



# Coal particle volatile combustion and flame interaction. Part I: Characterization of transient and group effects

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## ABSTRACT

The heat-up, devolatilization, ignition and volatile combustion of single coal particles and particle arrays in laminar and turbulent flow are investigated by direct numerical simulation (DNS). The first part of the paper considers the transient evolution and group effects in laminar flows, the second part will report the effects of particle Reynolds number and turbulence. The conditions for DNS are extracted from an accompanying large eddy simulation (LES) of a semi-industrial coal furnace. The DNS fully resolves the particle boundary layers, the flame thickness and the smallest flow scales. Particle heat-up is captured by solving for intra-particle heat transfer, while devolatilization and volatile combustion are described by specific particle boundary conditions and detailed homogeneous chemistry. The transient physico-chemical processes around the particle(s) are characterized for a single particle first, before the interactions of several particles are studied. The analysis of arrays of infinite particle layers shows a strong dependence of the flame interaction on the inter-particle distance  $L_x$ . In particular, different combustion regimes are observed for different  $L_x$  (for a fixed particle Reynolds number  $Re_p$ ), ranging from isolated burning of the particles for large  $L_x$  to group combustion for small  $L_x$ , and spanning a wide range of global equivalence ratios from very lean (large  $L_x$ ) to very rich (small  $L_x$ ). The regime transition affects the surface temperature and devolatilization rate history of the particles. Models for the mixture fraction distributions in the particle wake are provided, based on the analogous problem of droplet evaporation.

## 1. Introduction

Pulverized coal combustion (PCC) is a principal source of power and likely to remain so for decades due to its availability and relatively low cost. However, PCC produces pollutants, which affect ecosystems and contribute to global warming. Cleaner and more efficient technologies to burn coal can be developed through detailed experiments [1–4] and simulations that improve our knowledge of the physico-chemical processes governing PCC. Large eddy simulation (LES) for PCC is becoming increasingly popular [5–9] and is rapidly moving on from early simplified (jet-like) setups towards more realistic, swirl-stabilized coal combustors [10–16]. LES captures the largest turbulent scales, but does not resolve the small scale processes near the particle surface. However, the processes in the direct vicinity of individual particles and particle groups ultimately govern PCC flame ignition and stabilization, and accurate sub-grid closures for LES are required. Resolved simulation approaches such as resolved laminar flow simulations (RLS) and direct numerical simulations (DNS) help to study such near-particle processes in detail [17]. Resolved flow simulation studies of PCC have recently

been published, focusing on counterflow [18,19] and suspended particle [20] configurations, solid fuel clouds in turbulent flow [21–24] and entire turbulent laboratory scale burners [25,26]. These studies resolve the carrier (gas) phase, but rely on a Lagrangian point-particle framework for the solid phase, which leaves all particle boundary layers unresolved. PCC simulations that fully resolve the boundary layers have been performed assuming quiescent or laminar flow in 1D or 2D configurations. Goshayeshi & Sutherland [27] explored the effect of various devolatilization and gas-phase chemistry approaches by performing 1D simulations. McConnell et al. [28] analyzed the effect of furnace temperature and particle diameter on detailed char burnout calculations to investigate the efficacy of devolatilization and char conversion models. Nikrityuk et al. [29] analyzed a single carbon particle subject to oxidation in 2D. Farazi et al. [30] used 2D-RLS to study char combustion of single particles in various oxidizing environments and Sayadi et al. [31] extended the analysis to small particle clusters, exploring the effect of a wide range of parameters on char conversion characteristics. In preparation of the present study, Vascellari et al. [32] performed Lagrangian point particle simulations and RLS along with flamelet

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modeling to predict the ignition delay of single coal particles in a non-premixed Hencken burner. Tufano et al. [33] extended this work by conducting RLS of single coal particle ignition with improved pyrolysis boundary conditions and for non-unity Lewis numbers, later followed by detailed RLS of a series of particle ignition experiments in various gas atmospheres [34]. The RLS results showed a limited influence of detailed transport, but a strong effect of the heating rate history and gas phase chemistry on ignition delay. These results were recovered by Vascellari et al. [35], who used a flamelet/progress variable (FPV) approach to predict the flame structure during coal particle ignition. The present work applies DNS to examine particle heating, devolatilization, fuel-oxidizer mixing, ignition and volatile combustion in the immediate proximity of pulverized coal particles. Extending our previous study [34], here we

- obtain characteristic particle conditions from a reference LES of a semi-industrial coal furnace [15],
- explore transient effects at (mildly) larger particle Reynolds number,
- study particle arrays and characterize coal combustion regimes.

The DNS covers the volume of a single cell of the reference LES, fully resolving mixing, scalar dissipation and the transient evolution of the reacting scalar fields at the particle surface, and thereby provides detailed LES sub-grid information. For decreasing inter-particle distance, volatile flame interactions are observed, which are related to existing regime classifications [36].

