Soot Formation from Premixed Ethylene and Benzene Flames

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BACKGROUND and OBJECTIVES

Soot formation, caused by the incomplete combustion of hydrocarbons, has become the main theme of many research activities covering experimental, theoretical and computational efforts due to the health and environmental issues associated with its emissions to the atmosphere (Sarofim et al., 2002). Nevertheless, this is a complex process that involves a great number of chemical and physical steps; therefore, different analytical techniques need to be coupled to achieve a better understanding of the inception and growth of nanoparticles in flames.

The aim of this work is to characterize differences in size, composition, structure and morphologies of soot extracted from premixed aromatic (benzene) and aliphatic (ethylene) flames under similar conditions of C/O ratio and flame temperature and compare these results with computational data. This study will provide additional support to prior work on particle size distributions using nano-DMA.

EXPERIMENTAL SETUP

Model predictions of Particle Size Distributions

- GRI mechanism for C1 – C2 species
- Miller and Melius (1992) for C3 – C4 chemistry

The kinetic mechanism of C1 – C4 species includes 50 species and 250 elementary reactions

- PAH formation
  - C2H2 addition to aromatic rings (HACA mechanism)
  - Resonantly-stabilized free radical combination

- Aromatic growth
  - Radical-molecule addition reactions
  - Surface growth: acetylene addition on activated molecule

- Collisional coagulation

CONCLUSIONS

The data and gas-phase modeling results support findings presented in previous theoretical and experimental studies that benzene flames lead to early nucleation of particles. This is then responsible for the observed differences, particle size distribution and soot growth patterns in benzene versus aliphatic flames.

Gas precursor predictions for the benzene flame show that the precursor concentration of aromatics is higher as compared to ethylene flames. The results are well reproduced by the model.

The ethylene flame shows two modes in the size distribution functions with small particles (less than 10 nm) evident higher in the flame. The results are not well reproduced by the model.

Gas precursor predictions for ethylene suggest lower concentrations of aromatics and higher concentration of acetylene, suggesting that the formation pathways are different.

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