3.9 Subproject B3

3.9.1 General information about sub-project B3

3.9.1.1 Title

Direct numerical simulation and modeling of oxyfuel combustion processes Short title: Direct numerical simulation

3.9.1.2 Field classification

Combustion, Turbulence, Fluid Mechanics

3.9.1.3 Project Leadership

Pitsch, Heinz, Prof. Dr.-Ing.
*26.03.1966, deutsch
Institut für Technische Verbrennung
RWTH Aachen University Templergraben 64,
52056 Aachen
(+49 241) 80-94608
h.pitsch@itv.rwth-aachen.de

Is the position of any of the persons mentioned above limited ? *No*

3.7.1.4 Information on research legal matters

Please refer to the general information on page 67.

Summary

In simulations of fuel particle combustion, individual particles are typically described as point-like entities using Lagrangian methods to efficiently and accurately represent a large number of particles. The local interactions of particle combustion with both the flow and the oxidizing atmosphere surrounding the particles are important for the heat release rate and the formation of gas-phase species. However, these interactions are not considered in the film models commonly used for this type of modeling. In the first funding period of the project, fully resolved simulations of combustion of individual particles and particle groups in laminar flow were considered, and improved particle combustion models were developed for application in the point particle approach. So far, mainly cylindrical but also spherical particles have been considered.
In the second funding period, the focus is on a higher level of detail regarding particle structure and the interaction of particle combustion with turbulence. Initially, particle-resolved simulations of single particles and particle groups will be conducted, taking into account particle porosity and the interaction with chemical and transport processes within the particle, to subsequently incorporate these effects into the point particle model and overall model development in C2. Additionally, fully resolved three-dimensional simulations of reacting spherical and non-spherical particles in a turbulent flow field are planned to investigate the interactions between chemistry and turbulence. Furthermore, direct numerical simulations of devolatilization, coke combustion, and combined effects using the point particle approach in a turbulent planar jet will be conducted to examine the turbulence/particle/chemistry interaction with a realistic number of fuel particles under oxyfuel conditions. This will generate high-quality statistical data for different parameter variations.
Finally, the simulations initiated in the first funding period of a swirl-stabilized configuration, simulating the flame stabilization zone of a real combustion chamber, will be continued. This aims to investigate the details of flame stabilization in solid particle combustion and provide data for the analysis of combustion models developed in TP B6. The resulting data will be examined with

systematic analysis methods, such as the Optimal Estimator Method, focusing on interactions between particle combustion, particle dynamics, and molecular and turbulent mixing processes. The results will then be used in TP B6 for further model development.

3.9.3 Development of the sub- project to dte

3.9.3.1 Report and state of research

Objectives of the first funding period

In the first funding period of the project, models were developed to cover the entire spectrum of the smallest relevant scales of particles, boundary layers, and chemistry, up to the largest relevant scale, a modern swirl burner. Fully resolved simulations of individual particles (AP1) and particle groups (AP2) required for model development were successfully conducted with numerous parameter variations, and models were developed for application in the point particle approach. These models allow for the consideration of the influence of physical processes occurring at the micro level that are not resolved in the point particle approach. Furthermore, simulations of the experimental configuration used in TP A2 were conducted in accordance with AP1. During the remaining time of the first funding period, the models will be finalized. Direct numerical simulations (DNS) of particle-laden, planar, time-evolving free-jet flames (AP3) are currently underway. These simulations were started later than planned due to the extensive work on chemically reacting, particle-resolved simulations. However, analyses are expected to be completed by the end of the year.In accordance with the fourth work package, simulations of coal dust combustion in a swirl burner will be initiated towards the end of the first funding period (AP4), in which the developed point particle models will also be utilized. These simulations are planned to be continued and analyzed in the next funding period of the project.

Report on the first funding period

Resolved simulations of single particles (Ref. [1])

The interactions between the flow field and the combustion of a coal particle were investigated in temporally, spatially, and chemically fully resolved simulations. Particle-resolved simulations are

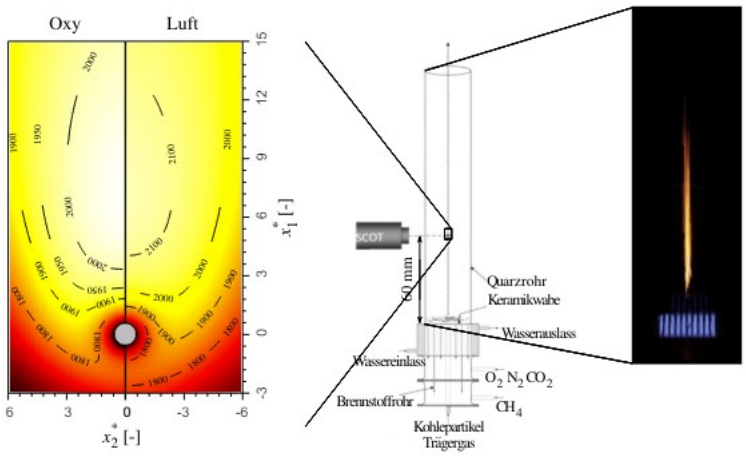


***Figure 1**:Right side: Representation of model validation. Flat flame burner from TP A2 with an image of a particle stream during coke combustion.*

typically conducted for spherical particles. However, microscopic images from TP A2 indicate that while this assumption may apply to some particles, others may be better approximated by cylinders, thus both forms should be examined as boundary structures. Initially, infinitely long cylindrical particles were investigated, as these can also be described for particle groups through 2D simulations. Subsequently, simulations for spherical particles were also conducted.For the simulations, an approach similar to that of Lee et al. [17] was used, marking the first time such a transient model for fully resolved simulations of coal combustion in an oxy-fuel atmosphere (CO2/O2 instead of N2/O2) was employed. The model was implemented in the institute's own simulation code CIAO, described in more detail in Refs. [4, 8], and can be used for both devolatilization and coke combustion. The implementation was validated based on the experiments conducted by TP A2 on coke combustion in both air and oxy-fuel atmospheres, showing good agreement with the experiments in both environments. Figure 3.26 illustrates the experimental setup and the calculated temperature distribution for both cases.

