknowledgements

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

Biomass pyrolysis: Critical issue on tar analysis

F. Cerciello[1], C. Ontyd[2], C. Russo[3], E. Freisewinkel[2], M.M. Oliano[3], O. Senneca[3], V. Scherer[2], M. Schieman[2], M. Muhler[1] and B. Apicella[3*]

*barbara.apicella@stems.cnr.it

[1] *Laboratory of Industrial Chemistry, Ruhr University Bochum, 44801 Bochum, Germany*
[2] *Institute of Energy Plant Technology, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[3] *Istituto di Scienze e Tecnologia per l'Energia e la Mobilità Sostenibili (STEMS)-CNR, 80125 Napoli, Italy*

The present work focused on the analysis of tar produced from fast pyrolysis in N_2 and CO_2 of lignin-rich lignocellulosic biomass named Walnut Shells. Heat treatments were carried out in a drop tube reactor (DTR) in a temperature range of 1100-1300 K, with a residence time between 0.1–0.4 s and a heating rate of 10^4 K/s.

In the DTR the volatiles generated by biomass pyrolysis were entrained in a hot gas stream and were collected at the reactor outlet by tar traps. The tar samples were recovered by washing the glass tube placed downstream of the DTR with acetone in ultrasonic bath. Initially, acetone was able to remove all the tarry material deposited from DTR. However, not all tar sample were completely soluble in acetone. Indeed, as soon as they were collected, a brown precipitate appeared in the acetone-solution for selected samples.

Analytical techniques as gas chromatography-mass spectrometry (GC-MS), size exclusion chromatography (SEC) and fluorescence spectroscopy were used for evaluating the chemical composition, the molecular weight (MW) distribution and the aromatic moieties of the tar, respectively. The concentration of aromatics, oxy-compounds and aliphatics detected by GC-MS was quantified using response factors calculated from the analysis of standard samples of known concentration. The GC-MS analysis turned out to be inadequate for a complete identification of the tar compounds in the acetone solution, due to the limited mass scanning mode (from 50 to 400 u) and also, for some samples, to the presence of an acetone insoluble brown precipitate. SEC was indeed necessary to complete the tar evaluation. Formation and growth of polycyclic aromatic hydrocarbons (PAHs) were relevant under DTR conditions. However, the chemical structure of the brown precipitate cannot be ascribed to the soot formation due to the different MW distrubution and to its fluorescence properties. The presence of large concentration of CO_2 in the pyrolysis atmospheres further promoted formation of this brown precipitate.

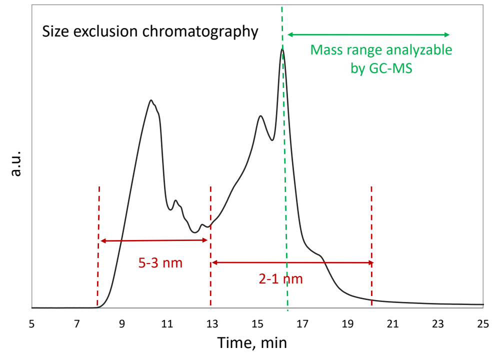


Figure 1. Size exclusion chromatography of biomass tar collected in the DTR.

Acknowledgements

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

Prediction of pyrolysis kinetics with models of different complexity for isolated biomass components

S. Pielsticker[1*], P. Debiagi[2], F. Cerciello[3], A. Coppola[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] *Simulation of Reactive Thermo-Fluid Systems (STFS), Technische Universität Darmstadt, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany*

[3] *Laboratory of Industrial Chemistry, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

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

Pyrolysis describes the thermochemical decomposition of organic materials in the absence of oxygen. Through the supply of energy (endothermic), chemical bonds break and a variety of different products is formed. During the pyrolysis of biogenic or fossil solid fuels, pyrolysis gases, liquid products called tar and a carbon-rich solid residue (char) are formed. Within pulverised biomass combustion, pyrolysis is the major decomposition process. As the pyrolysis products strongly influence subsequent processes like ignition, flame stability, and pollutant formation, an adequate mathematical modelling is required for simulations of combustion furnaces. Depending on the application and the required degree of detail, pyrolysis models of various complexity are available.

Within the present study, pyrolysis models of different complexity are investigated regarding their accuracy to predict the release of volatiles from the isolated extracted biomass components cellulose, hemicellulose and lignin. As model representatives of different complexity, the single first-order reaction (SFOR) model, the CRECK-S-B model [1] and the bio chemical percolation devolatilization (Bio-CPD) [2] model are selected. The SFOR model assumes the conversion as a single global reaction from solid to volatiles. Despite the simplification, it is often used in large-scale CFD simulations due to its low numerical cost. In contrast, the Bio-CPD model approximates the molecular structure of the solid, calculates the decomposition of molecular bonds, gives the fragment composition based on the percolation theory and provides the release of tar and light gas molecules using a vapour-liquid equilibrium calculation. These model complexities come along with a higher numerical effort but promise better precision. The CRECK-S-B model serves as an intermediate between both approaches and assumes the decomposition as a combination of different multi-step first-order reactions.

The performance and precision of all three models are evaluated based on experimental data from two different experimental setups – a thermogravimetric analyser and a fluidised bed reactor. The two different reactor systems represent different thermal boundary conditions and include low and high particle heating rates. To be able to evaluate the prediction of the reaction kinetics, time-dependent mass loss curves and volatile release profiles from ex-situ gas analysis are taken as reference values [3]. Additionally, predictions of light gas and tar fractions are compared for the CRECK-S-B and the Bio-CPD model and the relevance of secondary cracking reactions in the gas phase is evaluated. Significant differences are visible for the different models as well as for the different reactor setups. The discrepancies depend also on the complexity of the molecular structure of the biomass component.

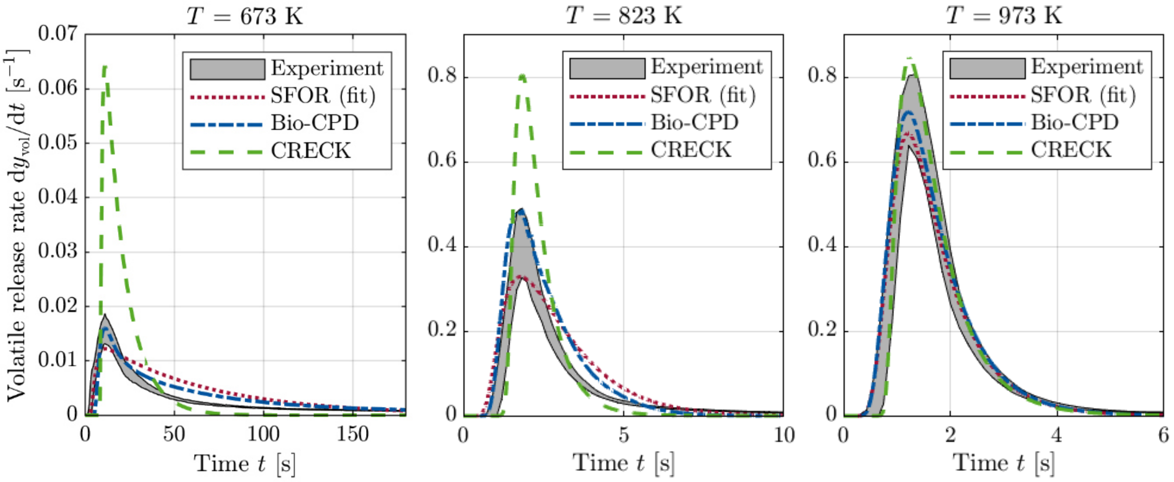


Figure 1. Experimentally derived volatile release rates in a fluidized bed reactor at different temperatures in comparison with predictions from SFOR, Bio-CPD and CRECK model.

Figure 1 shows exemplarily the total volatile release rate of pure cellulose during pyrolysis in the fluidised bed reactor at three different temperatures measured via ex-situ gas analysis in comparison with the model predictions from the SFOR model (calibrated to these experimental data), the CRECK model and the Bio-CPD model.

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

References

[1] Debiagi, P., Faravelli, T., Hasse, C., Ranzi, E., Kinetic modeling of solid, liquid and gas biofuel formation from biomass pyrolysis, in: Production of Biofuels and Chemicals, Vol. 10. Singapore: Springer Nature (2020), 31–76.
DOI: 10.1007/978-981-15-2732-6_2.

[2] Sheng, C., Azevedo, J. L. T., Modeling biomass devolatilization using the chemical percolation devolatilization model for the main components, Proceedings of the Combustion Institute 29 (1) (2002), 407–414,
DOI: 10.1016/S1540-7489(02)80054-2.

[3] Pielsticker, S., Gövert, B., Umeki, K., Kneer, R., Flash pyrolysis kinetics of extracted lignocellulosic biomass components, Frontiers in Energy Research 9 (2021), DOI: 10.3389/fenrg.2021.737011.

Release of nitrogen gas species during combustion and pyrolysis of walnut shells in an entrained flow reactor

C. Yildiz[1*], M. Richter[1], J. Ströhle[1] and B. Epple[1]

*coskun.yildiz@wihi.tu-darmstadt.de

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

In order to limit the global warming target to 1.5 °C, as set out in the Paris Agreement, it is mandatory to reduce carbon dioxide emissions (CO_2). The largest contribution to reducing the emissions can come from the energy and electricity sectors. One advanced method for achieving carbon capture, utilization, and storage (CCUS) is the oxy-fuel process. There are numerous of changes in the combustion behaviour of solid fuels, due to the change in atmosphere resulting from flue gas recirculation.

An entrained flow reactor is used to investigate the influence of oxy-fuel conditions on the release of nitrogen compounds contained in walnut shells. The reactor is operated under four different atmospheres for this study: N_2 and CO_2 to study the nitrogen release during devolatilization, air and oxy-fuel (combustion conditions) to study the influence of char conversion at different stoichiometric ratios. Additionally, the experiments were performed at different temperatures (1000 °C–1300 °C) and oxygen ratios (0.8–1.1). The heating rate of the particles corresponds to the conditions that can be achieved in real combustion plants. During the experiments, gases were sampled from the reactor and analyzed for the species HCN, NH_3, NO, NO_2 and N_2O using a Fourier transform infrared spectrometer (FTIR). The gas sampling is performed at two different positions in the reactor with a particle residence time of approximately 0.22 and 0.50 s.

The results show that atmosphere, temperature and air ratio have a significant influence on the release of these species. With increasing temperature in nitrogen atmosphere, the total release of the measured compounds decreases from 80 % (1000 °C) to 9 % (1300 °C) at a residence time of 0.22 s. NO is the main species measured at 1000 °C, which decreases from 250 ppm to 0 ppm (1200 °C). At the same time, the NH_3 concentration increases from 0 ppm (1000 °C) to 79 ppm (1200 °C), which suggests an interaction of these species. A similar behaviour with higher NH_3 and lower NO concentrations is observed in CO_2 atmosphere. CO_2 promotes the formation of NH_3 at high temperatures (1000–1300 °C) at both residence times.

In air and oxy-fuel atmosphere, 29–59 % of the nitrogen contained in the fuel is released as NO, depending on the oxygen ratio. An increasing oxygen ratio (0.8–1.0) increases the NO formation in both atmospheres. Combustion experiments with an oxygen ratio of 1.1 show lower NO concentrations in the oxy-fuel atmosphere. While no NH_3 is detected during combustion in air atmosphere at all oxygen ratios, a formation of NH_3 is detected under fuel-rich conditions up to 17 ppm. In air atmosphere N_2O is observed in small amounts (<1 ppm), while the amount in oxy-fuel atmosphere is up to 3 ppm. During all combustion experiments, no HCN and NO_2 are measured at all oxygen ratios.

Acknowledgements

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

Use of egg shells wastes for catalytic pyrolysis of lignocellulosic biomass

A. Maaoui[1,2], R. Chagtmi[1,2], F. Cerciello[3], A. Ben Hassen Trabelsi[1*],
M. Urciuolo, F. Stanzione[4], R. Migliaccio[4], O. Senneca[4] and B. Apicella[4]

*aidabenhassen@yahoo.fr

[1] *Laboratory of Wind Energy Control and Waste Energy Recovery, LMEEVED, Research and Technology Centre of Energy, CRTEn, B.P. 95, 2050 Hammam-Lif, Tunisia*

[2] *Department of Geology, Faculty of Sciences of Tunis, University of Tunis El Manar, 2092, El Manar II, Tunis, Tunisia*

[3] *Laboratory of Industrial Chemistry, Ruhr University Bochum, 44801 Bochum, Germany*

[4] *Istituto di Scienze e Tecnologia per l'Energia e la Mobilità Sostenibili (STEMS)-CNR, 80125 Napoli, Italy*

Catalytic pyrolysis of lignocellulosic biomass received considerable attention in the literature. Utilization of natural and waste materials as catalysts to improve the yields and quality of desired pyrolysis products is also an interesting option that deserves further investigation. In the present work Eggshell waste (EGW), a naturally calcium-rich material, is investigated as a catalyst for pyrolysis of two different (woody and a non-woody) Mediterranean biomass wastes: pine wood (PPC) and pomegranate peels (PGP).

Slow pyrolysis was carried out at a constant temperature of 500 °C, 10 °C/min heating rate, and 60 min residence time with 250 mL/min N_2 flow rate. The biomass samples were characterized in terms of proximate and ultimate analyses, mineral content, and high heating value (HHV). They were also analysed by FTIR spectroscopy, X-ray diffraction (XRD), and thermogravimetry. The bio-oils produced by pyrolysis of single fuels and mixtures with EGW (in the ratio 1:1) were characterized by GC-MS analysis and the quality in terms of chemical families was discussed.

Results revealed that PPC bio-oil composition is dominated by oxygenated aromatics (~53 %), retene derivative, and anhydrosugars compounds, while, PGP oil mostly contained fine chemicals with oxygen, in particular furfural (~50 %) and anhydrosugars (~20 %). Co-pyrolysis results suggest that the alkali and alkaline-earth metals (AAEMs) present in the EGW affect pyrolysis oil composition, indeed, GC-MS confirmed that the addition of EGW increased the content of oxygenated aromatics and reduced the amount of anhydrosugar, retene derivative, and aliphatic compounds for PPC-EGW.

Figure 1. Lignocellulosic biomass for bio-oil production

Acknowledgments
This work was supported and funded by the Ministry of Higher Education and Scientific Research (MESRST) in Tunisia and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – 215035359 – SFB/TRR 129 "Oxyflame".

10.18154/RWTH-2023-06259

Lagrangian point-particle models for non-spherical particles in turbulent flow

L. André[1*], T. Kiwitt[1], M. Meinke[1,2] and W. Schröder[1,2]

*l.andre@aia.rwth-aachen.de

[1] *Institute of Aerodynamics, RWTH Aachen University, Wüllnerstr. 5a, 52062 Aachen, Germany*
[2] *JARA-CSD, RWTH Aachen University, Seffenter Weg 23, 52074 Aachen, Germany*

Introduction

In many natural and technical environments, particle-laden flows are of importance. Applications are ranging from aerial pollutant transport, blood flow, over to solid-fuel combustion of biomass particles. The cost of fully resolving the dispersed phase is remarkably high due to the complex multi-scale nature of the flow and the small particle diameters generally involved. Hence the interest in accurate Lagrangian point-particle models. Commonly used models are often simplified by assuming very small particle diameters or an ideal spherical shape. However, these assumptions are rarely found in real applications. Since the complex turbulence modulation of such flows strongly depends on particle shape and size, these particle characteristics should be considered by the point-particle models to ensure more accurate predictions.

In this contribution, spherical (SLM) and ellipsoidal Lagrangian models (ELM) are assessed in anisotropic flow by comparison to highly resolved direct particle-fluid simulations (DPFS) of non-spherical particles with sizes in the order of the Kolmogorov length-scale η. Of particular interest are particle-laden pipe flows and free jets.

Numerical Methods

The highly resolved DPFS reference solutions are generated using a finite-volume solver and solution adaptive hierarchical Cartesian meshes. Particles are described using a signed distance function, i.e., an analytical level-set and are sharply resolved by a fully conservative cut-cell method.

The SLM is based on a simplified model of the Maxey-Riley equation. The model accounts for fluid inertia, but does not consider the actual particle shape. The commonly used ELM is derived under the assumption of creeping flow, consequently, does not account for fluid inertia. The ELM is therefore extended using newly derived correlations for drag, lift, and torque. Several thousand single particle simulations with varying aspect ratios and orientations were conducted and new correlations as a function of the particle Reynolds number, particle aspect ratio and orientation were derived [1]. Fig.1 shows the results for the drag coefficient. The dynamic equations of the ELM are modified to incorporate the new correlations.

Both, the DPFS and Lagrangian particle tracking (LPT) simulations, profit from a dynamic load balancing strategy, that enables highly efficient computations on high-performance computers (HPC).

Results and Discussion

In this contribution, prolates with aspect ratios in the range of $2 \leq \beta \leq 8$ and an equivalent particle diameter of $d_{eq} \sim \eta$ are investigated. Simulations using the different Lagrangian models are assessed by comparison to reference solutions generated by DPFS. A fully developed flow in a circular pipe and an axisymmetric round jet are analysed. The pipe flow serves as inflow condition to the jet and ensures realistic particle inflow conditions. The SLM and ELM with different correlations are analysed. Preferential particle compositions and orientations are investigated for anisotropic turbulent flow and a first assessment of the new ELM will be given.

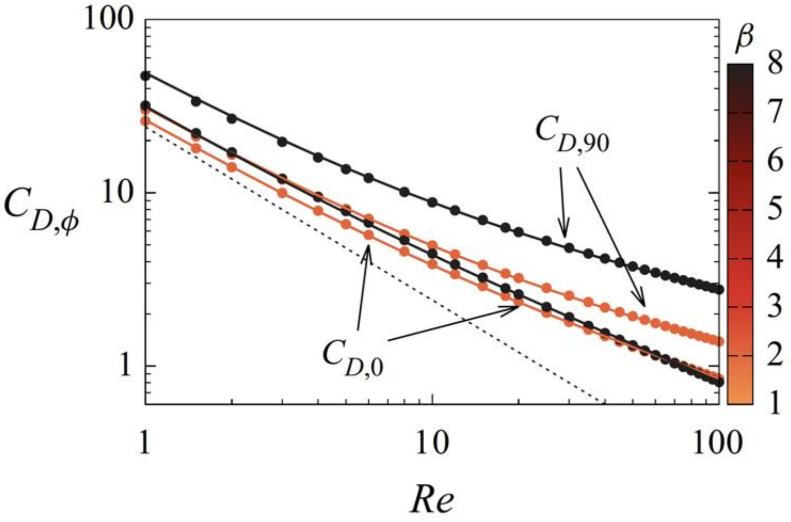


Figure 1. Newly derived drag coefficient $C_{D,\phi}$ with $\phi = 0°$ and $90°$ for aspect ratios $\beta = 2$ and 8 [1].

