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# Flamelet LES of a semi-industrial pulverized coal furnace

M. Rieth[a,*], F. Proch[a], M. Rabaçal[b], B.M. Franchetti[d], F. Cavallo Marincola[d], A.M. Kempf[a,c]

[a] Institute for Combustion and Gasdynamics (IVG), Chair for Fluid Dynamics, University of Duisburg-Essen, Duisburg 47048, Germany
[b] IDMEC, Mechanical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal
[c] Center for Computational Sciences and Simulation (CCSS), University of Duisburg-Essen, Duisburg 47048, Germany
[d] Thermofluids Division, Department of Mechanical Engineering, Imperial College London, London SW7 2AZ, UK

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ABSTRACT

The goal of this work is to introduce the flamelet model into large eddy simulation (LES) of realistic coal furnaces. A flamelet table based on two mixture fractions (for volatile and char off-gases) and enthalpy is generated and used in a massively parallel LES of the semi-industrial IFRF coal furnace (Weber et al. 1992 [1, 2]) for which comprehensive experimental data is available enabling the validation of the flamelet model under realistic conditions. Comparison between experiment and simulation is shown by means of averaged quantities of velocities, species concentrations and temperature. Overall good agreement between experiment and simulation could be obtained, giving evidence for the suitability of the flamelet model. The results of the LES are further analyzed, focussing on instantaneous particle and gas phase data to gain additional insight into the coal conversion process inside the furnace.



## 1. Introduction

Pulverized coal combustion (PCC) is currently among the major sources of energy supply and is expected to play an important role in the future due to coal being the most abundant fossil fuel. However, its combustion releases large amounts of carbon dioxide due to the high carbon content of the coal. Efforts being made to reduce the emissions of PCC, e.g. carbon capture and storage with oxy-coal combustion or co-firing coal with biomass, go along with penalties in power plant efficiency. This requires the combustion to be as efficient as possible and a highly optimized combustor design, supported by a comprehensive set of experimental and numerical data. However, comprehensive experimental studies of full scale combustors are infeasible. Even laboratory scale experiments suffer from some gas flame diagnostics being infeasible in PCC, e.g. due to scattering of laser light at coal particles and soot. Simulations promise to provide additional data which cannot be obtained from experiments, giving further insight into the physics of PCC. Large eddy simulation (LES), a technique successfully applied to gaseous flames, is a very promising approach for the simulation of PCC as the effect of unclosed terms is small compared to Reynolds-averaged Navier–Stokes simulations (RANS). However, further research effort is still needed, particularly on the description of the gas phase, on which this work concentrates by introducing tabulated flamelet chemistry into realistic LES of PCC.

Large eddy simulation of PCC has emerged around a decade ago with a study of a hypothetical solid fuel flame by Kurose and Makino [3]. This study employed a conserved scalar approach with an idealized single-step reaction. Sub-grid turbulence-chemistry interaction was modeled by a $\beta$-pdf for the species mass fractions, with the variance calculated with an algebraic model. Successive LES studies of coal flames have been mainly employing the eddy break-up model (EBU) or the eddy dissipation concept (EDC) to describe the gas phase [4–12]. These studies considered two or three reactions, of which one describes the conversion of volatiles to CO and $H_2$ or $H_2O$, and another the conversion of CO to $CO_2$. A third reaction is used to describe the conversion of a pilot gas such as $CH_4$ [8] or an intermediate species such as $H_2$ [7]. The volatile gas is treated as a postulate substance in these studies, since the exact composition of the volatile gases is unknown, and since a postulate substance can easily be used in the EBU/EDC framework.

Different to the commonly employed EBU or EDC description are the studies by Yamamoto et al. [13], Pedel et al. [14,15] and Muto et al. [16], where a relaxation model towards equilibrium, a mixture fraction based equilibrium approach and the scale similarity filtered reaction rate model is used, respectively. Yamamoto et al. argued that in their particular ignition experiment pyrolysis is more important than gaseous combustion to predict the flame.

