Sulfur chemistry in combustion processes

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Sulfur is present in the composition of many fuels, and their combustion can lead mostly to significant amounts of sulfur dioxide (SO_2) which is an undesired pollutant, and can produce significant operational problems if combined with other species or if converted to sulfur trioxide (SO_3), which is highly corrosive. Additionally, sulfur dioxide can affect the conversion of the fuel, the effectiveness of electrostatic precipitators and can interact with other pollutants generated during the combustion process, NO_x or unburned products, including hydrocarbons, polycyclic aromatic hydrocarbons and soot (Glarborg et al., 1996; Alzueta et al., 2001; Dagaut et al. 2003). Apart from SO_2, another important sulfur species that is of interest, mainly for the combustion of sulfur containing gases (e.g., sour gas, shale gas, gasification or refinery gases) and the Claus process, is hydrogen sulfide (H_2S). Hydrogen sulfide conversion chemistry is still significantly uncertain, but may be very relevant (Glarborg, 2007; Bongartz and Ghoniem, 2015).

The chemistry of sulfur in combustion and related processes appears, thus, to be of huge interest and exhibits unique and challenging features that deserve investigation. In this context, our objective is to study the conversion of sulfur compounds, H_2S and SO_2, but also other sulfur compounds of interest, such as CS_2, COS, mercaptanes, etc under conditions of interest for combustion processes. To achieve that objective, a combined experimental and kinetic modelling work is being performed. Experiments are carried out in well-controlled laboratory setups adressing the conversion of the sulfur species or evaluating the impact of the presence of sulfur species on the concentration of other pollutants, such as soot. The operating conditions considered include variation of pressure (between atmospheric and 60 bar), temperature (400-1500 K), stoichiometry (conditions ranging from pyrolyisis to very fuel lean conditions), and residence times (from few miliseconds to several seconds).

A detailed chemical kinetic mechanism to describe the conversion of sulfur compounds and the interaction bewteen those and hydrocarbons is being developed. The mechanism is built up taking as starting point reaction subsets of the species involved from literature and evaluating the performance of the mechanism with the experimental results. The mechanism is progressively updated and improved based on the experimental results and information for specific reactions and thermochemistry for species taken from literature. The mechanism developed is intended to be used for assessing the combustion phenomena occurring in the presence of sulfur compounds.

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