Acknowledgments

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 "Oxyflame". The support is gratefully acknowledged. Computing resources were provided by the High Performance Computing Centre Stuttgart (HLRS) and by the Jülich Supercomputing Centre (JSC) within a Large-Scale Project of the Gauss Centre for Supercomputing (GCS).

References

[1] Fröhlich K., Meinke M., and Schröder. W., Correlations for Inclined Prolates Based on Highly Resolved Simulations, J. Fluid Mech., 901, (2020).

10.18154/RWTH-2023-06259

Numerical study on the influence of conversion- and temperature-dependent particle radiative properties on pulverised solid fuel flames

H. Askarizadeh[1*], H. Nicolai[2], M. Koch[1], S. Pielsticker[1],
C. Hasse[2], R. Kneer[1] 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] *Department of Mechanical Engineering, Simulation of Reactive Thermo-Fluid Systems (STFS), Technical University of Darmstadt, Otto-Berndt-Straße 2, Darmstadt 64287, Germany*

In the context of pulverized solid fuel combustion (PSFC), radiation emerges as the most important mechanism of heat transfer. Consequently, it becomes essential to incorporate accurate radiation models in the numerical simulation of such systems. However, the presence of the discrete phase (solid particles) adds complexity to radiation modeling, as it necessitates the consideration of radiation interactions in both the solid and gaseous phases. From the literature, it can be inferred that the weighted-sum of grey gases model (WSGGM) has demonstrated sufficient accuracy in predicting gaseous radiative properties in PSFC [1]. On the other hand, radiative properties of the discrete phase have predominantly been assumed as constants, although properties such as scattering and absorption efficiencies of the discrete phase are subject to variations during the combustion process, depending on factors such as particle composition, diameter, and wavelength [1]. Detailed models have been explored only in a few studies [2, 3].

Incorporating a more detailed model that accounts for temperature- and conversion-dependent radiative properties introduces additional complexity to the simulations. Consequently, this study aims to investigate the significance of the disparity between the resulting temperature fields when considering variable versus constant radiative properties for the particles. To achieve this objective, a reference case is simulated, involving a pilot-scale combustion chamber with a 60 kW_{th} swirl burner. The numerical solution is conducted using Ansys Fluent. Given the swirling nature of the flame, the k-ϵ model with the renormalization group (RNG) theory of turbulence is employed. In order to capture the turbulence-chemistry interaction, the eddy dissipation concept is utilized. For solving the radiative transfer equation, the discrete ordinate model is employed, along with the domain-based WSGGM. To incorporate the variability of particle radiative properties, user-defined functions (UDFs) are implemented in the simulation, enabling the application of the desired variable particle radiative properties.

To emphasize the significance of incorporating variable radiative properties for the discrete phase using UDFs, the following steps are executed: Firstly, a reference case is simulated, considering a uniform particle size distribution with a diameter of $D_p = 80$ µm. The Baum and Street model [4] is employed for particle combustion, maintaining a constant diameter while gradually reducing particle density during the combustion process. To verify the external calculator of radiative properties in UDFs, constant radiative properties for particles are assumed based on an average particle temperature of 1200 K. Subsequently, two simulation cases are conducted: one with UDFs and another without UDFs, both employing the same radiative properties. The obtained results are then compared and presented in Figure 1(a). After successfully verifying the UDFs, the focus shifts to limiting the parameters that influence the temperature field. This is achieved by deactivating the kinetic models, thereby allowing radiation to be the sole mechanism responsible for temperature field variations resulting from radiation interactions between particles. The outcomes of this non-reactive flow scenario within the chamber are presented and compared to the reference case in Figure 1(b). In the third step, a simulation is performed considering a smaller particle size distribution ($D_p = 10$ µm), with radiation being the sole factor affecting the temperature field in the above introduced non-reactive flow scenario. The resulting temperature field is compared to that of $D_p = 80$ µm. The comparability of temperature fields for different particle size distributions relies on the similarity of the particle velocities, which is the case for $D_p = 10$ µm and 80 µm. The comparison depicted in Figure 1(c) underscores the significance of considering variable radiative properties in the numerical simulation of PSFC, as the temperature field for $D_p = 10$ µm exhibits substantial differences from that of $D_p = 80$ µm.

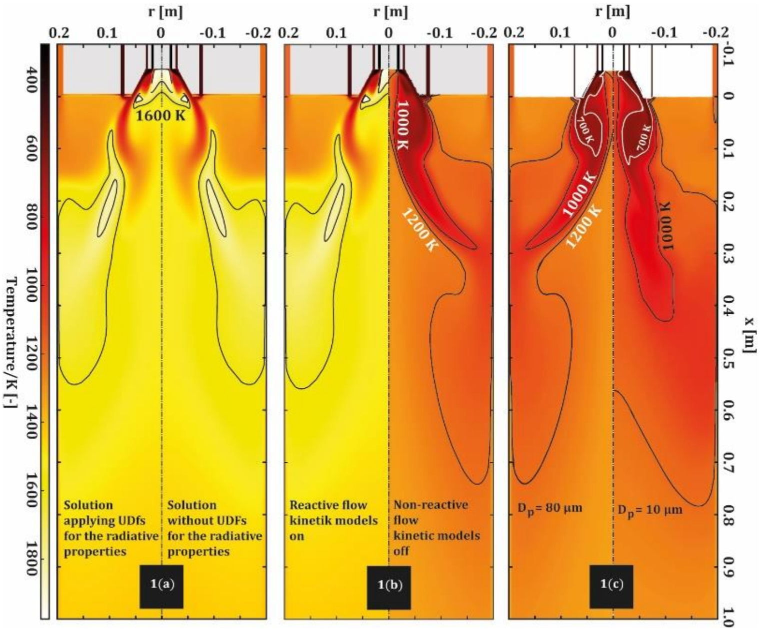


Figure 1. Importance of variable radiative properties in PSFC simulation: **(a)** UDF verification **(b)** Limiting influencing mechanisms by deactivating kinetics models to isolate radiation's impact on the temperature field. **(c)** Varying particle size distribution in non-reactive flow

Acknowledgements

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

References

[1] Koch M., Pielsticker S., Kneer R. Numerical investigation of the radiative properties of a fully resolved particle cloud. International Journal of Thermal Sciences 2023;185:108102.
[2] Yin C. On gas and particle radiation in pulverized fuel combustion furnaces. Applied Energy 2015;157:554–61.
[3] Nicolai H., Wen X., Miranda F. C., Zabrodiec D., Massmeyer A., Di Mare F. et al. Numerical investigation of swirl-stabilized pulverized coal flames in air and oxy-fuel atmospheres by means of large eddy simulation coupled with tabulated chemistry. Fuel 2021;287:119429.
[4] Baum M. M., Street P. J. Predicting the Combustion Behaviour of Coal Particles. Combustion Science and Technology 1971;3(5):231–43.

Comprehensive analysis of the effect of oxyfuel atmospheres on solid fuel combustion using large eddy simulations

L. L. Berkel[1*], P. Steffens[1], H. Nicolai[1], S. Gierth[1], P. Debiagi[1],
H. Schneider[2], A. Dreizler[2] and C. Hasse[1]

*Corresponding author: berkel@stfs.tu-darmstadt.de

[1] *Institute for Simulation of reactive Thermo-Fluid Systems, TU Darmstadt, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany*
[2] *Institute of Reactive Flows and Diagnostics, TU Darmstadt, Otto-Berndt-Str. 3, 64287 Darmstadt, Germany*

With increasing environmental concerns and energy demand, cleaner power generation technologies that reduce pollutants are required. Decreasing the released CO_2 with carbon capture and storage (CCS) technologies is a prominent option for reducing carbon emissions in the near future. Oxyfuel combustion in combination with CCS is a promising technology in which the N_2 in the combustion atmosphere is replaced by CO_2, producing flue gases that almost only consist of CO_2, facilitating CCS technologies. Nonetheless, the thermophysical characteristics of the combustion process change significantly as a result of high CO_2 concentrations. Therefore, an in-depth understanding is required to optimize process development and plant technology with oxyfuel conditions.

Solid fuel combustion modeling is challenging due to the multitude of physical phenomena involved at various scales. Complex processes like devolatilization and char surface reactions, are strongly coupled with the gas phase and require appropriate modeling for a 3D Computational Fluid Dynamics (CFD) simulation. Being a scale-resolving technique, Large Eddy Simulation (LES) coupled with a Lagrangian description of solid particles has become a feasible option due to the increasingly available computational resources. The large number of reactions involved in describing the multiphase system can still not be directly calculated in 3D CFD. Instead, a tabulated chemistry approach is developed for both single-phase and multi-phase conditions, including finite-rate chemistry effects. For the heat transfer calculations, the radiation is considered by using the discrete ordinates method and the weighted sum of grey gases model. This work focuses on a lab-scale swirled burner that is operated both in single-phase operating conditions (Methan: 20/31.5 kW_{th}) and multiphase operating conditions (Methane and Rhenish lignite: 40/63 kW_{th}), both in air and oxyfuel conditions. The overall numerical configuration is validated with extensive experimental data, including flow field and temperature information. Simulations are used for comprehensive analysis of the effects of oxyfuel conditions on flame characteristics. Initial temperature results are shown in Figure .

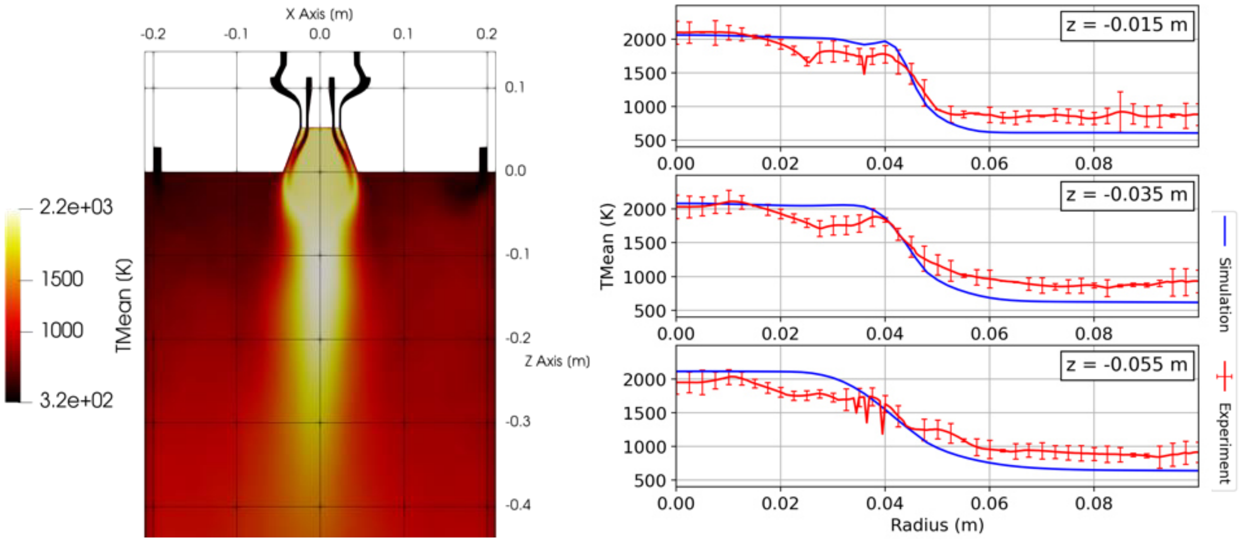


Figure 1. Mean temperature contour (left) and profiles at different heights (right) in the reactor.

Acknowledgements

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

BE4G ultra-low emissions biomass burner: Modelling procedure and full-scale test results

R. Dadduzio[1*], M. Penati[1], L. Bini[1], M. Rogora[1], M. Valenzano[1], A. Saponaro[2], O. Senneca[3], F. Cerciello[4], C. Ontyd[4], D. J. Brand[5], A. Uzair[6] and M. Torresi[6]

*ruggiero.dadduzio@acboilers.com

[1] *AC BOILERS S.p.A., Largo Buffoni n°3, 21013 Gallarate (VA), Italy*

[2] *Centro Combustione Ambiente S.p.A., Via Milano km 1600, 70023 Gioia del Colle (BA), Italy*

[3] *Istituto di Scienze e Tecnologia per l'Energia e la Mobilità Sostenibili (STEMS)-CNR, Piazzale Vincenzo Tecchio 80, 80125 Napoli (NA), Italy*

[4] *Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany*

[5] *Central Analytical Facilities (CAF), NMR unit, Stellenbosch University, Schumann Annex De Beer Street, 7600 Stellenbosch, South Africa*

[6] *Politecnico di Bari, DMMM, Via Re David 200, 70125 Bari (BA), Italy*

While the worldwide power demand continues to soar, the transition toward net zero carbon emission pushes the scientific and industrial communities to develop new and more efficient technologies for the energy production. Recent assessment reports on climate change urge the drastic replacement of fossil fuels with renewables as the main pathway to curb CO_2 emissions. Today, energy from renewables covers only a small portion of the demand, while often requiring, as for solar and wind, advanced energy storage technologies to guarantee flexibility. Pulverized biomass, when sourced responsibly, represents a sustainable and efficient complement to wind and solar, especially when applied to plants originally designed for coal. The broad expertise of AC Boilers and its Combustion Center (CCA) in pulverized fuel burner design and full-scale testing, laid the foundation for the development of the low emissions, high combustion efficiency, BE4G biomass burner, specifically designed for coal plant revamping. The innovative BE4G burner nozzle is designed to sustain the flame front in fuel-rich conditions, hampering at the same time the NO_x formation and slag deposit. The patent awarded BE4G primary duct guarantees the optimal fuel mixing, lowering the presence of unburnt carbon in the fly ashes. Extensive use of quality CFD studies boosted the design process while minimizing the need of long and expensive full-scale experimental tests. Starting from the experience gained over the years in the accurate characterization of pulverized solid fuels, the present paper describes in detail the modelling procedure which led to the novel burner design. An ad-hoc lab-scale experimental protocol is proposed as a means to provide reliable input data for the combustion model.

Acknowledgements

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

Chemical reactor network modeling of a self-sustained solid fuel combustion chamber under oxy-fuel atmospheres

S. Dübal[1*], L. L. Berkel[2], P. Debiagi[2], H. Nicolai[2],
T. Faravelli[3], C. Hasse[2] and S. Hartl[1]

*soeren.duebal@h-da.de

[1] *Optical Diagnostics and Renewable Energies (ODEE), Darmstadt University of Applied Sciences,*
Haardtring 100, 64295 Darmstadt, Germany

[2] *Simulation of reactive Thermo-Fluid Systems (STFS), Technical University of Darmstadt,*
Otto-Berndt-Str. 2, 64287 Darmstadt, Germany

[3] *Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano,*
Piazza Leonardo Da Vinci 32,20133 Milano, Italy

Oxy-fuel combustion is one of the most promising carbon capture and storage (CSS) technologies for reducing CO_2 emissions in power plants. In the oxy-fuel process, N_2 is replaced with CO_2 in the oxidizer, resulting in combustion products almost entirely composed of CO_2, facilitating its capture and storage or utilization. Recently both experimental and numerical studies were performed to gain a more detailed understanding of the combustion process. However, large scale CFD simulations coupled with detailed chemistry remain prohibitive and thus are not suitable for a standalone design of future power plants. Therefore, chemical reactor network (CRN) modeling as a scale-reduced approach is applied in this work. The framework used for solving chemical reactor networks, NetSMOKE, is based on OpenSMOKE++ libraries and utilizes single-phase and, recently introduced, two-phase reactor models.

Generating reactor networks requires information on the flow and temperature fields, which highly depend on the operating points of the system under consideration. However, in particular the investigation of different operating strategies is interesting in the design phase of power plants. Hence, exploring the predictability and understanding the limitations of a CRN approach is desirable. In the context of oxy-fuel combustion, the ratio of oxygen to recirculated flue gas is one of the main parameters of interest. Therefore, this work focuses on applying a multiphase reactor network on a self-sustained burner configuration representing a 40 kW Rhenish lignite swirl stabilized flame under oxy-fuel conditions with different oxygen concentrations. Differences in the flame structure between the considered operating points are highlighted, to test the robustness of the initial reactor network. Subsequently, the limitations and necessary changes in the network design are discussed and applied. Finally, sensitivities of the reactor temperature, to the formation of selected pollutants, are investigated.

This work demonstrates the general capabilities of the CRN approach to describe the complex physics involved in the conversion of solid fuels in oxyfuel atmospheres. Thereby, it presents a path towards computationally effective design and retrofit of power plants.

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

10.18154/RWTH-2023-06259

Modeling smoldering combustion of wood

A. Galgano[1]

agalgano@unina.it

[1] *Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli Studi di Napoli "Federico II", P.le Tecchio, 80125 Napoli, Italy*

A comprehensive solid-phase model is applied to simulate the glowing ignition and burning of thick wood samples in a conical heater with grain orientation parallel or perpendicular to incident heat fluxes in the range 18−40 kW/m^2, that is, in the absence of flame. The description of heat and mass transfer processes, at constant gas pressure, is combined with global volumetric rates of wood decomposition and char oxidation. Surface regression occurs for a limit value of char density while a critical surface temperature describes ignition. Good quantitative predictions are obtained for the ignition times (Fig.1) and the surface temperature and mass loss rate profiles during wood burning as the external heat flux intensity and the orientation of the wood fibers with respect to the incident radiation are varied. Given sample thicknesses of 40 mm, the process dynamics are characterized by the propagation from the surface toward the bottom of the sample of the decomposition and burning zones with the conversion that always consists of three main stages. The first short transients correspond to the formation of a relatively thin charred surface layer where glowing ignition occurs. The second much longer stage represents a pseudo-steady-state burning, where the rates of advancement of the various conversion zones are approximately constant as well as the surface temperature and the global rate of mass loss. The last short stage, resulting from the adiabatic bottom condition, is the enlargement of the decomposition zone to the entire sample so that char burning remains the sole process still under way. The first transient stage and the ignition times are noticeably affected by the external heating conditions whereas the characteristics of the pseudo-steady-state burning are mainly dependent on the char oxidation rate which, for the typical values of the kinetic parameters, is controlled by the rate of oxygen supply at the surface. Remarkable sensitivity of the model predictions to some input parameters is observed: in the first place, yields of the lumped classes of pyrolysis products and the global mass (oxygen)-transfer coefficient.