Furthermore, mass and energy exchange between the solid particle and the gas phase during combustion in an oxy-fuel atmosphere were investigated and compared with corresponding cases in an air atmosphere. For both atmospheres, an energy balance analysis revealed that the majority of heat release occurs not through heterogeneous reactions but through gas-phase reactions involving components released by heterogeneous reactions. Additionally, in an oxy-fuel atmosphere, both a lower coke combustion rate and an overall lower heat release rate compared to combustion in an air atmosphere were observed. Detailed chemical mechanisms were used to analyze the intermediate reactions involved. The lower coke combustion rate in an oxy-fuel atmosphere leads to increased activity of the reaction O2 + H → OH + O, resulting in oxygen deficiency for surface oxidation reactions and consequently lower heat release. The combination of lower heat release and higher specific heat capacity of the gas phase leads to lower temperatures in oxy-fuel compared to air atmospheres.
For the typical particle Reynolds numbers and local conditions considered here, the convective Damköhler number (Dakonv) of the particles is always greater than one, indicating that transport processes play an important role. Therefore, the interaction between transport processes and chemistry was investigated based on a series of simulations with varying particle Reynolds numbers (Rerel). Rerel was modified via the relative velocity U01. Figure 3.27 on the left shows a nonlinear trend, where the coke combustion rate increases with increasing Reynolds number until Rerel = 2,

after which it decreases again. Increasing Rerel leads to higher oxygen supply but reduces surface temperature due to increased convection, thus decreasing reaction rates. Above Rerel > 2, the reduction in surface temperature predominates, causing the coke combustion rate to decrease. This behavior was also observed under different oxygen concentrations. Figure 3.27 also shows that the coke combustion rate in an oxy-fuel atmosphere is always lower than in an air atmosphere for the investigated cases with the same oxygen concentration. The release, as shown in Figure 3.27 on the right, changes with Rerel similarly to the coke combustion rate. Heat release through homogeneous gas-phase reactions depends mainly on available oxygen in the atmosphere, coke combustion rate, and temperature. It is further observed that the reduction in temperature and coke combustion rate only surpasses the influence of higher oxygen concentrations on homogeneous reactions at Rerel > 4, resulting in an overall decrease in heat release.

In the model used here, the influence of porosity was accounted for by a constant effectiveness factor in the rates of heterogeneous reactions. This factor represents the ratio of the surface area available for heterogeneous reactions, including the particle's internal pore structure, to the nominal surface area of the particle without considering the pores. However, this ratio not only depends on the type of solid fuel but also changes with increasing porosity during particle combustion. Sensitivity analyses revealed that the effectiveness factor has a particularly strong influence on combustion behavior. Therefore, in the second funding period, improved models for the influence of porosity will be developed in close collaboration with TP A6.

The data and insights obtained from the simulations described here can further inform model development. This will be presented following the discussion of simulations of particle groups.

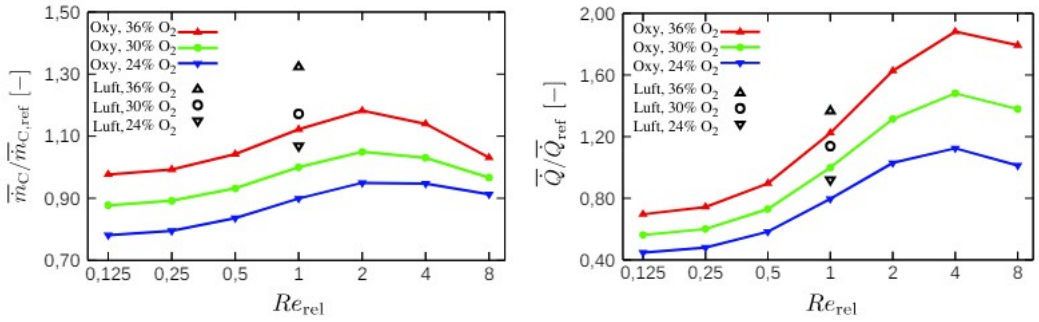


Figure 2 *Coke combustion rate and heat release rate as a function of particle Reynolds number in air and oxyfuel atmosphere. \(\dot{m}_{C,ref} \) and \(\dot{Q}_{ref} \) correspond to the respective values at (Re_{rel} = 1) and (XO_2 = 30%).:*

Resolved simulations of particle groups (Ref. [21])

Particle group combustion was also investigated through fully resolved simulations of various configurations. The parameter space for these simulations includes different gas compositions, particle Reynolds numbers, Damköhler numbers, particle spacings, particle numbers, and group arrangements, and was conducted for infinitely long cylinders, similar to single particle simulations. The particle spacing L was varied between 3 D_p and 9 D_p, where D_p represents the particle diameter. This corresponds to the range resulting from the typical particle number densities calculated by TP C2 for the 100 kW swirl burner used in TP C1 at Aachen. In most cases, the behavior of the first particle upstream is similar to that of a single particle, while particles downstream exhibit significantly different behavior. A reference case was defined with three horizontally arranged particles, L = 6 D_p, and Re_{rel} = 1. Figure 3.28 shows the heat release, temperature, and mass fractions of OH and O2 in the vicinity of the particles. The surrounding gas phase of the first particle contains significantly more oxygen than the surrounding gas phases of the rear particles, so the highest heat release rate is observed at the first particle despite higher temperatures at the rear particles.

With the same particle spacing, the influence of a Reynolds number change depends on the particle position. The coke combustion rate at the first upstream particle shows a maximum similar to that of

