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Book of Abstracts

EFFECTS OF PRESSURE ON LIGNOCELLULOSIC BIOMASS FAST PYROLYSIS IN CO₂ RICH ATMOSPHERE

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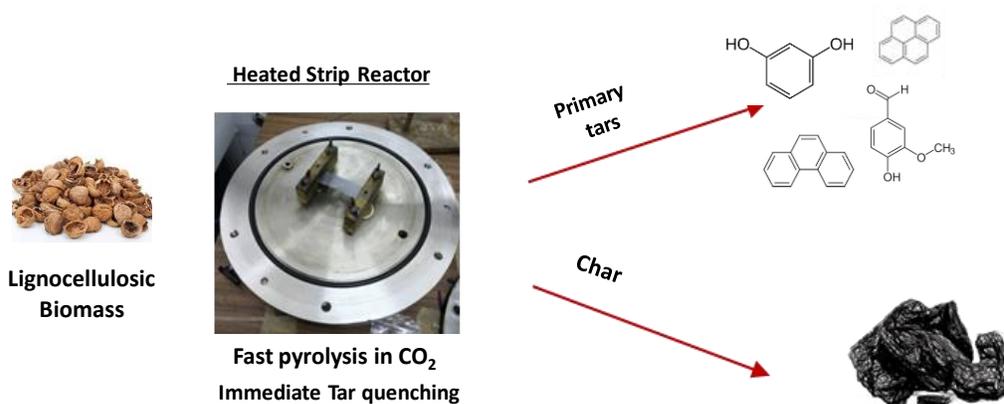
Abstract

The present work aims to characterize char and primary tar produced from a lignocellulosic biomass, namely Walnut Shells (with high content of Lignin), upon heating under the following conditions:

1. with very fast heating rates (10^4 K/s);
2. at high temperature (up to 1573 K);
3. at different pressure (up to 8 bar);
4. in CO₂ rich atmospheres.

It must be emphasised that, even though pyrolysis of biomass has been the object of extensive research over the last decades, experimental studies which combine the conditions reported in points 1 to 4 are relatively scarce. In the present work, these conditions are achieved by means of a special heated strip reactor, which allows not only heating the solid samples with temperature and heating rates (up to 10^4 K/s) similar to those of laminar flow reactors, but also quenching the volatiles as soon as they are emitted. Tars, after acetone extraction, are analysed by gas chromatography-mass spectrometry for quantitative determination of aromatic and aliphatic compounds. The focus posed on primary tar, i.e. on condensable volatile products collected immediately after their ejection from the particles, before they undergo secondary reactions in the gas phase, is indeed an important novelty addressed by the present work.

Chars structure and morphology are characterized by TGA, Raman spectroscopy and Scanning Electron Microscopy. Severe heat treatment and the presence of CO₂ in the atmosphere generate multiple char components. It is possible that the newly formed high reactive char component arises from interactions with CO₂ and subsequent crosslinking reactions within the solid matrix, whereas the less reactive component arises from thermal annealing and graphitization of the solid phase.



Investigation of biomass gasification process under various operating conditions inside entrained flow cyclone gasifier

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Abstract

Entrained flow gasification of biomass followed by the production of methane is an interesting possibility for synthetic fuels that has been particularly investigated in the Nordic countries. In order to optimize the efficiency of gasification plant, it is important to understand the influence of each effecting parameter.

In this work, numerical simulations of the biomass gasification process were carried out inside a 4.4 MW entrained flow cyclone gasifier constructed by Meva Energy AB at Hortlax, Piteå Sweden. Two important process variables were investigated i.e., the equivalence ratio (λ) and the fuel loading of gasifier. The fine grind wood pellets were used as a fuel feedstock and the process was characterized with respect to the resulting cold-gas efficiency, temperature and fuel conversion. Three-dimensional Reynolds-Averaged Navier – Stokes equations were solved together with the eddy-break up combustion model in conjunction with the modified $k - \epsilon$ model. The sub-models for drying, devolatilization, homogeneous and heterogeneous reactions were incorporated for the gasification model. The model was validated against the experimental measurements at different equivalence ratio in terms of gas – phase species at the outlet. The predicted results were in good agreement with the experimental data and model provides detailed information about the gas compositions and the temperature field. Systematic variation of both λ (0.25 – 0.45) and fuel loading (600 – 1200 kg/hr) will be carried out and goal is to determine the optimum value of λ for a given fuel loading rate.

Ignition and combustion of single pulverized biomass and coal particles in N₂/O₂ and CO₂/O₂ environments

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Abstract

The ignition and combustion characteristics of single particles of two biomass residues and three coals were evaluated in the hot combustion products of a CH₄ fired Hencken burner. Particles of corn straw and wheat straw residues, and lignite, bituminous coal and anthracite, all in the size range 125-150 μm, were injected upward through the central nozzle of the burner into combustion products with a mean temperature of 1550 K and a mean O₂ concentration of 15 mol.%. The experiments were carried out in N₂/O₂ and CO₂/O₂ environments. Temporally resolved CH* chemiluminescence images of the single burning particles were captured by an ICCD camera equipped with a 430 nm band-pass filter. The results show that the biomass and lignite particles ignited homogeneously, while the bituminous coal and anthracite particles ignited heterogeneously in both N₂/O₂ and CO₂/O₂ environments. For the biomass and lignite particles, the gas-phase combustion of the volatiles took place in an enveloping flame surrounding the particle, followed by the heterogeneous oxidation of the char. For the bituminous coal and anthracite particles, both the volatiles and char combustion processes occurred simultaneously. The biomass particles ignited earlier and were more combustible than the coal particles. For the three coals, the ignition delay time decreased almost linearly with the increase of their volatiles content. Moreover, the biomass particles exhibited shorter volatiles burnout times than the coal particles due to their lower absolute volatiles content. When N₂ was replaced by CO₂, the ignition of all solid fuels was delayed, and the burnout time of volatiles was lengthened. In addition, the combustion of all solid fuels was markedly less intense in the CO₂/O₂ environment than in the N₂/O₂ environment, due to the lower binary diffusivity of the O₂ in CO₂ and the higher volumetric heat capacity of the CO₂, as compared with N₂.

Keywords: Single particle, CH* chemiluminescence, ignition and combustion mode, oxy-fuel combustion

A fundamental physicochemical model of oxidation of carbonaceous materials

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Abstract

Combustion processes have been extensively described with detailed kinetic models in the past decades. The increase in computational power has allowed their application into realistic CFD simulation of complex reactors. Combustion of solid fuels involve complex multi-phase and multi-scale problems. Typically, a solid fuel undergoes a step of primary pyrolysis (devolatilization), releasing its volatile matter to the gas-phase. The remaining solid residue is a carbon-rich material with very complex chemical and physical structures, which is further converted by oxidation reaction, in a heterogenous reacting process. However, gas-phase kinetic mechanisms are available in a much higher level of detail than the heterogeneous gas-solid reactions. The present work focuses on the development of comparable detailed kinetics to bring the char oxidation process to a new level of detail and predictability. To this aim, char physical structure is described including porosity, surface area, density of active sites and their change along the conversion process. The chemical aspects of char are modeled considering a carbonaceous bulk structure, surrounded by a variety of surface reactive sites, which represent the chemical functionalities typically present in these materials. The chemical reactions and their kinetic parameters were developed by analogy to gas-phase reactions of aromatic species, taking into account the differences that take place between the homogeneous and heterogeneous processes. The resulting innovative model is able to describe the oxidation of not only natural graphite materials, but also complex amorphous chars from biomass and coals. This model is the first attempt to highlight the importance of chemical complexity of char in the oxidation process, addressing the problem with the development of detailed kinetics. The results of this work open path to further improvements in this model which can be extended to account for pollutants formation from nitrogen and sulfur contents and catalytic effect of alkali-metals.

Keywords: Kinetic Modeling, Oxy-Fuel, Coal,

Systematic Evaluation and Kinetic Modeling of Low Heating Rate Sulfur Release in Pyrolysis and Oxidation in Various Atmospheres

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Abstract

Coal combustion releases elevated amounts of pollutants to the including SO_x. During the pyrolysis step, sulfur present in the coal reacts and is released not only in the primary pyrolysis, but also in secondary gas-phase reactions and during the char oxidation. Many different chemical species such as H₂S, COS, SO₂, CS₂, thiols and larger tars are formed. These species are called SO_x precursors, as they are further oxidized in the gas-phase generating SO_x. Understanding the chemical processes taking place in the release of sulfur is crucial to the development of reliable kinetic models, which support the design of improved reactors for cleaner coal conversion processes, such as oxy-fuel combustion. In the present work, the release of sulfur from two bituminous coals, Colombian hard coal (K1) and American high sulfur coal (U2) was systematically analyzed in inert and oxidative atmospheres. Coal samples employed are of similar rank and have comparable amounts of volatile matter and ashes, whilst sulfur is three times higher in the U2. Low heating rate experiments were performed in a TG-MS, using N₂, CO₂, air and oxy-fuel (30% O₂/70% CO₂) atmospheres, allowing to track the mass loss and the evolution of many gas species (CO, CO₂, CH₄, SO₂, H₂S, COS, HCl and H₂O). The thermogravimetric analysis in these various atmospheres allowed to systematically analyze the different steps of coal conversion and the chemical paths leading to the formation of SO_x and its precursors. A kinetic model of sulfur release and conversion is proposed, in which sulfur in the raw coal is accounted as three organic functionalities (aliphatic, aromatic and thiophenic), and two inorganic forms (pyritic and sulphatic). Lumped molecular structures are assigned for all the sulfurated species. The kinetic model describes both devolatilization and oxidation of char-bound sulfur. Because homogeneous gas-phase reactions play an important role in the species formed for all non-inert atmospheres, a sulfur gas-phase mechanism was also employed (Alzueta et al, 2001). The presented sulfur model is fully compatible with the previously available coal conversion model (Sommariva et al, 2010), resulting in a comprehensive tool for coal conversion in various operating conditions.