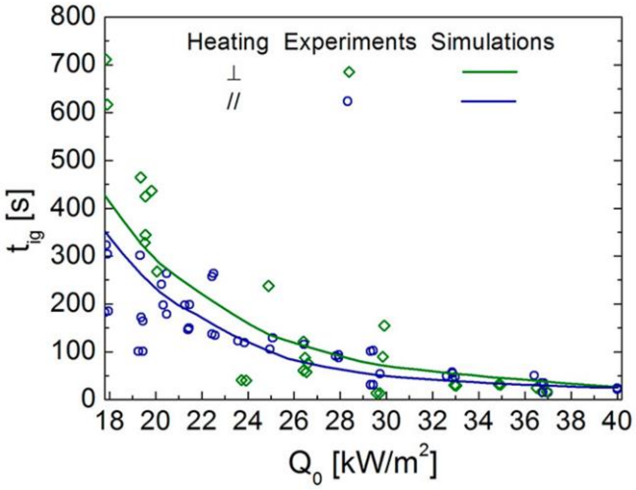


Figure 1. Predicted (lines) and measured (symbols) ignition time, t_{ig}, versus the intensity of the external heat flux, Q_0, for heating parallel (||) or perpendicular (⊥) to the wood grain.

Sensitivity analysis and uncertainty quantification of an axisymmetric reacting particle

A. Hassan[1*], L. Schumacher[1], V. Le Chenadec[2] and T. Sayadi[1,3]

*a.hassan@itv.rwth-aachen.de

[1] Institute for Combustion Technology, RWTH-Aachen University, Aachen, Germany
[2] Laboratoire Modélisation et Simulation Multi-Echelle, Université Gustave Eiffel, Champs-sur-Marne, France
[3] Institut Jean-le-Rond d'Alembert, CNRS/Sorbonne Université, Paris, France

Simulations of unsteady solid fuel particle combustion consist of the interaction of multiple complex phenomena, such as chemistry, turbulence, etc. In order to capture such interactions, models with variable fidelity are used. These models, in turn, rely on model parameters, which are determined by experiments or small-scale simulations. It is, therefore, essential to quantify the uncertainty of different quantities of interest with respect to these model parameters in order to achieve robustness. The first step in this process is to identify the most sensitive parameters of the model. The large size of the parameter space however makes the use of traditional methods such as brute force (finite difference) infeasible. Therefore, in this study, a semi-discrete adjoint method is used to extract such sensitivities. An adjoint-based method proves to be advantageous in this context since a single forward and backward simulation is sufficient for computing the gradients with respect to all model variables. Using this approach, the evolution of sensitivities is computed in time for a single unsteady axisymmetric particle going through devolatilisation. Methane mechanism is used to represent the reactions in the gas phase. Dominant model parameters are identified for multiple objective functions, such as particle temperature and gas phase ignition. The role of different devolatilisation models on the extracted sensitivities is also analysed. Finally, a linear adjoint approximation method (LAAM) [1] is used to quantify the underlying uncertainties in the model. This method is shown to be a cost-effective strategy in quantifying uncertainties in these configurations.

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

References

[1] A. Hassan, M. Sabry, V. Le Chenadec, T. Sayadi, Uncertainty quantification of kinetic models using adjoint-driven active subspace algorithms, Proceedings of the Combustion Institute, 2022, ISSN 1540-7489,

10.18154/RWTH-2023-06259

Coupling radiative properties with detailed char conversion kinetics

M. Koch[1*], S. Pielsticker[1], D. Tarlinski[2], V. Scherer[2] 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*

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

In pulverized fuel combustion systems, thermal radiation is the primary heat transfer mechanism. Thereby, particle radiation dominates, in most cases, gas radiation. 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 particles optical properties, characterized by the complex index of refraction (IOR). Within the conversion process, these optical properties change due to conversion in the particle morphology, material composition, and particle size. After pyrolysis, a solid fuel particle mainly consists of carbon and mineral components. During the char conversion, the carbon material is converted to gaseous products and released from the particle, while the minerals are transformed into ash. Depending on the reaction conditions, effects like ash film formation, particle swelling and particle shrinking occur.

To model the char conversion in dependency of the boundary conditions, the char conversion kinetics (CCK) model is used. It considers the solid fuel composition, gas and particle temperatures as well as oxygen transport within the particle pores and the boundary layer. Consequently, the conversion process can be categorized into three reaction regimes: In regime I, the conversion is limited solely by the intrinsic reaction rate of the char conversion reactions. Enough oxygen is available at all positions within the particle and the reactions evolve uniformly. In regime II, the conversion process is limited by the oxygen diffusion within the particle pores. Thus, the reactivity is higher at the particle surface than at the particle center. In regime III, the overall conversion process is limited by the oxygen transport through the boundary layer and the conversion process only takes place at the particle surface.

To quantify the effects of the structural changes during the conversion process on the radiative properties – absorption efficiency, scattering efficiency, and scattering phase function – the output data of the CCK model (particle size, ash fraction) are used as input values for a detailed radiative analysis using the discrete dipole approximation (DDA). For this purpose, the current diameter and composition are extracted from the CCK model at different conversion degrees. Depending on the described reaction regime, these data are then used to build artificial particles as shown in figure 1 with the following properties:

In regime I, the IOR of the particle m_{P} is calculated by applying equation (1),

$$m_{\mathrm{P}} = \sum m_{\mathrm{i}} \varphi_{\mathrm{i}} \tag{1}$$

with the index i denoting ash or the solid fuel and φ representing the volume fraction of the respective substance. In regime II, a thin ash layer covers the carbon core with IOR m_{ash}, and the remaining ash is used to calculate an appropriate IOR of the core by applying equation (1). In regime III, the particle is divided into two sections, a core with IOR m_{coal} and a coating with IOR m_{ash}.

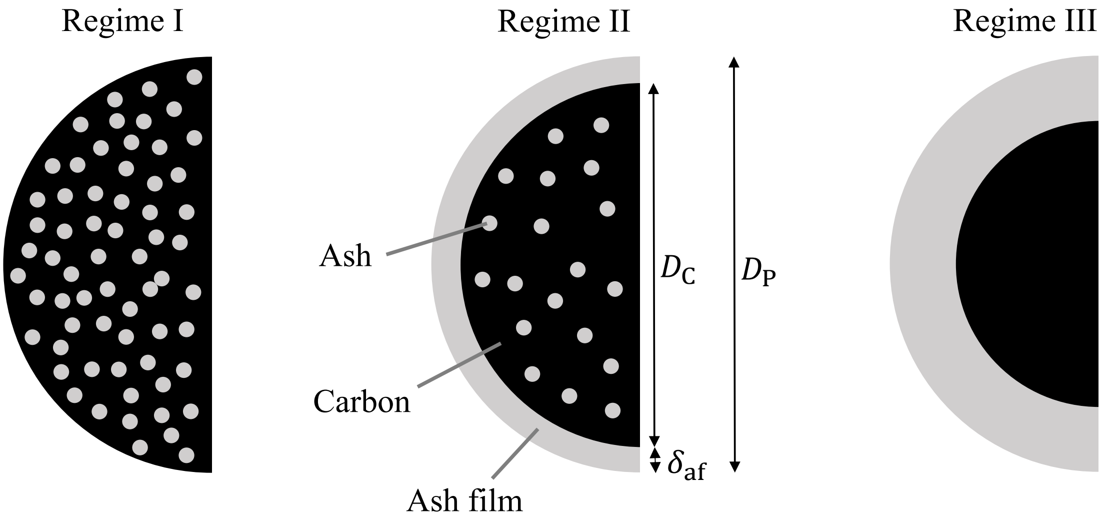


Figure 1. Illustration of the three regimes for a given burnout. The overall size of the particle is described by particle diameter D_P which is equal in each regime. In regime II and III, the particle is additionally described by an ash layer with thickness δ_af and core diameter D_C. In each regime, black illustrates carbon and grey illustrates ash.

Furthermore, a simplified approach currently used for large-scale CFD simulations is used to calculate the radiation properties depending on burnout. Within this approach, the IOR is suddenly changed from those of the raw solid fuel to those of pure ash when the particle reaches a burnout of 50 %.

In the last step, the radiative properties calculated by the detailed approach utilizing the CCK model are compared to the radiative properties calculated by the simplified model for CFD simulations. The goal is to decide whether a detailed differentiation of these regimes is necessary or not. Here, the burnout is varied for $0 < B < 1$ and the overall particle diameter for $1 < D_\mathrm{P}$ 50 µm.

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

Single particle conversion of woody biomass using fully-resolved and grid-independent Euler-Lagrange approaches

T. D. Luu[1,3*], J. Zhang[2], J. W. Gärtner[1], S. Meng[1,3],
O. T. Stein[1,3], A. Kronenburg[1], T. Li[2] and T. Løvås[2]

*tien-duc.luu@itv.uni-stuttgart.de

[1] Institut für Technische Verbrennung, Universität Stuttgart, Pfaffenwaldring 31, 70569 Stuttgart, Germany

[2] Department of Energy and Process Engineering, Faculty of Engineering, NTNU – Norwegian University of Science and Technology, Trondheim, Norway

[3] Present address: Engler-Bunte-Institut Verbrennungstechnik, Karlsruher Institut für Technologie, Engler-Bunte-Ring 7, 76131 Karlsruhe, Germany

It is expected that the global energy demand will continue to rise in the next few decades to meet the rising world population. Fossil fuels are still the most dominant global energy source, but due to their limited availability and environmental impact, the need for alternative energy sources increases. Solid biomass is considered as a promising renewable alternative to coal, however, the transition from coal to biomass raises substantial challenges, such as fuel preparation, combustion stability and corrosive pollutants. In the context of computational modelling, major challenges are the limited model fidelity of thermophysical sub-models specific to biomass and the relatively large diameter of biomass particles in pulverised fuel applications, which often invalidates the assumption of thermally thin particles. In the present study, the conversion of single woody biomass particles is studied using several complementary modelling approaches. The most detailed approach is a fully-resolved (FR) laminar flow simulation which is validated against experimental data. Subsequently, the FR data is compared to the results from two low-cost Euler-Lagrange (EL) approaches. For small ratios $d_p/\Delta x$ of the particle diameter d_p to the grid size Δx a standard point-particle EL approach is sufficient. However, for $d_p/\Delta x$ ratios near unity, the standard EL approach fails and is extended to consider *coarse-graining* (CG) methods.

The high-fidelity FR approach fully resolves the heat and mass transfer in the gas phase and across the particle boundary layer. Radiation is considered using the discrete ordinate method (DOM) with the weighted sum of grey gases model (WSGGM). The particle-interior conversion processes are described by a layer-based approach that is able to consider the drying, pyrolysis and char conversion of thermally-thick woody biomass particles in detail [1]. The particle-interior model releases light gases, tars and char off-gases to the gas phase, where a homogeneous kinetic mechanism with 33 species and 256 reactions describes tar decomposition and gas kinetics in detail. The FR approach is validated against the results from an experimental campaign conducted in a drop tube reactor, which studied the thermal conversion of various types of coal and biomass [2].

Since high-fidelity FR simulations cannot be conducted for millions of particles in industrial systems, reliable EL models for pulverised biomass conversion need to be developed. Within the EL approach, pulverised biomass is described by Lagrangian point-particles and the heat and mass transfer across the particle boundary layers need to be modelled. In a first step, for small ratios of $d_p/\Delta x$, we consider a standard EL approach, where the interaction of the particle with the gas phase is restricted to the Eulerian cell in which the particle resides, and we compare the EL results to the

FR data. For larger biomass particle diameters, i.e., for $d_p/\Delta x$ approaching unity, the standard EL approach will become invalid. Hence, the final set of EL simulations considers a coarse-graining approach [3]. The purpose of the CG method is twofold. With CG, the sampling of the gas phase quantities required to model the gas-solid interactions is improved by considering gas phase data from a larger region than the local Eulerian cell. Moreover, the Lagrangian heat and mass source terms do not only affect the local cell, but are distributed to a larger volume. The final coupled EL-CG approach is validated against the FR results.

References

[1] H. Ström, H. Thunman, *Combust. Flame* 160 (2013), 417-431.
[2] H. Tolvanen et al., *Fuel* 111 (2013), 148-156.
[3] J. Zhang et al., *Chem. Eng. J.* 387 (2020), 123964.

10.18154/RWTH-2023-06259

DEM/CFD-simulation of a generic lime shaft kiln: A numerical study on air-fired and oxy-fuel operation

H. Merten[1*], E. Illana[1], T. Bergold[1], S. Wirtz[1] and V. Scherer[1]

*merten@leat.rub.de

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

The chemical process of converting limestone to quicklime at an industrial scale is performed in lime shaft kilns which operate as a counterflow solid-gas heat exchanger. Since the process conditions within the shafts are almost non-accessible to measurements experimental data can be only obtained at the periphery of these reactors. Additional and far more detailed insight into the process can be obtained from corresponding numerical simulations. To this end, the Computational Fluid Dynamics (CFD) solver OpenFOAM coupled with a Discrete Element Method (DEM) code developed at LEAT has been employed for a numerical comparison of a generic lime shaft kiln operated in both, air-fired and Oxy-fuel operation.

While these kilns in industry can reach heights of up to 15 meters and production rates of 200 t/day (with a charging rate of around 340 t/day), the investigated generic reactor represents a simplified and downscaled geometry. In this system, limestone particles of a pre-defined size distribution are charged at the throat (diameter 0.64 m) of the kiln with a rate of 3.3 t/day. While the particles are slowly descending, they are heated by an uprising gas flow (pre-heating zone). In the actual process, the combustion of methane provides the energy for heating and calcining the particles. Within this DEM/CFD investigation, the combustion process is approximated by a simplified approach: hot exhaust gases are directly introduced into the kiln at the location of the burners. When the particles approach this high temperature area, the calcination rate increases. The final calcination degree of a lime particle depends on its size, the residence time in the kiln as well as on the local temperature and carbon dioxide concentration of the surrounding gas phase. The reaction progress inside the spherical particles is resolved spatially by a radial discretization.

In contrast to the air-fired operation of a lime shaft kiln in which methane is burned with air, the Oxy-fuel mode is defined by a combustion of methane with recirculated exhaust gas enriched by the required amount of oxygen. This operational mode is particularly relevant for calciners in sugar refineries where both, the lime and the carbon dioxide are required. As the kiln in Oxy-fuel operation contains an increased carbon dioxide fraction compared to air-fired operation, the necessary adaption of process parameters to ensure similar product quality will be presented.

Acknowledgments

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 422037413 – TRR 287.

Numerical study and burner optimization of the non-catalytic partial oxidation of natural gas

G. Gonzalez Ortiz[1]*, Y. Voloshchuk[1], B. Meyer[1], M. Gräbner[1] and A. Richter[1]

*gabriel.gonzalez-ortiz@iec.tu-freiberg.de

[1] *Institute of Energy Process Engineering and Chemical Engineering, TU Bergakademie Freiberg, Fuchsmühlenweg 9, 09599 Freiberg, Germany*

The present work studies the partial oxidation of natural gas by use of numerical modeling. The focus is to analyze the impact of the burner design on the oxidation zone and the burner optimization with focus on flame characteristics and syngas quality. For this, a comprehensive CFD model coupled with detailed chemistry is used to model both the turbulent combustion and gasification reactions. The CFD model is validated with experimental data obtained from the semi-industrial high-pressure POX plant in Freiberg. Here, large-scale process data for conventional POX burner designs and for high-velocity regimes with different feedstock and oxidizer velocities were utilized. Furthermore, different reaction mechanisms for the CFD model are evaluated. A systematic evaluation of the influence of swirl, feedstock, and oxidizer velocities, as well as the feed composition on the overall process characteristics is performed. The numerical calculations demonstrate how different burner concepts impact the flame structures, which in turn affects temperature distribution and recirculation zones in the reactor, leading to a different conversion process of the initial feedstock. The expected impact of swirl on the natural gas conversion was confirmed for conventional and for diluted feedstocks. Finally, a burner optimization was performed and the potential for improving the feedstock conversion and the product quality is demonstrated, which gives a clear indication for potential improvements in industrial processes.

10.18154/RWTH-2023-06259

Large eddy simulation of a 40 kW self-sustained pulverized biomass combustion chamber using tabulated chemistry

P. Steffens[1*], L. L. Berkel[1], S. Gierth[1], P. Debiagi[1], B. Özer[2],
A. Maßmeyer[2], H. Nicolai[1] and C. Hasse[1]

*steffens@stfs.tu-darmstadt.de

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

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

In order to fight climate change, a drastic cut of atmospheric CO_2 emissions is needed. The emissions of combustion-based energy production systems can be greatly reduced through carbon capture and storage (CCS) technologies. When CCS methods are combined with biomass combustion, CO_2 can be permanently removed from the atmosphere. One promising technology for CCS is oxyfuel combustion. By replacing N_2 with CO_2 in the oxidizer, the combustion products are almost entirely composed of CO_2, facilitating its capture and storage or utilization. However, the substitution of N_2 by CO_2 in the oxidizer significantly influences the thermo-physical characteristics of the combustion processes and still needs to be understood. Therefore, process analysis and development require further collaborative experimental-numerical studies. The first step to understanding oxyfuel biomass combustion requires the investigation of biomass combustion in air and the comparison with coal. For coal combustion, comprehensive analysis and model evaluation have been performed recently. They serve as the basis for the present work.

Numerical modeling and simulation of pulverized biomass combustion is still a significant challenge, given the wide range of multiscale physical phenomena involved. Since these phenomena are complex and strongly coupled, developing appropriate models is crucial for accurate 3D CFD simulations. Due to the increased availability of computational resources, scale-resolving simulation techniques like Large Eddy Simulation (LES), coupled with a Lagrangian description of the solid particle dynamics, have become feasible for the simulation of large-scale systems. In this work, a fully coupled model is employed to simulate a 40 kW self-sustained pulverized walnut shell flame obtained with a swirl-stabilized burner in an OpenFOAM-based simulation framework (OxySim-129). Considering the large number of reactions required to describe the combustion of volatiles and gaseous char products in the gas-phase, a tabulated chemistry approach is developed to capture finite rate chemistry effects in the simulation. The overall model is validated with experimental data of the flow field. Subsequently, the numerical model is employed to comprehensively study flame stabilization, local oxidation behavior and particle trajectories. Finally, results are contrasted with previously attained data of coal combustion in the same setup to evaluate the maturity of our current biomass models and to understand the influence of the fuel on the combustion process.

Acknowledgements

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 “Oxyflame”. Simulations were performed on the computing resources granted by Lichtenberg High-Performance Computer Darmstadt.

Enhancement of a detailed char conversion model for biomass combustion in oxy-fuel atmospheres

D. Tarlinski[1*], E. Freisewinkel[1], D. Golab[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*

For retrofitting or new design of burners and combustion chambers, Computational Fluid Dynamics (CFD) simulations are an important instrument. CFD simulations require predictive char burnout models. The Carbon Conversion Kinetics model (CCK model) is the most detailed char burnout model. The CCK model has been calibrated for oxy-fuel atmospheres [1,2] and is an advanced version of prior models like CBK, CBK/E and CBK/G.

