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Correlation effects between turbulence and the conversion rate of pulverized char particles

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ABSTRACT

The effect of turbulence on heterogeneous reactions on the surface of char particles embedded in a turbulent oxidizer, consisting of oxygen and carbon-dioxide, is in this work studied numerically. It is shown that for a small Damköhler number (**Da**), which is the ratio between a turbulent and a chemical time scale, the char conversion rates are somewhat *increased* by the turbulence. This is found to be due to the increased mass transfer rate to the char particle surface that is caused by the turbulence-induced relative velocity between the char and the oxidizer. For large Damköhler numbers, however, the char conversion rate is strongly *reduced* due to particle clustering. This reduction is explained by the fact that when particles are clustered in densely populated particle clusters, the transfer of oxygen to the particles in the centre of the clusters is reduced since the oxygen is consumed by the particles closer to the external surface of the cluster. At the same time, high concentrations of oxygen exist in the voids between the particle clusters. This oxygen cannot take part in the conversion of the char until it is transported to the char surface. The effects of turbulence on the heterogeneous reaction rates are furthermore modelled based on Direct Numerical Simulation (DNS) data for a simplified reacting gas particle system.

1. Introduction

Numerical simulations are an important tool in predicting the performance, and planning the operation, of industrial applications involving heterogeneous reactions, such as pulverized coal combustion (PCC) or biomass gasification. To increase efficiency and decrease the environmental impact of new systems and optimize existing ones, more insight into the details of combustion processes is essential. Since combustion processes are a complex interaction of physical and chemical effects such as mass, momentum, heat and species transfer over a wide range of scales, also in conjunction with chemical reactions, detailed simulations of even just components of an industrial combustion system are challenging in respect to computational costs. This restricts simulations of industrial scale combustion systems to be very coarse and use empirical models. This is especially true if a lot of cases have to be simulated for a parametric study.

A common approach used in industry and research is the Reynolds-Averaged Navier Stokes (RANS) model [1,2]. The evolution of the particle position in turbulence can be accounted for by, among others, stochastic tracking [3], or by solving a joint PDF that is derived from probabilistic models of both the fluid and particles [4]. To account for the interaction between the turbulent flow field and chemistry, closure models for RANS have been developed that use transported PDF methods for both gas and particle phase attributes [5,6] and show good agreement with measurements of the semi-industrial IFRF furnace No.1. However, the effect of clustered particles due to turbulence on the reaction rates is not explicitly accounted for.

Recently, the first Large-Eddy simulations (LES) are employed for pilot scale systems [7–9]. The work of Stein et al. [8] presents a joint effort of three different research groups to present a comprehensive LES of pulverized coal combustion. For two of the three groups, particle dispersion is also taken into account with a stochastic component. Combustion of char is modelled using the kinetic diffusion rate model introduced by Baum and Street [10] or an intrinsic model presented by Smith [11]. For all three approaches, the obtained velocity fields show good agreement with experimental data, but there are some differences regarding the temperature and species data. The simulation of Watanabe et al. was able to predict the coal burnout along the central axis of a lab-scale coal jet flame to within measurement error, and could reproduce unstable combustion performance for a large-scale coal burner [9]. Watanabe et al. also combines LES with a flamelet model model [12] to investigate ignition and extinction of lab-scale

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and industrial-scale burners, and coal burnout along the central burner axis is in good agreement with measurements for the lab scale burner. Ignition limits for the industrial scale burner obtained from the simulation compare well with flame images from the actual burner, and the simulation is able to successfully predict a sharp decrease in flame stability near the ignition limit.

These modelling approaches require subgrid models that account for flow and chemistry effects on scales that are smaller than what is resolved by the simulation. The subgrid models used in RANS and LES are developed by theoretical and statistical analysis of the basic processes of combustion, studying lab scale systems or numerical experiments using Direct Numerical Simulation (DNS), where all relevant turbulent scales are resolved. Although they are computationally expensive [13], DNS provide a way to non-intrusively study turbulent combustion systems and yield flow statistics that are difficult or impossible to obtain in real experiments [14]. This accurate description of the flow in DNS makes it especially suitable to study turbulent flows in detail. The insights gained can then be utilized to develop models and correlations that can be used in simulations of industrial systems.