Keywords: Kinetic Modeling, Coal, Pollutants, Sulfur, SO_x

Evaluation of Multiple Test-rig and Comprehensive Kinetic Model of Coal Conversion in Inert, Air and Oxy-Fuel Conditions

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Abstract

Oxy-fuel combustion is one of the most promising clean coal conversion technologies. Clear physical differences are present when CO₂ is used as diluent instead of N₂ due to the change in heat and mass transfer properties of the gas mixture. Additional complex reacting paths are present because of the reactivity of CO₂ with the fuel. A better understanding of the overall process is possible when separately evaluating the coal conversion in increasing levels of complexity. In the present work, a bituminous Colombian coal is pyrolyzed and oxidized in a combination of experimental test-rigs. By employing the same fuel in different test-rigs, different effects can be observed, similarities highlighted and experimental uncertainties reduced. For this aim, thermogravimetric analyzer (TGA), fixed-bed reactor (FixBR), drop-tube reactor (DTR), flat-flame burner (FFB) and fluidized-bed reactor (FBR) were used to investigate the coal conversion in a wide range of heating rates, peak temperature, atmosphere composition and residence times. The collection of experimental data obtained in these campaigns allowed a consistent outlook of both devolatilization and oxidation rates, together with product distribution and effect of the different operating conditions. Supported by these data, a comprehensive kinetic model is proposed, corresponding to an updated and calibrated version of the model presented by Sommariva et al. (2010). A characterization step, requiring the ultimate analysis of the sample, describes the coal as a combination of a few reference coals. The resulting coal conversion is obtained as a linear combination of the conversion of each reference coal. The model seamlessly describes coal devolatilization and char oxidation both in low and high heating rates, in inert, air and oxy-fuel atmospheres. Detailed kinetic mechanisms for secondary gas-phase reactions can be easily coupled to describe the evolution of volatiles. The resulting kinetic model can be directly coupled to CFD simulations or employed for calibration of simplified kinetic models.

Keywords: Kinetic Modeling, Oxy-Fuel, Coal,

The effect of large steam addition on the NO_x formation during oxy-combustion of bituminous and subbituminous coals

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Oxy-steam combustion consists on the replacement of carbon dioxide by steam in the firing atmosphere, then avoiding the CO₂ recycling from the flue gases in oxy-combustion plants. The use of steam as temperature moderator offers some advantages, like a reduction of the boiler sizes, the avoidance of air in-leakages and the decoupling of the furnace operation from the CO₂ loop.

So far, few studies are available addressing the effect of large steam addition in O₂/CO₂ atmospheres and mostly focused on the ignition behaviour of the oxy-fired fuels. In our work, the effect of steam addition (up to 40% vol.) on the NO_x formation during the oxy-combustion of **two different coals** has been experimentally investigated. The selected coals have a similar volatile content, but very different **heating value** and sulfur and ash contents.

The experiments are carried out in a lab-scale facility at the *University of Zaragoza* (Spain), consisting in an entrained flow reactor able to fire pulverized solid fuels in O₂/N₂, O₂/CO₂ and O₂/CO₂/H₂O atmospheres. Besides the effect of steam addition (10—40% vol.), different oxygen ratios (1.15—1.35) and oxygen concentrations (21%—35% vol.) have been also tested. On-line measurements of flue gas composition are gathered, including CO₂, CO, O₂, SO₂, NO and NO₂ concentrations at the exit of the facility. Fly solid samples are also collected and analysed.

The results show the role of oxygen on NO_x formation, enhancing the fuel-NO_x production when the atmosphere is enriched in O₂. As concerns the role of steam, a decrease of NO_x formation is detected when steam is supplied in comparison to the dry atmospheres. But this trend is reversed in some cases for the largest steam concentrations, pointing out a value that minimizes the NO_x formation. These observations depend not only on the fuel, but also on the %O₂ in the atmosphere. Discussion of this behaviour is presented in relation to the variables affecting the conversion of the particles, providing new insights in the way towards the oxy-steam concept.

Investigation of the catalytic influence of doped metals on the pyrolysis product distribution and resulting char of hydrothermally derived model fuels

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Introduction: The application of carbon capture and storage techniques may provide one possibility to achieve negative CO₂ emissions for pulverized solid fuel combustion. Modeling primary and secondary pyrolysis as well as char combustion behavior assists the determination of the optimal operation conditions for the combustion of different coals and biomasses with deviating mineral contents.

Aim: Evaluation of the catalytic influence of minerals on pyrolysis as step of pulverized solid fuel combustion to provide model validation data.

Methods: Hydrothermal carbonization (HTC) of microcrystalline cellulose (MCC) was used to synthesize a mineral-free model fuel, which was subsequently impregnated with K, Na, Fe, Mg, or Ca as sulfates. This procedure enabled us to study the catalytic influence of the loaded minerals which are also found in natural coals and biomasses while changes due to different counter ions are excluded. A special pyrolysis-GC/MS-GC/TCD with Deans switch heart cutting was used for the quantification of light permanent gases and the simultaneous qualitative analysis of larger tars evolving after flash pyrolysis in helium. In addition, a flat flame burner was used to prepare metal sulfate-doped chars, whose composition, structure and oxidation kinetics was studied in detail.

Results: First, we demonstrated the advantages of a coupled pyrolysis-GC/MS-GC/TCD system for the analysis of solid fossil fuel pyrolysis separating the whole spectrum of pyrolysis products from small permanent gases to heavy tars with high resolution in one run. Flash pyrolysis studies of the doped fuels clearly revealed a decreasing CO/CO₂ ratio and a simultaneously increasing CO/CH₄ ratio for most metal sulfates identifying gasification and steam reforming or solid decomposition as catalyzed reactions. Further, the application of different pyrolysis conditions and the characterization of the resulting chars verified the impact of higher heating rates during the thermal treatment resulting in decreased thermal stability and increased char oxidation rates.

Conclusion: The consistent study of samples doped with different metal sulfates enabled the identification of the catalytic effects of these minerals on a model fuel, suitable to represent both a lignite and a thermally treated biomass for the modeling of pulverized solid fuel combustion.

Direct numerical simulation of solid fuel ignition and combustion in laminar and turbulent jets in oxy-atmosphere

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This work aims to numerically investigate the group particle ignition and volatile combustion in oxy-atmosphere. Coal combustion is modeled in an Euler-Lagrange framework using point particle approximation for the dispersed solid phase. The devolatilization process and chemistry are modeled using the chemical percolation devolatilization (CPD) model coupled with finite rate chemistry (Farazi et. al., Fuel 241, 2019). The effect of particle number density on ignition dynamics, the shape of the volatile flame, and other combustion characteristics are investigated in different oxy-atmospheres. When the cold particles are injected into the hot atmosphere, they absorb significant amount of energy from their surrounding gas and their temperature starts to increase while the surrounding temperature decreases. Figure 1 shows the configuration which is used in all of the simulations in the laminar conditions. Particles are injected in the mid-section of the inlet using a carrier gas with an initial temperature equal to the hot ambient. After injection, particles start to heat up and release volatile gases to the surroundings. The diffusion flame of volatile gases and oxygen is firstly ignited at a location of proper mixing and high temperature. The ignition location is affected by the particle-gas and particle-particle interactions. After investigating the laminar jet, a simulation will be performed for a turbulent case and results will be compared to the laminar case to asses the effect of flow field on the ignition and combustion behavior.

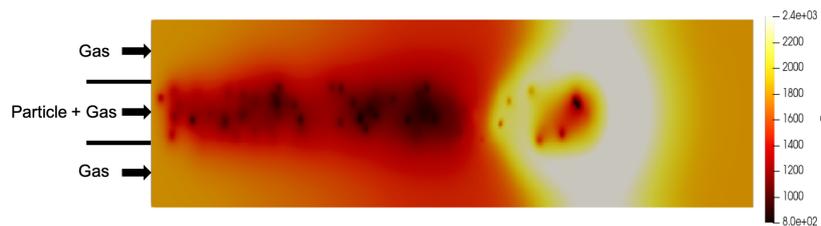


Figure 1: Group particles in a laminar slab condition

Bio-dust Combustion for Heat and Power Production

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Abstract

The presentation deals with the research efforts to facilitate an efficient conversion of coal-fired power plants to biomass, retaining a high electrical efficiency with a broad fuel-band. This effort has specifically addressed challenges related to biodust combustion on central power plants, including agricultural biomass quality, fuel characterization, burner design, ash transformation, deposition, and use of additives to mitigate ash related problems. The activity, which has involved experiments in laboratory, semi-industrial and full scale (power plants) in addition to a wide range of modeling, has resulted in significant new knowledge on fuel analysis and characterization methods, fuel pretreatment, biomass devolatilization and combustion, and inorganic chemistry, including aerosol formation, deposit build-up, and corrosion management. Devolatilisation studies were conducted in entrained flow reactors, on a grid heater, and in a single particle combustion reactor to investigate the influence of fuel type, heating rate, and maximum temperature on char yield, char morphology and char reactivity. The obtained chars were characterized with respect to morphology and TGA used to determine reactivity towards oxygen, assisted by FTIR and Raman spectroscopy. The data obtained from full-scale tests were the first reported worldwide for the near-burner region in a full-scale furnace combusting bio-dust, using high speed thermal flame imaging, FTIR/UV fiber-optics and extractive measurements for gas composition and temperatures, particle sampling, Laser Doppler velocity measurements, and spectral heat flux measurements. The flame structures observed at the two campaign units tested were very different in terms of flame stabilization and structure, making the data sets very valuable for design purposes and for CFD model validation. The activity has improved our capability to model wood combustion considerably and the results are important both scientifically and industrially.

Comparison of scattering phase functions of reacting and non-reacting pulverized fuel particles

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In pulverized fuel combustion systems, thermal radiation is one of the main heat transfer phenomena. Besides emission and absorption, scattering at particle surfaces is the third observable effect. To describe the angular dependent redistribution of the scattered radiation, the scattering phase function is used. This function is affected by several parameters as fuel particle composition, particle diameter, burnout process and the wavelength of the incident radiation.

In the current work, the scattering properties of cold and burning particles are compared. Therefore, two independent experimental setups, determining the scattering field function of contactless particles, are applied. In the first experimental setup, observing cold fuel particles, the particles are acoustically levitated and irradiated by an angle adjustable infrared source. A monochromator is used to select specific wavelengths from the determined scattered radiation spectrum. The second setup, observing burning fuel particles, consists of a flat flame burner providing a burning particle streak under conditions typical for pulverized coal combustion ($d_p \sim 100 \mu\text{m}$) and high heating rates ($10^4\text{-}10^5 \text{ K/s}$) under controlled oxy-fuel combustion conditions. A broadband light source emitting radiation in the visible and infrared region can be rotated around this streak. An FTIR (Fourier-Transform-Infrared Spectrometer) detects the spectrally resolved scattered radiation of the particle streak "in-flight". For particle diameter and number density measurements, a camera-based system is used.

