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Growth Mechanism of Soot Particles in Inverted Gravity Diffusion Flames

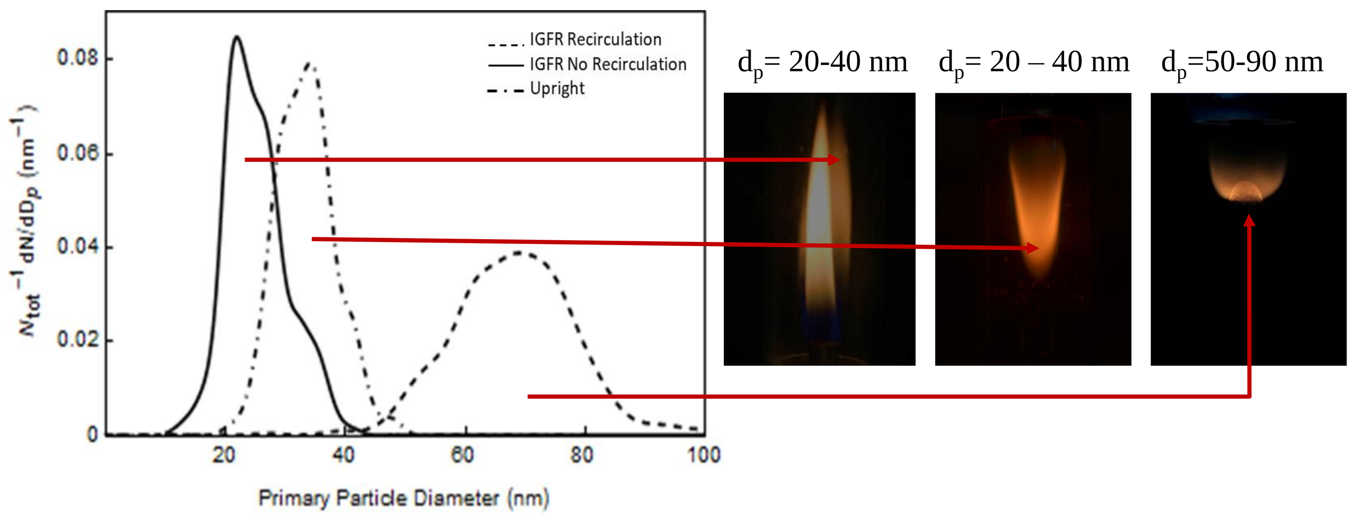
Kartik Tiwari[1], Justin Davis[2], Jay Rutherford[3], Igor V. Novosselov[1,2]

[1]Mechanical Engineering, University of Washington; [2] Department of Molecular Engineering, University of Washington; [3]Department of Chemical Engineering, University of Washington