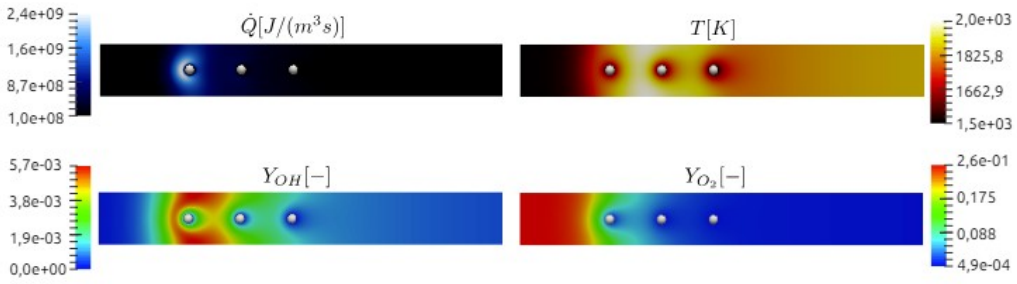


Figure 3 *Heat release rate \(\dot{Q} \), temperature \(T \), OH and \(O_2 \) mass fractions \(Y \) near the particle at a particle distance of \(6 D_p \) and \(Re_{rel} = 1 \). The particles are approached from the left.*

single particles, after which an increase in the Reynolds number leads to a reduction in the coke combustion rate. However, the coke combustion rate at the second and third particles increases monotonically with Re_{rel}. At $Re_{rel} = 8$, the third particle shows its highest coke combustion rate due to the increased oxygen concentration and temperature at the surface. Further studies of various parameters have shown that the coke combustion rate of downstream particles increases with increasing Reynolds number regardless of particle spacing and oxygen concentration in the atmosphere. Figure 3.29 also shows that an increase in the Reynolds number enlarges the flame front and leads to a different flame structure. At small particle spacings, an increased Reynolds number leads to particle group combustion, while at larger particle spacings, each particle behaves similarly to a single particle.

For all particle spacings, an increase in Re_{rel} leads to a shift of the temperature peak towards the outlet. To compare the heat release at different particle spacings while keeping the Reynolds number constant, the volume-averaged heat release was calculated, as shown in Figure 3.30. It is evident from this that a denser particle cloud at lower Reynolds numbers results in a decrease in heat release, while dense particle clouds at higher Reynolds numbers lead to particle group combustion and thus significantly higher heat release. The curve for single particles corresponds to the limiting case for infinitely large particle spacings. Further parameter studies were conducted and analyzed to

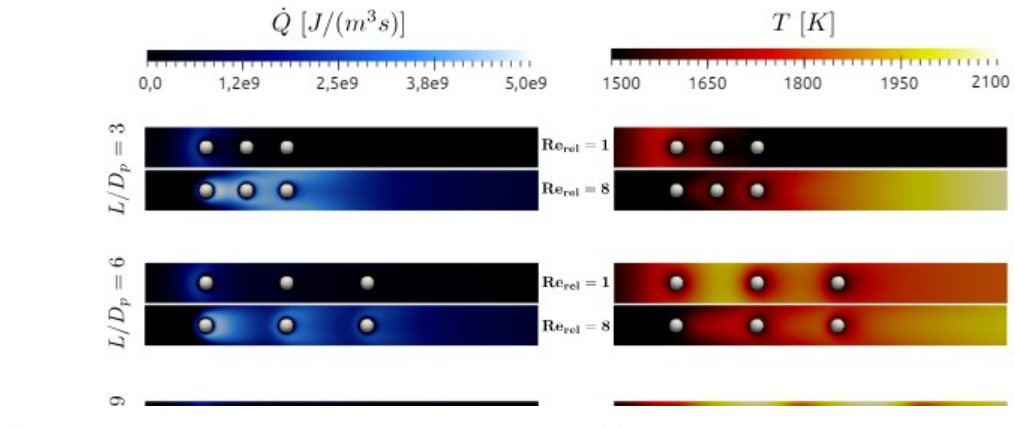
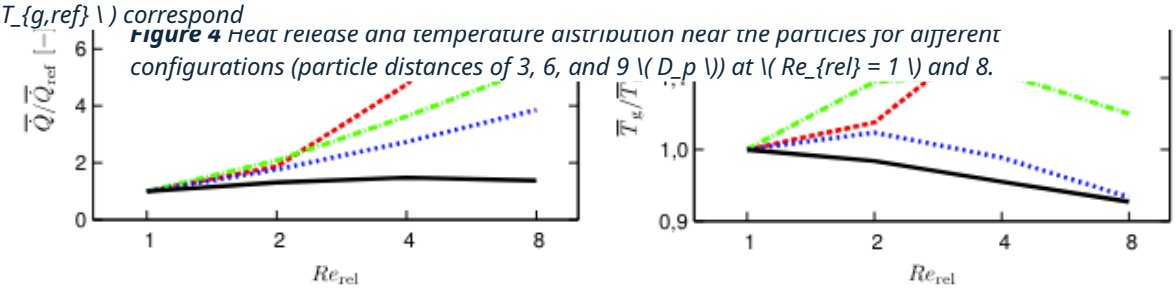


Figure 5*: : Volume-averaged heat release and temperature for different particle distances and (Re_{rel}). In each case, the gas temperature (T_g = 1496K \) and oxygen mass fraction (Y_{O_2} = 30%). (dot{Q}_{ref}) and(T_{g,ref} \ ) correspond*

Figure 4 *Heat release and temperature distribution near the particles for different configurations (particle distances of 3, 6, and 9 \(D_p \)) at \(Re_{rel} = 1 \) and 8.*



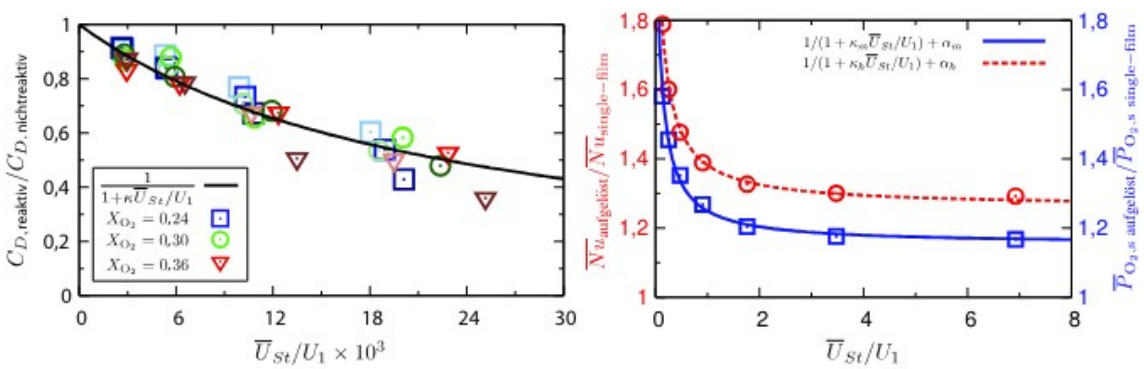
incorporate the results regarding particle interaction into the model development for the point particle approach.