First results will be presented comparing scattering data of coal and biomass. Raw fuel and the corresponding ash will be investigated at room temperature using levitated particles. In the flat flame burner, ash from both fuels will be injected into the hot atmosphere to measure scattering at elevated temperature. Fuel particles will be used to determine the influence of burnout.

Oxyfuel bubbling fluidized bed combustion in laboratory and pilot scale

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This paper presents our bubbling fluidized bed oxyfuel combustion research and development activities in the scale of 30 and 500 kW thermal power load. Based on years of practical experiences, in this paper are discussed specific features from more general point of view, concerning fluidization in the oxyfuel mode compared to air mode and transition between them – minimum fluidization velocity and thermal conditions. Generally, changing from air to oxyfuel combustion mode in the bubbling fluidized bed is connected with different thermal conditions, causing drop of the bed temperature when attempting to keep the fluidization velocity. Other issue addressed in the paper is expressing concentrations of pollutants in the CO₂ stream and particular features affecting CO, NO_x and SO₂ formation in the bed. The paper presents general approach for numerical evaluation of the process and shows experimental validation, which enables to identify potential weak points of the scale-up, one of which is significant effect of false air intake into the combustor on the output CO₂ concentration and content of non-condensable gases. The correlation of CO₂ concentration with the ratio of false air was obtained, providing CO₂ concentration decrease with percentage of false oxygen in the total oxygen supply. In the end, this turns out to be the key factor affecting quality of the final CO₂. The scale-up of the experiments also shown different behaviour of pollutant formation, and pointed out the importance of common gas leakages and pressure conditions in the combustor, that are normally not relevant in the air combustion mode.

CHEMICAL CHALLENGES IN COMBUSTION OF BIOMASS FUELS

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Abstract

Biomass fuels differ in many ways from the conventional fossil fuels used in combustion processes, such as coal. They often have high moisture contents, lower heating values, and a variety of minor constituents, such as chlorine, sulfur, phosphorus, nitrogen, and a variety of ash-forming metals. Design of the combustion devices and choice of their operating parameters are very dependent on the detailed properties of the biomass fuel or fuels to be used, especially the chemical aspects of the fate of the minor constituents and impurities.

This paper reviews some of the chemical details that are important to take into consideration. The focus of the paper is in large, industrial scale combustion technologies for biomass and biomass derived waste fuel. We will discuss biomass particle burning, in particular biomass char oxidation at varying conditions, including oxy-combustion conditions. We will report advanced in-furnace measurements of nitrogen species in a large scale furnace with heavy air staging, and the novel modelling work to explain the measured data. Further, we will discuss recent results in superheater fouling and corrosion due to biomass ashes.

The effect of Stefan flow on the gasification of suspended char particles

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Abstract

Biomass will play a major role in replacing fossil fuel as a source of carbon neutral and sustainable fuel. Biomass gasification and oxy-fuel combustion are attractive techniques for its utilization.

Char conversion is the rate limiting step in gasification. Complete char conversion is necessary for high efficiency. Char gasification is a complicated process since it is in the regime II which is controlled by both kinetics and diffusion. Therefore, it is hard to model using simple methods and it is important to study more about char gasification in detail.

This study aims to study the char gasification using a simulation model resolving both particle interior and surrounding boundary layer. Numerical simulations will be carried out both inside and outside a single char particle. Char particle is treated as a porous media and thermal equilibrium is assumed between fluid inside the particle and char.

Heat (Nu no.-Nusselt number) and momentum transfer (C_D -drag coefficient) between the particle and the surrounding fluid will be calculated including Stefan flow created by the reactions. Those drag coefficients and Nu no.s will be compared with models developed considering uniform Stefan flow around a particle.

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Influence of non-sphericity and wavelength dependency on the scattering phase function of pulverized fuel particles

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The scattering phase function is important to describe the radiative heat transfer of particles in pulverized fuel combustion. For coal and ash particles the scattering phase function is often modelled with Mie-Theory, which assumes perfect sphericity and homogeneity of the particles. In this context, wavelength of the radiation source, the complex index of refraction and the diameter D_p of the investigated particles are input parameters which need to be defined prior to calculation.

In a first attempt, the scattering phase function was measured for coal particles illuminated by a helium-neon laser with a wavelength of $\lambda = 632.8$ nm for different scattering angles. For correct measurements of the optical properties, the particles need to be contactless. An acoustic levitator was designed for the particle capture. Since the particles are not perfectly spherical, D_p was set to the longest cross-sectional length. Afterwards, the measurements were fitted by an optimal phase function calculated by the Mie-theory (figure 1). The measured forward scattering peak is well represented, while the difference between experimental and calculated phase function increases for increasing scattering angle. A similar behaviour was noticed for prolate ellipsoids. Therefore, the difference between measurements and calculations could arise from the non-sphericity.

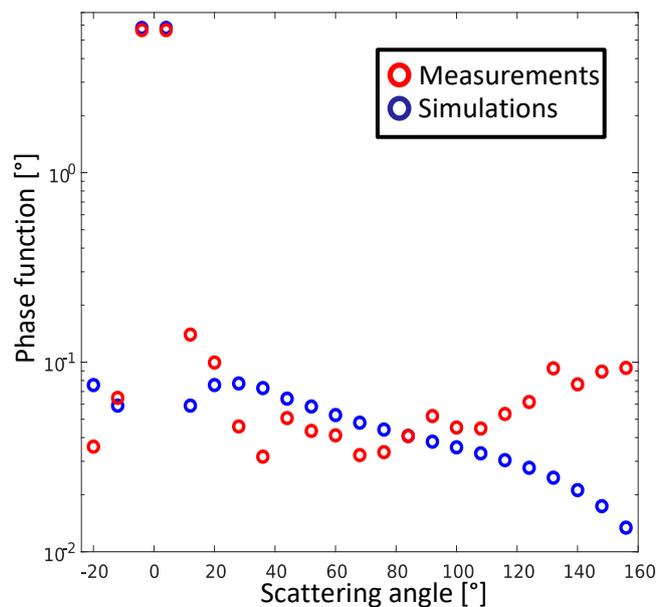


Figure 1: Measured and calculated phase function

In this study, the influence of the non-sphericity is investigated in a more detailed way. For this purpose, the cross-sectional lengths of the investigated particles are measured and summed up by a form-factor. Thus, the particles are described by an ellipsoidal form. The scattering phase function is then computed depending on different form-factors. For the calculation of the non-spherical particles, the Discrete-Dipole Approximation is used. Here, each particle is represented by a finite number of dipoles, where the total number of dipoles is defined by the volume of the particle and the wavelength of the radiation. Therefore, also the effect of different wavelengths on the phase function is investigated. Afterwards, a correction factor for the Mie-theory is developed. For the validation, the scattering phase function is measured for different particles and different wavelengths.

Development of drag correlations for ellipsoidal particles using fully resolved simulations

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A popular method to analyze particle dynamics in turbulent flows is the Lagrangian point-particle method where the motion of the particles is modeled via semi-empirical expressions. For heavy rigid particles, these expressions are mostly reduced to the drag force. In the case of spherical particles, a huge data base and an established "standard drag curve" is available. Such a data base is missing for non-spherical particles. Available ellipsoidal Lagrangian point-particle methods are largely restricted to vanishing particle Reynolds numbers.

In this contribution, correlation functions for the drag, lift, and torque acting on a fixed non-spherical particle in uniform flows are presented. Therefore, a numerical parameter study is performed, which covers the range $Re_p \leq 100$ for aspect ratios $1 \leq \beta \leq 8$ and inclination angles $0 \leq \Phi \leq 90$. In total, more than 4,000 simulations are performed to provide sufficient data points for the models. A conservative discretization on locally refined Cartesian meshes is used, where the fluid-solid interface is sharply resolved via a cut-cell representation [1]. Figure 1 shows one of the conducted simulations, i.e., an ellipsoidal particle with $\beta = 1.5$, $Re_p = 100$, and an inclination angle $\Phi = 45^\circ$. The generated data set is used to derive a drag correlation based on correction functions for analytical solutions valid for creeping flow conditions.

For the final contribution, it is planned to expand a common ellipsoidal Lagrangian point-particle model by the semi-empirical correlations for the drag, lift, and torque acting on the particle, and to provide a validation against large-scale benchmark simulations of fully-resolved particle-laden turbulence [2]. It is expected that the correlations significantly improve the accuracy of ellipsoidal point-particle models.

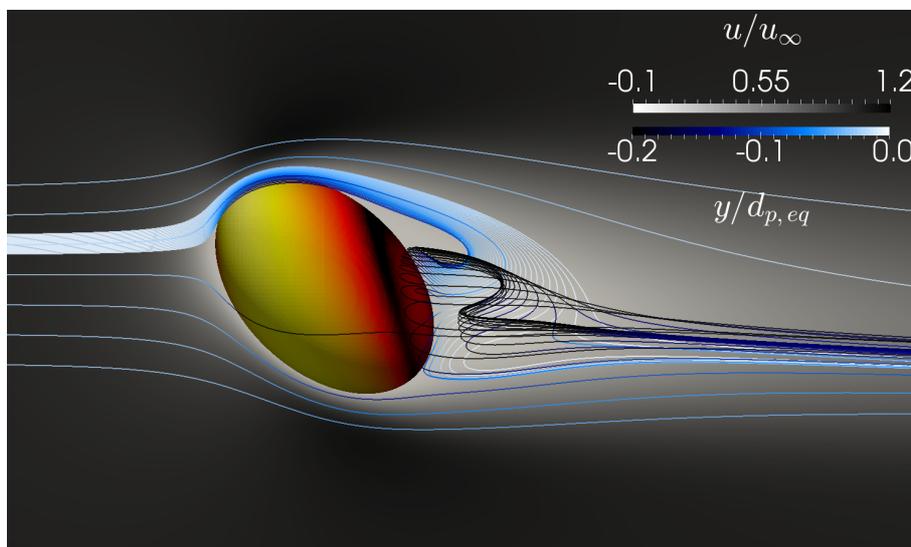


Illustration 1: Visualization of an ellipsoidal particle in a uniform flow field with $\beta = 1.5$, $Re_p = 100$, and an inclination angle $\Phi = 45^\circ$. Stream tracer are injected to visualize the particle wake.

