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Coal particle volatile combustion and flame interaction. Part II: Effects of particle Reynolds number and turbulence

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ABSTRACT

Direct numerical simulation (DNS) is performed to characterize volatile combustion of isolated coal particles and closely spaced particle ensembles in laminar and turbulent flow. In part I of the paper the transient evolution of devolatilization and group flame effects were studied, Tufano et al. (2018). This analysis was limited to laminar flows and relatively low particle Reynolds numbers Re_p. Here, we investigate the effect of large Re_p and considerable levels of turbulence on the devolatilization and burning behavior of the particles. The complex physico-chemical interactions during PCC are characterized for laminar flow conditions first, before arrays of infinite particle layers are subjected to turbulence. Increasing Re_p in laminar flow leads to delayed ignition of single particles with local extinction due to high upstream scalar dissipation rates and the formation of wake flame structures downstream of the particle. An attempt is made to recover the single particle results with a standard steady laminar flamelet approach, which is shown to work well at low Re_p, but fails at high Reynolds numbers, where multi-dimensional effects occur and must be incorporated into flamelet modeling. It is found that applying standard film theory to model the effect of convection on devolatilization rates can lead to qualitatively wrong trends and up to 66% error in the peak devolatilization rate compared to the DNS results at $Re_p = 8$. The analysis of particle arrays in laminar flow shows a strong dependence of flame interactions on the values of Re_p due to the different extent of the particle wakes. The occurrence of significant levels of turbulence introduces a wide range of additional chemical states due to the randomness of the turbulent fluctuations that can either act to increase or decrease the local strain, in turn weakening or enhancing particle interactions. For the studied conditions turbulence slightly promotes the mass release from the most upstream particle set, but considerably delays the volatile release from the downstream particles, which is explained by the different extents and degrees of interaction of the up- and downstream volatile flames. The present results are considered useful for the development of LES sub-grid scale combustion models for pulverized coal flames, such as flamelets and others.

1. Introduction

Solid fuels are a primary source for power generation. Pulverized coal combustion (PCC) is the key technology for energy conversion, due to the abundance and limited cost of coal. However, burning coal threatens the environment and may intensify global warming. Detailed experiments [1–4] and simulations can provide fundamental insights in the physico-chemical processes involved in PCC, and are essential to pursue innovative and less polluting techniques to burn coal. Large eddy simulation (LES) has been extensively applied for the prediction of PCC in basic (jet-like) setups [5–9] as well as more practical swirl-stabilized coal combustors [10–16]. LES resolves the large turbulent eddies and reverts to modeling of the small scale processes in the direct vicinity of individual particles and particle groups, although the small scales may considerably influence PCC flame ignition and stabilization. Resolved simulation approaches such as resolved laminar flow simulations (RLS) and direct numerical simulations (DNS) allow for detailed investigations of near-particle processes [17]. Recent publications focus on resolved flow simulation of PCC, studying counterflow [18,19] and suspended particle [20] setups, solid fuel clouds in turbulent flow [21–25] and entire burners at the laboratory scale [26,27]. All these studies commonly resolve the gas phase, but use point-particles to describe the solid phase and do therefore not resolve the boundary layers around individual coal particles. PCC simulations with full resolution of the particle boundary layers have primarily been performed assuming quiescent or laminar flow in 1D or 2D configurations [28–32]. A preparatory study for the present work by Vascellari et al. [33] combined Lagrangian point-particle simulations, RLS and flamelet modeling to

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predict the ignition delay time of single coal particles in a Hencken burner. Tufano et al. extended this work by performing RLS of an experimental campaign for single coal particle ignition in N_2- and CO_2-atmospheres [34]. The main RLS findings were recovered by Vascellari et al. [35], using a flamelet/progress variable (FPV) approach to predict the flame structure during coal particle ignition. Part I of the present work identified relevant PCC conditions from the reference LES of a pilot-scale furnace [15] and studied the transient behavior and near-particle scalar profiles of single particles and particle arrays that undergo heating, pyrolysis and volatile combustion by DNS [36]. The main focus of that work was the analysis of various coal combustion regimes that may result from a wide range of relative inter-particle spacings L_x/D_p. The work was confined to low particle Reynolds numbers Re_p and laminar flow conditions, but analysis of the reference LES revealed that high Re_p and locally turbulent flow do occur in industrial PCC furnaces. As a result, we extend the previous work by

- exploring the effects of high particle Reynolds numbers on single particles and closely spaced particle ensembles,
- investigating the limits of conventional flamelet modeling and standard film theory on highly strained envelope flames,
- studying the effect of locally turbulent flow on volatile flame interaction and devolatilization.

2. Modeling

The DNS modeling strategy has already been described in part I [36,34], such that only the main modeling characteristics are repeated here. The conservation equations of momentum, enthalpy, total and species mass are solved for the gas phase in their general formulations, assuming variable density, a single gas phase diffusion coefficient, unity Lewis number, and Prandtl/Schmidt numbers of 0.7. The solid particles are assumed to be homogeneous spheres of constant size. Heat transfer inside the coal particles and heat exchange between the particles and their surroundings are included in the model. Radiative effects within the gas are included by the P1-approximation [37,38], assuming unity gas emissivity ($\epsilon_{gas} = 1$), whereas particle emissivity is neglected after a sensitivity study did not reveal any significant influence over the full range $0 \leqslant \epsilon_p \leq 1.0$. Devolatilization is described by a single kinetic rate, Arrhenius-type expression with rate parameters obtained from FG-DVC [39] and fitted to pyrolysis kinetics measurements specific to the employed coal (Saar hvBb, Table 1).