Model development for the point particle approach (Ref. [2] and [21])

For further investigation of coal particle combustion, an Eulerian approach for the gas phase and a Lagrangian approach for the particle phase are assumed. Here, fuel particles are treated as point particles, requiring models to describe the interaction of particles, chemistry, and flow. The influence of particles on the balance equations in the gas phase is accounted for through source terms for species, mass, momentum, and energy. Additionally, conservation equations for mass, momentum, and energy are solved for each particle, yielding particle position, velocity, and temperature. The modeling approaches developed in this project for various physical phenomena regarding particle-gas phase interaction are described below.

Particle trajectories are calculated based on the forces acting on the particles. Primarily, this includes air resistance resulting from particle interaction with the gas phase. Air resistance depends on the Stefan flow generated by surface reactions. However, this effect is usually neglected in simulations of reactive coal particles. In this project, the influence of surface reactions on the flow around the coal particle for different gas compositions and Reynolds numbers was investigated to develop an improved model for the drag coefficient depending on the Stefan flow and thus the surface reaction rate. Surface reactions lead to a Stefan flow velocity USt directed from the particle towards the gas phase, affecting the surrounding flow. To quantify the influence of surface reactions, the ratio of the surface-averaged Stefan flow velocity to the relative velocity, USt/U1, is introduced as a dimensionless parameter. USt/U1 reaches its maximum value for a gas phase with the lowest particle Reynolds number and the highest oxygen content. The drag coefficient CD was then calculated for each particle for both reactive and non-reactive cases. The drag coefficient decreases due to surface reactions, with this effect being more pronounced for lower particle Reynolds numbers and higher oxygen content. As shown in Figure 3.31, the ratio of drag coefficients for the reactive and non-reactive cases, CD,reactive/CD,non-reactive, exhibits an almost universal, reciprocal behavior depending on USt/U1 for all cases. An empirical relationship between CD,reactive/CD,non-reactive and USt/U1 is extracted to represent the obtained results, which can now be used for oxy-fuel coal combustion simulations using a point particle approach to consider the influence of the Stefan flow on the particle drag coefficient.

In many experimental and numerical studies based on the point particle approach, temperature and oxygen concentration on the particle surface are calculated using simplified models, such as the single film model. The single film model is based on a non-reactive, quiescent gas phase and does not resolve temperature and oxygen concentration gradients at the surface. Heat flows due to conduction and convection are jointly calculated based on the Nusselt number Nu via E = Nu λ/Dp(TP − Tg). Typically, the Nusselt number is solely given as a function of the Reynolds number, neglecting the influence of the Stefan flow. In this TP, particle-resolved simulations were conducted where the initial particle temperature, gas phase temperature, and gas phase composition were set according to the measurements from the flat flame burner experiment of TP A2.



The resulting heat flux through conduction and convection was then converted into an effective Nusselt number using the correlation mentioned above. Figure 3.31 on the right shows the ratio of the effective Nusselt number calculated from the resolved simulation to the Nusselt number used in the single film model, as well as the resulting empirical correlation. It is observed that the effective Nusselt number is always greater than that calculated from the single film model. The ratio increases as expected for large relative flow velocities, as the single film model assumes a quiescent gas phase to calculate heat fluxes. Similarly, exploiting the analogy between heat and mass transport, the oxygen partial pressure at the surface $P_{O2,s}$ was compared between the resolved simulation and single film model. Again (see also Figure 3.31 on the right), it is observed that the oxygen partial pressure at the surface calculated in the single film model is significantly lower than that established in the resolved simulation. The correlation functions for both quantities have the same form as the function used to correct the drag coefficient. These correlation functions were incorporated into the models for mass, momentum, and heat exchange in the point particle approach. The improved models can now be used in large-scale simulations, such as in TP B6. Additionally, they are to be applied to the experimental data from TP A2 to obtain more accurate reaction rates. At the end of the first funding period of the project, the developed models for further investigations based on the point particle approach will be finalized. To examine the influence of these models, simulations of a planar, turbulent jet with and without particle loading will be conducted and analyzed in the remaining time of the first funding period. In the jet without particle loading, a fuel mixture representing the devolatilization products of coal particles in an oxy-fuel atmosphere will be injected and burned instead of coal particles. The jet with particle loading will provide data for the analysis and validation of models for turbulent particle combustion.

Highlights

Particle-resolved simulations of chemically reacting particles are scarcely documented in the literature, and particularly, the model development based on these data has not been pursued in the past. The single-particle simulations described here for coke burnout in air and oxy-fuel atmospheres using heterogeneous and detailed gas-phase kinetics, and the resulting model development, therefore represent an important step towards improving point-particle models for simulating coal dust combustion.

State of Research

The importance of porosity and particle internal processes for particle combustion has been thoroughly documented in the literature. Hecht et al. [15, 16] conducted simulations where steady-state equations for mass, energy, and chemical components were solved for a reacting porous particle. This demonstrated that for models that do not account for flows within the particle interior, intrinsic reaction rates need to be adjusted by corrections to reaction rate coefficients and reaction orders. Additionally, Richter et al. [24], as a simple model of a porous particle, investigated the heat and mass transfer of an agglomerate consisting of 185 spheres and showed that chemical reaction models must account for accurate predictions of particle internal processes.

The relative velocity between particles and the gas phase leads to apparent turbulent fluctuations, even in laminar flows. However, this is typically not considered in simulations using the point-particle approach, as simplified models for particle drag are employed. Nevertheless, these models lead to deviations, particularly in turbulent flows. Since the proposal for the first funding period, several studies have been published, but most of them focus on non-reacting particles. For instance, Mehrabadi et al. [20] developed a model based on fully resolved simulations to assess the influence of slip Reynolds number and solid mass fraction on the Reynolds stresses in the gas phase. The heat transfer between particles with constant temperature and the surrounding gas phase was

investigated by Tenneti et al. [25] based on fully resolved simulations. Typically, models for heat transfer assume a constant mean flow temperature. However, it was shown in the mentioned study that the mean flow temperature becomes inhomogeneous when streams of particles are encountered. A model was developed that provides statistically homogeneous Nusselt number even for inhomogeneous flow temperatures. Both examples consider chemical reactions and thus do not account for the Stefan flow. However, devolatilization and ignition on individual coal particles were recently calculated by Tufano et al. [26] in particle-resolved simulations. Nonetheless, the effects of particle structure and porosity, which are to be investigated in this TP, were not addressed.