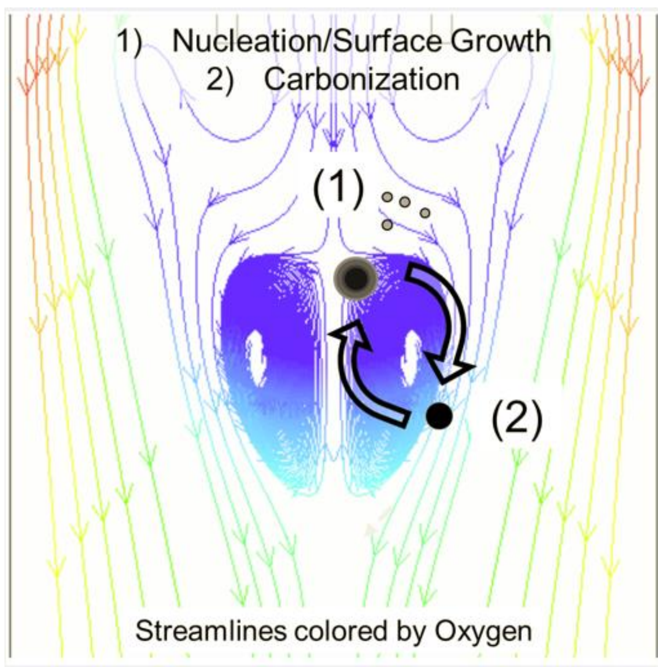
Novosselov Research Group

Contact: Prof. Igor Novosselov – IVN@uw.edu

ABSTRACT



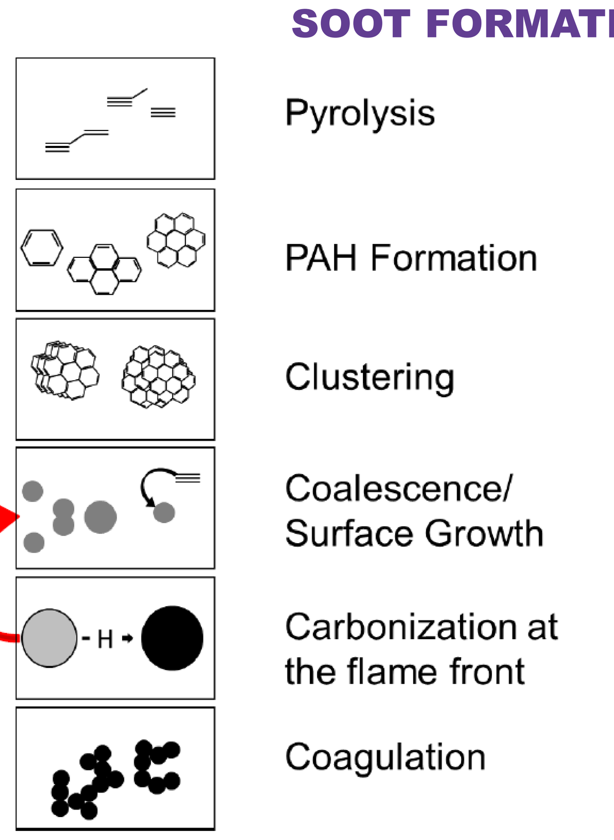
- The recirculating inverted flame gives larger primary particle diameter due to recirculation between fuel rich and post flame region.
- The PAH mass fraction of the soot produced by inverted recirculating flame is also significantly higher, suggesting the particle growth through PAH addition.

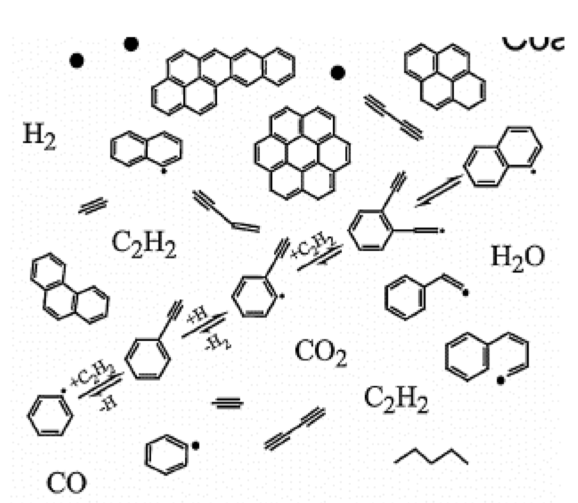


INTRODUCTION

- 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





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.
3. 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*

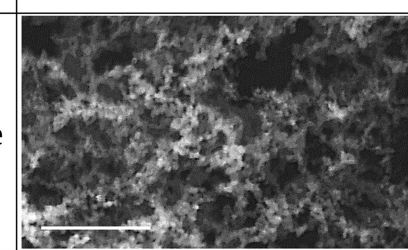
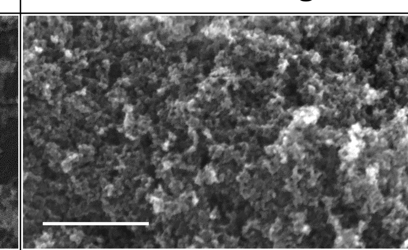
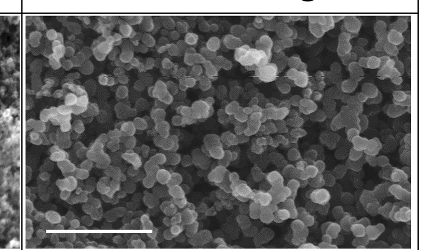
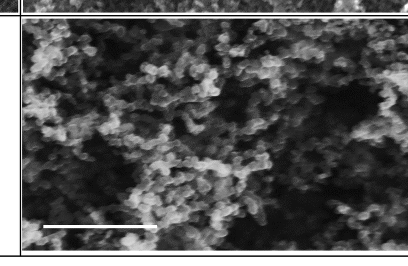
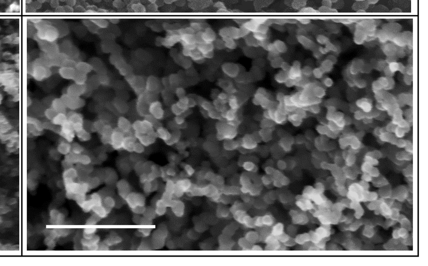
	Upright	Inverted Non-Recirculating	Inverted Recirculating
Methane			
Propane	NA		

