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Simulation of an Oxyfuel Pilot-Scale Pulverized Coal Flame to Quantify the Effect of Boudouard-Reaction

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Oxyfuel combustion in a pilot-scale coal flame (~40kW$_{th}$) has been investigated using Computational Fluid Dynamics (CFD) to quantify the effect of the Boudouard reaction on the combustion process. Oxyfuel combustion is a technically feasible option for use of fossil fuel without releasing CO_2 into the atmosphere (Carbon Capture and Storage; CCS). It is characterized by replacing air as oxidizer with pure O_2, which is diluted with recycled flue gas to achieve technically manageable flame temperatures. This produces flue gas mainly consisting of CO_2 and H_2O. Through condensation, H_2O can be easily separated. The remaining gas is nearly pure CO_2 that is ready for sequestration or further use as raw material.

Many aspects of the combustion process change in oxyfuel conditions due to high concentrations of CO_2 in the gas phase. The difference in material properties of CO_2 compared to N_2 comprise of increased heat capacity, lower diffusivity of O_2, increased density, and high absorption of infra-red radiation. As a consequence, the flame temperature is decreased, fluid momentum is higher, and radiative heat transfer is increased. Furthermore, CO_2 is more chemically active than N_2 and can interact with solid carbon contained in the fuel through the Boudouard reaction: $CO_2 + C_{(s)} \Leftrightarrow 2\,CO$. This reaction can promote the solid fuel burnout but being endothermic, it can also lower the temperature of the fuel particle and thus restrain the chemical reactions. Studies on this subject are contradictory, some stating a promotion of the combustion process and others finding a slow-down; for an overview, see [1]. As a large number of opposed effects influences oxyfuel combustion, a study must include them all simultaneously. CFD simulation provides this capability and furthermore allows to "switch-off" individual effects. The influence of a single effect, such as Boudouard reaction, can be thus quantified.

The simulated pilot-scale flame has been studied both experimentally and numerically by the Institute of Heat and Mass Transfer (WSA) at RWTH Aachen University[2]. Experimental data from Toporov et al.[2] are used to validate the CFD simulation. The simulation is carried out with the open source CFD software OpenFOAM. Results for different char combustion models, with and without Boudouard reaction, are compared. The validation shows that the accuracy of the simulation is comparable to state-of-the-art results published in literature. The variation of char combustion models shows that the Boudouard reaction promotes the combustion process in regions with low concentration of O_2 in the gas phase. In those regions, particle burnout increases and flame temperature is reduced. Further downstream, the particle burnout is similar with and without consideration of Boudouard reaction.

REFERENCES

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