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Influence of oxygen and water vapor on the thermochemical conversion of fossil, biogenic and surrogate fuels

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The combustion of solid fuels under oxyfuel conditions involves a variety of special aspects, which clearly separate this process from conventional air combustion. Two of these are varying oxygen contents and potentially higher amounts of water vapor in the oxidizing gas atmosphere. To account for these differences in numerical models of full boiler simulations, it is desirable to use experimentally verified kinetic submodels, applicable for both fossil and alternative fuels. Therefore, the influence of both oxygen and steam partial pressure on the conversion rates of three different pulverized fuels is investigated experimentally. Chosen fuel particles are Rhenish lignite, torrefied beech wood and a surrogated fuel from municipal waste, so that they can be related to the classes of fossil, biogenic and refuse derived fuels.

For measurements of the conversion rates, a small-scale fluidized bed reactor is utilized. This reactor allows high heating rates ($\sim 10^4$ K/s), unlimited residence times of the particles and the investigation of reactions under a well-defined gas-atmosphere. Due to multiple thermal mass flow controllers and a separate water vapor dosing system, different amounts of oxygen and water vapor can be set independently of each other. In this study the oxygen concentration was varied between 5 and 100 % and the H₂O concentration between 0 and 20 %, respectively. The carrier gas and reaction products are monitored by online FTIR gas analysis.

Experimental results are evaluated by different kinetic approaches and compared to literature.

Experimental and numerical investigation of solid fuel particle group combustion under air- and oxy-atmospheres

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ABSTRACT

The application of combustion for power generation or heat production needs to be well-controlled to achieve clean and reliable output. When pulverized solid fuels, coal and biomass are considered, which are still important nowadays and in the future, the ignition and volatile combustion phase play an essential role in flame stability and pollutant formation. For the fundamental understanding of complex processes of solid fuel combustion, collaborations of experimental and numerical studies are desired, which assist to design more sustainable furnaces. In this work, the ignition and volatile flame of high-volatile bituminous (hvb) coal particle groups are experimentally and numerically investigated in a laminar flow reactor.

In the experiments, simultaneous volumetric laser induced fluorescence imaging of OH (OH-LIF) using a novel laser scanning technique is combined with tomographic particle tracking velocimetry (TPTV) providing fundamental insights into flame topologies. The quasi-instantaneous 3D OH-LIF measurements are performed by raster scanning the laser beam from a 10 kHz dye laser across the probe volume using an acousto-optic deflector (AOD). Three-dimensional volatile flames of coal particle groups are visualized using volumetric reconstruction of OH-LIF signals from 10 parallel planes. Time- and space-resolved particle trajectories are evaluated from 10 kHz TPTV measurements using a Lagrangian particle tracking approach (Shake-the-Box). Numerical simulations are performed taking real operating conditions from experiments into account. An extended Flamelet generated manifold model accounting for the complex mixture of gases being released during devolatilization is applied to capture the gas-phase chemistry. The interactions of the gas phase with particles is modeled within a fully coupled Euler-Lagrange framework.

This study includes parametric variation of the particle size and combustion atmospheres. The ignition and volatile flame transition with increasing particle number densities (PNDs) is analyzed and compared with single particle measurements. The inter-particle and particle-gas interactions are investigated utilizing particle trajectories which interact with the evolution of the flame structure. The coupled effects of gas temperature and mixture fraction on group particle flame topology are discussed by combining experimental and numerical observations. This collaborative study sheds new light on the fundamental physical and chemical processes of group particle combustion in air- and oxy-atmospheres.

Strategy and Practices of China's Clean and Efficient Coal Power

Dr. Pisi Lu

China is the largest coal power producer in the world. How to make coal power clean and efficient has been a great challenge to this country. In the past twenty years, China government has adapted a serial of policies to promote new technologies development and demonstrations. It has enacted laws and regulations to address coal power efficiency and pollutant emission issues. With over twenty years efforts, its coal power unit efficiency has improved from the lower of thirties percent to above the middle of forties percent level. Its current environment regulations for new coal-fired power units are the most stringent ones in the world, which basically requires the new coal-fired power units reach the same pollutant emission standards as gas power. In this presentation, we will review China's clean and efficient coal power strategy and discuss its practices by using a few specific projects as examples including new constructions projects and retrofitting projects.

Investigation of soot formation characteristics during oxy-coal combustion in reducing-to-O₂/CO₂ ambiences

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Abstract

Soot formation in oxy-coal combustion plays a dominant role in the radiative heat transfer, but the effect of the O₂/CO₂ ambience remains unclear. In this paper we apply a novel two-stage flat flame burner to provide a flexibly-adjustable reducing-to-O₂/CO₂ ambience that is ubiquitously encountered in real combustors. We incorporate the *in-situ* visible light, LII and Mie scattering diagnostics with online measurement of particle size distribution and off-line soot sampling. We find that the peak of LII signals appears later than that of Mie scattering, indicating the LII signal is free of the scattering interference and the soot formation takes place when the coal particle ignites. Moreover, the consistency between the LII and SMPS results verifies LII provides reliable concentrations of primary soot particles. Through a comparison of various operating conditions, the O₂/CO₂ ambience is found to delay the ignition in the flue gas temperature of 1500 K. Furthermore, the O₂/CO₂ ambience is found to promote soot formation under 1500 K by advancing the soot incipient time and elevating the peak value of LII signals. Because the temperature is well controlled in our experiments, we postulate the chemical effect to be mainly responsible for this phenomenon.

Stability analysis of 60 kW coal flames under air and oxyfuel-conditions

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The successful short-term implementation of oxyfuel combustion by retrofitting existing conventional boilers, or employing conventional existing designs in future applications depends to a large degree on how similar oxyfuel flames behave compared to the originally designed air flames of these boilers. Thus, it is of high relevance to understand the impact of changes in viscosity, momentum or flame boundary conditions on flame stability when transitioning from air to oxyfuel combustion.

For this, the present study aims to examine the relationship between spatio-temporal fluctuations in the flame and changing composition of the oxidizer mixture under well controlled experimental conditions. Therefore, three measurement techniques, each providing high temporal resolution data are employed: i) time dependent local velocity measurements (laser Doppler velocimetry) ii) flame temperature (high data rate two-color-pyrometry) and iii) high speed flame imaging. Measurements were conducted for three pulverized coal swirl flames (Rhenish lignite) confined within an experimental combustion chamber (60 kW_{th}) with same stoichiometry and same thermal output. The chosen oxidizer mixtures were: a) air (conventional) and b,c) two different oxyfuel atmospheres with 21 and 25 vol.% O₂ in CO₂ respectively.

The combined preliminary analysis of the temporally high-resolution data series shows that the substitution of conventional-air by oxyfuel combustion can introduce differences in fluctuation patterns of the flames which can be attributed to the coal particle entrainment and early mixing with the oxidizer in the combustion chamber. The differences in mixture viscosity and momentum associated to oxyfuel conditions seem to have a stabilizing effect when transitioning from air to oxyfuel combustion in swirl burners due to an enhanced mixing of the reactants in the flame zone.

Evaluation of a moving reference frame approach for the numerical analysis of pulverized coal combustion

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Abstract

A moving reference frame approach is employed to investigate the small scale structures of the *Central Research Institute of Electric Power Industry* (CRIEPI) pulverized coal jet flame with very highly resolved LES at reasonable computational effort. The coaxial burner with a hydrogen supported pulverized coal flame is modelled using the in-house code *PsiPhi*. A newly implemented four-dimensional flamelet table, adapted to the lab-scale flame, is introduced. The flamelet/progress-variable (FPV) approach, studied by Rieth *et al.* in the context of pulverized coal combustion (PCC), is used for modelling the complex multiphase flow. In an *a priori* step, a simulation of the whole burning region is performed. The simulation is validated by comparing temperature of the gas phase, radial and axial velocity components, as well as gas composition against experimental data.

In an *a posteriori* step, the moving reference frame approach is introduced. Since the flame spreading in radial direction is small in the investigated case, this method poses a promising approach to reduce computational effort. The domain covers a small cross-sectional area of the burner volume with periodic boundary conditions applied in axial direction. A reasonable domain length is kept for statistical analysis.

The applicability of this method is discussed with the analysis of velocity and temperature of the gaseous as well as of the particle phase. The flame structure is analysed using mole-fraction profiles along the centerline.

This approach allows the detailed investigation of the flame without the necessity of modelling the whole burner volume which strongly decreases the computing time, while promising reasonable results in terms of particle devolatilization and flame propagation.

Keywords:

Flamelet, LES, FPV, Pulverized coal combustion

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Large Eddy Simulation of a semi-industrial pulverized coal combustion chamber under oxyfuel atmospheres using tabulated chemistry

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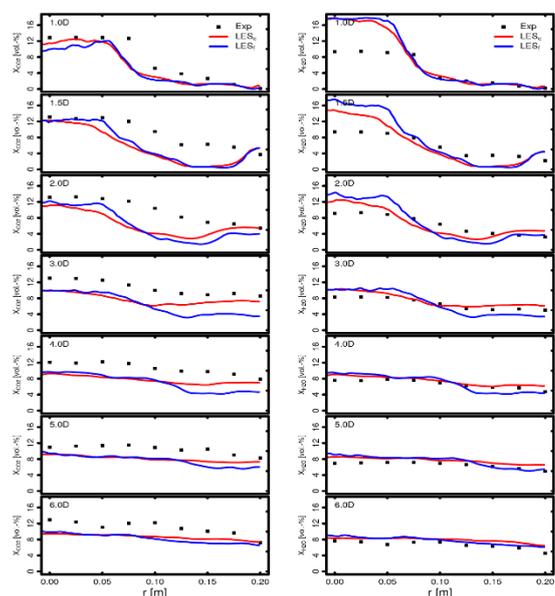
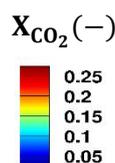
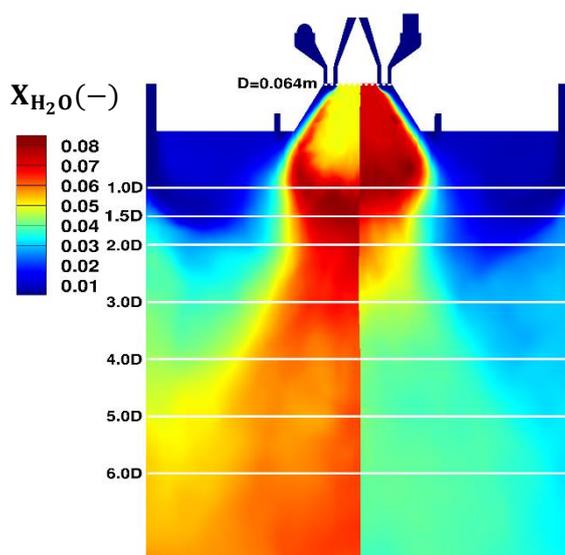
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In order to meet climate change goals and limit global warming, a drastic reduction of CO₂ atmospheric emissions of hydrocarbon fuel-based power plants and industrial processes is required. Under the current global socio-economical context, carbon capture and storage (CCS) technologies present themselves as one of the most plausible alternatives for short-term CO₂ emission reduction from industrial combustion applications. For instance, oxyfuel combustion is one of such technologies which can, by replacing N₂ with CO₂ in the oxidizer, generate product gases almost entirely composed of CO₂, therefore facilitating its capture or utilization. However, the substitution of N₂ by CO₂ in the oxidizer can significantly influence the thermophysical characteristics of the combustion processes, which still need to be understood. Therefore, process analysis and development require more collaborative experimental-numerical studies.

