Numerical Simulations about the Partial Oxidation of a Moving Single Carbon Particle in Steam Atmosphere with varying H_2O/O_2 content

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Chemically reacting coal particles have been extensively studied over the last one hundred years due to the practical importance of coal by production of energy and chemicals (e.g. see [1] or [2]). In spite of the numerous works about the modeling of particle combustion, works about the influence of the water and oxygen content in the ambient air in combination with convection are rare.
Motivated by this fact the purpose of this paper is to study numerically the influence of the gas composition and Reynolds number on the carbon consumption.
In our work we consider a spherical particle placed in a hot ambient gas. To model the chemistry 3 heterogeneous and 3 homogeneous semi-global reactions are employed. The range of parameters considered in this study are $10^{-5} \leq Y_{H2O,In} \leq 0.5$, $0.055 \leq Y_{O2,In} \leq 0.233$, $1000K \leq T_{In} \leq 3000K$ and $0 \leq Re \leq 50$, where Y_{H2O}, Y_{O2}, T and Re are the ambient water mass fraction, the oxygen mass fraction, the temperature and the Reyolds number, respectively.
The software used in this work was validated against an analytical solution for a diffusion combustion of carbon particles. Excellent agreement between both was yield.
Based on the numerical results for a coal particle of 2 mm diameter, we found that the carbon consumption and the surface-average mass fractions for CO and CO_2 are almost unchanged for $Y_{H2O} \leq 10^{-2}$, whereas the reduction of O_2 in the ambient gas leads to a reduction of the surface-average for CO and CO_2 and the carbon consumption for all analysed cases. For cases with reduced O_2 content in the atmosphere the influence of the water mass fraction to all analysed parameters becomes stronger compared to cases with high O_2 content.
Furthermore the increase of H_2O in the ambient gas leads to a splitting of the CO_2 and temperature flamesheets that surround the particle for $T_{In} \geq 2500K$. The effect is enhanced by a reduction of O_2.

References

[1] Caram, H. S., Amundson, N.R. "Diffusion and reaction in a stagnant boundary layer about a carbon particle", *Ind. Eng. Chem. Fundam,* 16: 171–181 (1977)

[2] Libby, P.A., Blake, TH.R. "Burning carbon particles in the presence of water vapor", *Combustion and Flame* 41: 123–147 (1981)