As biomass is important in future energy supply, the enhancement of the CCK model for biomass as a fuel is necessary. Biomass shows a different behaviour than coal in the char burnout phase. Therefore, it is required to edit, add and improve sub-models in the CCK model. During char conversion, diffusion processes, reactions on the particle surface, changes in the solid (diameter and density), thermal annealing and ash inhibition do have an effect on burnout. All these effects have to be checked based on detailed experimental data.

Therefore, the results of the CCK model are compared to optical measurements for various types of biomass in a flat flame burner. The data set of biomass includes new measurements and already published data in [3]. It comprises eight oxy-fuel atmospheres. The biomasses examined were torrefied miscanthus and walnut shells. The data set of the optical measurements provides single particle temperature, equivalent circular diameter (ECD), particle shape, aspect ratio of the particle and the ratio of self-luminous to non-emitting particles as a function of the residence time. The setup of the Stereoscopic Camera system for Optical Thermography (SCOT) and the evaluation of the optical measurements are presented in the literature [3,4]. Besides the data from the optical measurements, analyses of solid samples with various degrees of burnout are also available for validation of the CCK model. Analyses of the solid samples include ash content and the elemental release of carbon, hydrogen and nitrogen.

Figure 1 shows the results of the original CCK model (Figure 1, left side) and the modified CCK model (Figure 1, right side) in comparison with the experimental data achieved. The atmosphere was 10 $\%_{Vol}$ oxygen, 10 $\%_{Vol}$ water vapor and 80 $\%_{Vol}$ of carbon dioxide. In addition, the results for the carbon content of collected samples at different burnout stages will be presented in comparison with the burnout predicted by the CCK model.

The calibration of the model includes the modification of the CCK model constants of the surface reaction kinetics. Since biomass has higher contents of volatiles compared to coal, the CPD model plays an important role. Therefore, CPD models from the current literature [5,6] were implemented into the CCK model for validation and comparison.

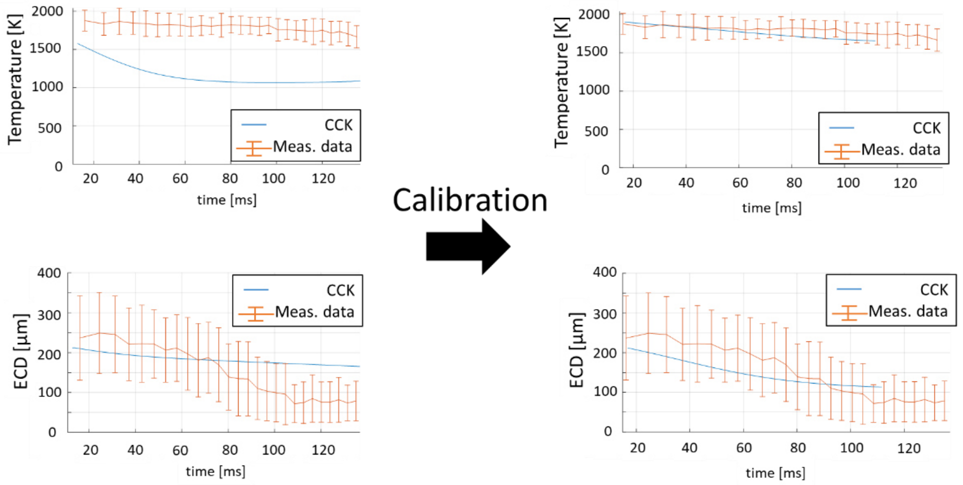


Figure 1. Comparison of measurement data with the results of the original (left) and the calibrated (right) CCK model for an oxy-fuel atmosphere with 10 %$_{Vol}$ oxygen

In future work, a thermal annealing concept for lignocellulosic biomass from the literature [7] will be implemented for comparison the original CCK thermal annealing model.

Acknowledgements

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

References

[1] Holland T, Fletcher TH. Comprehensive Model of Single Particle Pulverized Coal Combustion Extended to Oxy-Coal Conditions. Energy Fuels 2017;31(3):2722–39. https://doi.org/10.1021/acs.energyfuels.6b03387.

[2] Holland T, Fletcher TH. Global Sensitivity Analysis for a Comprehensive Char Conversion Model in Oxy-fuel Conditions. Energy Fuels 2016;30(11):9339–50. https://doi.org/10.1021/acs.energyfuels.6b02190.

[3] Vorobiev N, Valentiner S, Schiemann M, Scherer V. Comprehensive Data Set of Single Particle Combustion under Oxy-fuel Conditions, Part II: Data Set. Combustion Science and Technology 2020:1–16. https://doi.org/10.1080/00102202.2020.1754207.

[4] Vorobiev N, Valentiner S, Schiemann M, Scherer V. Comprehensive Data Set of Single Particle Combustion under Oxy-fuel Conditions, Part I: Measurement Technique. Combustion Science and Technology 2020:1–22. https://doi.org/10.1080/00102202.2020.1743696.

[5] Lewis AD, Fletcher TH. Prediction of Sawdust Pyrolysis Yields from a Flat-Flame Burner Using the CPD Model. Energy Fuels 2013;27(2):942–53. https://doi.org/10.1021/ef3018783.

[6] Vizzini G, Bardi A, Biagini E, Falcitelli M, Tognotti L. Prediction Of Rapid Biomass Devolatilization Yields With An Upgraded Version Of The Bio-CPD Model. Proceedings of the Combustion Institute, Italian Section, Turin 2008.

[7] Senneca O, Ontyd C, Cerciello F, Schiemann M, Scherer V. Extension of the Thermal Annealing Concepts Developed for Coal Combustion to Conversion of Lignocellulosic Biomass. Energy Fuels 2020;34(3):3661–70. https://doi.org/10.1021/acs.energyfuels.9b03172.

Evolution of oxygen functional groups during char burnout

Ö. Yönder[1]*, G. Schmitz[2] and C. Hättig[1]

*oezlem.yoender@ruhr-uni-bochum.de

[1] *Lehrstuhl für Theoretische Chemie I, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

[2] *Lehrstuhl für Theoretische Chemie II, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

Char burnout is the rate limiting step of solid fuel combustion reactions. Oxygen functional groups (OFGs) within char play an important role. They either already exist in the solid fuel and facilitate initiation reactions or they are formed as intermediates that open up fast reaction pathways with low barriers. This study aims to provide an atomistic level understanding of evolution of OFGs during char burnout. One of the major motivations behind this study is to provide functional group specific reaction mechanisms which can be used to develop predictive physico-chemical models of char oxidation such as in a recent study by Locaspi et al [1]. For our investigation of char burnout reactions at the OFGs, we use an automated reaction discovery tool based on reactive molecular dynamics simulations using ReaxFF and quantum mechanical refinement of the reactions using density functional theory (DFT) and correlated wavefunction calculations (coupled cluster) [2]. The model OFGs contain aldehydes, carboxylic acids, anhydrides, quinones, dioxins, furans, pyrones and lactones. We have observed that the OFGs convert into each other such as in the example mechanism shown in Figure 1 for phenanthrene-2-carbaldehyde, which converts into phenanthrene-2-carboxylic acid and phenanthren-2-ol.

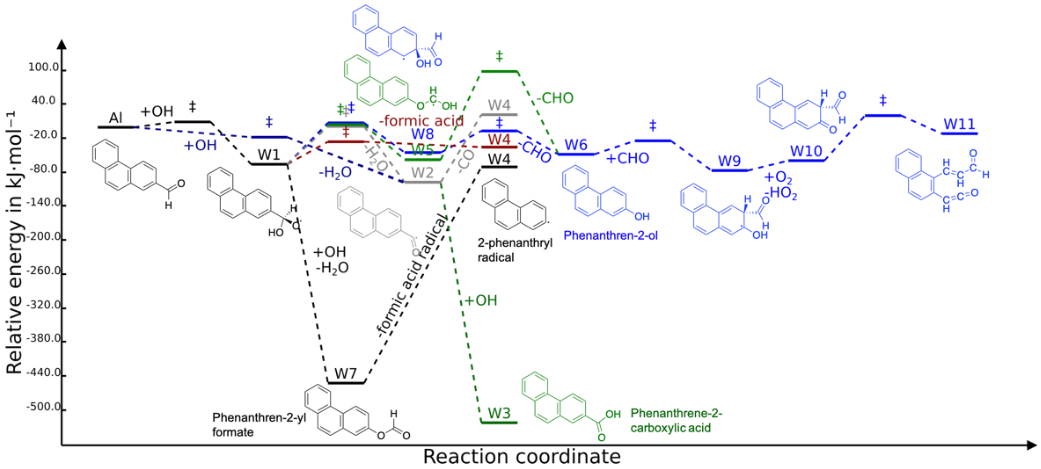


Figure 1. The initial steps of phenanthrene-2-carbaldehyde combustion. The electronic reaction energies are given at TPSSh-D3/TZVP level of theory including zero-point vibrational energies.

Acknowledgements

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

References

[1] A. Locaspi, P. Debiagi, M. Pelucchi, C. Hasse, and T. Faravelli, "A Predictive Physico-chemical Model of Biochar Oxidation," *Energy & Fuels, vol. 35, no. 18, pp.* 14894-14912, 2021, doi: 10.1021/acs.energyfuels.1c01559

[2] G. Schmitz, Ö. Yönder, B. Schnieder, R. Schmid, and C. Hättig, "An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants," *J. Comput. Chem.*, vol. 42, no. 32, pp. 2264–2282, Dec. 2021, doi: 10.1002/jcc.26757.

Oxidation of chars with high alkali content

Carmen Branca[1*]

*carmen.branca@stems.cnr.it

[1] *Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili, Consiglio Nazionale delle Ricerche, Piazzale Tecchio 80, 80125 Napoli, Italy*

Oxidation reactivity of lignocellulosic char is highly dependent on the formation conditions and the substrate's physicochemical properties. A key role is played by alkali and alkaline earth metals which catalyze the gasification and oxidation reactions, with potassium being the most effective for reducing the burnout temperature. The extent of these catalytic effects depends on both the content and the chemical state of the compounds. In this study, the effects of both potassium compounds (additives KOH, K_2CO_3, $KC_2H_3O_2$ and KCl) and content in char (up to about 5 wt%) have been examined, by means of dynamic thermogravimetry. Char is produced from the catalytic pyrolysis of beech wood particles first impregnated by means of aqueous solutions, containing the potassium compounds in proper amounts, and then dried. Scanning Electron Microscope (SEM) images of the char particles show high local concentrations of deposits of the additive (Figure 1A).

An important aspect of this study is that the char samples are representative of those produced in practical applications, also incorporating the effects of the thermal conditions of formation, affected by the nature and content of the additive. Wood chars are produced from packed-bed pyrolysis at a heating temperature of 605 K. The conversion is characterized by significant temperature overshoots (up to 130 K), owing to the enhancement in the reaction exothermicity induced by the loaded potassium, which locally causes very high self-heating rates of the substrate, as testified by the presence of cluster of bubbles, consequence of the release of volatile products across a molten phase, on the char structure (Figure 1B). As the nature/content of additives in wood is varied, the morphological structure of the chars is also partly modified. Therefore, in consequence of the additive loading, both the formation temperature and the structure of the chars vary, in this way affecting the subsequent oxidation.

The detailed dynamics of char conversion have been analyzed through the introduction of several characteristic parameters (rates of volatile release, temperatures, and mass fractions) leading to identifying the factors controlling the various reaction zones, to identify the possible conversion regimes as the additive content/nature is varied and to ascertain whether optimal potassium contents exist for enhanced carbon conversion. The thermogravimetric curves (heating rate of 5 K/min) show that in all cases, for temperatures up to 750 K, chars undergo a kinetically controlled stages of oxidative devolatilization and oxidation, but the quantitative features depend on the additive. For the untreated wood char, complete oxidation takes place within a relatively narrow temperature range (from about 670 to 740 K) with a well-defined peak rate. As the K content increases, the temperature range of interest tends to enlarge, leading to two conversion zones each characterized by a shoulder/peak rate (Figure 2). These features can be attributed to a shift from a thermal activation to a mixed catalytic-thermal activation of the oxidation reactions. For relatively low K contents, the wider conversion temperature range is delimited by continuously decreasing values of the ignition and the burnout temperatures, the more the basicity of the additive is high. However, for potassium contents above certain threshold limits, effects appear first of saturation and then of inhibition. Moreover, small amounts of char are always oxidized during ash cooking, at high temperatures, well above 750K, with very slow rates.

In conclusion, potassium enhances the char oxidation rates only for relatively low contents, up to maximum contents around 1–2 wt%, resulting from alkaline catalysis and modifications in the char structure, caused by interactions between additives and wood during both aqueous impregnation and pyrolysis.

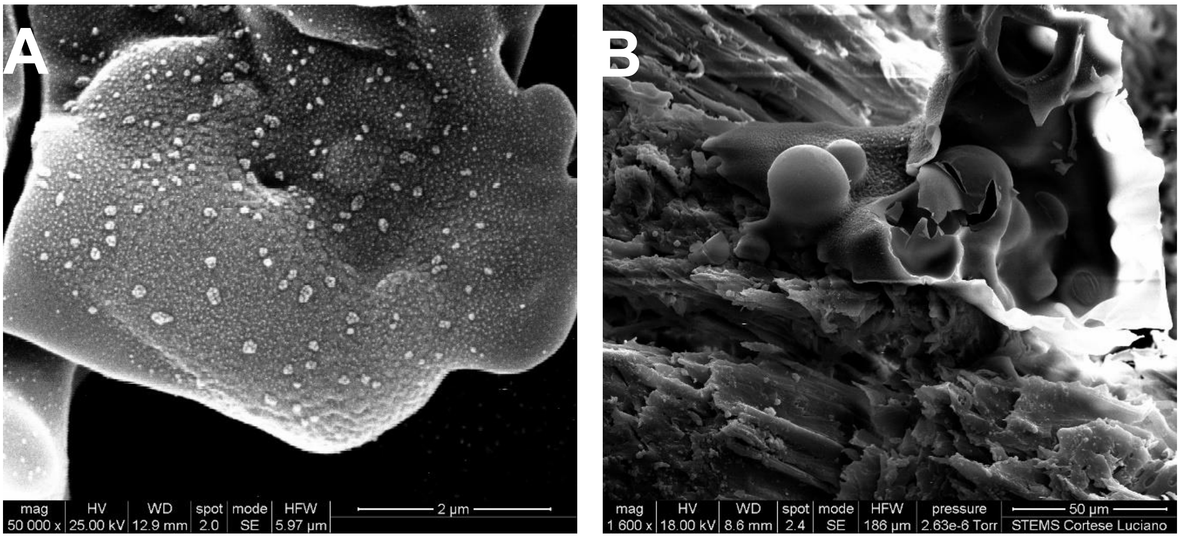


Figure 1. SEM images of the pyrolysis chars produced from K loaded wood showing significant deposits of the original/modified additive (A), and the formation of a molten phase with cluster of bubbles (B).

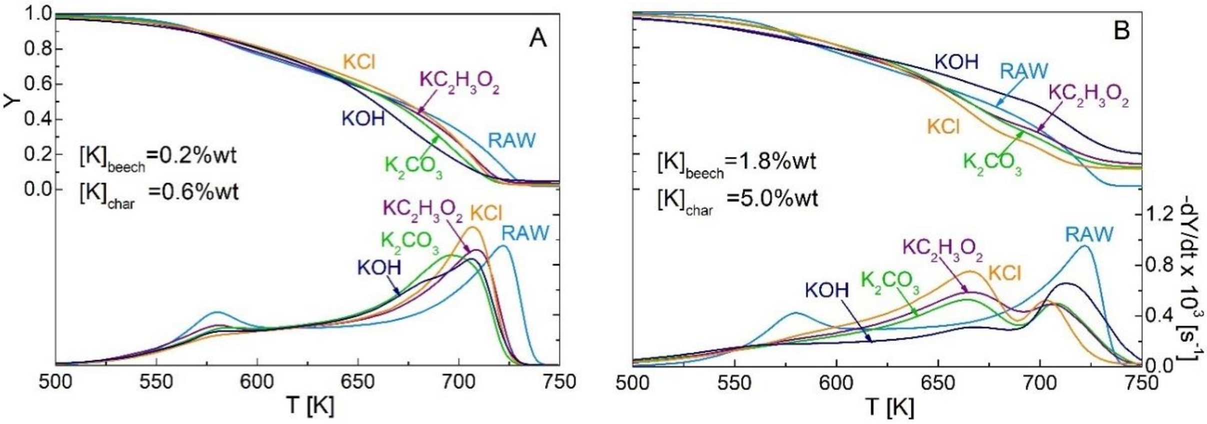


Figure 2. Thermogravimetric curves (heating rate 5 K/min) versus temperature for the conversion in air of chars generated from potassium-loaded beech wood for various potassium contents and additives KOH (A), K_2CO_3 (B), $KC_2H_3O_2$ (C) and KCl (D).

Mass transfer around freely moving active particles during fast heterogeneous chemical reaction in dense gas-fluidized bed

L. Molignano[1,2], M. Troiano[1,3], R. Solimene[3*], S. Tebianian[2],
J.-F. Joly[2], F. Scala[1] and P. Salatino[1]

*roberto.solimene@stems.cnr.it

[1] Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli Studi di Napoli Federico II, Piazzale Tecchio 80, 80125, Napoli, Italy

[2] Direction Conception Modélisation Procédés, IFP Energies Nouvelles, Rond-point de l'échangeur de Solaize, 69360, Solaize, France

[3] Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili, Consiglio Nazionale delle Ricerche, Piazzale Tecchio 80, 80125, Napoli, Italy

Fluidization technology offers attractive solutions for efficient thermochemical conversion of solid fuels. Fluidized bed combustion of solids is a mature technology, widely practiced worldwide for direct exploitation of biomass, with only moderate effort required to retrofit fossil fuel-based fluidized bed boilers to biomass-fired ones.

The operating temperature of fluidized bed combustors is, frequently, high enough for intrinsic kinetics not to be the rate-controlling step of the conversion. This aspect makes the process more sensitive to bed hydrodynamics: for fast heterogeneous chemical reactions, the apparent reaction rate depends on mixing/segregation patterns of the fluidizing gas, determined by the bubbling pattern, and by mass transfer around the active particles. Knowledge about the last-mentioned aspects is, thus, a key prerequisite for successful design and operation of such converters. However, there are still broad areas of uncertainties regarding fluidized beds hydrodynamics, mixing, heat and mass transfer phenomena.

Hydrodynamics in dense gas-fluidized beds of Geldart group B granular solids is most typically represented according to the simple "two-phase theory". Mass transfer between the bubble and the emulsion phases is governed by a gas interchange coefficient which takes into account gas cross-flow between the phases, as well as diffusional terms. Mass transfer between the bulk of the fluidized bed and an active particle is expressed, accordingly, in terms of a Sherwood number, Sh, by a Frössling-type correlation:

$$Sh = 2.0 \cdot \varepsilon_{mf} + K \cdot \left({}^{Re_{mf}}\!/_{\varepsilon_{mf}} \right)^{1/2} \cdot Sc^{1/3}$$

where ε_{mf}, is voidage at minimum fluidization conditions, K a fitting parameter, Re_{mf} is the Reynolds number at incipient fluidization referred to the active particle, and Sc is the Schmidt number. The reference to properties of the bed at incipient fluidization arises from the assumption that active particles mostly reside in the emulsion phase, and by the additional hypothesis that, according to the two-phase theory, the emulsion phase voidage is equal to the bed voidage at incipient fluidization ε_{mf}.

