P125

EFFECT OF CO_2 ATMOSPHERE ON SOOT FORMATION DURING COAL VOLATILES COMBUSTION

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1. Introduction

Coal combustion with O_2/CO_2 is one of several promising new technologies associated with CO_2 reduction in the atmosphere. As coal heats up, the volatile components of the coal will diffuse into the gas stream. These volatiles consists hydrocarbon compounds with significant number of polycyclic aromatic hydrocarbon (PAH). This PAH molecules are considered to form subsequent higher PAH molecules and soot. The oxidation of PAH and soot has been occurred during secondary gasification and therefore forming H_2 and CO. In this paper the authors predicted the soot and PAH concentration profiles in a wide range of reaction conditions.

2. Simulation

A PFR mechanism for reaction of coal volatiles is developed in our previous study for O_2/CO_2 gasification and validated [1, 2]. In this paper inlet gas species considered are H_2, CH_4, H_2O, CO, CO_2, some smaller aliphatic hydrocarbon, 37 PAH and inert species N_2 that is obtained from the pyrolysis of coal. PAH of increasing size are mainly formed by sequences of chemical reactions of radicals of smaller PAH with acetylene, PAH or PAH radicals. PAH having molecular weight higher than 2000 is being considered as soot particle. Particle sizes increase further by collision of growing soot particles. Soot oxidation involves loss of CO and a fraction of the next smaller soot/PAH. The reaction mechanism consists of 276 species and 3793 reactions that are taken from MIT combustion research website [3]. The inlet boundary conditions for O_2 and CO_2 mass fraction are 0.007 and 0.02241 respectively.

2. Result and Discussion

Figure 1 shows that mass fraction of soot and PAH (Total) decreases significantly when the high temperature is maintained. This figure also shows that at high temperature and high CO_2 inlet almost all soot and PAH reduces due to following reaction.

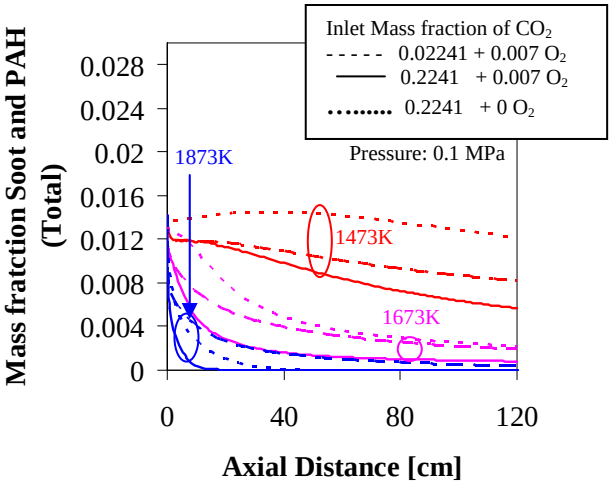

Figure 1: Concentration profiles of Soot and PAH (Total) under various temperature and CO_2 inlet conditions

$$PAH/SOOT + O/OH \longrightarrow CO + H/H_2/H_2O$$

It has also been found that at high temperature only CO_2 (without O_2) can oxidize all soot and PAH. Figure 2 shows the effect of O_2 and CO_2 at lower temperature (1373K) for 10 times of the default concentration for each. It has been found at that temperature O_2 can completely reduce the total of soot and PAH but CO_2 cannot. This is because at lower temperature addition of smaller hydrocarbon with soot and PAH becomes dominant rather than the decomposition/oxidation of soot and PAH. Also the oxidizing species e.g., O or OH are not sufficient at lower temperature.

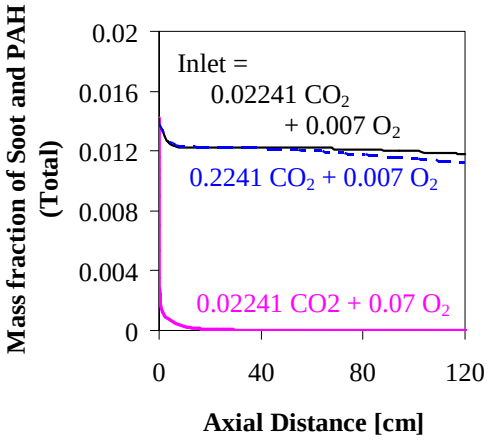

Figure 2: Effect of O_2/CO_2 on concentration profiles of Soot and PAH (Total) at temperature 1373K and pressure 0.1 MPa

4. Conclusion

The effect of O_2/CO_2 on coal volatiles combustion in a Plug Flow Reactor has been studied both in low and high temperature. At higher temperatures CO_2 have large effect on soot and PAH reduction. On the other hand O_2 shows good prediction of soot and PAH at lower temperature. Therefore regarding CO_2 reduction in the atmosphere and for reduction of soot and PAH in the outlet of the reactor, the temperature should be maintained at >1673K and the inlet CO_2 should be also high. At high temperature O_2 can also be replaced by CO_2.

References

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