Coal and biomass combustion in turbulent free jet flames will be investigated in TP B3 using DNS. Hara et al. [14] examined the devolatilization behavior in a turbulent free jet flame with ground coal at a Reynolds number of Re = 2544 using DNS. It was found that the reactions of volatile components occur partially within a premixed inner flame zone and partially with coke combustion (mainly oxidation of CO) in an outer diffusion flame layer. The DNS conducted here considers planar free jet flames. This configuration allows relatively high Reynolds numbers above the mixture transition, as demonstrated in our simulations of a non-premixed free jet flame using a gaseous fuel and very detailed chemistry with a jet Reynolds number of 15000 [3], significantly higher than that of the round free jet flame by Hara et al. [14].

In addition to these DNS studies, several LES investigations of coal combustion in turbulent flames are documented in the literature. Although they employ models for closing turbulent combustion, which precludes their use as DNS data for validating other models, they reveal interesting relationships that can be further explored through DNS. For instance, Bai et al. [11] analyzed LES results of a turbulent free jet flame with ground coal in a hot vitiated co-flow at a Reynolds number of Re = 28284. It was observed that the reaction zone becomes more continuous downstream and encompasses a large number of particles. Additionally, it was demonstrated that the combustion is dominated by non-premixed combustion. Three different flame structures were identified, termed as "Interspersed," "Striped," and "Stable Flame." The latter predominates mainly downstream and contributes nearly 70% to the total heat release. The most reactive zone exhibits the highest scalar dissipation rate and the lowest vortex strength, with the scalar dissipation rate being reduced not only by turbulent mixing between gas and fuel but also by the devolatilization process. Another example is the investigation of the swirl-stabilized coal burner IFRF No. 1 using LES by Olenik et al. [23]. These authors observed a lower volatile combustion rate in the inner recirculation zone due to oxygen deficiency, which they attributed to the Eddy Break-Up (EBU) model used and speculated that more realistic results could be achieved with an improved combustion model.

3.9.3.2 Project-related own publications

Peer-reviewed publications and book releases

Own publications resulting from the sub-project

[1] Farazi, S., Sadr, M., Kang, S., Schiemann, M., Vorobiev, N., Scherer, V., Pitsch, H., Resolved simulations of single char particle combustion in a laminar flow field, Fuel (2016) (accepted)* .

[2] Farazi, S., Sayadi, T., Pitsch, H., Numerical analysis of the drag force acting on the reactive single char particle under oxy-fuel condition, Proc. of the China National Symposium on Combustion (2016).

[3] Bisetti, F., Attili, A., Pitsch, H., Advancing predictive models for particulate formation in turbulent flames via massively parallel direct numerical simulations, Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 372 (2022) (2014).

[4] Desjardins, O., Blanquart, G., Balarac, G., Pitsch, H., High order conservative finite difference scheme for variable density low Mach number turbulent flows, Journal of Computational Physics 227 (15) (2008) 7125–7159.

[5] Jocher, A., Foo, K. K., Sun, Z., Dally, B., Pitsch, H., Alwahabi, Z., Nathan, G., Impact of acoustic forcing on soot evolution and temperature in ethylene-air flames, Proceedings of the Combustion Institute (2016) (available online).

[6] Knudsen, E., Shashank, Pitsch, H., Modeling partially premixed combustion behavior in multiphase LES, Combustion and Flame 162 (1) (2015) 159–180.

[7] Luo, K., Pitsch, H., Pai, M. G., Desjardins, O., Direct numerical simulations and analysis of three-dimensional n-heptane spray flames in a model swirl combustor, Proceedings of the Combustion Institute 33 (2) (2011) 2143–2152.

[8] Trisjono, P., Kang, S., Pitsch, H., On a consistent high-order finite difference scheme with kinetic energy conservation for simulating turbulent reacting flows, Journal of Computational Physics 327 (2016) 612–628.

[9] Trisjono, P., Kleinheinz, K., Hawkes, E. R., Pitsch, H., Modeling turbulence–chemistry interaction in lean premixed hydrogen flames with a strained flamelet model, Combustion and Flame 174 (2016) 194–207.

[10] Trisjono, P., Pitsch, H., Systematic Analysis Strategies for the Development of Combustion Models from DNS: A Review, Flow, Turbulence and Combustion 95 (2) (2015) 231–259

3.9.4 Planning the sub-project

3.9.4.1 Goals

The overarching goals of the second funding period are (i) the development of point-particle models that can be used in Lagrangian methods to describe reacting solid fuel particles, (ii) the analysis of turbulence/particle/chemistry interactions using DNS, and (iii) the further development of multiscale models for the turbulent combustion of solid particles. To this end, the important effect of porosity in particle-resolved simulations will initially be considered and investigated. Furthermore, particle-resolved simulations of solid fuel combustion in turbulent flows are planned. The influences of particle geometry, particle structure, and particle porosity, as well as turbulence in the surrounding gas phase on combustion using detailed chemical mechanisms, will then be considered in the developed models. DNS of turbulent free jets with the joint consideration of all relevant chemical processes will be conducted to investigate the turbulent combustion of solid particles, analyzed, and compared with the combustion of gaseous fuels. Special attention will continue to be given to flame stabilization. DNS

of the stabilization zone of a swirl burner will be conducted to better understand the processes important for this. The Optimal Estimator Analysis of the DNS data will identify the best parameters to be used for the parametrization of the models. The DNS data will further be used for a posteriori validation of the models derived in TP B6. The insights gained will ultimately contribute to the development of the multiscale models.