There is extensive evidence from the literature that fluidization patterns of dense gas fluidized beds may largely depart from the basic two-phase theory, as regards both the split of fluidizing gas between the bubble and the emulsion phases, and associated bubble flow patterns, and the voidage in the emulsion phase. Key reaction engineering parameters, like the extent of gas bypass in the emulsion phase, visible bubble flow and bubble rise velocity, mass transfer around fluidized particles, emulsion-bubble interphase mass transfer, are affected accordingly.

In the present study, a dedicated experimental campaign is directed to assess the influence of gas flow distribution on the mass transfer around active particles when a fast chemical reaction, namely the catalytic oxidation of carbon monoxide at 450 °C over Pt-loaded alumina spheres, takes place. A dense gas-fluidized bed of grey quartz sand solids belonging to group B of Geldart classification was previously characterized at the temperature of interest using custom-made capacitance probes. In particular, spatial maps of time-resolved pointwise values of the bed voidage were obtained. In the present study, gas mass transfer from the bulk of the bed towards the surface of Pt-loaded alumina is measured during the reactive experiments, in which grey quartz sand is used as fluidization medium, and worked out to calculate the corresponding Sherwood number. Results from mass transfer tests are fully consistent with the experimental findings obtained from the hydrodynamic characterization of the bed. It is shown that more accurate estimates of the active particle Sherwood number are obtained if the Frössling equation is implemented using the actual voidage and superficial gas velocity of the expanded emulsion phase, previously measured through the capacitance probes, rather than emulsion-phase properties corresponding to incipient fluidization.

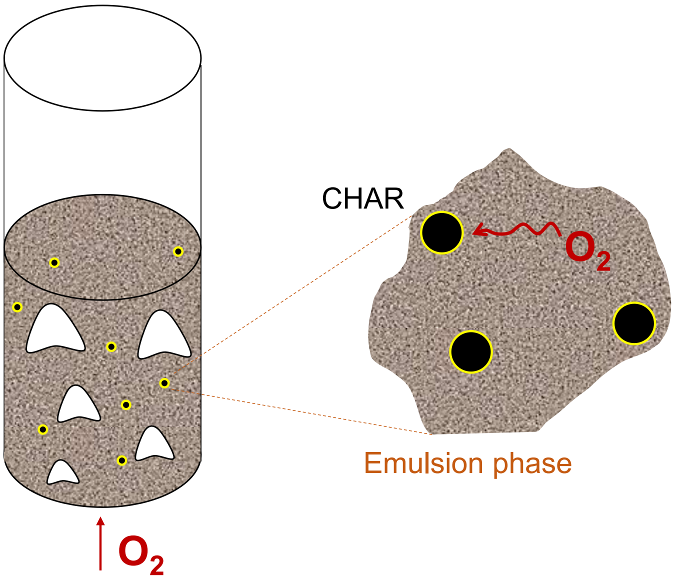


Figure 1. Scheme of oxygen mass transfer in the emulsion phase of the dense fluidized bed towards the surface of char particles.

Experimental investigation of RDF combustion for the optimisation of CFD simulations of oxy-fuel-fired cement kilns

R. Solana Gómez[1*], R. Streier[2], S. Pielsticker[1], R. Kneer[1] and V. Scherer[2]

*solana.gomez@wsa.rwth-aachen.de

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

[2] *Institute of Energy Plant Technology, Ruhr-Universität Bochum, Universitätsstraße, 44780 Bochum, Germany*

The cement industry is one of the major drivers of oxy-fuel technology in Europe. The operation of an oxy-fuel cement kiln in southern Germany has been announced recently by the research company CI4C (Cement Innovation for Climate) [1]. For the design of oxy-fuel kilns, reliable CFD simulation models of the complex combustion behaviour of refuse-derived fuels (RDF) are needed.

RDF comprises a large variety of materials with different physical and chemical properties. In addition, RDF particles are relatively large with a size in the centimetre range that requires consideration as thermally thick particles [2]. In this study, five model fractions of RDF, namely beech wood, cardboard, cotton, polyvinyl chloride (PVC) and polyethylene (PE) are analysed. These examinations are done in two different reactors, a fluidised bed reactor (FBR) to determine intrinsic reaction kinetics with pulverised RDF and a single-particle reactor to examine the effective reaction kinetics of the centimetre-sized original RDF particles.

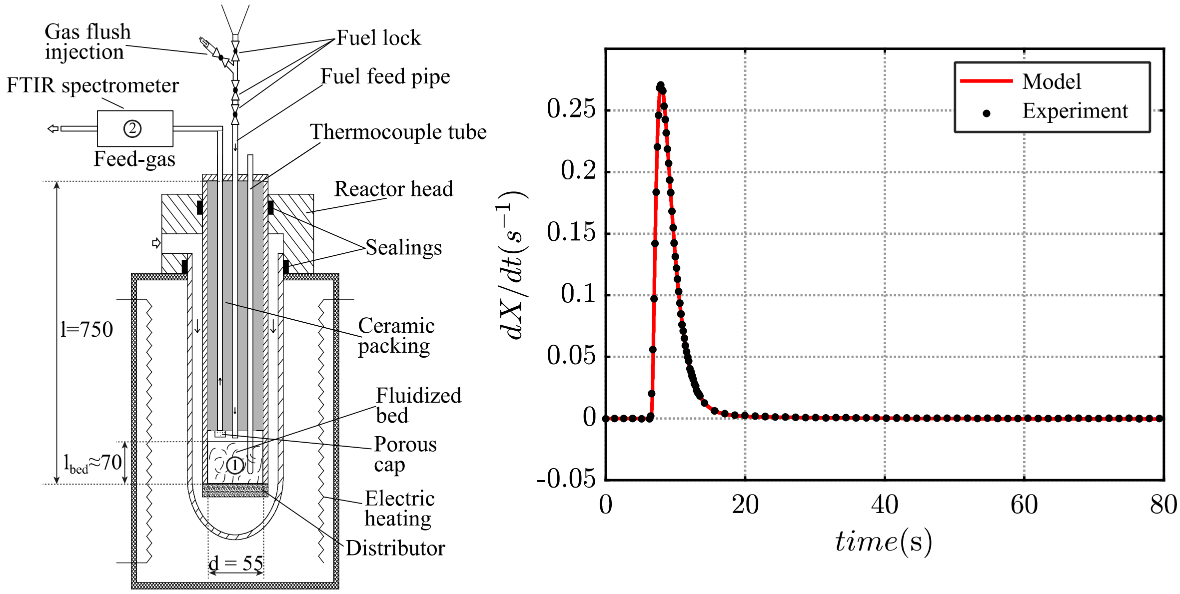


Figure 1. Scheme of the FBR [3] and exemplary mass release rate of cotton at 700 °C normalized with sample mass

The FBR, which is optimised for fast response behaviour [3], is used to derive pyrolysis kinetics for the different fuels. Milled samples of small particles, up to around 100 µm in size, are pyrolysed in a nitrogen atmosphere at different temperatures and the resulting reaction gases are measured *ex-situ* by means of FTIR-spectroscopy. A scheme of the entire experimental setup is shown in Fig. 1. The gathered data allow for a reconstruction of the volatile mass release rates. A two-step reaction model is fitted to the experimentally determined release rates (see Fig. 1), while an Arrhenius approach describes the reaction behaviour depending on temperature.

To examine the conversion of the thermally thick RDF particles, a single-particle reactor is used. With the single-particle reactor, the combustion of RDF particles in their original size is optically recorded at different temperatures (up to 1300 °C) and oxygen contents. Two RGB cameras observe the various conversion steps of the RDF particles from two different angles of view (see Fig. 2) [4]. This allows for the determination of characteristic times scales of conversion such as ignition delay time, time for volatile combustion and char burnout.

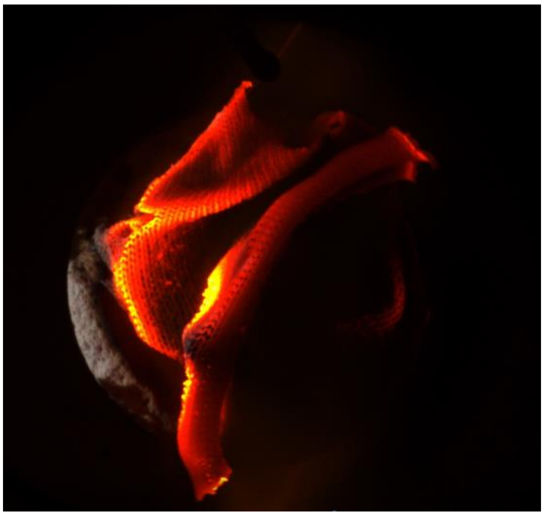


Figure 2. Char burnout of a cotton particle observed with RGB camera in single-particle reactor.

The current contribution will present the obtained experimental results and will give an outlook on how these data will be incorporated into respective models for the thermal conversion of RDF under oxy-fuel conditions in cement rotary kilns.

Acknowledgements

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

References

[1] https://www.cemnet.com/News/story/172829/polysius-wins-ci4c-order-for-oxyfuel-system-at-mergelstetten.html
[2] Streier R, Veckenstedt I, Deck T, Lampe K, Scherer V. Analysis of the impact of RDF combustion on cement clinker quality in a superstoichiometric oxy-fuel atmosphere by CFD simulations. MCS 12, Luxor 2023.
[3] Pielsticker S, Schlögel KU, Kreitzberg T, Hatzfeld O, Kneer R. Biomass pyrolysis kinetics in a fluidized bed reactor: Measurements and plausibility verification for reaction conditions. Fuel 2019;254:115589. https://doi.org/10.1016/j.fuel.2019.05.172
[4] Liedmann B, Arnold W, Krüger B et al. An approach to model the thermal conversion and flight behaviour of Refuse Derived Fuel. Fuel 2017;252-271.

10.18154/RWTH-2023-06259

Reaction kinetics for pressurized gasification of high-temperature biomass char with steam and mixtures of steam with CO_2

S. Walker[1*] and T. Kolb[1,2]

*stella.walker@kit.edu

[1] *Karlsruhe Institute of Technology (KIT), Engler-Bunte-Institute, EBI, Fuel Technology, Engler-Bunte-Ring 3, 76131 Karlsruhe, Germany*

[2] *Karlsruhe Institute of Technology (KIT), Institute of Technical Chemistry, ITC, Gasification Technology, 76131 Karlsruhe, Germany*

High pressure entrained flow gasification (EFG) of biogenic suspension fuels is part of process chains that deliver non-fossil synthesis gas as a source of hydrogen and as a feedstock for base chemicals and fuels. During fuel conversion in EFG, the suspension fuel droplets are rapidly heated up, the liquid phase undergoes evaporation and cracking reactions whereas char undergoes secondary char pyrolysis and subsequently gasification in a CO_2- and H_2O-rich atmosphere. The gasification step is known to be the rate-limiting step during fuel conversion. Reaction kinetics of secondary char gasification in mixed atmospheres at elevated pressures are therefore necessary for EFG reactor design.

Secondary chars were produced in lab-scale experiments at conditions similar to EFG conditions, i.e. high heating rates and high temperatures. The chars were characterized with respect to specific surface area, ash dispersion on the char surface and the graphitization of the carbon matrix. A non-linear correlation between the temperature of secondary pyrolysis and specific surface area and ash dispersion was found, while graphitization increased monotonically with pyrolysis temperature. From reaction kinetic experiments, it could be deduced that especially catalytically active calcium species on the char surface affect gasification reactivity in CO_2 [1, 2].

Experimental investigations of heterogeneous reaction kinetics in the chemically controlled regime of char gasification in H_2O and H_2O-CO_2-mixtures at different partial pressures are necessary to clarify the influence of char properties on gasification reactivity in H_2O and H_2O-CO_2-mixtures. A differentially operated pressurized fixed-bed reactor developed for this purpose is presented. Reaction kinetics in various gas atmospheres can be investigated at temperatures up to 900 °C and at pressures up to 20 bar. Steam can be applied at partial pressures up to 12.5 bar. The product gas phase analysis allows for calculation of carbon conversion rate. Reaction kinetic experiments with one type of secondary beech wood char in steam indicate that the reactive surface area is not saturated in the investigated pressure range. In mixed gasification atmosphere, an increasing dominance of steam on the reaction rate with increasing steam partial pressure could be observed.

References

[1] Schneider, Christoph, Stella Walker, Aekjuthon Phounglamcheik, Kentaro Umeki, and Thomas Kolb. Effect of calcium dispersion and graphitization during high-temperature pyrolysis of beech wood char on the gasification rate with CO_2 [online]. *Fuel.* 2021, 283(3), 118826. Available from: 10.1016/j.fuel.2020.118826.

[2] Schneider, Christoph, Michael Zeller, Daniel Böhm, and Thomas Kolb. Influence of pressure on the gasification kinetics of two high-temperature beech wood chars with CO_2, H_2O and its mixture [online]. *Fuel.* 2021, 299(3), 120523. Available from: 10.1016/j.fuel.2021.120523.

Effects of pyrolysis reactor types on the bioproduct compositions of tannery fleshing waste

R. Chagtmi[1,2], A. Maaoui[1,2], F. Cerciello[4*], A. Ben Hassen Trabelsi[1], B. Apicella, F. Stanzione[3], R. Migliaccio[3], M. M. Olliano[3], M. Urciolo[3] and O. Senneca[3]

*francesca.cerciello@ruhr-uni-bochum.de

[1] *CRTEn: Research and Technology Centre of Energy, Technopark Borj-Cédria, B.P 95, 2050, Hammam Lif – Tunisie*
[2] *FST: Faculty of Sciences of Tunis, University Tunis El Manar*
[3] *STEMS, C.N.R., P.le Tecchio, 80125 Naples, Italy*
[4] *Laboratory of Industrial Chemistry, Ruhr University Bochum, 44801 Bochum, Germany*

The discharge of huge quantities of fleshing waste by the leather industries has raised serious concerns about its impact on the environment [1]. Quantitatively, one ton of raw material yields up to 800 kg of production-related wastes and by-products [2]. This study aims to investigate the effects of pyrolysis types (slow and fast) on the bioproduct compositions.

The Tannery fleshing waste was dried under air (TFW-OD) and greenhouse (TFW-GD), the dried samples were characterized using several techniques: proximate analyses (moisture, volatile matter, ash, fixed carbon), elemental analyses CHNO, HHV, FTIR, and XRD. Pyrolysis was conducted using two different reactors: a fixed bed reactor and a heated strip reactor. In the fixed bed reactor, the final temperature was 500 °C, the heating rate was 10 °C/min and the residence time 60 min. In the heated strip reactor, 1000 °C was the final temperature, 1000°C/s was the heating rate, and 3 seconds was the residence time. The produced biochars were characterized by proximate analyses, elemental analyses CHN-O, FTIR, XRD, and the bio-oils were characterized by GC/MS.

As far as biochars are concerned, both slow and fast pyrolysis TFW-GD bio-chars have a comparable carbon content of around 30 wt.%, the carbon content of chars from slow and fast pyrolysis of TFW-OD is instead quite different (41.07 vs 28.12 wt. %). All chars are rich in Ca, Si, and Mg, even though differences in the mineralogical form are observed between OD and GD samples due to the occurrence of saponification reaction. On the whole, all biochars are interesting for agronomical and environmental uses (biofertilizer, bioadsorbents, or for soil remediation).

Bio-oils collected by slow and fast pyrolysis are quite different in terms of share of aromatic vs. aliphatic compounds, the fast pyrolysis tars being all richer in aromatics. However, the large presence of N and O in both aliphatic and aromatic compounds calls for further upgrading before utilization of these products of TFW pyrolysis as biofuels.

Acknowledgments
This work was supported and funded by the Ministry of Higher Education and Scientific Research (MESRST) in Tunisia and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – 215035359 – SFB/TRR 129 "Oxyflame".

References

[1] P Puhazhselvana, A Pandia, P B Sujirithaa, G S Antonya, S N Jaisankarb, N Ayyaduraia, P Saravananc NRK. Recycling of tannery fleshing waste by a two step process for preparation of retanning agent. Process Saf Environ Prot 2022;157:59–67. https://doi.org/10.1016/j.psep.2021.11.003.

[2] Yilmaz O, Cem Kantarli I, Yuksel M, Saglam M, Yanik J. Conversion of leather wastes to useful products. Resour Conserv Recycl 2007;49:436–48. https://doi.org/10.1016/j.resconrec.2006.05.006.

Fast pyrolysis of biomass of different type and origin: Effect on bio-oil and char

A. Maaoui[1,2], R. Chagtmi[1,2*], F. Cerciello[3], B. Apicella[4], R. Migliaccio[4],
F. Stanzione[4], M. M. Oliano[4], A. Ben Hassen Trabelsi[1] and O. Senneca[4]

*chagtmiraouia@gmail.com

[1] Laboratory of Wind Energy Control and Waste Energy Recovery, LMEEVED, Research and Technology Centre of Energy, CRTEn, B.P. 95, 2050 Hammam-Lif, Tunisia

[2] Department of Geology, Faculty of Sciences of Tunis, University of Tunis El Manar, 2092, El Manar II, Tunis, Tunisia

[3] Laboratory of Industrial Chemistry, Ruhr University Bochum, 44801 Bochum, Germany

[4] Istituto di Scienze e Tecnologia per l'Energia e la Mobilità Sostenibili (STEMS)-CNR, 80125 Napoli, Italy

Pyrolysis is considered the most promising approach to convert biomass and to generate valuable bio-oils and biochars. This study aimed to investigate fast pyrolysis of different types of wastes from Mediterranean biomasses (Opuntia Ficus Indica, Pomegranate, Aleppo Pine Cones, and *Pinus Pinea* Cones) and compare the quality of bio-oils and chars.

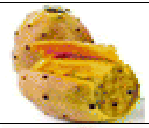
Biomasses were characterized by proximate and ultimate analyses, FTIR spectroscopy, X-ray diffraction, thermogravimetric and calorimetric analysis. Fast pyrolysis experiments were carried out in a heated strip reactor with a heating rate of 10^3 K/s and holding time of 3 s at 1000 K. Tar products were readily quenched and collected on a cold pyrex bridge, positioned above the sample holder at near ambient temperature, so as to minimize secondary reactions. Tar samples were characterized by GC-MS analysis and the quality in terms of chemical families was discussed. Char samples were recovered from the strip and analysed by SEM, elemental analysis, and XRD.