Only recently, Watanabe & Yamamoto [17] introduced the flamelet model with volatile and char off-gases for the simulation of PCC. A two-dimensional jet was studied with direct numerical

* Corresponding author.
*E-mail address:* martin.rieth@uni-due.de (M. Rieth).

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simulation and the flamelet model was compared to finite rate chemistry. Despite having been only tested on a very simplified case, the flamelet model promises significant improvement of the description of the gas phase when applied to the LES of real PCC configurations. Previously, Williams et al. [18] reported the use of the flamelet model for volatile combustion and recently, Vascellari et al. [19] and Xu et al. [20] investigated flamelet approaches for resolved single coal particle simulations. They obtained very good agreement between finite rate chemistry and flamelet approaches.

The flamelet model, mainly developed by Peters [21], has been applied in the LES of gaseous flames with great success, as illustrated by the reviews by Pitsch [22] and Janicka & Sadiki [23]. The flamelet model assumes the chemical time-scales to be small compared to the turbulent time-scales, such that reactions occur only in thin layers embedded in the turbulent flow field [21]. These thin layers maintain their structure in the turbulent flow field and can be described one-dimensionally as a function of mixture fraction. The interaction between the turbulent flow field and the flamelet structure is described by the scalar dissipation rate, which acts as a diffusion coefficient in the flamelet equations.

This study applies the flamelet model to the LES of PCC in a semi-industrial coal furnace experiment by Weber et al. [1,2], which is a test case that features a good compromise between realistic PCC conditions and comprehensive experimental measurements to validate the approach. The furnace has only recently been studied by means of LES by Olenik et al. [11], who employed the EBU model to describe the gas phase reactions. Flamelet solutions for the reaction of the three streams of oxidizer, pyrolysis gases and char off-gases are tabulated and additionally parameterized by enthalpy and the variance of the sum of the mixture fractions. To our knowledge, this is the first LES of PCC employing the flamelet model.

The remainder of this work is structured as follows. A description of the solid phase, coal and radiation modeling is given in the next sections, which is followed by the description of the combustion modeling approach employing the flamelet model. This is followed by the description of the numerical method and an outline of the experiment. Finally, results from the computations conducted will be presented and the work concluded in the summary.

## 2. Coal particle and radiation modeling

Coal particles are treated in a Lagrangian manner following the laws of motion for dispersed flow and the fundamental processes of heat exchange with their surroundings. However, specific models are required to describe the processes coal undergoes as it is being converted in a combustion system. The conversion of coal is mainly governed by the two steps of devolatilization and char combustion, where first matter bound in the coal volatilizes and combusts in the gas phase. In the second step, the remaining porous char structure further combusts with oxygen diffusing into the pores and oxidizing the carbon left in the coal. Both processes are of fundamental importance for the gas phase combustion model since they provide the source terms in the equations governing the gaseous phase.

### 2.1. Particle motion

The coal particles are treated in a Lagrangian manner, their motion being described by the balance of the particle's inertial forces with the forces acting on it. Similar to previous LES studies of PCC or particle-laden flows [9,24], simplifications are made regarding the forces acting on the particles. This leaves only drag, gravity and buoyancy forces and a force representing the influence of the unresolved flow scales acting on the particle in Eq. (1):

$$d\mathbf{u}_p = \frac{\tilde{\mathbf{u}} - \mathbf{u}_p}{\tau_p} dt + \left(1 - \frac{\bar{\rho}}{\rho_p}\right)\mathbf{g}dt + \sqrt{C_0 \frac{k_{sgs}}{\tau_t}} d\mathbf{W} \tag{1}$$

