MODELLING OF FURNACES AND COMBUSTION SYSTEMS

(644) - (*) - FLAMELET LES OF OXY-COAL SWIRLING FLAMES USING DIRECTLY COUPLED SEAMLESS MULTI-STEP KINETICS FOR HOMOGENEOUS AND HETEROGENEOUS SOLID FUEL KINETICS

Hendrik Nicolai (Germany)[1,2]; Paulo Debiagi (Germany)[1]; Johannes Janicka (Germany)[2]; Christian Hasse (Germany)[1]

1 - Institut for Simulation of reactive Thermo-Fluid Systems, Technische Universität Darmstadt, Otto-Berndt-Strasse 2, 64287 Darmstadt; 2 - Institut for Energy- and Powerplant Technology, Technische Universität Darmstadt, Otto-Berndt-Strasse 3, 64287 Darmstadt

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The reduction of industrial emissions into the atmosphere is an essential criterion for technical plants in energy or process engineering. In addition to pollutants, the focus is primarily on reducing CO_2. The subsequent capture of CO_2 within the framework of CCS (Carbon Capture and Storage) processes represents a promising approach for combustion applications, whether classically operated with fossil fuels or alternatively with biomass. To avoid the expensive separation of CO_2 and N_2 in the flue gas, the oxy-fuel process was developed in which the nitrogen is removed by air separation before combustion and replaced by CO_2. Thereby, the ratio of CO_2 to O_2 can be adjusted and thus facilitates a flexible operation of the furnace. However, replacing N_2 with CO_2 also has a strong influence on combustion characteristics. To enable reliable predictions for this oxy-fuel processes, the development of models must rely on a close cooperation between experiments and numerical simulation. In particular, novel models must adequately describe the interactions of the turbulent-chemically reacting gas phase, the heat and mass transfer, and the particle chemistry.

Regarding the first two points, flamelet modeling approaches combined with large eddy simulation (LES) have shown promising results in recent years. However, in many studies, these advanced methods are combined with strongly simplified solid fuel kinetics models. These simplified models require an a priori calibration for predictive simulations, resulting in a limited range of application. Established detailed solid kinetics models can be used directly in simulations, but these were mostly developed for specific phases of the solid's conversion (devolatilization or char oxidation). Therefore, for application in the overall process, elaborate interfaces would have to be created to allow a coupled use of the models. However, recent developments in the field of solid kinetics have, for the first time, resulted in a seamless modeling approach, so-called CRECK-S model, for the entire particle conversion process, which is ideally suited for coupling into computational fluid dynamics (CFD). In this model, the employed coal is mapped onto a set of reference coals using proximate and ultimate analysis. Then, a detailed multi-step mechanism (22 solid species and 46 reactions) describes the decomposition of these reference coals during both devolatilization and char oxidation.

In this work, the fully coupled model, previously only validated on academic test cases, has been applied in the pilot-scale facility located at WSA-RWTH-Aachen for which detailed in-reactor data were measured. First, the overall model is validated against measurements. After the initial validation, two additional operating points with different O_2 to CO_2 ratios, were simulated. Subsequently, the predictiveness of this model is investigated over all three operating conditions. Moreover, a comparison to simplified models is carried out, demonstrating the increased predictive capabilities by employing seamless solid fuel kinetics.

In summary, this paper presents a holistic model for the simulation of oxy-fuel combustion chambers based on LES, tabulated chemistry, and directly coupled multistep kinetics. The developed model is applied to different operating conditions in a pilot-scale pulverized coal combustion chamber to assess the predictive capabilities of the approach.

Palavras-chave : Pulverized coal combustion, CFD, LES, detailed solid fuel kinetics, Flamelet