The results show that the bio-oils and char composition vary sensibly:

- Aleppo pine cones and *pinus pinea* cones, the hardest of the examined biomasses, upon fast pyrolysis produce a bio-oil that is made of oxygenated aromatic compounds and a bio-char with high carbon content (>60 %), which could be envisaged for soil amendment and carbon sequestration.
- Pyrolysis of Opuntia Ficus Indica wastes (peels and cladodes) generates chars with comparably lower carbon content, but particularly rich in potassium (K) and calcium (Ca).
  The bio-oil from the peels is still rich in aromatic compounds, similar to APC and PPC, while the bio-oil from the cladodes is almost exclusively made of anhydrosugars.
- Pyrolysis of pomegranate peels generates a carbon-rich char, as APC and PPC, but the bio-oil is rich in anhydrosugars and also furfural.

From the morphological point of view, all bio-chars seem to be made up of agglomerates of irregular elongated or semi-spherical shaped particles with large macropores.

Acknowledgments
This work was supported and funded by the Ministry of Higher Education and Scientific Research (MESRST) in Tunisia and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – 215035359 – SFB/TRR 129. Authors acknowledge Mr Luciano Cortese for SEM analysis.

Biomass			**Main components in bio-oil** 	**%Carbon in bio-char** 
Opuntia Ficus Indica cladodes		**OFIC**	anhydrosugars	19
Opuntia Ficus Indica peels		**OFIP**	oxygenated aromatic compounds	35
Pomegranate peels		**PGP**	furfurals and anhydrosugars	>60
Aleppo pine cones		**APC**	oxygenated aromatic compounds	>60
Pinus Pinea cones		**PPC**	oxygenated aromatic compounds	>60

Fast pyrolysis

Heated Strip Reactor
1000K
3s

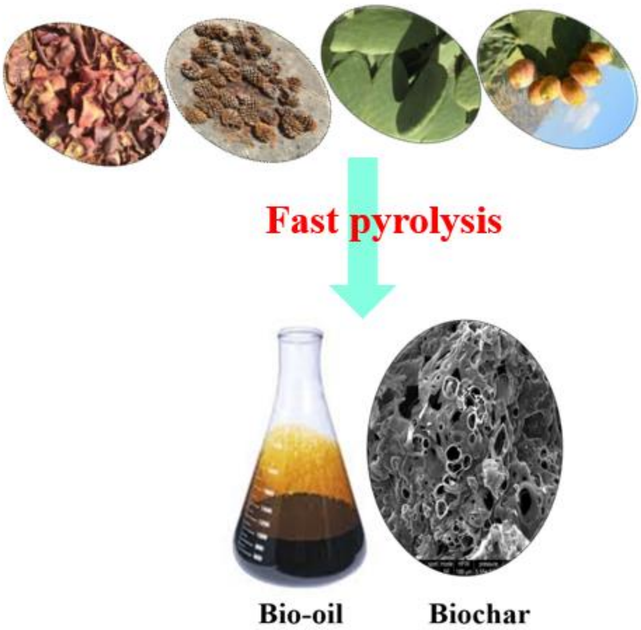


Figure 1. Mediterranean biomass for pyrolytic oil and char production

An experimental study of the stability and nearfield structure of oxyfuel jet flames at elevated pressures

M. Bukar[1*], S. Basnet[1], B. Wu[1] and G. Magnotti[1]

*muhammad.bukar@kaust.edu.sa

[1] *Clean Combustion Research Centre, King Abdullah University of Science and Technology, 23955, Thuwal, Saudi Arabia*

Oxy-fuel combustion at high pressures is considered one of the promising carbon capture technologies (CCT), which has the potential to reduce emissions (both CO_2 and NO_x) while at the same time increasing the thermodynamic efficiency of the system. It involves burning fuel in pure oxygen (obtained from an air separation unit) at high pressures in a CO_2-enriched environment.

In this study, we present experimental results of the flame stability limit and the nearfield structure of oxy-methane jet flames from 2–5 bar. The oxidizer is an equimolar mixture of CO_2 and O_2. Two sets of cases were studied: one where pressure increase was achieved by keeping the fuel Reynolds number constant and the other where the velocity was kept constant while increasing pressure. Stability limits (lift-off and reattachment velocities) are reported for various co-flow velocities. Natural flame luminosity imaging with a DSLR camera and combined CH* and CO_2* chemiluminescence using an ICCD (PIMAX 4) are used to characterize the near-field structure of the flame. The ICCD camera was equipped with a 104 mm UV lens (f# 4.5) and a narrow band-pass filter (430 nm± 5nm) to strengthen the relative contribution of CH* over CO_2*. The images obtained from the ICCD camera were first background subtracted and then subjected to the Abel inversion method to obtain two-dimensional images which are then further post-processed to study the nearfield structure. The study investigates the effect of fuel velocity and pressure on the flame attachment height, attachment radius, and CH* thicknesses. The DSLR images complement the study with qualitative information on the flame appearance, and sooting propensity. Preliminary results show that at constant Reynolds number, the attachment height decreases with pressure for all cases considered while the attachment radius increased with pressure increase. At constant velocity, however, both the attachment height and radius were observed to decrease with increased pressure.

Particle dynamics within a high-velocity biomass-laden jet investigated by two-phase velocimetry at low to ultra-high repetition rates

C. Geschwindner[1*], K. Westrup, A. Dreizler[1] and B. Böhm[1]

*geschwindner@rsm.tu-darmstadt.de

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

The combustion of pulverized biomass in oxy-fuel environments in combination with carbon capture and storage facilities has the potential to generate negative carbon dioxide (CO_2) emissions. A promising pathway for the realization of this technology is the retrofit of coal power stations, in which the introduction of aspherical biomasses causes complex particle-turbulence interactions, which need to be investigated to understand the coupling between the movement of complex particle shapes and the surrounding turbulent carrier phase.

To enable the experimental investigation of particle-laden turbulent jets at high flow speeds and optical magnifications, a flexible repetition rate two-phase velocimetry laser diagnostics system was introduced and demonstrated by Geschwindner et al. [1], in which the pulse picking of a fiber laser was utilized for limited field-of-view time-resolved and statistical particle image velocimetry. With this approach, the movement of individual biomass particles was spatially and temporally captured at unprecedented resolutions. The simultaneous recording of the particle shapes using diffuse back-illumination allowed for an estimation of the particle Reynolds number by measuring the slip velocity and the particle size in a nonreactive turbulent jet at a jet exit velocity of 41.75 m/s ($Re_{jet} = 7500$).

In this study, we present detailed results of this experimental study focusing on the dynamics of walnut shell and miscanthus particles sieved in a size range of 90-125 µm within the intermediate region of the turbulent jet. As all biomasses within this investigation show Stokes numbers far greater than 1, particles drag behind the flow within the pipe but decelerate slower than the surrounding phase as the jet expands axially. This behaviour causes an inversion of the direction of the particle wakes within the intermediate region of the turbulent jet, which is highly relevant for the transport of volatiles away from the particles. The slip velocity field is evaluated with respect to the orientation, size and shape of biomasses highlighting the aerodynamic effects of different particle geometries on the multi-phase dynamics of the particle-laden turbulent jet.

Acknowledgements

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

References

[1] Geschwindner, C.; Westrup, K.; Dreizler, A.; Böhm, B. (2022): Pulse picking of a fiber laser enables velocimetry of biomass-laden jets at low and ultra-high repetition rates. *Proc. Combust. Inst.* 39, DOI: 10.1016/j.proci.2022.07.138

10.18154/RWTH-2023-06259

Characterization of the ignition and combustion behaviour of biogenic residues

M. Giesen[1*], D. Bernhardt[1] and M. Beckmann[1]

*matteo.giesen@tu-dresden.de

[1] *Chair for Energy Process Engineering, TU Dresden, George-Bähr-Str. 3b, 01069 Dresden, Germany*

In the development of burners and combustion chamber systems, increasing efficiency, reducing emissions, and extending travel times continue to be the important objectives. In addition, questions of fuel and load flexibility are increasingly playing a role. The higher the demands placed on the systems, the more precisely they must be designed for the respective application (fuel, output, flexibility, emission, etc.). This means that beyond laboratory tests and experience from already similar practical plants, fuel-technical tests on pilot plants and mathematical models must increasingly support the design. Nowadays, biomasses, process residues and by-products as well as waste are increasingly used in existing combustion plants as substitute fuels for mono-combustion or together with fossil fuels for co-combustion. However, this is not readily possible due to changes in fuel properties. In this case, the laboratory tests of the new fuels or fuel mixtures can provide the first information on the possible changed combustion behaviour. To date, however, there is no standardised measurement method for determining the reaction kinetic properties. Therefore, special attention should be paid here to the investigation of the ignition and combustion behaviour of pulverised fuels. Investigations on the ignition and burning behaviour are often performed for single particles or particle clouds.

A method for the examination on single particles is using a drop tube reactor like the FIELD-tube [1]. Using the FIELD-tube, the combustion behaviour, which represents the temporal course of the combustible components in fuel particles during the combustion process, dependent on external conditions like heating rate, gas composition, particle size as well as the fuel composition can be determined. The combustion curves obtained not only allow the reactivity of fuels to be compared with each other, but also the determination kinetic parameters for the subsequent computer-aided combustion simulations. combustion simulations. The high number of dependent variables leads to considerable measuring insecurities, high costs and difficulties in representative application to inhomogeneous or time-varying fuels such as biomasses. Using single particle methods, the essential influencing factor of particle-wall and particle-particle interactions can’t be regarded.

To consider these essential processes in the combustion of particle clouds the Zelkowski ignition oven method can be used [2]. In this method, the ignition delay time measuring the change in light intensity and its dependence on the mentioned parameters can be estimated. The ignition delay time plotted against the combustion gas temperature results in the ignition hyperbole which can be used to derive the burner design and settings. In this contribution, the ignition oven method will be discussed using experimental data. In further research, the ignition oven method should be combined with near infrared spectroscopy to obtain temporal and spectral data of the ignition and combustion behaviour of powdered fuels and using a statistical-empirical model a standardised method should be developed.

References

[1] Field, M. A.: Rate of combustion of size-graded fractions of char from a low-rank coal between 1200 K and 2000 K. British Coal Utilization Research Association, 1969.

[2] Zelkowski, J.: Kohlecharakterisierung und Kohleverbrennung, Kohle als Brennstoff, Physik und Theorie der Kohleverbrennung. VGB PowerTech e.V. Essen, VGB - B 008. 2. Edition, 2004.

An experimental study on oscillating behaviour of the radiation spectrum of self-sustained biomass flames at different thermal loads

B. Özer[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 assessment of the transient behavior of solid fuel flames with different thermal loads is essential to understand the sensitivity and scalability of experimental results. Therefore, the present study aims to experimentally examine the spatio-temporal fluctuations in self-sustained pulverized biomass swirl flames. Moreover, the impact of the periodic and non-periodic fluctuations in the particle feeding line on the transient flame behavior is investigated. Experiments are conducted using a pilot-scale down-fired cylindrical combustion chamber in the test facility of the Institute of Heat and Mass Transfer (WSA) at the RWTH Aachen University. Four different flame conditions with four different thermal loads (60, 80, 100, and 120 kW) are investigated under a conventional air atmosphere. For the experiments, ground walnut shells with a volumetric particle size range of 100–250 µm have been used, whereby 65 % of the particles have been in the size range < 15 µm.

Two experimental methods, each providing high temporal resolution data, are synchronously employed: i) narrow-angle spectrometer measurements to determine the transient behavior of flame radiation and ii) a beam extinction method to measure the fluctuations in particle feeding. The narrow-angle spectrometer measurements are performed at six different axial distances from the dump plane of the burner such that the transient behavior of the different sections of the flame can be differentiated. Although the narrow-angle spectrometer lacks spatial resolution, fluctuations in the flame radiation can be categorized based on the spectral bands of different species (e.g., sodium and potassium). Also, solid particle temperatures are estimated by performing a fit of the Planck function over the corrected flame spectra. For the beam extinction method, the attenuation of a collimated laser beam passing through the transparent section of the particle feeding line is captured and directly linked (via Lambert-Beer's law) to the particle number concentration of particles.

The described methods allow to compare the transient behavior in the particle feeding line and in the solid particle temperature for the studied flames by means of flicker frequency (weighted averaged frequency of fluctuations) and fluctuation amplitude. Moreover, the impact of arbitrary short-term changes in particle feeding line on the flame radiation will be quantified using wavelet coherence analysis.

Acknowledgements

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

Investigations on solid fuel particle porosities and their influence on the particle radiation interaction

L. Pörtner[1*], M. Koch[2], E. Freisewinkel[1], S. Pielsticker[2],
M. Schiemann[1], R. Kneer[2] and V. Scherer[1]

*poertner@leat.rub.de

[1] *Institute of Energy Plant Technology, Ruhr-University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[2] *Institute of Heat and Mass Transfer, RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*

The interaction of radiation with solid fuel particles in combustion systems is an important heat transfer phenomenon for the adequate modelling of the combustion process. Detailed knowledge of the single particle properties allows for a valid description of the underlying processes. Typically, a solid fuel particle is not a homogeneous solid mass but is interspersed with pores whose percentage and shape vary during the conversion process. The total porosity, defined as the ratio of the particle pore volume and the solid structure volume, serves as an important characterization feature for this purpose.

Experimental investigations on single Columbian bituminous coal char particles show a conversion-dependent internal particle structure. Thin film particle REM images of raw coal and char samples, produced by a drop tube reactor presented in [1], are analysed, showing particle porosities, differing from conventional porosity measurements. While these methods, using e.g. N_2 or CO_2 adsorption, determine values of 0–0.4 [2, 3], the optical analysis leads to particle porosities of 0.5–0.8. The difference in these results is caused by the limits of the adsorption methods: As the adsorption only detects open particle pores close to the particle surface, the optical analysis also captures closed pores of the internal particle structure. Figure 1 shows an original and a processed REM image of a particle thin film with a calculated porosity of 0.75.

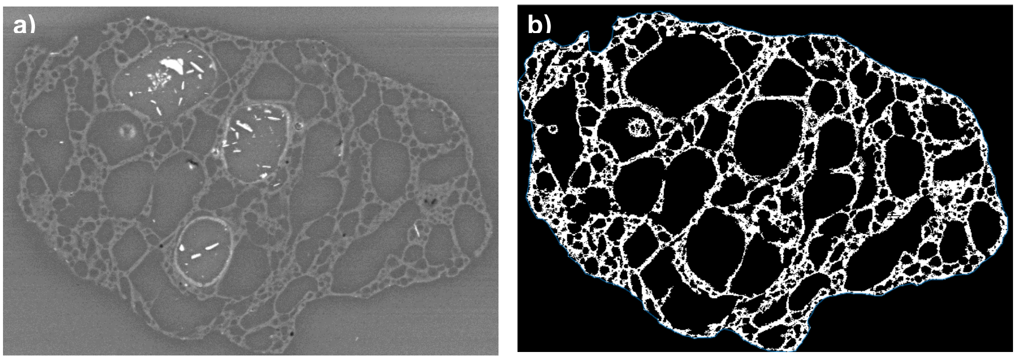


Figure 1. Images of a single coal char particle thin film: **a)** raw REM image, **b)** analysed structure image (white: particle structure, black: empty space)

As known from adsorption experiments of [2], the porosity of coal char particles increases with advancing conversion. Considering this evolution, simulations using the generalized multiparticle Mie theory (GMM) [4], are performed to investigate the impact of the porosity on the particle radiation interaction. As Mie theory is only valid for spherical particles, clusters of monodisperse spheres are generated to represent spherical coal particles of a total diameter $D_P = 50$ µm. To investigate the largest possible porosity range, hcp-lattice-based (hcp $\widehat{=}$ hexagonal close-packed) sphere clusters are designed. The control of the total particle porosity defined as the ratio of the 50 µm total diameter, spherical particle volume and the sum of all single sphere volumes, is managed by randomly removing single spheres from the cluster, resulting in a porosity increase. Figure 2 exemplarily presents two clusters of different porosity.

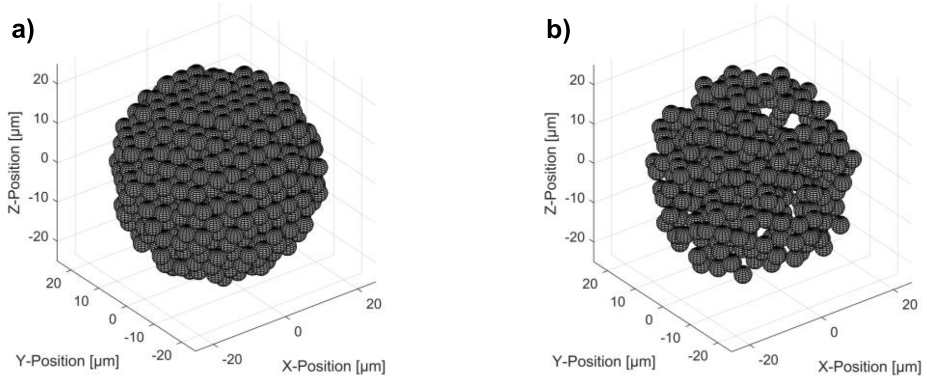


Figure 2. Images of two hcp-lattice based sphere clusters with a total diameter of 50 µm and sphere diameter of 4 µm: **a)** porosity = 0.5, **b)** porosity = 0.8

Following, simulations of the particle radiation interaction are performed, investigating particles with varying porosities of 0.5–0.9, irradiated by an electromagnetic wave ($\lambda = 3$ µm). Analysis of the determined particle radiation interactions from GMM identifies trends of increasing absorption and decreasing scattering coefficients with decreasing porosity. By variation of the single sphere diameter, saturation effects of both coefficients with decreasing sphere diameter can be observed, indicating the need for highly resolved structure simulations.

Caused by cluster system complexity at higher resolutions, resulting in time-consuming calculations of the GMM, the faster Discrete Dipole Approximation (DDA) is used to validate the received GMM data, prove the porosity impact and extend the dataset. In the DDA, the particle structure is modelled by point dipoles. As long as the distance between neighbouring dipoles d is lower than $d \leq \lambda/10$, the DDA is able to calculate radiation interaction with solid fuel particles with $D_\mathrm{P} = 50$ µm.

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

References

[1] Heuer S., Senneca O., Wütscher A., Düdder H., Schiemann M., Muhler M., Scherer V.: Effects of oxy-fuel conditions on the products of pyrolysis in a drop tube reactor. Fuel Processing Technology 2016;150:41–9.
[2] Heuer S., Wedler C., Ontyd C., Schiemann M., Span R., Richter M., Scherer V.: Evolution of coal char porosity from CO_2-pyrolysis experiments. Fuel 2019;253:1457–64.
[3] Vorobiev N., Valentiner S., Schiemann M., Scherer V.: Comprehensive Data Set of Single Particle Combustion under Oxy-fuel Conditions, Part II: Data Set. Combustion Science and Technology 2020;5(1):1–16.
[4] Xu Y.L: Electromagnetic scattering by an aggregate of spheres. Appl. Opt., AO 1995;34(21):4573–88.