In this equation, $\mathbf{u}_p$ is the particle velocity vector, $\tilde{\mathbf{u}}$ the filtered Eulerian phase velocity vector at the particle location, $\tau_p$ the particle relaxation time, $\bar{\rho}$ the filtered Eulerian phase density at the particle location, $\rho_p$ the density of the particle, $\mathbf{g}$ the gravitational acceleration, $C_0$ a model constant, $k_{sgs}$ the sub-grid kinetic energy of the Eulerian flow field, $\tau_t$ the particle-turbulence interaction time-scale and $\mathbf{W}$ a Wiener vector process. The particle relaxation time $\tau_p$ represents the time-scale on which the particle is able to adjust to the flow field, as modeled by Eq. (2) depending on the particle Reynolds number $\mathrm{Re}_p = \bar{\rho}|\tilde{\mathbf{u}} - \mathbf{u}_p|D_p/\mu$, with $\mu$ being the dynamic viscosity of the gas phase and $D_p$ being the particle diameter.

The calculation of $\tau_p$ is based on the analytical solution for Stokes flow, $\tau_{p,\,\mathrm{St}}$ (derived for $\mathrm{Re}_p$ approaching zero). The Schiller–Naumann correlation [25,26] is used for the drag coefficient, incorporated in the calculation of $\tau_p$. The correlation is valid up to $\mathrm{Re}_p = 1000$, which is sufficient in this case.

$$\begin{aligned} \tau_p &= \frac{\tau_{p,\mathrm{St}}}{f_1} \\ \tau_{p,St} &= \frac{\rho_p D_p^2}{18\mu} \\ f_1 &= 1 + 0.15\mathrm{Re}_p^{0.687}, \quad \mathrm{Re}_p \leq 1000 \end{aligned} \tag{2}$$

The last term in Eq. (1) represents the force due to the interaction of sub-grid motion and particle, modeled as a Wiener process [27]. The sub-grid kinetic energy is estimated following Bini & Jones [27], Eq. (3), with the turbulent kinematic viscosity $\nu_{\mathrm{sgs}}$, the filtered strain rate tensor $\tilde{S}_{i,j}$, the Smagorinsky model constant $C_S$ and the cell width $\Delta$.

$$k_{\mathrm{sgs}} = (2\Delta\nu_{\mathrm{sgs}}\tilde{S}_{ij}\tilde{S}_{ij})^{2/3} = \left(\frac{\nu_{\mathrm{sgs}}}{C_S^{4/3}\Delta}\right)^2 \tag{3}$$

The particle-turbulence interaction time-scale, used in Eq. (1), is calculated by Eq. (4) [27] with $\alpha = 0.8$ [28]. The modeling constant $C_0$ is set to unity [27].

$$\tau_t = \frac{\tau_p^{2\alpha}}{(\Delta/\sqrt{k_{\mathrm{sgs}}})^{2\alpha-1}} \tag{4}$$

The particle position $\mathbf{x_p}$ evolves according to $d\mathbf{x_p} = \mathbf{u}_p dt$.

### 2.2. Coal composition and volatile gas properties

As the coal particle is heated up, matter bound in the coal breaks down and is released as volatile gas [29]. The process of devolatilization is complex and involves processes of cracking of labile bonds inside the coal structure, formation and re-attachment of metaplast and vaporization of light gases and tars. The products of devolatilization are light gases, tars and the char remaining in the coal particle. The exact composition of the gases released during devolatilization is unknown, but can be modeled under mass balance considerations using the data from proximate and ultimate analysis and assuming that the coal is pure carbon and ash after devolatilization. The ultimate and proximate analysis of the Saar hvBb coal fired in the experiment is given in Table 1 [1].

In the computation, coal is solely composed of volatile matter (VM), fixed carbon (FC) and ash. The low moisture content of 2% and sulphur content of 1% was neglected. The yield of volatile gases is usually higher than the amount of volatiles obtained by proximate analysis under rapid heating conditions, reflected in a higher initial amount of volatile matter of the particles in the computation, $m_{\mathrm{VM},0} = m_{\mathrm{VM},0}^{\mathrm{prox}} \cdot Q$ [29]. Devolatilization measurements