## 2. Modeling

The gas phase conservation equations for momentum, enthalpy, total and species mass in their variable density formulations are solved. Differential diffusion was found to have a negligible impact [33], such that a single gas diffusion coefficient ( $D_i = D$ ) equal to the thermal diffusivity ( $Le = 1$ ) and Prandtl/Schmidt numbers of 0.7 are assumed. The particles are treated as homogeneous spherical solids of constant size. Their interior heat transfer is described by the following equation,

$$\rho_c c_{p,c} \frac{\partial T}{\partial t} + \nabla \cdot (-k_c \nabla T) = \frac{\dot{m}_v}{V_c} \Delta h_v, \quad (1)$$

where  $\rho_c$ ,  $c_{p,c}$ ,  $k_c$ ,  $V_c$  are the density, heat capacity, thermal conductivity and volume of the particle,  $\dot{m}_v$  is the volatile mass flow rate and  $\Delta h_v$  is the heat of devolatilization, with  $c_{p,c} = 1200 \text{ J}/(\text{kgK})$ ,  $k_c = 0.3 \text{ W}/(\text{mK})$  and  $\Delta h_v = 0.267 \text{ MJ}/\text{kg}$  [34]. At the particle surface, the following boundary condition describes the heat exchange between gas and solid phase

$$k_c \frac{\partial T}{\partial r} \Big|_{\text{coal}} = k_g \frac{\partial T}{\partial r} \Big|_{\text{gas}} + Q_{r,p}, \quad \text{with} \quad Q_{r,p} = -\frac{\epsilon_p}{2(2-\epsilon_p)} (4\sigma T_p^4 - G_p), \quad (2)$$

where  $Q_{r,p}$  is the surface radiative heat flux,  $\epsilon_p$  the particle emissivity,  $\sigma$  the Stefan-Boltzmann constant and  $G$  the incident radiation calculated by the P1-approximation [37,38]. Coal particle emissivity is commonly assumed to be near unity during devolatilization and to reduce to  $\approx 0.5$  [39,15] and lower [40] during char conversion. Sensitivity studies within the full range  $0 \leq \epsilon_p \leq 1.0$  did not reveal any significant influence for the particle configurations considered here. Thus, the term  $Q_{r,p}$  in Eq. (2) is omitted from the present DNS, albeit a stronger impact could be expected for cases with heterogeneous chemistry. However, as gas phase radiation had a (mild) cooling effect on our previous results [34], it is included here, assuming unity gas emissivity ( $\epsilon_{\text{gas}} = 1$ ). Devolatilization is described by

$$\dot{m}_v = A_v e^{-\frac{E_v}{R_u T_p}} (\dot{m}_v^* - \dot{m}_v), \quad (3)$$

with the universal gas constant  $R_u$ , the final and instantaneous volatile

**Table 1**

Proximate and ultimate analysis (dry, ash-free) of the employed coal [43].

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	32.32 MJ/kg [44]	S	1.00

**Table 2**

Assumed volatile matter composition [mass%].

CO	C <sub>2</sub> H <sub>4</sub>	CH <sub>4</sub>	H <sub>2</sub>	N <sub>2</sub>	C <sub>6</sub> H <sub>6</sub>
37.70	37.00	0.50	0.20	2.20	22.40

yields  $\dot{m}_v^*$  and  $\dot{m}_v$  and the volume-averaged particle temperature  $\bar{T}_p$ . The pre-exponential factor  $A_v$  and activation energy  $E_v$  have been calculated by FG-DVC [41] and fitted to pyrolysis kinetics measurements specific to the employed coal (Saar hvBb, Table 1), resulting in  $A_v = 20,820 \text{ s}^{-1}$  and  $E_v = 46.96 \text{ kJ}/\text{mol}$  [42].

The volatile yield is calculated based on  $\rho_c = 1000 \text{ kg}/\text{m}^3$  and the coal's proximate analysis (Table 1), and Q-factor correction lead to a final yield of 59.2%. Mass transfer across the particle surface is computed as

$$\dot{m}_i = Y_i \dot{m}_v - \rho_g A_c D_g \frac{\partial Y_i}{\partial n}, \quad (4)$$

with the total mass flow rate  $\dot{m}_i$  of species  $i$ , gas density  $\rho_g$  and diffusivity  $D_g$  at the particle surface, and the particle surface area  $A_c$ . A detailed volatile composition including both light gases and larger hydrocarbons to represent tar is used [15] and listed in Tab. 2.

Gas phase chemistry is based on the detailed POLIMI\_TOT\_1407 [45,46] scheme for C<sub>1</sub>-C<sub>4</sub> species and C<sub>6</sub>H<sub>6</sub>, which has been reduced to a skeletal mechanism with 52 species and 452 reactions [34]. Heterogeneous char reactions are ignored, assuming consecutive and independent stages of coal combustion, with the present focus on ignition and volatile burning. Additional information on the models and equations used in the DNS are documented in our previous paper [34].

## 3. Computational configuration

The DNS configuration reproduces the typical conditions that coal particles experience inside a furnace after injection, where they undergo heat-up, devolatilization, ignition and combustion. The volatile combustion regime ranges from single envelope flames around individual particles to group flames around sets of particles or particle clouds. The present DNS considers single particles and sets of particles arranged in regularly spaced arrays.

### 3.1. LES data extraction for DNS

To identify relevant conditions for our DNS setup, we evaluate gas phase statistics and time histories of coal particles from the LES of a semi-industrial coal furnace (IFRF furnace #1) by Rieth et al. [15]. Figure 1 (background) shows a snapshot of gas temperature inside the furnace from LES, with a zoom into the upstream near-quarl region, where axial velocities and gas-particle relative velocities are shown. On the right of Fig. 1 the typical quantities extracted from LES and used to set up the DNS are shown schematically. For selected regions of interest, the LES provides information on the typical gas composition around the particles, as well as quantities that characterize gas-particle

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