Combined flow, temperature and soot investigation in oxy-fuel biomass combustion under varying oxygen concentrations using laser-optical diagnostics

H. Schneider[1*], H. Hamel[1], J. Hebel[1], J. Emmert[1], B. Böhm[1],
S. Wagner[1], R. Kneer[2] and A. Dreizler[1]

*hschneider@rsm.tu-darmstadt.de

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

[2] *Institute of Heat and Mass Transfer, RWTH Aachen University, Augustinerbach 6, 52056 Aachen, Germany*

Electric power generation and heat supply will be spread over many, mostly renewable technologies to significantly lower greenhouse gas emissions in future. While renewable energy sources like solar and wind power suffer from short- and long-term fluctuations, biomass combustion can produce large amounts of power and heat independent of seasonal and weather conditions.

Applying carbon capture and storage (CCS) technologies to biomass combustion will result in negative CO_2 emissions concerning the atmosphere and therefore biomass energy with carbon capture and storage (BECCS) has a great potential to even reduce CO_2 concentration in the atmosphere. One promising concept to efficiently capture and store CO_2 after the combustion process is burning biomass in an oxy-fuel atmosphere. Thereby large amounts of exhaust gases consisting mostly of CO_2 are recirculated into the combustion chamber and pure oxygen is added.

With oxy-fuel combustion, the oxygen concentration can therefore be easily adjusted. To investigate the influence of the oxygen concentration in an oxy-fuel atmosphere on flame stabilization and the combustion process of biomass particles, different operation conditions inside a gas-assisted, swirled combustor are studied. The combustor operates flames in the power range up to 70 kW_{th} and offers full optical access to the combustion process. The oxygen concentration under oxy-fuel conditions is varied between 27 vol.% and 36 vol.% and a comparable operation condition in air is investigated. To gain a deeper understanding of fluid-mechanical, particle-dynamical and chemical processes underlying pulverised solid fuel combustion under varying oxy-fuel conditions, a large dataset is measured using laser-optical diagnostics. The dataset includes chemiluminescence imaging of CH*, flow velocities of the gas and solid phase, gas temperatures and qualitative soot measurements including visualisation of polycyclic aromatic hydrocarbon (PAH) occurrences as soot precursors.

First, the oxygen influence on the single-phase combustion (methane combustion) is analysed in the near-nozzle region. A comparison of the gas temperature map and the flow field of an oxy-fuel operation condition with 33 vol.% oxygen concentration is shown in Figure 1. In a second step, biomass particles are added to the single-phase operation conditions.

In this study, a comprehensive analysis of the influence of oxygen concentration on oxy-fuel combustion in the near nozzle is presented. Flame stabilization is investigated using information on CH* chemiluminescence, gas flow velocities, particle velocities and gas temperatures. The combustion process of biomass particles and the formation of pollutants is analysed using qualitative soot and PAH measurement data in combination with information on flow and temperature.

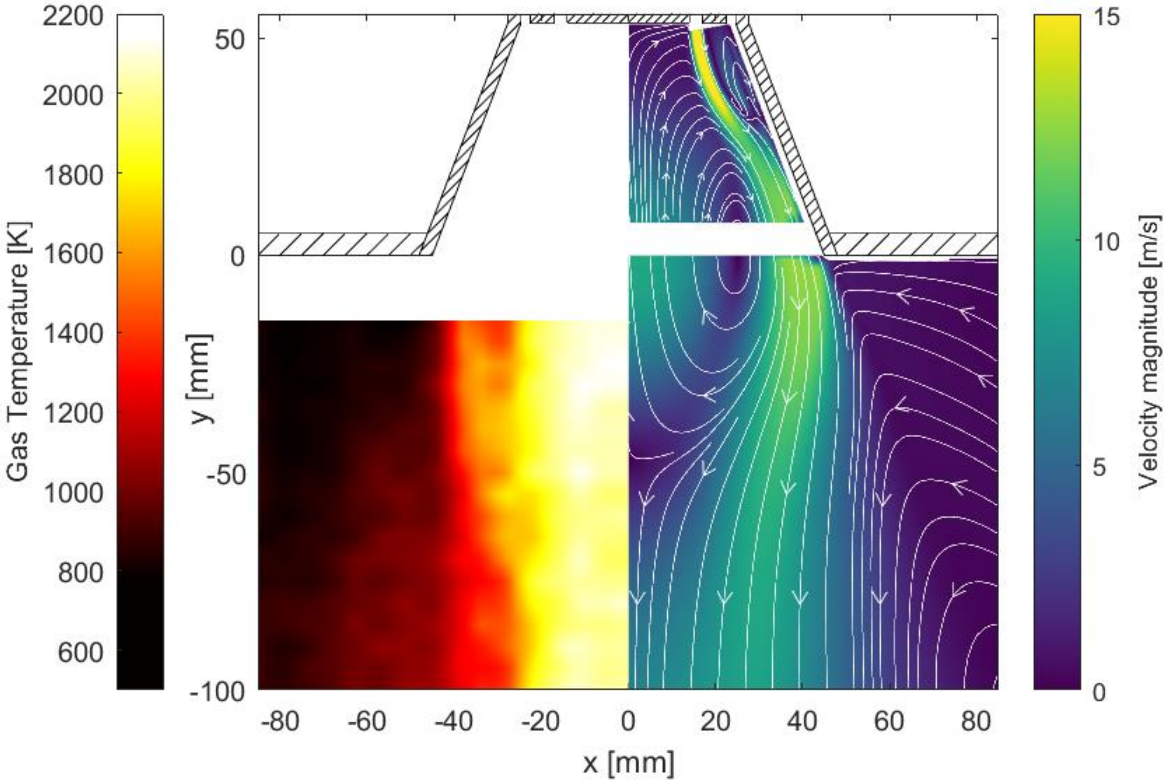


Figure 1. Flow field and temperature map of single-phase combustion for oxy-fuel combustion with 33 vol.% oxygen concentration. Left: Gas temperature map. Right: Flow field of the gas phase. Areas marked in white were not measured due to limitations of the measurement method or optical access.

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

Investigation of oxygen-enriched biomass flames in a lab-scale entrained flow reactor

M. D. B. Takehara[1*], M. A. Chishty[1], K. Umeki[1] and R. Gebart[1]

*marcelo.takehara@ltu.se

[1]*Division of Energy Engineering, Luleå University of Technology, Luleå, Sweden*

Introduction

Enriched air combustion using pulverized biomass fuel is an effective method to improve char combustion and improve flame stability. Moreover, understanding the impact of O_2 addition is an important step toward oxyfuel combustion, one of the most promising technologies for bioenergy with carbon capture and storage (BECCS). Our previous studies focused on flow manipulation methods, e.g., swirling co-flow and acoustic forcing, to enhance particle dispersion during biomass combustion and gasification. This work aims to extend the understanding of the effect of different manipulation methods on oxygen enrichment combustion at different levels in a lab-scale entrained flow reactor. Visual observation of the flame structure is assessed by high-speed imaging and emission characteristics by a flue gas analyser and particle emission characterization.

Methodology and Results

The experiments were carried out in an atmospheric down-fired entrained flow reactor with a 400 mm inner diameter and 950 mm length (Figure 1a). The refractory lining was electrically heated to temperatures up to 900 °C to enable ignition and to represent conditions close to large industrial-scale reactors. A 30 kW_{th} burner with an adjustable swirl and acoustic forcing system was top mounted to the reactor. Pulverized biomass (sawdust and pine bark from forest residue) feeding was controlled by a screw feeder and mass flow controllers adjusted the air supply for transport and secondary swirling air. Oxygen enrichment was controlled by an additional flow controller and mixed with the secondary air. The acoustic oscillations were imposed by a synthetic jet actuator mounted perpendicular to the feeding line. 2000 post-processed flame visualizations by high-speed cameras provided information on flame morphology, including lift-off distance by ignition point identification. Particle samples were collected from the bottom hopper and the surface of quartz filters after iso-kinetic sampling and characterized to verify carbon burnout.

The reference case (Table 1) considered air-combustion of 1 kg/h pine bark (particle size in the 0–400 µm range and presented relatively high CO emissions (above 2,000 mg/m^3 at 6 vol.% O_2) due to the relatively low reactor temperature and particle at large size ranges. Flame observations presented the ignition point located around 330 mm from the injection in the reactor. Maintaining the gas bulk velocity (Case A), an oxygen enrichment from 21 to 27 % reduced the CO emission by 43 %, and the lift-off height reduced by 15 %. As suggested by the literature, oxygen enrichment improves char oxidation and gas-phase reactions. NO emission slightly increased during the experiments with oxygen enrichment.

Considering the constant global equivalence ratio from the reference case (Case B), an experiment was carried out by decreasing the secondary air flow rate and performing oxygen enrichment to 27 %. A lower co-flow bulk velocity of 0.9 m/s decreased the mixing characteristics, resulting in 30 % higher CO emissions than the base case. Due to the impact on particle dispersion without additional operating modifications, acoustic forcing was implemented in Case B. Preliminary results with acoustic forcing indicated a reduction from the CO emissions, however not achieving the base case condition with higher velocity secondary co-flow (1.4 m/s). Investigations with different operating conditions (swirl intensity and acoustic settings) and particle size will be further evaluated in this work, bringing new insights into the effect of different manipulation methods on oxygen enrichment combustion.

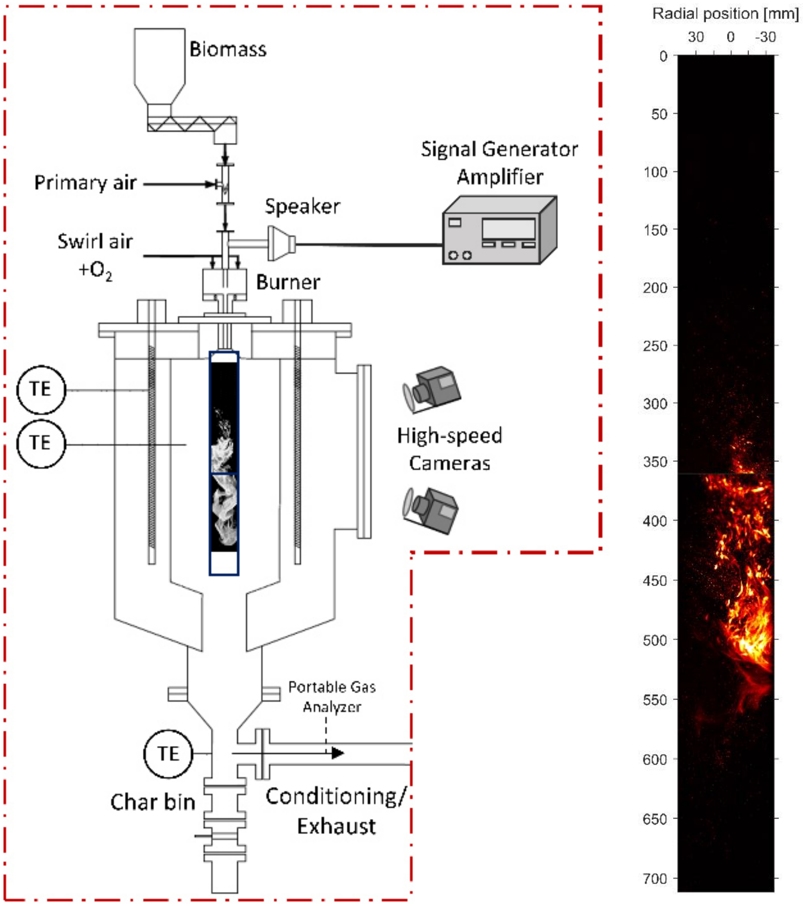


Figure 1. (left) Representation of the experimental setup
(right) Flame visualization example, instantaneous snapshot.

Table 1. Operating conditions.

	Ref. Case	*Case A_Oxy27%*	*Case B_Oxy27%*
m_biomass (kg/h)	1.0	1.0	1.0
O_2_total (%mol.)	21.0	28.0	28.0
λ_$_{I+II}$ (-)	1.0	1.3	1.0
v_$_{II}$ (m/s)	1.4	1.4	0.9

Structural char models including oxygen functional groups

V. Angenent[1] and R. Schmid[1*]

*rochus.schmid@rub.de

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

For a molecular understanding of coal combustion, realistic coal and char models are essential. We developed a top-down method for the construction of char models consisting of stacked carbon layers with defects. We start with stacked meshes templating the carbon layer. Then carbon atoms are pre-positioned on these and surrounded with hydrogen atoms. In an MD simulation, the atoms are rearranged. Afterwards, small molecules and unfavourable arrangements, such as three and four membered rings, are removed and dangling bonds are saturated with hydrogen atoms. In the final step, we add oxygen functional groups to the structural model. We have generated several models one containing more than 20.000 atoms.

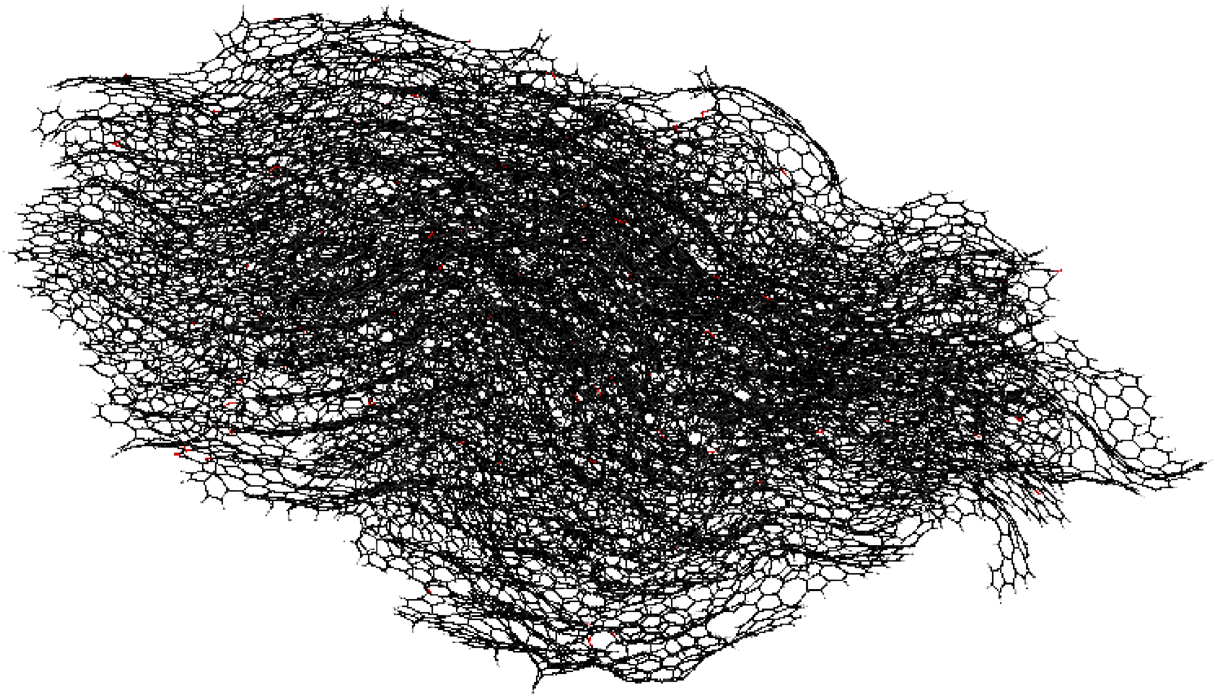


Figure 1. Structural char model: Stacked, defective carbon planes with oxygen functional groups.

Acknowledgements

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

Modeling homogeneous ignition processes of clustering solid particle clouds in isotropic turbulence

P. Farmand[1*], H. Nicolai[2], L. Berger[1], A. Attili[3], C. Hasse[2] and H. Pitsch[1]

*p.farmand@itv.rwth-aachen.de

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

[2] *Technical University of Darmstadt, Department of Mechanical Engineering, Simulation of reactive Thermo-Fluid Systems, Otto-Berndt-Straße 2, 64287 Darmstadt, Germany*

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

This work aims to numerically investigate the ignition and combustion of pulverized solid fuels in turbulent conditions and assess different modeling strategies relevant to large-eddy simulations (LES). Direct numerical simulations (DNS) of igniting coal particles in turbulent conditions employing detailed kinetics for solid and gas phases were performed to assess models in the context of flamelet tabulation methods for LES. Pulverized fuel combustion was modeled using the point-particle approximation to represent the dispersed phase in an Eulerian-Lagrangian framework.

Isotropic turbulence was employed to investigate the influence of particle clustering on the ignition process. The investigation showed that particles face different slip velocities due to turbulent flow fluctuations when exposed to turbulence. Due to having higher density than the surrounding gas, solid particles do not necessarily follow the flow. This behavior at small Stokes numbers can lead to particle clustering and a change in ignition behavior.

This change in the ignition process of a clustering particle cloud in isotropic turbulence was studied using DNS to identify the affecting parameters.

The DNS dataset was used as a benchmark for assessing the reduced-order flamelet models usually employed in the LES of pulverized fuel combustion. To this end, the thermo-chemical states were extracted from the DNS at different time instants to be used as a reference to assess the reduced-order models in LES, focusing on the ignition process. The flamelet model performance in predicting the selected quantities of interest were assessed in comparison with the DNS data. The error decomposition is performed using the optimal estimator concept to obtain the errors involved in the functional model. Finally, the distribution errors are assessed to find the best presumed subgrid PDF shapes for the input variables and the model performance in predicting the quantities of interest.

Acknowledgements

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

10.18154/RWTH-2023-06259

Exploring formation of N-containing pollutants in pyrrole counterflow diffusion flame

B. Chen[1*], S. Faller[1], A. Nobili[2], M. Pelucchi[2] and H. Pitsch[1]

*b.chen@itv.rwth-aachen.de

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

[2] *CRECK Modelling Lab, Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milan, Italy*

Biomass waste conversion through direct combustion (energy production) or pyrolysis (bio-oils production) are novel concepts to reduce CO_2 emissions and mitigate the climate change. However, the high nitrogen content in the biomass feedstock might result in elevating the emission of N-containing pollutants, which are highly harmful to humans and the environment. In this work, we studied the combustion chemistry and the formation of N-containing pollutants in counterflow diffusion flames fuelled by pyrrole, a biomass tar surrogate component that accounts for the majority of nitrogen in biomass tar. To investigate the influence of methane addition in a co-firing process, we also looked into the addition of methane with either the same location of stagnation plane (constant Z_{st}) or constant equilibrium temperature (T_{eq}) as the pure pyrrole flame. 29 species were identified and measured in all three flames, including 10 N-containing pollutants. Compared to the experimental data, numerical simulations using the kinetic model from the CRECK group can capture most of the species profiles well, except for some under-predictions of the N-containing pollutants, e.g., NO, NO_2, and C_2H_3CN. The mole fractions of hydrocarbons, e.g., C_2H_2, C_3H_4, and C_4H_4, increase with methane addition, but for N-containing species, their mole fractions do not change much. This indicates that formation of N-containing species depends less on the flame temperature or hydrocarbons in the species pool, but more on the reactivity of the pyrrole molecule itself. The experimental measurements and modeling results presented here may guide further kinetic model development for improved understanding of the combustion chemistry of pyrrole and related formation of N-containing pollutants.

