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Highly resolved flamelet LES of a semi-industrial scale coal furnace

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Abstract

A highly resolved large eddy simulation (LES) of the semi-industrial IFRF coal furnace [1,2] employing the steady flamelet model is presented. The flamelet table is based on mixture fractions of volatile and char off-gases as well as on enthalpy and scalar dissipation rate. Turbulence–chemistry interaction is treated with an assumed pdf approach, with the variance obtained from a transport equation. Radiation is computed by the discrete ordinates method and the grey weighted sum of grey gases model. The simulation is conducted with the massively parallel "PsiPhi" code on up to 1.7 billion cells and with 40 million particles. Results are processed and compared against the comprehensive set of experiments to (i) validate the new flamelet model and the simulation method and to (ii) gain further insight into the combustion process that is not available from the experiment. The simulation results show that the flamelet LES approach can successfully describe the flow field and combustion inside the furnace; major species and velocities are found in good agreement with the experiment.

The results are further analyzed with a focus on the processes of particle heating, devolatilization, char combustion and flame stabilization in a highly turbulent environment. Additionally, the relative importance of scalar dissipation rate is highlighted, showing a large separation of mixing scales between volatile and char off-gas combustion due to the long residence time and generally much lower scalar dissipation rates than typical for lab-scale experiments.

Keywords: Turbulent combustion; Large scale; Flamelet model; Pulverized coal combustion; Large eddy simulation

1. Introduction

World's energy demand relies and will rely on burning fuels in the foreseeable future, with coal remaining attractive due to its abundance. The move toward more efficient and less polluting plants

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drives research efforts into fields like oxy-coal or biomass combustion [3].

Experiments are invaluable for the design and validation of efficient combustion systems, but are increasingly supported by simulations. One of the most promising tools for accurately predicting pulverized coal combustion (PCC) is large eddy simulation (LES). It offers superior predictions of flow and scalar fields, accurately considering gas phase combustion and turbulent transport. This has become the weakest link in (RANS) coal simulations, since advanced coal sub-models have become available. The first application of LES to coal combustion has been reported by Kurose and Makino [4] followed by several studies on lab-scale jet flames [5–11], lab- and pilot-scale furnaces and test facilities ($\leq$1.0 MW$_{th}$) [12–17] and semi-industrial furnaces [18] like the 2.5 MW$_{th}$ swirled IFRF experiment [1,2] studied in this work. Although we find that LES is the most promising tool for predictive PCC simulations, there are several recent Reynolds-averaged/transported probability density function (RANS/PDF) based studies that were capable of reproducing PCC experiments very well [19–23], but usually in simulations with non-swirled flow fields.

Most of the reported LES studies rely on early turbulent combustion models (eddy break-up and eddy dissipation), but there is a need to advance the gas combustion models in PCC LES to the state-of-the-art as in pure gas flames to capture turbulence-chemistry interaction phenomena, which are important for flame stabilization and pollutant formation. The flamelet model [24] is particularly promising for PCC applications due to its numerical efficiency and wide success in the field of turbulent combustion LES [25,26]. After the first application of the flamelet model to volatile combustion by Williams et al. [27], Vascellari et al. [28] and Xu et al. [29] investigated flamelet methods for resolved single coal particle simulations. Recently, Watanabe and Yamamoto [30] presented a flamelet model that can be applied to turbulent PCC simulations taking volatile and char combustion into account. Their testing in a two-dimensional simulation of a coal jet showed a good agreement compared to data obtained with finite rate chemistry.

This work applies the flamelet model to the LES of the semi-industrial IFRF coal furnace studied experimentally by Weber et al. [1,2], introduces efficient subgrid modeling and validates the model under realistic conditions and against a comprehensive set of measurements.

2. Gas phase and radiation modeling

The flamelet model is based on two mixture fractions, similar to previous work on split injection in Diesel engines [31,32], RANS/PDF of PCC [21] and the recently introduced flamelet model for PCC [30].

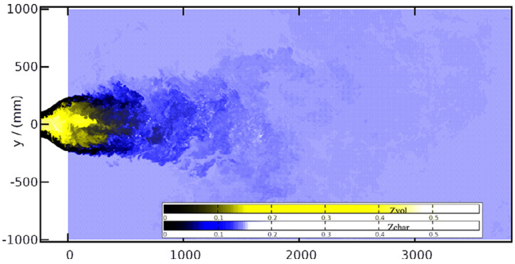

Fig. 1. Mixture fraction for volatile (yellow) and char off-gases (blue) on the 2.5 mm grid showing approximately half of the domain in axial direction (1600 × 816 of a total of 2624 × 816 cells). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The two mixture fractions are defined by the amount a respective mass flow contributes to the mixture in a three-feed system expressed in terms of mass flows of oxidizer ($\dot{m}_{\mathrm{ox}}$), volatiles ($\dot{m}_{\mathrm{vol}}$) and char off-gas ($\dot{m}_{\mathrm{char}}$: pure carbon released, $\dot{m}^*_{\mathrm{char}}$: CO/N$_2$ released from char combustion) in steady state:

$$\begin{aligned} Z_{\mathrm{vol}} &= \dot{m}_{\mathrm{vol}}/(\dot{m}_{\mathrm{vol}} + \dot{m}_{\mathrm{char}} + \dot{m}_{\mathrm{ox}}) \\ Z_{\mathrm{char}} &= \dot{m}^*_{\mathrm{char}}/(\dot{m}_{\mathrm{vol}} + \dot{m}_{\mathrm{char}} + \dot{m}_{\mathrm{ox}}) \end{aligned} \tag{1}$$

Both mixture fractions evolve by Favre-filtered transport equations containing source terms for the mass leaving the coal particles, Eq. (2), with $\alpha =$ vol, char.

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{Z}_\alpha + \frac{\partial}{\partial x_j}\bar{\rho}\tilde{u}_j\tilde{Z}_\alpha = \frac{\partial}{\partial x_j}\left(\bar{\rho}D_{\mathrm{eff}}\frac{\partial \tilde{Z}_\alpha}{\partial x_j}\right) + \bar{\rho}\dot{S}_{\tilde{Z}_\alpha} \tag{2}$$

Subgrid fluxes are closed with the Smagorinsky model [33] ($C_S = 0.173$), assuming a turbulent and laminar Schmidt number of 0.7. The fact that char combustion consumes oxygen is considered in the definition of the mixture fractions, Eq. (1), and source terms, Eqs. (3), as further discussed in Section 3.

Instead of solving two-dimensional flamelet equations to provide the flamelet table, the present approach relies on one-dimensional steady non-premixed counter-flow flames solved in physical space. This is justified if the fuel streams interact only weakly in flamelet space [34], which can be assumed to be the case here, where volatile and char combustion are mainly consecutive processes, as illustrated in Fig. 1 and discussed in Section 5.

We use scalar dissipation rate as a steady flamelet table parameter, as opposed to a progress variable [30]. This is motivated by the fact that the unstable branch of the S-curve does not play a role

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