Numerical modeling and simulation of pulverized coal combustion is still a significant challenge, given the wide range of multiscale physical phenomena involved. Since these phenomena are complex and strongly coupled, appropriate models need to be developed, which are crucial for 3D CFD simulations. To this end, due to the increasing computational power available, 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 60 kW Rhenish lignite swirl flame, under oxyfuel conditions, in a semi-industrial configuration. Considering the large number of multiphase reactions required to describe the chemical processes, these cannot be directly computed. Therefore, a tabulated chemistry approach is developed to capture finite rate chemistry effects in the simulation. In addition, radiative heat transfer is calculated by solving the full radiative heat transfer equation applying the weighted sum of grey gases model for spectral resolution. The overall model is validated employing detailed experimental data of flow fields, particle temperature and local gas species concentrations. Subsequently, the numerical model is employed for the comprehensive study of flame stabilization, local oxidation behavior and particle trajectories to provide valuable insights into the oxyfuel combustion process under realistic conditions.



Direct, absolute and selective NO₂ measurements as from fuel combustion process emissions using dTDLAS

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Abstract:

Nitrogen dioxide (NO₂) is an air pollutant produced from fuel combustion, that has a great risk to human health. The standard reference method (SRM) for NO₂ emissions is based on chemiluminescence, as called for by the European standard EN 14211:2012. However, using chemiluminescence, NO₂ is measured only indirectly, i.e. NO₂ is calculated as the difference between total nitrogen oxides (NO_x) and nitrogen monoxide (NO) after conversion of NO₂ to NO. This conversion of NO₂ to NO does partly convert other species (NO_y) different to NO, thus causing an overestimation in the NO₂ results [1]. Therefore, there is an increased need to develop accurate and reliable measurement methods for direct NO₂ measurements, enabling the development of new standards and the drafting of future legislations. Next generation laser spectroscopic techniques such as direct tunable diode laser absorption spectroscopy (dTDLAS) offers the capability of direct and selective NO₂ measurements. dTDLAS is a variant of the known laser absorption spectroscopy by means of compact semiconductor diode lasers which combines this spectroscopic technique with a special, first principles data evaluation approach to directly extract metrologically traceable absolute gas species concentrations [2-4]. A dTDLAS spectrometer directly providing SI-traceable gas concentration shall be referred to as an “Optical Gas Standard” (OGS).

Here, we present our new interband cascade laser-based dTDLAS approach for direct and selective NO₂ amount fraction quantification. We report directly measured NO₂ concentration results to demonstrate the capability of the spectroscopic system as an independent “calibration free” sensor. The feasibility of the spectrometer being operated as a field OGS, and the options of upgrading the spectrometer for simultaneous NO/NO₂ measurements in a complex gas matrix, as, e.g., in car exhaust gas matrix, are discussed.

Part of this work has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme. (<https://msu.euramet.org/>) [5]. PTB is member of European Metrology Network (EMN) for Climate and Ocean Observation.

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Influence of water vapour on tar and gas formation during biomass pyrolysis under N₂ and CO₂ atmosphere in a drop tube reactor

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Under oxy-fuel conditions, wet-recycling of exhaust gas leads to an elevated concentration of H₂O in the combustion chamber. This is especially the case for the combustion of biomass fuels due to its higher moisture content. Despite the relevance for the oxy-fuel process, the information on the influence of the higher water content on pyrolysis, volatile release and secondary pyrolysis in the literature is scarce.

For this reason, a series of tests with walnut shells was carried out, chosen as an example of an agricultural waste fuel. The experiments were carried out in a drop tube reactor to achieve temperatures and heating rates similar to pulverized fuel combustion conditions. Particles and pyrolysis gases were collected with a moveable oil cooled and quenched sample probe. In addition to the particles ($d_p > 1 \mu\text{m}$), tars were collected with a tar trap and volatiles are analysed by online FTIR spectroscopy. The FTIR is calibrated for 36 species, leading to the possibility of a detailed analysis of released volatiles during pyrolysis. Initial tests in pure atmospheres of CO₂ and N₂ build the reference for experiments in atmospheres with 5 wt% and 15 wt% H₂O in CO₂ and N₂, respectively. For all atmospheres, experiments with 4 different sample probe positions were carried out, leading to residence times of about 0.05 s to 0.15 s.

First results show a clear tendency towards higher hydrocarbon content in the volatiles with increasing water content. The increase in the relative content of heavier hydrocarbons increases up to a factor of 10. The biggest difference can be seen in sulphur compounds. While the content of detectable sulphur compounds in the pyrolysis gases in the water-free atmospheres is only 1 wt%, their proportion in 15 % H₂O is about 40 wt%.

Reactivity of mineral-free and doped synthetic chars in O₂-, CO₂- and H₂O-containing atmospheres

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The reactivity of synthetic chars in different atmospheres related to air (O₂/He) and oxyfuel conditions (CO₂/He, H₂O/He, O₂/CO₂) was investigated by thermogravimetric analysis applying a magnetic suspension balance. The mineral-free model char was derived from cellulose by hydrothermal carbonization at 200 °C and subsequent pyrolysis at 800 °C in flowing N₂. Afterwards, the char was doped with 20 wt% of different mineral model compounds by the tight-contact method. The metal oxides and carbonates used for this doping procedure were selected according to the high abundance of the corresponding metals in the ash of natural coals. Isothermal measurements of the char samples were performed to obtain the relative reactivities as a function of the applied atmosphere and the added mineral. For the mineral-free char, a variation of the partial pressures revealed a positive reaction order with respect to O₂, CO₂, and H₂O as reactive gases. The char reactivity in oxidative reaction atmospheres was distinctly higher than in gasification atmospheres. Comparing the gasification processes, the reaction proceeded faster in H₂O/He than in CO₂/He. The similarity of char conversion in O₂/He and O₂/CO₂ atmosphere in the low-temperature regime was in good agreement with the observed low conversion in CO₂-containing atmospheres especially at low temperatures. Doping of the char affected the char conversion qualitatively similar in the investigated atmospheres. In all reactive compositions, K₂CO₃ and Na₂CO₃ were found to have the highest catalytic influence. Increased char reaction rates were also observed applying Fe₂O₃ and CaO as dopants, while there was no significant acceleration of the reaction in the case of added MgO, SiO₂, and Al₂O₃.

Effects of the spatial heterogeneity of gas matrix and thermal boundary layers on absolute TDLAS HCl measurements in hot flue gases

Zhechao Qu, Jarvis Nwaboh, Olav Werhahn and Volker Ebert

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Abstract:

EU are setting increasingly stringent Emission Limit Values (ELVs) for key air pollutants and regulating emissions from combustion/industrial processes. Accurate measurement of emissions to the atmosphere is vital to control and reduce air pollution. Optical methods offer promising tools to investigate the dynamic release of molecular species from combustion environments. The EMPIR IMPRESS 2 project [1] goes beyond state of the art in measuring the emissions of critical pollutants (e.g. HCl) with lower ELVs.

Tunable diode laser absorption spectroscopy (TDLAS) [2-4] is frequently applied in combustion research and industry for open path in situ gas analysis [5]. While, TDLAS is a line-of-sight (LOS) technique, especially for combustion diagnostics, the effects of spatial heterogeneities (e.g. temperature, gas matrix) along LOS should be considered for spectral fitting and concentration quantification [6], and efforts are needed to reduce the heterogeneity effects on TDLAS measurements.

A direct TDLAS (dTDLAS) based HCl spectrometer [7] has been developed in PTB recently, and a simulation model was built for analysing thermal boundary layers effects. Here, the key point of this presentation is to extend the simulation model for a better understanding of the spatial gas matrix heterogeneity effects on HCl-dTDLAS measurements in i.e oxy-flame.

Acknowledgement

This work was supported by IMPRESS2 within EMPIR. This project has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.

PTB is member of the European Metrology Network (EMN) for Climate and Ocean Observation (<https://www.euramet.org/european-metrology-networks/?L=0>).

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- [7] Z. Qu, O. Werhahn and V. Ebert, PTB OAR DOI: 10.7795/810.20191105

Effects of the spatial heterogeneity of gas matrix and thermal boundary layers on absolute TDLAS HCl measurements in hot flue gases

Zhechao Qu, Javis Nwaboh, Olav Werhahn and Volker Ebert

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Abstract:

European Directives are coming into force setting increasingly stringent Emission Limit Values (ELVs) for key air pollutants and regulating emissions from combustion processes. Accurate measurement of emissions to the atmosphere is vital to control and reduce air pollution. Optical methods offer promising tools to investigate the dynamic release of molecular species from combustion environments. The IMPRESS 2 project [1] goes beyond state of the art in measuring the emissions of critical pollutants (e.g. HCl) with lower ELVs.

Tunable diode laser absorption spectroscopy (TDLAS) [2-4] is frequently applied in combustion research and industry for sampling-free and in situ gas analysis [5], but its application is normally limited to uniform conditions along the line-of-sight (LOS). However, in many applications, for example, combustion diagnostic measurements, heterogeneities (e.g. temperature, gas matrix) along the LOS may occur. In those conditions, the effects of heterogeneities should be considered for spectral fitting and concentration quantification [6].

A direct TDLAS (dTDLAS) based HCl spectrometer [7] has been developed in PTB recently. Here, the key point of this presentation is a better understanding of the effects of spatial gas matrix heterogeneity on the absolute accuracy of this spectrometer. A simulation model will be used here to analyze the effects of spatial heterogeneities on dTDLAS HCl concentration measurement.