3.9.4.2 Methods

Methods for Particle-Resolved Direct Numerical Simulations

Direct numerical simulations of flows with particles require both the numerical resolution of turbulence and the resolution of the length and time scales of the particles, including the associated energy, mass, and momentum boundary layers. Such so-called Particle-Resolved Direct Numerical Simulations (PR-DNS) are intended to be conducted in this project. However, they are only feasible for limited systems [1, 12] and involve several challenges, such as describing the boundary conditions at the particle surfaces. Various approaches have been proposed in the literature to address these challenges, including Immersed Boundaries, Body-Fitted Boundaries, and others. These challenges and the impractical computational expense for technical combustion systems make the use of DNS with a point-particle approach—known as Point Particle Direct Numerical Simulations (PP-DNS)—attractive. However, for the point-particle DNS approach, models for interaction with the gas phase must be provided that reflect the influence of chemistry. Such models will be developed here using the results of particle-resolved DNS, with the kinetics of solid fuel combustion from TP A1 and A2, and the kinetics of gas-phase reactions from TP B1. Particle-resolved DNS has already been conducted during the first funding period, albeit under laminar conditions. This corresponds to the case where the particles are small compared to the Kolmogorov length. Here, particle-resolved DNS will be performed in turbulent flows. For this purpose, an Immersed Boundary Method combined with Overset Grids will be used. These methods have already been developed and implemented for the Low Mach solver CIAO [4, 8] used during the first funding period.

Systematic DNS Data Analysis

Various systematic procedures will be employed for DNS data analysis to support model development. Examples include Correlation Analysis [19], which can determine the required number of parameters in a model, the Optimal Estimator method [22], which will be further described below, and a posteriori LES, which can estimate the actual error propagation of model assumptions. An overview of different analysis methods is provided in Trisjono and Pitsch [10]. As an example, the Optimal Estimator method [10, 22] will be described in more detail here. This is a powerful analysis tool for selecting model parameters and evaluating the quality of a model's formulation. Within the Optimal Estimator method, the absolute error of a model for a quantity g is divided into two components. One component, called the Irreducible Error, corresponds to the modeling error that results solely from the choice of parameters φ used in the model. An estimation for this is based on the Optimal Estimator, which represents the best possible model for a given dataset and parameter set φ. Reducing the Irreducible Error

is only possible through adjusting the parameter selection. The other component corresponds to the error that arises solely from the formulation of the model based on the given parameters.This method has been successfully applied in the applicant's group in various modeling studies, such as in the modeling of scalar variance [13] or the modeling of turbulent premixed combustion [9].

3.9.4.3 Work program

The work program for the proposed funding period is divided into four work packages. The schedule is presented in Table 3.35. Table 3.36 illustrates the interfaces with the project partners in the Collaborative Research Center (SFB).

AP1: Particle-resolved simulations considering the influence of particle porosity

During the first funding period of the project, particle-resolved DNS was conducted, and models for mass, momentum, and energy transfer necessary for the point particle approach were developed. In sensitivity studies, the critical influence of particle structure, particularly porosity, on physical and chemical processes was observed. The porosity of the particles, typically considered only as a factor, not only increases the surface area available for heterogeneous reactions but also allows oxygen diffusion into the particle, enabling volumetric combustion. Depending on the oxygen concentration in the particle boundary layer, the depth of oxygen penetration into the porous particle varies, affecting the proportion of participating surface in the chemical reaction. Analyzing the depth of penetration is a crucial aspect for representing carbon consumption based on intrinsic kinetics.To investigate this effect further, additional simulations will be conducted using models for porosity from TP A6 and TP A2 for spherical and cylindrical particles. TP A6 conducts a detailed investigation of diffusion in porous coal particles. Based on the resulting outcomes, kinetic parameters for coke combustion reactions will be formulated in TP A2, considering the influence of porosity. In this project, the modified kinetic mechanisms will be applied in particle-resolved DNS of both individual particles and particle groups to quantitatively assess the influence on combustion behavior at high resolution and provide data for model development. The ultimate goal is to develop models considering the influence of porosity, which will subsequently be utilized in TP B6 and C2.

AP2: Particle-resolved simulations of solid fuel combustion in isotropic turbulence

In the first funding period of this project, the influence of gas flow on particle combustion within a laminar regime was investigated and modeled. This is sufficient when the particle diameters are small compared to the small turbulent scales. In the second funding period, the interactions between particles, turbulence, and chemistry during particle combustion will be examined for larger particles. The hypothesis here is that the turbulent flow field leads to a higher coke combustion rate and a higher rate of heat release, depending on the intensity of turbulence at the scale of the particle diameter. In this work package, three-dimensionally chemically and spatially fully resolved coal particles (particle-resolved DNS) will be considered in isotropic turbulence. Approximately 10 to 100 particles moving in the flow will be used. Important

parameters include the ratios of particle spacing and Kolmogorov length to particle diameter, as well as a Damköhler number formed with the Kolmogorov time. Additionally, ellipsoids will be used as representative non-spherical fuel particles to represent biofuels. The influence of turbulence on heterogeneous and homogeneous reactions will be investigated and modeled using simulation results.
In point-particle DNS, the Schiller-Naumann correlation is typically used to determine the drag between particles and the gas phase. It is assumed that the particles are smaller than the Kolmogorov length, and the phenomena resulting from the shearing of the fluid around the particles are ignored. However, in the present application, the particle sizes are comparable to the Kolmogorov length in the unladen flow, and by ignoring the above-mentioned phenomena, the forces exerted by the particles on the gas phase are underestimated. Accordingly, corrections to the point-wise drag forces will be derived, taking into account the influence of chemistry and turbulence.
Finally, in a posteriori simulations, the models developed in the first funding period and here in AP1 and 2 for point particle simulations will be validated and checked for accuracy. The flow simulation still uses DNS resolution, but particle dynamics are described using a Lagrange method. The models developed in this work package will also be passed on to TP B6 and C2 after validation. An exchange of the parameters used will take place with TP B7.

AP3: DNS, a priori and a posteriori analysis of particle combustion in turbulent flow

In this work package, further point-particle DNS of a planar jet will be conducted, and the data will be analyzed together with the results of simulations from the first funding period, followed by a posteriori LES. In the simulations of the first funding period, ignition and devolatilization on one hand and coke combustion on the other hand were considered separately. The focus for the second funding period is on simulations of the entire combustion process and thus on the interaction of the processes. For these simulations, the point-particle models provided in this subproject and from TP B2 will be used. The reduced reaction mechanisms for gas-phase chemistry in the oxyfuel atmosphere will be provided by TP B1. Furthermore, simulations for biofuels in an oxyfuel atmosphere will be conducted. For this purpose, non-spherical particles described aerodynamically by the results from B2 and chemically by the results from AP2 will be used. Another focus of this work package is the detailed analysis of the interactions between turbulence and chemistry during combustion in an oxyfuel atmosphere with a large number of particles. For this purpose, the DNS data will be analyzed using various methods as described above. The Optimal Estimator method will identify parameters that are particularly suitable for modeling. Through a posteriori analysis of the models developed in TP B6, validation and opportunities for model improvement will be provided.