It is known that turbulence affects combustion systems on different scales, from the recirculation zone behind a bluff body burner to the flow far downstream. Turbulence is also essential for mixing and transport of physical quantities, such as energy and species composition, which in turn have an influence on the reaction rates. For the case of homogeneous combustion, the interaction between turbulence and combustion has been studied extensively, and consequently a large variety of models have been developed. For premixed flames e.g., models that are based on the interaction of scales [15], probabilities to find either burned or unburned gases [16,17], or geometrical descriptions of the flame [18,19] can be used. In the case of non premixed flames with infinitely fast chemistry, one can use a presumed Probability Density Function (PDF) [20] or the Eddy Dissipation Concept (EDM), where the reactions are limited by either a deficiency of fuel, oxidizer or energy [21], or the Conditional Moment Closure (CMC), where all variable parameters are conditionally averaged on flow parameters such as the mixture fraction [22,23]. If the chemistry is not assumed to be infinitely fast, the reaction rates may be obtained from flamelet libraries based on presumed PDFs of unsteady flamelets to account for transient effects [24] or local chemical equilibrium if the chemical time is still much smaller than the convective or diffusive time scales [25]. Each of these models have individual strengths and shortcomings making them applicable to different combustion conditions. The review paper by Veynante and Vervisch [26] and the book by Poinsot and Veynante [27] provide an excellent overview over the state of homogeneous combustion research and the models for turbulence chemistry interaction in use and development.

Combustion of solid matter adds more complexity to the phenomena of turbulence chemistry interaction due to the multi phase nature of the problem. Depending on the composition of the fuel, each particle has to undergo drying, devolatilization/pyrolysis and finally heterogeneous combustion, all of which have to be accounted for in a complete description of the combustion process [28]. Compared to the heating and devolatilization processes, and even the conversion of devolatilized fuels, the combustion of fuel through heterogeneous reactions is slow [29,30], which makes an accurate prediction of the process all the more crucial for achieving good combustion efficiency. The interested reader is referred to the article of Eaton et al. [31] for a review on models used in pulverized coal combustion. However, to the authors' knowledge, there is no turbulence-chemistry model connecting the effect of turbulence to the process of conversion of a dried, devolatilized char particle, which is the objective of the present work.

A reacting particle and the surrounding turbulent flow are interacting on different scales, and these effects can increase or decrease the reaction rate depending on turbulence intensity. At the scale of a particle, the flow around the particle is responsible for transporting reaction products away from the particle surface, and bringing reactants to it. Additionally, turbulence increases heat transfer from and to the particle, leading to a change in the speed of reaction [32]. On larger scales, turbulence leads to a preferential concentration of particles [33,34], where particles form dense particle clusters, separated by voids where nearly no particles are present. This can separate the solid fuel from the gaseous oxidizer. Describing the shape and size of these particle clusters and voids is a major research field in itself [35].

Annamalai and Ramalingam [36] performed a theoretical study of the combustion behaviour of clusters of coal particles in a quiescent flow and identify three distinct regimes, which are defined by low, medium or high particle concentrations inside the clusters. The Individual Particle Combustion (IPC) regime is characterized by that the distances between particles are so high that their interaction can be neglected. For medium particle concentrations, the particles on the outside of the clusters consume the oxidizer fast enough so that particles on the inside of the cluster react under fuel-richer conditions, which is called Group Combustion (GC). Finally, for high particle concentrations, the outermost shell of particles consumes all the oxidizer which is transported to it, effectively preventing oxidizing species transport to the internal particles. This combustion regime is called Sheath Combustion (SC), as only the sheath of the particle cluster is reacting. These regimes were found to have different combustion rates [36]. It is reported that in the IPC, a decrease in particle size (by particle break up, leading to a increase in particle number) results in an increase in the surface specific burning rate. In the SC regime, a decrease in particle size may result in a decrease of the surface specific burning rate. A similar finding is reported by Reveillon and Demoulin [37], who examined the evaporation behaviour of droplets in turbulent flows and found that the evaporation rate inside droplet clusters is slower than on the outside. This is due to the fast saturation of the fluid inside the droplet clusters and the slow mixing of saturated and unsaturated fluid.

Due to the increase of available computing power, DNS of pulverized coal jets under highly turbulent conditions have recently been published, providing insights into this complex phenomenon. Luo et al. performed a DNS of a pulverized coal jet flame [29] for a Reynolds number of around 30000 and compare their results qualitatively with experiments. They identify GC regimes at the jet nozzle and IPC regimes further downstream in the jet. The same numerical approach has been used to investigate the flame structures in a pulverized coal jet flame [38]. It is found that pulverized coal flames feature both premixed and non-premixed combustion, with non-premixed combustion dominating. A lab-scale pulverized coal jet flame was studied by Hara et al. [39], who propose a simple global reaction scheme that takes into account the effects of devolatilization products on the homogeneous reactions. A good agreement on the particle motion between simulation and experiments is reported. Moreover, they find different combustion regimes in the inner and outer flame layer. Brosh and Chakraborty investigated the effect of equivalence ratios and velocity fluctuations on pulverized coal combustion [40] and ignition [41] and found that the premixed combustion regime (which is more similar to IPC and GC than to SC) is more prominent for higher turbulent velocity fluctuations and vice versa. Moreover, an increase in velocity fluctuations is beneficial for mixing, but too high velocity fluctuations lead to flame extinction by increasing the heat transfer from the flame kernel. However, the published studies focus either on early stages of the combustion, where devolatilized fuel is the main driver of combustion [40], or on flows