Mass transfer across the particle surface is computed accounting for the convective contribution of devolatilization and the diffusion of species towards the particle and within the gas phase. A detailed volatile composition including both light gases and larger hydrocarbons to represent tar is used [15] and listed in Table 2.

The POLIMI_TOT_1407 [42,43] scheme for C_1-C_4 species and C_6H_6, reduced to a 52 species and 452 reactions skeletal mechanism [34], is used to describe homogeneous chemistry. Heterogeneous reactions involving the residual char are ignored since the focus of the present study is ignition and volatile burning in convective environments.

3. Computational configuration

The DNS is performed for single coal particles and small ensembles of regularly spaced particles. The aim of reproducing the typical heat-up, devolatilization, ignition and combustion conditions that characterize coal particles inside a furnace is pursued by identifying the relevant conditions from the LES of a semi-industrial coal furnace (IFRF furnace #1) [15]. The data extraction technique is based on the analysis of the gas phase statistics and time histories of coal particles from the reference Euler–Lagrange LES, to set the initial and boundary conditions for the DNS, as has been extensively reported in part I. Here, to select a suitable range of particle Reynolds numbers to be studied, probability density functions (PDFs) and cumulative distribution functions (CDFs) of the devolatilizing particle ensemble inside the burner quarl from the LES were inspected. It was found that more than 90% of the particles are subjected to particle Reynolds numbers of less than 8, with 60% of the particles facing a range $1 \leqslant Re_p \leqslant 8$. The reference LES data also revealed that some particles may face substantially higher Re_p. But according to the CDF these occurrences are rather rare events with, for example, an extremely low probability ($\approx 2{\cdot}10^{-5}$) of particles facing $Re_p \geqslant 100$. For completeness we have tested a DNS case with $Re_p = 100$. The case revealed that, in such highly convective environments, the local strain rate is too high for ignition to occur and the particle is surrounded by areas of extremely high scalar dissipation rate that prevent any chemical reaction in the direct particle vicinity. Hence, we limit the presentation of our results to the range $1 \leqslant Re_p \leqslant 8$. To evaluate the presence of locally laminar or turbulent flow around the particles, the ratio of the sub-grid turbulence intensity u'_{sgs} to the relative velocity U_{rel} in the LES was considered. It was established that 95% of the particles experience ratios u'_{sgs}/U_{rel} smaller than 0.97 and the most likely value of the normalized sub-grid turbulence intensity was 0.25. As a consequence, only laminar flow conditions were considered in part I. However, some particles facing sub-grid turbulence intensities of up to $u'_{sgs}/U_{rel} \approx 15$ were also found in the LES. These regions of high sub-grid turbulence intensity are mainly located in the highly sheared region between the two outer streams with large forward momentum and the inner quarl zone governed by recirculation in IFRF furnace #1 [15]. To reflect such occurrences of turbulence in the direct vicinity of the coal particle surface a study of fully-resolved turbulent flow around groups of coal particles is conducted, cf. Section 4.2. The turbulent inflow conditions for DNS are obtained by generating artificial turbulence based on a von Karman spectrum using inverse Fourier transforms according to the method of Billson et al. [44]. Turbulence generation is controlled by fixing the bounds of the desired turbulence spectrum by the integral length scale L and a total kinetic energy level representative of a velocity fluctuation level u', taken as the sub-grid velocity fluctuation from the LES u'_{sgs}. The range of integral scales that can be covered in the DNS is limited by the domain size and we set L to correspond to half the cross-stream (y-) extent of the DNS domain. Moreover, with the fully Eulerian approach used here, resolving the particles and the boundary layers around them but fixing their position in space, the energy levels of the flow can be strongly decreased by the "screen effect" [45]. Increasing the integral length scale may not affect the energetic structure of the flow any more, once the integral length scale is larger than the particle spacing. This is due to the mutual influence of neighboring particles with fixed positions, which limits the effective integral scale to the particle spacing. This intrinsic limit of the approach was confirmed by Wang et al. [46] who performed fully-resolved simulations of fixed arrays of evaporating droplets and found that the mixture fraction distribution, its conditional scalar dissipation and PDF are all independent of the largest turbulent length scales, which are limited by the inter-droplet spacing. In order to capture more realistic

Table 1
Proximate and ultimate analysis (dry, ash-free) of the employed coal [40].

Proximate Analysis		Ultimate Analysis	
Volatile matter	37.00	C	79.30
Fixed carbon	52.50	H	4.70
Moisture	2.00	O	13.70
Ash	8.30	N	1.30
LHV	32.32MJ/kg [41]	S	1.00

Table 2
Assumed volatile matter composition [mass%].

CO	C_2H_4	CH_4	H_2	N_2	C_6H_6
37.70	37.00	0.50	0.20	2.20	22.40