AP4: DNS of particle combustion in a swirl burner under oxyfuel conditions

In this work package, particle combustion in a swirl burner under both air and oxyfuel conditions will be investigated to consider the influence of different flame stabilization mechanisms in the combustion model. The focus is on the flame stabilization zone to obtain data on the interaction of turbulence with devolatilization, coke combustion, particle dynamics, and gas-phase mixing processes for further model development and validation. The hypothesis here is that similar to previous work on DNS [7] and LES [6] of droplet combustion in swirl-stabilized flames, partially premixed and, especially, locally premixed combustion play an important role in the combustion of solid particles and are responsible for the majority of heat release. The influence of thermal radiation in the primary zone will be estimated and, if necessary, considered in the simulations. Suitable models are already available in the simulation code to account for both emission and absorption [5, 18].
The simulations will be conducted using point-particle DNS to obtain complete data with high accuracy. The configuration of the swirl burner from TP B4 will serve as the basis for the simulations. This configuration is based on the 100 kW burner used in C1, but the geometry has been modified to allow simulation on a structured grid. This geometry will be largely adopted but adapted for DNS purposes. The relevant dimensionless parameters will be determined from simulations in TP C2. To enable DNS, the dimensionless parameters, such as the Reynolds number, will be adjusted accordingly to reduce the computational time requirement to an acceptable level. By the end of the first funding period, a reference case under oxyfuel conditions will be calculated as planned

Outlook for the 3rd funding period

The overarching goal of this subproject is the development of predictive and validated models for the combustion of solid fuels in turbulent flows to predict static and dynamic combustion processes, including pollutant formation. In the 3rd funding period, there will be an increased focus on particle-resolved DNS, even in more complex turbulent flows. Here, the investigations will particularly address pollutant formation, with different fuels being used. Models for soot formation and the formation of gaseous pollutants such as NOx, chlorine, and sulfur components will be initially examined both a priori and a posteriori, and if necessary, improved. Additionally, dynamic processes such as ignition behavior and flame stability will be investigated using DNS and then modeled jointly with TP B6.

	2017/2	2018	2019	2020	2021/1
AP1 Partikelaufgelöste Simulationen unter Berücksichtigung des Einflusses der Partikelporosität					
AP2 Partikelaufgelöste Simulationen der Feststoffverbrennung in isotroper Turbulenz					
AP3 DNS, *a priori* und *a posteriori* Analyse der Partikelverbrennung in turbulenter Strömung					
AP4 DNS der Partikelverbrennung in einem Drallbrenner unter Oxyfuel-Bedingungen					

Literatur

[11] Bai, Y., Luo, K., Qiu, K., Fan, J., Numerical investigation of two-phase flame structures in a simplified coal jet flame, Fuel 182 (2016) 944–957.

[12] Balachandar, S., Eaton, J. K., Turbulent dispersed multiphase flow, Annual Review of Fluid Mechanics 42 (1) (2010) 111–133.

[13] Balarac, G., Pitsch, H., Raman, V., Development of a dynamic model for the subfilter scalar variance using the concept of optimal estimators, Phys. Fluids 20 (2008) 035114-1–035114-9.

[14] Hara, T., Muto, M., Kitano, T., Kurose, R., Komori, S., Direct numerical simulation of a pulverized coal jet flame employing a global volatile matter reaction scheme based on detailed reaction mechanism, Combustion and Flame 162 (12) (2015) 4391–4407.

[15] Hecht, E. S., Shaddix, C. R., Lighty, J. S., Analysis of the errors associated with typical pulverized coal char combustion modeling assumptions for oxy-fuel combustion, Combustion and Flame 160 (8) (2013) 1499–1509.

[16] Hecht, E. S., Shaddix, C. R., Molina, A., Haynes, B. S., Effect of CO_2 gasification reaction on oxy-combustion of pulverized coal char, Proceedings of the Combustion Institute 33 (2) (2011) 1699–1706.

[17] Lee, J., Tomboulides, A. G., Orszag, S. A., Yetter, R. A., Dryer, F. L., A transient two-dimensional chemically reactive flow model: fuel particle combustion in a nonquiescent environment, Symposium (International) on Combustion 26 (2) (1996) 3059–3065.

[18] Liu, F., Guo, H., Smallwood, G. J., Effects of radiation model on the modeling of a laminar coflow methane/air diffusion flame, Combustion and Flame 138 (2004) 136–154.

[19] Maas, U., Thévenin, D., Correlation analysis of direct numerical simulation data of turbulent non-premixed flames, Proceedings of the Combustion Institute 27 (1998) 1183–1189.

[20] Mehrabadi, M., Tenneti, S., Garg, R., Subramaniam, S., Pseudo-turbulent gas-phase velocity fluctuations in homogeneous gas-solid flow: fixed particle assemblies and freely evolving suspensions, J. Fluid Mech 770 (2015) 210–246.

[21] **Sayadi, T.**, **Farazi, S.**, **Pitsch, H.**, Transient multiple particle simulations of char particle combustion, Fuel (submitted)*.

[22] Moreau, A., Teytaud, O., Bertoglio, J.-P., Optimal estimation for large-eddy simulation of turbulence and application to the analysis of subgrid models, Phys. Fluids 18 (2006).

[23] Olenik, G., Stein, O. T., Kronenburg, A., LES of swirl-stabilised pulverised coal combustion in IFRF furnace No. 1, Proceedings of the Combustion Institute 35 (3) (2015) 2819–2828.

[24] Richter, A., Nikrityuk, P. A., Meyer, B., Three-dimensional calculation of a chemically reacting porous particle moving in a hot O_2 / CO_2 atmosphere, Heat and Mass Transfer 83 (2015) 244–258.