This work was supported by IMPRESS2 within the EMPIR.

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Spectral modeling of an oxy-fuel pulverized coal fired boiler considering non-gray gas and particles

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Thermal radiation through gases and particles matter is the dominant mode of heat transfer in pulverized fuel fired boilers. Radiation influences ignition, flame temperatures and consequently the formation of soot. Due to the combustion of pulverized biomass or coal with recycled flue gas and pure oxygen, the amounts of carbon dioxide and water vapor in the flue gas of the power plant boiler are increased in comparison to the air-fired process. Both molecules show strong absorption and emission characteristics in the infrared wavenumber region providing enhanced thermal heat radiation on the evaporator tubes along the furnace walls. To precisely predict the thermal radiation, the non-gray behavior of gas and particle radiation has to be accounted for.

In this study, results from a CFD simulation of a 250 MW_{el} and 15 x 15 x 90 m dimensioned coal fired industrial boiler are used as boundary conditions for a radiation simulation. This simulation is based on temperature, species, pressure and particle distribution from the CFD simulation. The radiation heat flux is calculated

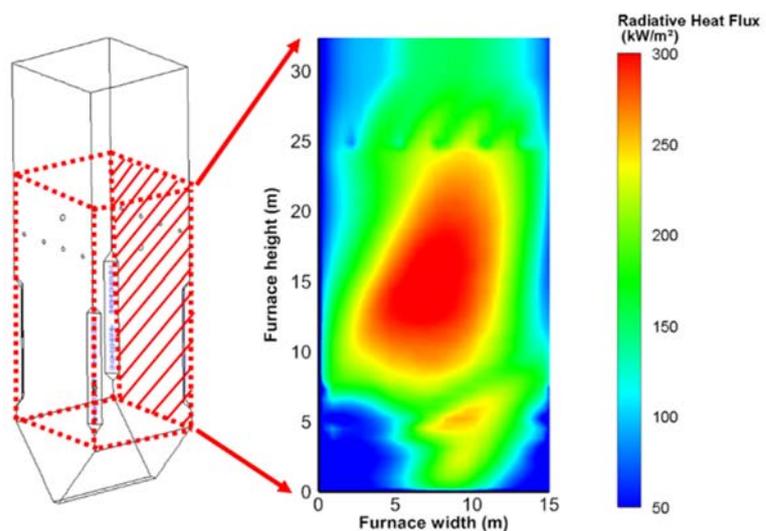


Figure 1: Radiative heat flux at the sidewall of an industrial furnace. Radiative heat flux calculated with NBCKM and Henyey-Greenstein (HG) phase function for particle scattering.

with a Narrow Band Correlated-k Model (NBCKM). To consider non-gray particles, different scattering phase functions are evaluated. A study of the mesh size from 31,250 up to 250,000 cells shows a slight difference in the calculated radiative heat flux.

Experimental assessment of the release of Nitrogen, Sulfur and Chlorine species during pyrolysis of coal and torrefied biomass in CO₂ atmosphere

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In oxyfuel combustion, the substitution of nitrogen in the combustion atmosphere by carbon dioxide is accompanied by a considerable change in the combustion behaviour of the solid fuel. The release of minority species, such as sulphur, nitrogen and chlorine compounds from the fuel plays an essential role in the design process of oxyfuel power plants, since significant corrosion and emission issues arise from these species.

In this study, the release of nitrogen, sulfur and chlorine species during pyrolysis of US-american bituminous coal with high sulphur content (U2) and a torrefied biomass was studied in an entrained flow reactor. With the entrained flow reactor, particle heating rates comparable to those observed in a full-scale furnace can be achieved. Pyrolysis experiments were performed at different temperatures in carbon dioxide atmosphere. Gas samples were extracted from the reactor at different heights and thus, different particle residence times. The gas samples were analysed for their H₂S, SO₂, COS, NH₃, NO, N₂O and HCl content using mass spectrometry and FTIR spectroscopy. Furthermore, solid particle samples were taken from the reactor and analysed using an elemental analyser to determine the composition (C, H, N, S) of the char particles after pyrolysis.

The results showed that the formation and release of the considered minority species changes with temperature and differs between the two fuels used for the experiments. It was found that the N₂O concentration decreases rapidly with increasing temperature, while the NO concentration increases. The release of NH₃ increased with increasing temperature, whereas the release of HCN decreased. Compared to the bituminous coal, more N₂O and NH₃ and less HCN was released during pyrolysis of the torrefied biomass. Moreover, the concentrations of SO₂, COS and HCl were higher during pyrolysis of the U2 coal.

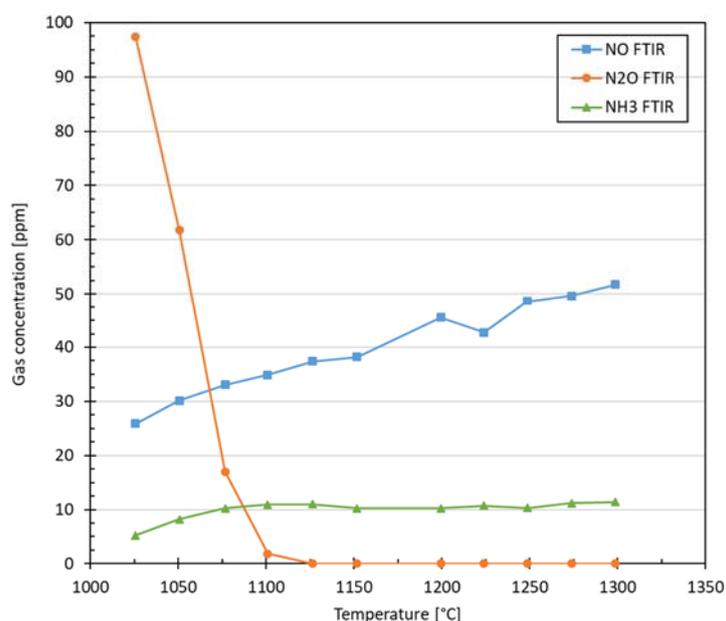


Figure 2: Concentrations of nitrogen species during pyrolysis of U2 coal in CO₂ atmosphere

Abstract Submission

TITLE OF TALK:

Visualization and analysis of solid fuel particle trajectories in a gas-assisted oxy-fuel combustion chamber

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Solid fuel combustion plays a major role in electric power generation. The oxy-fuel process is an approach to lower CO₂ emissions in future. As in conventional pulverized fuel combustion, trajectories of solid fuel particles contain useful information to support our understanding of flame stabilization, burnout behavior and burnout rate for oxy-fuel combustion. To investigate the particle trajectories a high-speed PTV setup was applied to a 40 kW_{th} gas-assisted oxy-fuel combustion chamber (PTV: Particle Tracking Velocimetry). The test rig is equipped with a swirl burner and offers excellent optical access through quartz glass walls and a quartz glass quarl. In this study three operational conditions, one air and two oxy-fuel atmospheres, were examined. As pulverized solid fuel, Renish lignite and torrefied biomass were used. The investigation focuses on the near-nozzle regime, which is important for flame stabilization and the combustion of volatiles.

Visualization of particle trajectories by a single camera gives access to the particle's velocities and accelerations in a two-dimensional projection. The pulverized solid fuel enters the quarl through an orifice in the burner nozzle. Close to the burner nozzle the particle mass flow is too dense to extract individual particles. In this region investigations on the jet dynamics with a specific focus on the shear layer between gas phase and the particle phase have been conducted. Further downstream and inside the characteristic central recirculation zone of the swirl burner a multitude of individual particle trajectories in terms of velocity, acceleration and direction were recorded and analyzed statistically. Most particles follow the main gas flow downstream, which surrounds the central recirculation zone. Especially particles inside the recirculation zone show a wide range of velocities, directions and accelerations, so that large slip velocities can be assumed in this region.

Determination of Temperature and Concentration of Major Combustion Species in Fuel-Rich Methane Flames under Elevated Pressure

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Abstract

Combustion processes with pure oxygen (oxy-fuel) instead of air as oxidant are attractive e.g. for high temperature thermal or thermochemical and gasification processes. In such applications, the absence of nitrogen leads to many advantages such as improved flame characteristics, lower exhaust gas volumes, reduced costs, increased flexibility and improved product quality.

An example for the use of partial oxidation (POX) of methane is the production of high purity synthesis gas with a high amount of hydrogen, which can subsequently be used in downstream synthesis processes as the Fischer-Tropsch or methanol synthesis. On an industrial scale, such processes are often carried out under elevated pressure.

In case of such methane/oxygen flames (premixed, fuel-rich in the equivalence ratio range of $2.5 < \phi < 3.0$, without any dilution of the oxidizer and elevated pressure and preheating temperature) experimental data are scarce.

In the present work, temperature and concentration profiles of major combustion species of premixed fuel-rich laminar CH₄/O₂-Flames under elevated pressures (1 to 5 bar_a) and preheating temperatures up to $T_P = 573$ K were experimentally determined for the first time, to the authors knowledge. A new burner and modular test rig were developed to be able to use optical (tunable diode laser absorption spectroscopy – TDLAS) and invasive (GC/MSD) measurement techniques. The TDLAS setup was used to determine temperature and H₂O concentration profiles. For the determination of major combustion (CH₄, O₂, H₂, CO and CO₂) species, a quartz probe was inserted into the flame and the sample was analysed by a GC/MSD.

The system pressure shows a high impact on the local development of the H₂-CO-rich synthesis gas. Additionally, peak concentrations and maximum temperatures are influenced by the pressure. The concentration and temperature profiles were compared with detailed reaction mechanisms.

Reaction Kinetics of Pulverized Fuels in Combustion and Gasification Atmospheres

3rd International Oxyflame Workshop, 4.–5.3.2020

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Modeling reaction kinetics of solid fuels in combustion and gasification atmospheres plays an important role in reactor design and optimization. A better understanding of the underlying fundamentals is essential – in particular at operating conditions relevant to large-scale industrial applications, e.g., at high temperatures.

This presentation gives an overview of these fundamentals with focus on entrained flow reactors, including different modeling approaches, experimental test procedures, and laboratory analyses. Two investigations are discussed in detail: The role of gasification reactions during pulverized fuel combustion at different wall temperatures and stoichiometries, and the conversion of different solid fuels at elevated pressures during oxygen-blown entrained flow gasification. Both examples cover CFD modeling as well as experimental results.

