Modeling the reaction mechanism of dispersed porous particles

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The basic knowledge of the combustion process resides among calculations of the combustion time, the gas temperature to predict NO formation and the particle temperature to predict the melting phenomenon of ash. The theme of the research is modeling of combustion behavior of porous coal particles surrounded with gaseous environment to calculate the heat and mass transfer coupled with chemical reaction within the porous particle as well as in the gas around the particle. This research work also comprises the experimental studies of behavior of different coals under same conditions. The behavior of coal particle under combustion conditions depends on its porous structure, porosity, internal surface area and the way how these parameters are influenced with temperature variations. During combustion, the continuous shrinkage of particle surface because of many heterogeneous reactions and temperature variations due to CO oxidation in the gas, results in structural changes of porous structure inside the particle. As the reactant first diffuses to macro-pores at particle surface then to micro-pores connected to these macro pores, these structural changes affect the reactivity of process. On the way to accomplish assigned task, we have modeled gas phase to generate concentration profiles of CO, CO$_2$ and O$_2$ and gas temperature profile along the distance from the particle surface. From experimental work, we came to know about the real behavior of coal particle in presence of CO$_2$ and it helps us to know the reaction kinetics of Boudouard reaction (C+CO$_2$→2CO) which is not widely studied by researchers.
Concentration Profile for O2, CO and CO2
(Particle Diameter 2 cm)

GAS TEMPERATURE PROFILE ALONG THE DISTANCE
FROM COAL PARTICLE SURFACE

References: