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Full Length Article

Application of Bound-to-Bound Data Collaboration approach for development and uncertainty quantification of a reduced char combustion model

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ABSTRACT

The development of efficient industrial oxy-coal boilers can be significantly aided by Computational Fluid Dynamics (CFD) tools, as far as fidelity in modeling coal combustion is also complemented by feasible computational costs. Reduced and predictive models are the most suitable for this application scale. Reduced models feature predictivity when they are validated against a broad range of experiments and targeted by Uncertainty Quantification (UQ) procedures. This work proposes a numerical procedure that uses Bound-to-Bound Data Collaboration (B2B-DC) to derive a reduced char combustion model describing transport phenomena and reactions between char carbon and O_2, CO_2 and H_2O, in both conventional and oxy-conditions. The approach determines the consistency between a numerical model and an experimental dataset. The latter is made up of the experiments carried out in an optically accessible laminar entrained flow reactor, operated by Sandia National Laboratories. The procedure follows five steps towards predictive modeling capability, namely: quantification of the uncertainty in the experiments, via instrument verification and modeling; development of a physics model and continuous improvement of its fidelity, via model-form uncertainty; identification of the uncertain and most sensitive parameters and of their prior bounds; sampling of the initial uncertain parameter space and training of a surrogate model; validation of the physics model via inference from the data. The last step, also known as inverse problem, is performed by applying the Bound-to-Bound Data Collaboration approach. A char combustion model is found consistent with the experimental data and its validity stands for conventional and oxy-combustion conditions. It accounts for heterogeneous reactions at the particle surface, mass transport of species in the particle boundary layer, pore diffusion and surface area changes. The consistent reduced model overcomes the differences in mass transport and kinetics observed in the experimental campaign. A reduction of the initial degree of uncertainty in both model and experiments is achieved.

1. Introduction

Carbon Capture and Sequestration (CCS) technologies have become increasingly remarkable to meet regulatory targets for reduced emissions of greenhouse gases. Among the several practices, oxy-fuel combustion is likely the most promising one due to the minimization of energy penalty associated with the investment and operational costs [1]. A lot of current research on oxy-fuel combustion has been focused on firing coal power plants. The main feature of oxy-coal combustion is well known: the replacement of air in the combustion system with a mixture of O_2 and recycled flue gases, mostly CO_2 and H_2O. A high amount of CO_2 at the outlet increases its removal efficiency, but modifies the combustion process [2,3] and, as a result, changes are seen in flame and particle temperatures, heat transfer, gas diffusion, char burnout and emissions [4–8]. Ultimately, conclusions on the effects promoted by oxy-fuel conditions cannot be asserted, despite the extent of studies of oxy-coal combustion. These effects, particularly regarding the enhancement of char burnout, showed dependence on coal rank [9–11], oxygen concentrations [12,13], carbon dioxide concentrations [14], steam concentrations [15], residence times and temperatures

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Nomenclature

Roman Symbols

A_l	pre-exponential factor of the l-th reaction [g/cm^2/s/atm]
c	mixture molar concentration [kmol/m^3]
$c^g_{O,l}$	molar concentration of l-th oxidizer at the gas phase [kmol/m^3]
c_p	particle specific heat [J/mol/K]
$c_{O,l}$	molar concentration of l-th oxidizer at the particle surface [kmol/m^3]
d_p	particle diameter [m]
E_l	activation energy of the l-th reaction [J/mol]
f_p	fraction of heat from the external surface reactions absorbed by the particle [–]
h^*	heat transfer coefficient [J/s/m^2/K]
k_c	mass transfer coefficient [m/s]
k_l	rate coefficient [m/s]
M	mixture molecular weight [kg/kmol]
m_A	ash mass [kg]
M_H	char molecular weight [kg/kmol]
m_H	char mass [kg]
m_p	particle mass [kg]
r''_l	char l-th reaction rate per unit area [kg/m^2/s]
r''_V	devolatilization rate [kg/m^2/s]
$r''_{H,EXT}$	char external reaction rate per unit area [kg/m^2/s]
$r''_{H,INT}$	char internal reaction rate per unit area [kg/m^2/s]
S^R_{EXT}	particle external reactive surface area [m^2]
S_g	particle internal surface area per unit mass [m^2/kg]
S_{EXT}	particle external surface area [m^2]
T_g	gas temperature [K]
T_p	particle temperature [K]
T_w	wall temperature [K]
V_p	particle volume [m^3]
x_H	char mass fraction [–]

