Growth Mechanism of Soot Particles in Inverted Gravity Diffusion Flames

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ABSTRACT

The recirculating inverted flame gives larger primary particle diameter due to recirculation between fuel rich and post flame region.

The PAH mass fraction of the soot produced by inverted recirculating flame is also significantly higher, suggesting the particle growth through PAH addition.

INTRODUCTION

Combustion-generated aerosols are one of the major components of PM (around 10-50%) and can cause significant lung inflammation, cardiovascular diseases, neurological diseases, and cancer.

The morphology of the particle presents ambiguity in the light absorption and scattering by atmospheric aerosols, which is a source of uncertainty in climate models.

There is need to understand the particle’s physical and chemical properties.

Even decades of research on soot formation, there are some uncertainties in the soot nucleation and nascent particle coalescence.

SOOT FORMATION PROCESS

Pyrolysis
PAH Formation
Clustering
Coalescence/Surface Growth
Carbonization at the flame front
Coagulation

HACA mechanism for growth of PAHs

PROJECT OBJECTIVES

Hypothesis:
Particle carbonization in the flame front and subsequent particle exposure to the high concentration PAH region in the fuel rich pre-flame zone leads to surface growth by the formation of a liquid hydrocarbon layer on the surface, followed by a phase change in the stoichiometric flame region [1].

Procedure:
1. Experimentally observe and measure flame conditions leading to particle growth with gaseous CxHy fuels.
2. Examine size and structure of nanoparticles
3. Analyze the chemical composition of soot particles using GC-MS for 16 EPA priority PAHs.
4. Model the three flames using CFD to gain insight on variables that play a major role in particle growth
4. Distinguish between recirculating and other flame conditions on particle formation

EXPERIMENTAL

Table 1: SEM images of the soot produced by the three flames at 15000 magnification. Scale bar correspond to 500 nm. Particles generated by the inverted recirculating flame with both the fuels are larger in size.

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<tr>
<th></th>
<th>Upright</th>
<th>Inverted Non-Recirculating</th>
<th>Inverted Recirculating</th>
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<tbody>
<tr>
<td>Methane</td>
<td>25 nm</td>
<td>68 nm</td>
<td>33 nm</td>
</tr>
<tr>
<td>Propane</td>
<td>NA</td>
<td>43 nm</td>
<td>52 nm</td>
</tr>
</tbody>
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Table 2: The primary particle diameters for the three flame configurations with Methane and Propane.

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Numerical

- Two-dimensional axis-symmetric CFD analysis with GRI 3.0 mechanism [2] and soot particle dynamics modeled by method of moments is used to give flow pattern, species profile, and temperature profile in the reactor.

CONCLUSIONS

- Recirculating flame produces soot with larger primary particle diameters and higher PAHs mass fraction.
- CFD simulations show that the particles recirculate between fuel rich region and stochiometric region.
- The concentration of C_2H_2 and H radical is also lower for the recirculating flame suggesting the unsuitability of HACA mechanism to explain particle growth.
- The surface growth of particles should occur by liquid PAH deposition as they re-enter the fuel pyrolysis region after carbonization through the flame front.

FUTURE WORK

- Perform CFD simulations with higher PAH species and surface growth mechanism to predict primary particle sizes for the three flame configurations.
- Analyze the morphology of the particles using TEM imaging.

ACKNOWLEDGMENTS

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REFERENCES