[25] Tenneti, S., Sun, B., Garg, R., Subramaniam, S., Role of fluid heating in dense gas-solid flow as revealed by particle-resolved direct numerical simulation, Heat and Mass Transfer 58 (1-2) (2013) 471–479.

[26] Tufano, G. L., Stein, O. T., Kronenburg, A., Frassoldati, A., Faravelli, T., Deng, L., Kempf, A. M., Vascellari, M., Hasse, C., Resolved flow simulation of pulverized coal particle devolatilization and ignition in air- and O_2/CO_2-atmospheres, Fuel 186 (2016) 285–292.

3.9.5 Position within the SFB/Transregio 129

The simulations conducted in B3 provide insights for both model development and data for model validation. The analysis of the data also provides clues for modeling in other projects. Additionally, the subproject incorporates models for the combustion chemistry of solid fuels from A1 and A2, which will be shared with C2 along with the models developed in B3 for point-particle simulations. Contribution to data analysis is made by conducting simulations of experiments conducted in A2. Together with B1 and B2, B3 bridges the gap between experiments and model development for single-particle combustion on one side and more complex, simplified, and realistic LES approaches on the other side. Close collaboration is intended with B6 in the area of model development and validation. Methodologically, there are connections to B2, from which the models developed there will be adopted. Furthermore, the project has important connections with B8, as the same codes and methods are used there for implementing error estimation through adjoint methods.

A1	*For the direct numerical simulation of coal combustion in TP B3, the kinetics used from A2 are supplemented with sub-models for increased pressures and oxygen volume fractions from A1. B3 assists in numerically and physically validating these sub-models.*
A2	*The simulations in B3 are supported by measurement data from A2 regarding coke combustion, temperatures, particle diameter, shape, and orientation. Models are developed in A2 and tested by B3 for their applicability.*
B1	B1 stellt B3 die Messdaten der Experimente zur Optimierung des Mechanismus zur Verfügung und erhält im Gegenzug den weiterentwickelten Code zur Simulation des heterogenen Koksabbrands zur Validierung.
B2	*Lagrange models for particle dynamics and heating are provided to B3. Source terms for the effective heat input due to surface reactions are determined by B3 and integrated into the simulations of B2; exchange via numerical methods.*
B8	*B8 adopts the flow configuration from B3 for a single particle in both laminar and turbulent flow, providing sensitivities and uncertainties regarding the models used in the simulations.*
C2	*Collaboration on group combustion modeling, exchange of numerical methods, and models for point-particle simulations for reacting particles.*
A3	*The reaction mechanisms developed by TP A3 for the release of minority species under oxyfuel conditions will be integrated into the model for the release of S, Cl, and N.*
A6	*A6 provides the sorption and diffusion data for integration into the burnout models in A2 for further transfer to B3. Together, the burnout model will be examined regarding the sorption effects.*
B4	Projekt B4 liefert die Brennergeometrie und relevante dimensionslose Kennzahlen der durchgeführten Experimente als Grundlage für Simulationen in B3.
B6	About C2: Development of a group combustion model. Evaluation of

	resistance, heat, and mass transfer based on reactive DNS simulation data.
B7	*The experimental results from B7 and numerical results from B3 are jointly interpreted. B3 conducts simulations based on the experimental parameters from B7 and supports B7 in selecting refinement parameters.*
A7	*Providing material parameters (thermal conductivity, heat capacities) for particle modeling and collaborating on optimizing simplified reaction models.*
C1	*The particle volume flows determined using LDA contribute to the validation of the models developed in project B3.*
C5	*The simulations of particle swarms (both spherical and non-spherical) conducted by B3 can be compared with the temperature, shape, and orientation data obtained from the present experiment.*

3.9.6 Distinguishing from other funded projects

A clear distinction of subproject B3 exists from all currently funded projects of the Institute for Technical Combustion (see Section 1.5) both in terms of methodology and work objectives.

		2017/2		2018		2019		2020		2021/1	
Personalmittel	**%**	Anz.	Betrag	Anz.	Betrag	Anz.	Betrag	Anz.	Betrag	Anz.	Betrag
Doktorand	100%	1	30.900	1	61.800	1	61.800	1	61.800	1	30.900
Summe			30.900		61.800		61.800		61.800		30.900
Sachmittel			Betrag		Betrag		Betrag		Betrag		Betrag
Geräte bis 10.000 Euro, Software und Verbrauchsmaterial			2.500		5.000		5.000		5.000		2.500
Sonstiges			0		0		0		0		0
Summe			2.500		5.000		5.000		5.000		2.500
Investitionsmittel			Betrag		Betrag		Betrag		Betrag		Betrag
Geräte zwischen 10.000 und 50.000 Euro			0		0		0		0		0
Geräte über 50.000 Euro			122.600		0		0		0		0
Summe			122.600		0		0		0		0
Summe insgesamt			156.000		66.800		66.800		66.800		33.400

(Alle Beträge in Euro)

	Nr.	Name, akad. Grad, Dienststellung	engere Fachzugehörigkeit	Institut der Hochschule*	Mitarbeit** (h/Woche)	Kategorie	Finanzierungsquelle
Vorhandenes Personal							
Wiss. Personal	1	Pitsch, H., Univ.-Prof. Dr.-Ing., Lehrstuhlinhaber	Verbrennung	ITV, RWTH Aachen	5		RWTH
	2	Attili, A., Dr., Wiss. Mitarb.	Verbrennung	ITV, RWTH Aachen	8		RWTH
	3	Goeb, D., M.Sc., Wiss. Mitarb.	Verbrennung	ITV, RWTH Aachen	2		RWTH
Nichtwiss. Personal	4	N.N., Stud. Hilfskraft		ITV, RWTH Aachen	8		RWTH
Beantragte Personalmittel							
Wiss. Personal	5	Farazi, S., M.Sc., Wiss. Mitarb.	Verbrennung	ITV, RWTH Aachen	40	Doktorandin	
Nichtwiss. Personal	6	N. N., Stud. Hilfskraft		ITV, RWTH Aachen	19	SHK	

* Außeruniversitäre Einrichtungen sind am geplanten SFB/Transregio 129 nicht beteiligt, ** (beratend: B)