Investigation of turbulent solid fuel combustion using a comprehensive Euler-Lagrange framework with detailed homogeneous and heterogeneous kinetics

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November 29, 2019

Abstract

A comprehensive Euler-Lagrange framework for coal particle combustion using detailed multi-step heterogeneous kinetics is presented. The heterogeneous kinetics (*POLIMI model*) involve 37 species (22 solid species and 15 gas species) and 49 reactions to describe pyrolysis [1] as well as char oxidation, gasification and annealing [2] for a wide range of coals. The porous structure of coal particles is considered and the heterogeneous reactions are assumed to occur throughout the entire particle by a volume-based approach. The ODEs of the heterogeneous kinetics are integrated on each Lagrangian coal particle and predict the conversion of the raw coal components to light volatile hydrocarbons, heavy tar species and char off-gases. Hence, the composition of the solid components and the released gas changes dynamically in space and time providing high fidelity predictions of solid fuel combustion. The homogeneous conversion of the released species is described by a detailed gas phase mechanism with 76 species and 973 reactions derived from the complete POLIMI v1407 kinetic model. The novel Euler-Lagrange approach is validated against fully-resolved single particle simulations in laminar flow [3] that predict the experimental ignition delay times of Pittsburgh seam high-volatile bituminous coal particles in air and oxy atmospheres [4]. Subsequently the new modelling framework is employed within carrier-phase direct numerical simulations (CP-DNS) of pulverized coal combustion in a three-dimensional turbulent mixing layer [5]. The latter configuration includes the additional physics of turbulence and particle group combustion by mixing solid fuel particles suspended in a primary oxidiser stream with the products from lean volatile combustion in a secondary stream. The CP-DNS data is analyzed in terms of mixing, ignition and combustion characteristics and comparisons to simpler modelling approaches are made.

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Carrier-phase DNS of NO_x formation in pulverized coal flames with fuel-bound nitrogen

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November 29, 2019

Abstract

Carrier-phase DNS (CP-DNS) of detailed NO_x formation in pulverized coal flames with fuel-bound nitrogen is conducted. The CP-DNS setup is a 3D temporally evolving mixing layer, where Lagrangian coal particles initially distributed randomly in a transport stream of air in the upper half of the domain are mixed with hot products from the lean combustion of coal volatile matter in a lower stream. A Colombian bituminous coal with significant amounts of fuel-bound nitrogen is used. Fuel-NO_x formation based on both nitrogen in the volatile matter (volatile-N) and char-bound nitrogen (char-N) is considered. The nitrogen in the volatile matter considers three fuel-NO_x precursors, namely the light gases NH₃ and HCN, and a lumped nitrogenated tar (tar-N) represented by pyridine (C₅H₅N). The devolatilization of the NO_x precursors and further hydrocarbon volatiles is based on the detailed multi-step kinetics model of Sommariva et al. (*Fuel* 89:318-328, 2010). The detailed pyrolysis model is run in a pre-processing step to determine the volatile composition for the CP-DNS using realistic particle heating rates from the mixing layer. The devolatilization rates predicted by the detailed pyrolysis model are fitted to a two-step competing rate model used for the Lagrangian coal particles in the CP-DNS. The release of char-N is associated with the heterogeneous oxidation of carbon and provides a second source of fuel-bound nitrogen in the system. A tailor-made comprehensive homogeneous mechanism based on detailed chemical kinetics, including all standard pathways of NO_x formation in gas-phase combustion, as well as a pyridine sub-mechanism, is adopted. Based on the CP-DNS database the principal mechanisms of NO_x formation from coal are investigated by analysing the turbulent flow field, reaction chemistry, and their interactions through chemical time scale and reaction paths analysis. The CP-DNS provides a detailed database for future combustion model development for example in the LES framework.

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Oxidation characteristics of hydrothermally derived model fuels doped with minerals in a laminar flow reactor

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The composition of solid carbonaceous fuels depends on their origin and rank. The variance of the content and composition of ash influences the combustion behaviour of these fuels. It is well known that alkali, alkaline earth and transition metals catalyse carbon conversion. Hence, it is highly relevant to quantify the catalytic effects of these metals on char burnout under realistic conditions.

A microcrystalline cellulose (MCC) is used to synthesize a reference mineral-free model fuel by hydrothermal carbonization (HTC). This model fuel is doped with minerals such as potassium, iron or magnesium as sulfates.

The temperature of single mineral-free and mineral-doped model fuel particles is measured as an indicator whether catalytic effects influence the oxidation behaviour. Therefore, pyrometric measurements of the char burnout are carried out in a laminar flow reactor under conditions typically for pulverized coal combustion ($d_p \sim 100 \mu\text{m}$) and high heating rates (10^4 - 10^5 K/s) under controlled oxy-fuel conditions. The feed rate is limited to avoid particle-particle interaction. The camera-based pyrometry system SCOT (stereoscopic camera system for optical thermography) is used to measure the temperature as well as the size, shape, and velocity for a statistically significant number of particles. SCOT operates on the principle of the two-colour pyrometry with intensified CCD cameras as detectors. The particle temperature is measured at different residence times from ignition to a significant char burnout.

The influence of the minerals on the particle temperature is discussed and implemented in existing reaction models which provide carbon conversion rates and heat release from the particle.

Investigation of particle temperature and burnout process of single and group particle combustion under oxyfuel conditions

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Models for carbonaceous fuel particle combustion have to provide carbon conversion rates and the heat release from the particle to the surrounding. To verify and calibrate these models the temperature and the burnout progress must be known.

Since pulverized fuel particles are in the range up to 100 μm , non-invasive methods like ratio pyrometry are the only technique for particle temperature measurements. Therefore, the temperature is measured in an optically accessible laminar flow reactor under conditions typical for pulverized coal combustion, i.e. high heating rates (10^4 - 10^5 K/s). The radiation temperature and size of the reacting particles are recorded in situ with a two-colour pyrometry system.

In addition to the optical measurement the burnout process is determined. Therefore partially reacted coal particles are extracted from the reactor by a sampling probe. Fast quenching of all gas-particle reactions is mandatory to determine the sampling point. The collective samples are analysed regarding their ash content and elemental composition. Thus the evaluated data provide knowledge about the burnout process and the release of particular elements such as carbon, hydrogen and nitrogen.

Although single particle studies are highly relevant for the study of ignition and combustion of dilute particle streams, particle group effects are very important to get a more realistic knowledge about particle combustion. Therefore, an understanding of the ignition and combustion at different particle number density (PND) is needed.

To compare the ignition delay time for single and group coal particle combustion with the particle temperature and burnout process the laminar flow reactor experiments for single particle combustion are expanded to higher feed rates. The experiments are implemented under controlled oxyfuel conditions for a Colombian coal. The influence of PND on the particle temperature and burnout process is discussed. Laser induced fluorescence data of OH (OH-LIF) for the same reactor and operational conditions are compared to the temperature data.

Evolution of micro- and mesopore structure during pyrolysis of coal and biomass in different atmospheres

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During pyrolysis, gasification, and combustion of solid fuels, char morphology changes and becomes in general more porous since the volatiles are released, and the reacting carbon develops more open and wider pores. This evolution of porosity, as well as the formation of macro-, meso- and micropores, are important information for, e.g., reliable models for char conversion. In oxy-fuel atmospheres, the formation of pores is in general more pronounced than in air atmospheres, since CO₂ also converts the solid fuel by gasification. The change of morphology during pyrolysis of a highly volatile bituminous Colombian coal and grounded walnut shells was investigated. Walnut shells were chosen as an example of an agricultural waste fuel. As walnut shells and Colombian coal particles show nearly spherical particle shape, experimental conditions are quite comparable. To achieve temperatures and heating rates similar to pulverized fuel combustion conditions, a drop tube reactor was used to produce chars under defined conditions. Reactor temperatures for the Columbian coal were 1300 K and 1475 K, and experiments with the walnut shells were conducted at 1125 K and 1300 K. A moveable oil cooled and quenched sample probe allows for collecting samples in different conversion stages. Since a direct measurement of the particle temperature and residence time is not possible due to the experimental setup, the temperature curves and the residence time of the particles in the reactor are calculated with the assistance of CFD simulations.

By conducting volumetric adsorption measurements with CO₂ at 273.15 K and N₂ at 77 K on the differently pyrolyzed chars, a micropore (Dubinin-Astakhov) and a meso- to macropore (BET) analysis were conducted. For both analyses, pore sizes, pore volume, surface area and porosity were determined and compared. The influence of pyrolysis gas, temperature, and residence time on the evolution of the different pores are discussed. In general it was observed, that at the beginning of pyrolysis, the evolution of micropores was pronounced. With ongoing pyrolysis, micropores expand to bigger micropores, but new micropores are formed as well.

Evaluation of flamelet model for laminar pulverized coal combustion in air and oxy-fuel atmospheres with pollutant formations

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In this work, the suitability of the flamelet models for pulverized coal combustion in air and oxy-fuel atmospheres is evaluated in a laminar counterflow configuration. The pollutant formations, including NO_x and SO_x , are considered. Particularly, both char-N and volatile-N are considered for NO_x formation, while volatile-S is considered for SO_x formation. The flamelet predictions are compared to the detailed chemistry solutions in *a priori* analyses. A newly developed oxy-fuel chemical reaction mechanism is employed, which contains 129 species and 911 elementary reactions. For both NO_x and SO_x formations, two different flamelet models are evaluated, with the species mass fractions either being extracted from the flamelet library (M1) or being obtained with the corresponding transport equations (M2). Figure 1 compares the pollutant mass fractions obtained from the detailed chemistry (DC) simulations and the different flamelet models along the central axis of the counterflow for air (left) and oxy-fuel (right) conditions. It can be observed that for NO_x species, M1 performs slightly better than M2 around the peak value regions for both air and oxy-fuel conditions. The good performance of M1 is considered due to the fast production rates of NO_x , which justifies the suitability of the flamelet models. For SO_x species, M1 performs very well in the entire computational domain while the peak values of Y_{SO} and Y_{SO_2} are over-predicted by M2 and the peak value of Y_{SO_3} is under-predicted.

