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Collaboration of simulations and experiments for development and uncertainty quantification of a reduced char combustion model

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Abstract

Computational fluid dynamics (CFD) plays a decisive role in the development of cost-effective oxy-coal combustion technologies to improve process efficiency and to decrease pollutant emissions. The implementation of detailed physical models describing coal devolatilization, char oxidation, gas-phase reactions and pollutant formation ensures accurate CFD simulations of coal combustion but is still challenging for large-scale combustors due to the significant computational efforts required, especially in the framework of Large Eddy Simulation (LES). The development of reduced physics model with quantified model-form uncertainty is needed to overcome the challenges of performing LES of industrial coal-fired boilers. Reduced models must reproduce the main features of the detailed models and the capability of bridging scales and being predictive. A tight coupling of simulation and experiments is necessary to ensure predictivity with uncertainty quantification for a reduced model. This work proposes a combined experimental/numerical methodology that uses global sensitivity analysis to rank fundamental input parameters of a reduced char oxidation and gasification model describing reactions between char carbon and O_2, CO_2 and H_2O reagents in both air and oxy-coal conditions. A careful evaluation of uncertainty in the data, in the model form and in the model parameters is performed. The reference dataset, consisting of the experiments carried out in a laminar entrained flow reactor operated by Sandia National Laboratories, has been exploited. The methodology is based on the use of so-called instrument models to include all the physical sub-models and the sources of uncertainty considered in the experiments and in the numerical simulations and affecting the main quantities of interest, e.g. reaction rates. The quantified uncertainty in the instrument models provides the range of uncertainty for the reduced char combustion model. Then, the reduced model with quantified uncertainty will be validated against the experimental data. The reduced model capability to address heterogeneous reaction at the particle surface, mass transport of species in particle boundary layer, pore diffusion and internal surface area changes will be assessed.

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1. Introduction

In the recent years oxy–fuel combustion has appeared to be one of the most promising technologies in terms of optimization of produced energy, investment and operational costs and carbon footprint [1]. The main feature of oxy–fuel combustion is the elimination of air from the system and its replacement with a mixture of recycled flue gases, mostly CO_2 and H_2O, and O_2. As a consequence, the flue gas contains high amount of CO_2, which significantly increases its removal efficiency. On the other hand, the combustion process can be altered due to different physical and chemical properties of diluents such as CO_2 and H_2O with respect to N_2 [2]. Flame and particle temperatures, heat transfer, emissions and burnout can change [3,4] because of different gas properties and/or combustion mechanisms. It was observed that char conversion profiles for air and oxy–fuel experiments were similar in conditions where combustion was primarily controlled by chemical kinetics, while at higher temperatures a faster conversion was found in air [5,6]. Experiments conducted under oxy-fuel conditions in reactors such as drop-tube furnaces or entrained flow reactors, show that particle temperatures and reaction rates are lower in oxy–fuel conditions than in O_2/N_2 mixtures. These results can be explained by the diffusion limitation of oxygen through the particle boundary layer in CO_2-enriched environments [5-8]. Nevertheless, ultimate conclusions on the effect of the gaseous atmospheres on char burnout cannot be drawn, despite the number of studies of oxy-coal combustion. Indeed, it was also observed that changes in coal burnout, when switching from air to oxy-fuel combustion, can be coal dependent, proving that some coals can be more suitable for oxy-fuel combustion [9,10].
Predictive CFD simulations are valuable tools in evaluating and deploying oxy-fuel technologies, either for retrofit or for new construction. However, accurate predictive simulations require physically realistic sub-models with low computational requirements. In the case of char combustion, comprehensive char oxidation and gasification models have been developed and describe multiple reaction and diffusion processes [11-14]. Since comprehensive models can require significant computational efforts, especially for Large Eddy Simulation (LES) of real combustion systems, simplified models have been proposed to improve computational capability. A tight coupling of simulation and experiments is necessary to ensure predictivity with Uncertainty Quantification (UQ) for a reduced model. The modeling of experiments involves the use of a physics model and of a so-called instrument model, representing the prior engineering knowledge about the derivation of the quantities of interest, e.g. reaction rates, from raw measurements. Moreover, an instrument model includes all the physical sub-models and the sources of uncertainty affecting the main quantities of interest.
In this work a simplified char combustion model and an instrument model of a specific experimental dataset was subjected to global sensitivity analysis in an effort to rank fundamental input parameters in order of importance. The analysis provided useful information about both instrument model and physics model that will aid the future UQ procedure, leading to models improvements and to consistency between experiments and modeling.

Nomenclature

m_p	particle mass [kg]
S_{EXT}^R	external surface area available for reactions [m^2]
r_H	char reaction rate [$kg/m^2/s$]
d_p	particle diameter [m]
x_H	char mass fraction [-]
θ	particle porosity [-]
ρ_p	particle density [kg/m^3]
ϕ_l	stoichiometric coefficient for oxidizer *l* [kmol char/kmol oxid.]
M_H	char molecular weight [kg/kmol]
$c_{O,l}$	molar concentration of oxidizer *l* at the particle surface [$kmol/m^3$]
m_H	char mass [kg]
$\rho_{H,b}$	char bulk density [kg/m^3]
m_A	ash mass [kg]