Greek Symbols

β	distributed activation energy coefficient of the oxidation reaction [J/mol]
η	effectiveness factor [–]
ϕ_l	stoichiometric coefficient for the l-th reaction [kmol char/kmol oxid]
ψ	random pore model structural parameter [–]
ρ_p	particle density []
$\rho_{A,mat}$	ash material density []
$\rho_{H,mat}$	char material density []
σ	Stefan-Boltzmann constant [J/s/m^2/K^4]
τ	tortuosity of particle pores [–]
θ	particle porosity [–]
ε	particle emissivity [–]

Miscellaneous

$\Delta h_{RXN,l}$	heat of the l-th reaction [kJ/kg]

[16–18].

CFD codes are valuable tools for the study and optimization of oxy-coal combustion in lab, pilot and industrial scale plants. Predictive simulations demand physically accurate sub-models with low computational efforts. In the case of char combustion, comprehensive models have been proposed, which consider either bulk partial pressure of main reacting species or their surface pressures and the effects of evolving char properties [19–24]. While these models describe the char combustion process in a fairly precise way, they might require significant computational costs, especially for Large Eddy Simulation (LES) of industrial coal-fired systems. Reduced-order models have been proposed to improve computational capability and to lose the minimum amount of accuracy. Uncertainty Quantification (UQ) is required for a reduced-order model. UQ's main goal is analyzing the propagation of model uncertainties to model predictions, therefore UQ has somehow become analogous to predictive modeling. A model is intended to be predictive if its outcomes are accompanied by rigorously determined uncertainty bounds: a model is more predictive if it provides more narrowly bounded interval estimations. This paper presents a procedure for the development of the simplest char combustion model that, once validated against an experimental database, will ensure predictivity for the specific conditions explored by the experiments. The procedure starts with the identification of a body of evidence, covering the broadest range of physics and spanning relevant time and length scales,

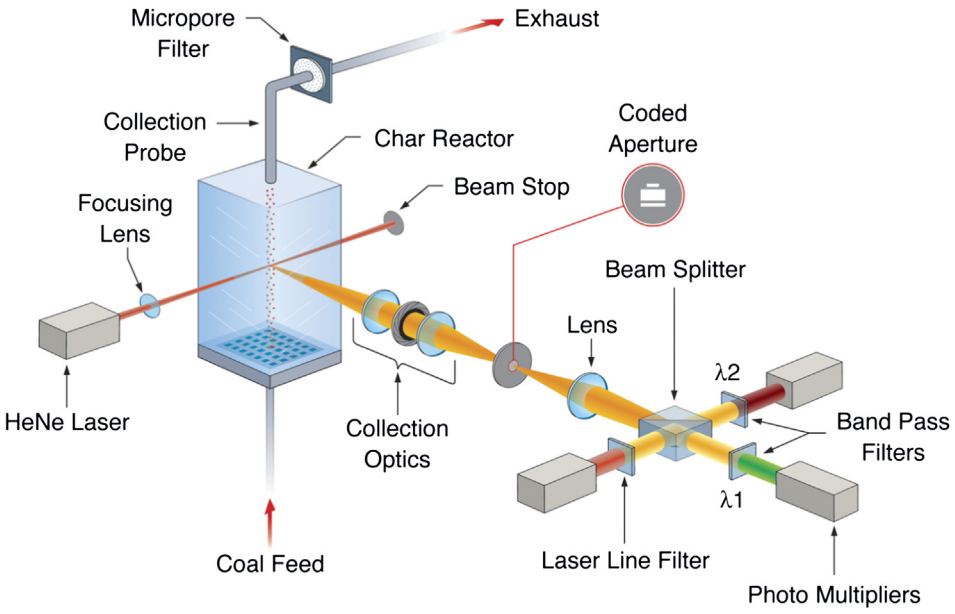

Fig. 1. Optically accessible laminar entrained flow reactor. Particles fed into the center of a flat-flame Hencken burner react as they travel upwards in a quartz chimney. A laser scatters off individual particles when they are in the focus plane of the optics. The particle temperature is measured by use of two-color pyrometry, performed at 550 and 700 nm. The particle size is determined by a coded aperture approach [22].