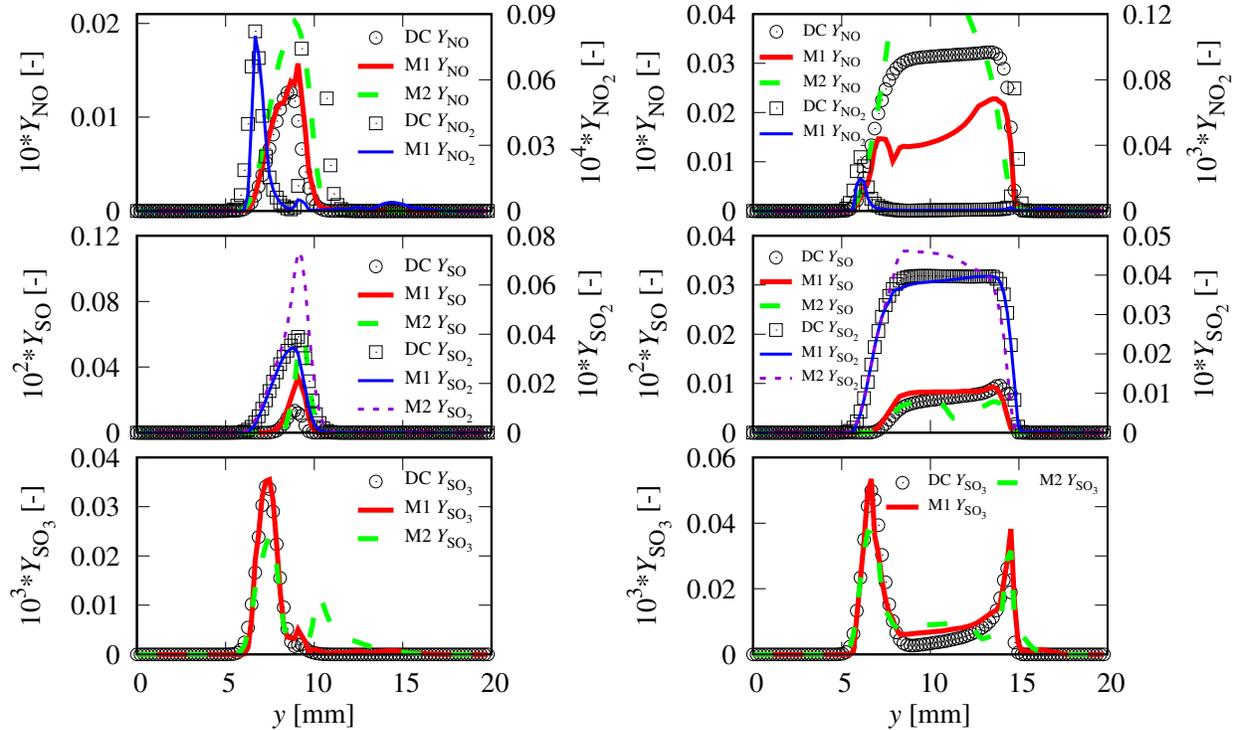


Fig. 1. Comparisons between the detailed chemistry (DC) solutions and *a priori* flamelet predictions along the central axis of the counterflow in (left) air, and (right) oxy-fuel atmospheres.

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Automated generation of char conversion reaction networks

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Char conversion is most of the time described by the Char Burnout Kinetic (CBK) model family, which simplifies the char oxidation reactions to a three-step mechanism. Such an approach is very useful in order to predict the kinetics of a solid fuel combustion when there is experimental data to be fitted. On the other hand, a detailed chemical reaction kinetics model which describes the reactions at different active sites, due to morphological features as well as different functional groups, would give insights about the processes and might help understanding the factors which affects the combustion rates of different fuels. Here, we will present an automated workflow of the software ChemTraYzer which combines the simulation and analysis reactive force field ReaxFF trajectories and automated submission of the quantum mechanism calculations for better resolution of potential energy surfaces. The results of the quantum mechanics calculations are then used to calculate thermodynamic properties of the molecular system such as NASA polynomials and reaction rates.

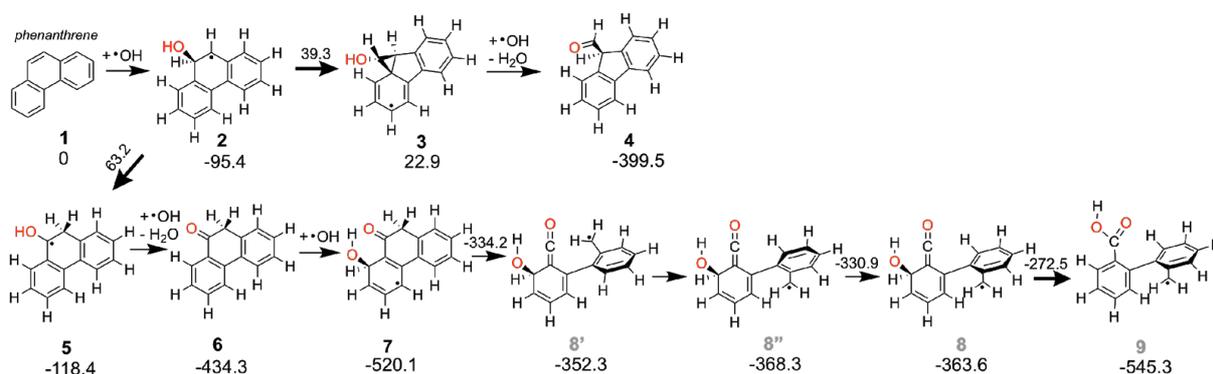


Figure 1: Some of the reactions observed during the ReaxFF simulations and detailed using density functional theory (TPSSH-D3/def-TZVP). The relative energies are shown under the molecules and given in kJ/mol.

Experimental study of the staged supply of oxygen in the oxy-fuel combustion in a bubbling fluidized bed

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This paper presents a comprehensive experimental study of the NO_x reduction by oxygen staging in the oxy-fuel combustion of wooden pellets in a 30 kW_{th} bubbling fluidized bed experimental facility. A number of experiments was performed examining the impact of relevant operational parameters on the level of NO_x reduction in comparison to oxy-fuel mode without oxygen staging. Various secondary/primary oxygen ratios were examined while keeping overall concentration of oxygen in dry flue gas at the same level. In these experiments, a constant ratio of O₂/CO₂ in fluidizing gas or a constant fluidized bed temperature were kept. However, it was not possible to keep both of them constant at the same time, since the bed temperature can be controlled only by changing the FGR or the fluidization gas flow. Additionally, the impact of the overall oxygen stoichiometry and fluidized bed temperature was studied.

The results showed that the secondary oxygen can be used with advantage to reduce the NO_x emissions. Previous experiments revealed that the NO_x formation tends to be sensitive towards the O₂ concentration in the fuel-rich region and towards the bed temperature, where a higher excess of oxygen and a higher temperature enhance the NO_x formation. In the case of oxygen staging, the conversion of fuel-bound nitrogen to NO_x is reduced due to a decrease of the O₂ partial pressure in the fluidized bed. Within the experiments, the NO_x reduction of nearly 50 % was achieved in comparison with a case without oxygen staging at similar conditions. In all operation regimes, the NO_x reduction efficiency increased with the increment of the secondary/primary oxygen ratio. The experiments also showed that the oxygen staging is a promising path to provide convenient conditions for the application of a SNCR in the freeboard, due to the possibility to reach an optimum temperature window by burning there the fuel volatiles, thus efficiently increasing the freeboard temperature. For the secondary/primary oxygen ratio about 1 and fluidized bed temperature 880 °C, the freeboard temperature higher than 950 °C was achieved at all conditions.

Numerical simulation of swirl oxy-coal combustion in a 60 kW Test Facility using the SST k- ω turbulence model

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Combustion of solid carbonaceous fuels plays a significant role in the global supply of electric energy. Although replacing fossil fuels through renewable sources has nowadays become more important than ever, mostly because of global warming, a sudden substitution is not possible. Therefore, a considerable fraction of energy production will be remaining in the near future dependent on combustion of solid fuels. In this regard, decreasing the pollution caused by coal combustion has gain a vital importance and been the impetus of a great number of scientific works over recent decades.

Oxy-combustion is one of the rethought combustion technologies, in which carbon dioxide can be cost-effectively sequestered. Nevertheless, the chemical and physical concepts behind the heterogeneous oxidation of carbon, which takes place at high temperature and pressure/or in rich CO₂ environments, are not still fully understood.

In this regard, this study aims to develop a detailed numerical simulation of turbulent oxy-combustion employing the SST k- ω model in the commercial Ansys Fluent 17.1 CFD package. Different stages in the combustion of solid carbon; such as drying, pyrolysis and char burnout, are implemented through user defined functions as well as particle tracking and gas and particle radiations. The results involve comparisons between different RANS models, turbulence-chemistry

interaction models, pyrolysis and char burnout models and the influence of a spectral absorption coefficient. For validation the velocity field is presented in Figure 1, showing good agreement between simulations and measurements carried out by the Institute of Heat and Mass Transfer in a 60 kW test facility at RWTH Aachen University.

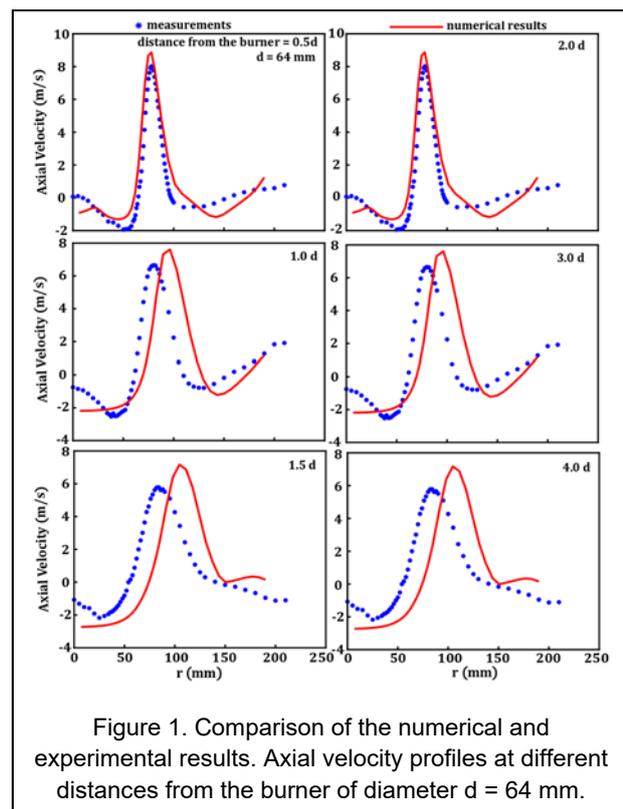


Figure 1. Comparison of the numerical and experimental results. Axial velocity profiles at different distances from the burner of diameter $d = 64$ mm.