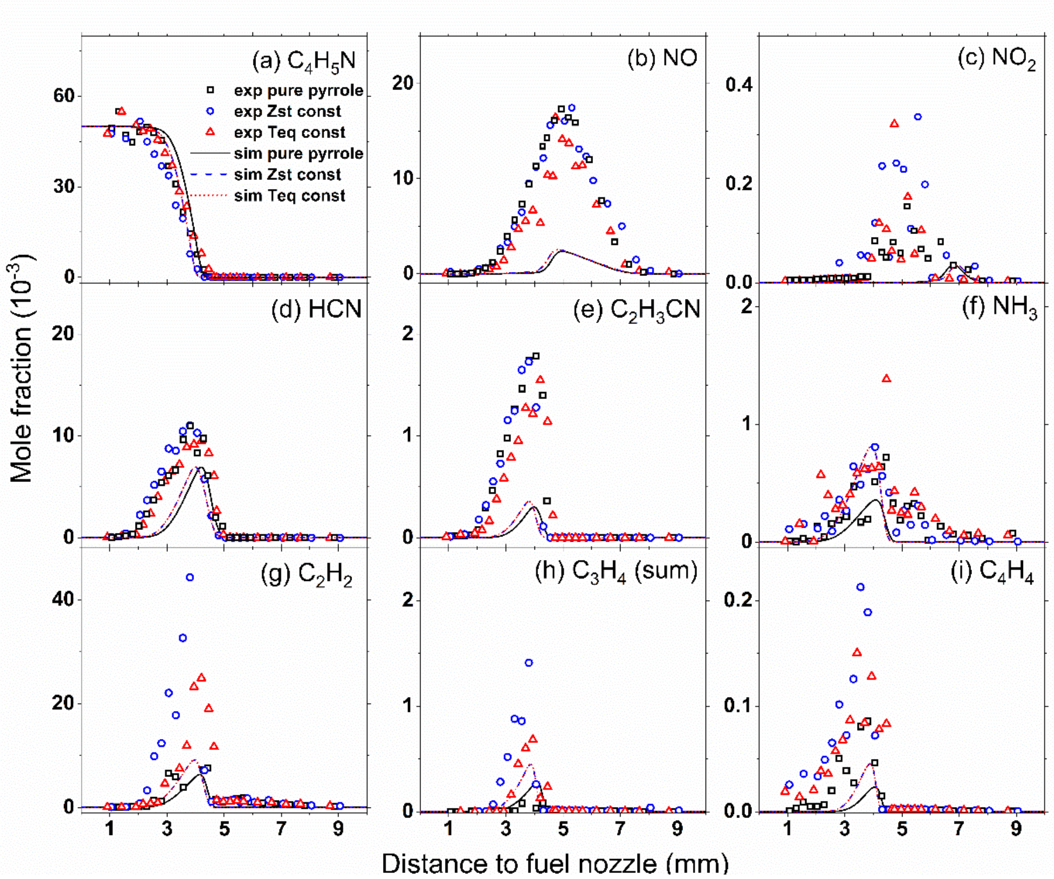


Figure 1. Important species profiles in counterflow diffusion flame fuelled with pure pyrrole, pyrrole + methane with constant Z_{st}, and pyrrole + methane with constant T_{eq}.

Acknowledgements

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

Correlation of chemical and structural pore properties and H_2O vapor adsorption in biomass char particles

T. Eisenbach[1*], C. Pflieger[2], C. Wedler[3], M. Muhler[2], R. Span[1]

*t.eisenbach@thermo.rub.de

[1] *Thermodynamics, Ruhr University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[2] *Laboratory of Industrial Chemistry, Ruhr University Bochum, Universitätsstraße 150, 44780 Bochum, Germany*
[3] *Department of Chemical Engineering, Imperial College London, London, SW7 2AZ, UK*

The rate of char conversion as a subprocess of solid fuel combustion may be limited by diffusion of reactive gases in the porous structure of the particles. For biomass combustion in an oxyfuel atmosphere, it is crucial to understand the diffusion behavior of CO_2, H_2O, and O_2. In general, the diffusion and adsorption of gas-phase molecules in porous chars depend on temperature, pressure, pore morphology, and chemical constitution of the fuel. The adsorption process of H_2O vapor in particular is strongly influenced by oxygen functional group (OFG) accumulation on the pore walls, the available pore surface area, and the associative character of the adsorbate favouring multilayer adsorption. Therefore, this study focuses on the pore size distribution (PSD) analysis and OFG quantification for two biomass chars in correlation with kinetic adsorption measurements of H_2O vapor, intending to provide a comprehensive basis for adsorption kinetics and diffusion modeling. This physics-based prediction of mass transport and diffusion properties can contribute to an improvement of char burnout kinetic and char conversion kinetic models.

The investigated chars were a mineral-free model char (MH800) obtained from microcrystalline cellulose by hydrothermal carbonization and subsequent pyrolysis at 800 °C as well as a torrefied beechwood char (TB), gasified at 1000 °C in a CO_2/N_2 atmosphere. The PSDs of both chars were analyzed by the two-dimensional non-local density functional theory (2D-NLDFT), considering the adsorption isotherms for N_2 and CO_2 in a simultaneous dual gas analysis. The pore surface areas summarised in Table 1 were calculated from the resulting PSD using the pore diameter-related IUPAC classification of ultra-micro pores (ul), micropores (mi), and mesopores (me) [1]. The quantification of individual OFGs was achieved by temperature-programmed desorption measurements. While heating 100 mg of sample to 800 °C with a low heating rate of 5 K min^{-1}, the effluent gas curves of H_2O, CO_2, and CO were monitored and deconvoluted into Gaussian contributions of individual OFG decomposition. Since carboxylic groups have a particularly strong influence on H_2O vapor adsorption, these contributions are summarised in addition to the overall quantities of OFGs in Table 1.

Table 1. Results for the pore regime-related surface area [1] and the OFG quantification.

	PSD			OFG	
char	A_{me} [m^2/g]	A_{mi} [m^2/g]	A_{ul} [m^2/g]	overall [mmol/g]	carboxylic [mmol/g]
MH800	39.3	225.1	286.6	1.546	0.185
TB	42.6	42.3	438.4	2.061	0.283

The kinetic adsorption measurements were performed in a gravimetric sorption analyser [2]. It is based on a magnetic suspension balance weighing the adsorption of molecules on a sample in a temperature-controlled measuring cell. The H_2O vapor pressure is set by a temperature-controlled vapor-liquid equilibrium (VLE) cell. Overall, adsorption kinetics were measured for both chars along three isotherms (T_{ads} = 25.4 °C, 35.3 °C, and 48.8 °C) at different relative pressures p/p_{sat}, where p_{sat} corresponds to the vapor pressure at adsorption temperature. A few selected results are shown in Figure 1.

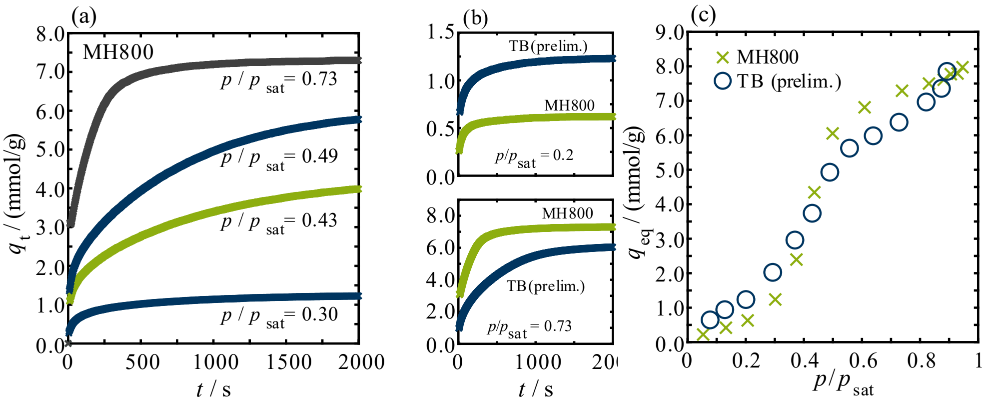


Figure 1. (a) Adsorption kinetics at T_{ads} = 25.4 °C for MH800 **(b)** comparative kinetics **(c)** equilibrium loadings.

The results of the PSD analysis show a distinct dominance of ultra-micro pores in the TB char, while the proportion of microporous surface area is significantly lower compared with the MH800 char. Typical for chars, both materials are of a comparable low functionalisation degree. However, the results for the TB char show a higher content of both carboxylic groups and overall OFGs. The adsorption isotherms for both investigated chars can be characterized as type V, which is an expected adsorption behavior on mostly hydrophobic, (ultra-) microporous carbons. At the first stage of adsorption at low relative pressures, ultra-micro pores and OFGs are known to act like initial adsorption sites [3]. This can be ascribed to the TB isotherm showing higher loadings in correlation to the char's ultra-micro pore fraction and OFG quantity. However, in the medium relative pressure range the significantly higher fraction of micropores in the MH800 char might support the formation of pore-spanning clusters and determine the steep increase of the isotherm (see Figure 1c). The kinetic adsorption behavior with respect to the results in Figure 1a and 1b are in good agreement with comparable investigations in the literature and will be discussed in detail in the conference presentation. Considering the formation of OFGs as intermediates as well as the evolution of a microporous structure during pyrolysis and char conversion processes, the associated influence on the diffusive behavior of the reactive component H_2O in the porous structure of particles is an important subject of research.

Acknowledgements

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

References

[1] Wedler C, Span R. A pore-structure dependent kinetic adsorption model for consideration in char conversion – Adsorption kinetics of CO2 on biomass chars. Chemical Engineering Science 2021;231:116281

[2] Rösler M, Wedler C. Adsorption kinetics and equilibria of two methanol samples with different water content on activated carbon. Adsorption 2021;27(8):1175–90

[3] Liu L, Tan SJ, Horikawa T, Do DD, Nicholson D, Liu J. Water adsorption on carbon - A review. Advances in colloid and interface science 2017;250:64–78

Thermochemical conversion of sewage sludge for energy and resource recovery: Opportunities for hydrogen and bio-materials production

A. Ben Hassen Trabelsi[1*]

*aida.benhassen@crten.rnrt.tn

[1] *Research and Technology of Energy CRTEn, Technopôle Borj-Cédria, B.P N°95, 2050, Hammam Lif – Tunisia*

In Tunisia, sewage sludge (SS) waste production is estimated to 1.9 million tons/year in 2009 and it is estimated to 2.5 million tons/year in 2016 [1]. Despite the large SS quantities generated yearly, no specific treatment is implemented. Actually, the major part of the generated SS (around 76 %) is stockpiled on wastewater treatment plants and only 24 % are landfilled in sanitary landfills. However, the high organic content (approximately 60 % on a dry basis), and the high calorific value of SS, their energy and materials recovery constitutes an interesting alternative to convert such carbonaceous materials into higher value products (bio-fuels, hydrogen, biomaterials). In this context, this work aims to convert Tunisian SS wastes into gaseous biofuels (Hydrogen rich gas mixture) and into residual biomaterials via thermochemical processes (gasification and pyrolysis).

In this study, pyrolysis and gasification experiments of pre-treated SS were conducted using two different laboratory-scale reactors [2] to produce a gas mixture rich with Hydrogen and biomaterials. The obtained results revealed the opportunity of the application of these two processes for the energy and material recovery of Tunisian SS. The produced syngas should be used either as a fuel or as an intermediate in the production of liquid fuels and chemicals. We suggest its reuse to supply a part of the energy needed in the heating part of the reactor in order to enhance the energy balance of the process.

With the pyrolysis process, the SS are converted into three fractions: liquid products or bio-oil, solid residue or bio-char and gaseous or syngas whereas with gasification, the organic compounds are converted into non-condensable combustible gases (syngas); condensable gases (tars) and solid residue (ash). The produced combustible gases from both pyrolysis and gasification can be not only applied to run internal combustion engines to generate electricity and used as substitute for fuel oils in direct heat application, but also used to produce chemicals which are useful as chemical feedstock for industries or be used to power hydrogen fuel cells [3].

The comparison of the chemical composition and characteristics of syngas evolved from pyrolysis and gasification of SS wastes, separately, has been the focus of this work. The released gases from SS pyrolysis and gasification present relatively high heating values (up to
9.96 MJ/kg for pyrolysis and 8.029.96 MJ/kg for gasification) due to their high contents of H_2 (up to 11 and 7 wt%, resp.) and CH_4 (up to 17 and 5 wt%, resp.). The yields of combustible gases (H_2 and CH_4) show further increase with pyrolysis. Moreover, the main characteristics of liquid biofuels and residual biomaterials from SS gasification have been investigated experimentally and then compared to those of pyrolysis.

The thermo-chemical conversion of SS through gasification and pyrolysis has been recognized as an efficacious and safer alternative process, since it leads to efficient pathogens, odors and toxic compounds removal and ensures human health and environmental protection and namely to hydrogen and biomaterials recovery.

References

[1] Office National de l'Assainissement, 2010. La valorisation énergétique des boues issues des stations d'épuration de l'ONAS, Rapport interne, pp 167-190.

[2] Aida Ben Hassen Trabelsi, Amina Ghrib, Kaouther Zaafouri, Athar Friaa, Aymen Ouerghi, Slim Naoui,1and Habib Belayouni, 2017. Hydrogen-Rich Syngas Production from Gasification and Pyrolysis of Solar Dried Sewage Sludge: Experimental and Modeling Investigations https://doi.org/10.1155/2017/7831470

[3] Balat B., Balat M., Kirtay E., Balat H. (2009). Main routes for the thermo-conversion of biomass into fuels and chemicals. Part 2: Gasification systems. Energy Convers. Manag., 50, 3158-3168

Ignition and flame structures of single coal and walnut shell particles in N_2/O_2 and CO_2/O_2 atmospheres – Particle size effect

T. Li[1*], P. Farmand[2], H. Pitsch[2], A. Dreizler[1] and B. Böhm[1]

*tao.li@rsm.tu-darmstadt.de

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

[2] *Institute for Combustion Technology, RWTH Aachen University, Templergraben 64, 52056 Aachen, Germany*

This study investigated coal and walnut shell particles with a combined experimental-numerical approach, focusing on ignition and flame structure evolution in N_2/O_2 and CO_2/O_2 atmospheres. Single-particle combustion characteristics were experimentally studied in high heating rate conditions enabled by a laminar flow reactor. High-volatile bituminous (hvb) coal and walnut shell particles were sieved to different diameter d_{prt} ranges, summarized in Table 1. The current study compared an N_2/O_2 atmosphere with a CO_2/O_2 atmosphere with the same O_2 mole fraction of 20 vol% and an initial gas temperature of 1800 K.

Table 1. Solid fuel particles used in this study.

hvb coal	C1	C2	C3
d_{prt} [µm]	90–106	106–125	160–200
walnut shell	W1	W2	W3
d_{prt} [µm]	90–125	106–125	160–200

In the experiments, gas-phase reactions of single-particle flames were visualized by planar laser-induced fluorescence of OH radicals (OH-LIF) at a frame rate of 1 kHz. Both ignition delay time t_{ign} and flame stand-off distance r_{f} were evaluated by tracking the OH-LIF intensities in the vicinity of particles from the unburnt stage to a well-developed enveloping volatile flame. These combustion parameters were further correlated with particle diameter d_{prt}, which was in-situ measured by the diffusive backlight-illumination (DBI) technique. The DBI system allows for particle size, shape, and velocity measurements at sufficient spatiotemporal resolutions.

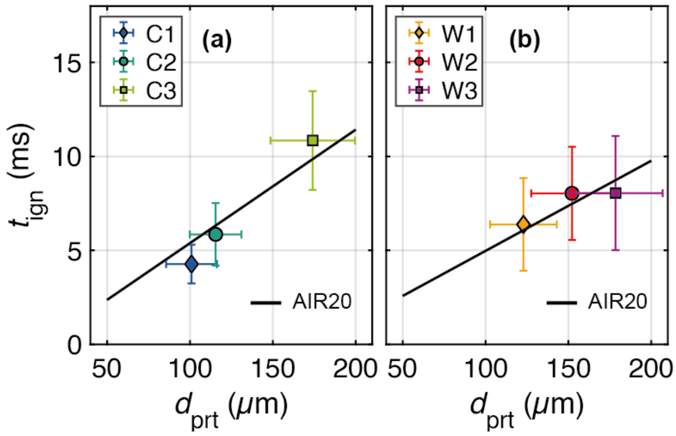


Figure 1. Ignition delay time t_{ign} with increasing particle diameter d_{prt} for **(a)** hvb coal (C1–C3) and **(b)** walnut shell particles (W1–W3) in the AIR20 atmosphere.

Figure 1 shows the statistical results of ignition delay time for investigated coal (C1–C3) and walnut shell (W1–W3) in an N_2/O_2 atmosphere with 20 vol% O_2 (AIR20). Horizontal and vertical error bars represent the standard deviations of d_{prt} and t_{ign} measurements, respectively. Both coal and walnut shell particles show delayed ignition with increased particle size. Additionally, walnut shell particles ignite slightly earlier than coal particles, especially at large diameters.

Detailed numerical simulations were performed to understand the particle size effect on the ignition characteristics, considering the experimental boundary conditions such as gas temperature, composition, and velocity. The coal and biomass combustion process is modelled in an Eulerian-Lagrangian framework using the point-particle approximation of the dispersed solid phase. The numerical methodology is first validated against experimental results of ignition delay times and is then used to explore additional combustion parameters. It was found that the different heating rate associated with the particle size is the major contributor to the ignition characteristics. A deeper analysis of the gas-phase radicals, such as OH radicals, provides further insights into different volatile combustion between coal and walnut shell 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”.

Imprint

Conference
4th International Workshop on Oxy-Fuel Combustion – Book of Abstracts
March 22nd–23rd, 2023
Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS)
Italian National Research Council (CNR).
Naples, Italy

Editors
Stefan Pielsticker
Anna Maßmeyer
Viktor Scherer
Heinz Pitsch
Andreas Dreizler
Osvalda Senneca
Reinhold Kneer

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

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

First published 2023

Available via the institutional repository of RWTH Aachen University:
DOI: 10.18154/RWTH-2023-06259