Table 2: *The primary particle diameters for the three flame configurations with Methane and Propane.*

	Upright	Inverted Non-Recirculating	Inverted Recirculating
Methane	33 nm	25 nm	68 nm
Propane	NA	43 nm	52 nm

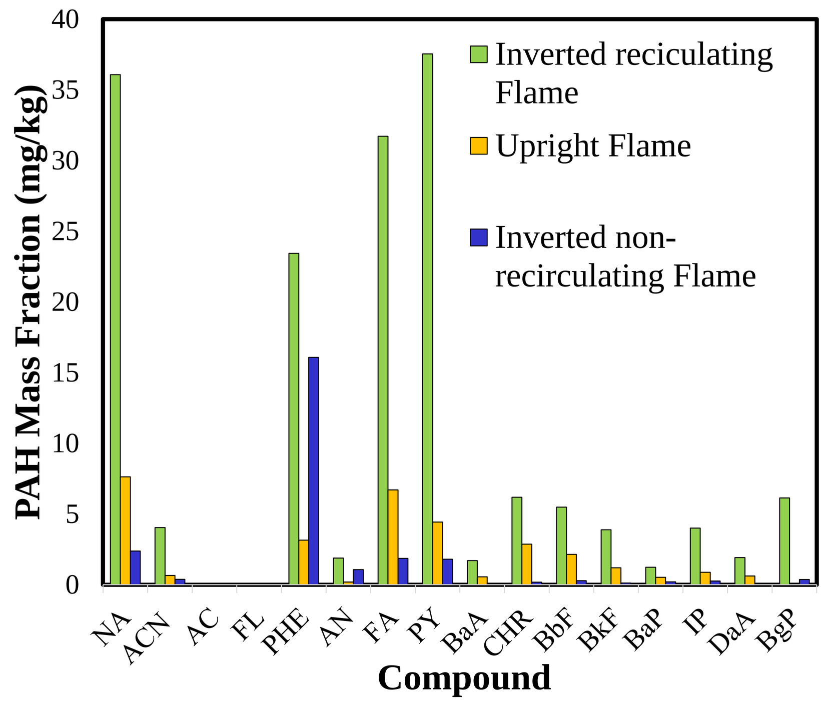


Figure 3: *Mass fraction of 16 EPA priority PAHs in the soot samples collected from the three flames characterized using GC-MS analysis. The mass fraction of PAHs is highest for inverted flame with recirculation.*

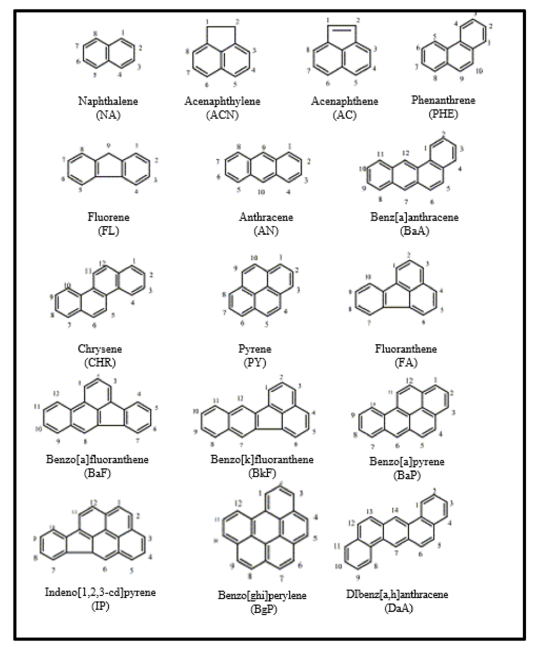


Figure 4: *Structures and nomenclatures of the 16 PAHs on the EPA priority pollutant list.*

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.

Table 3: *Comparison between experimental and computational boundary conditions*

	Non-Recirculating		Inverted Recirculating	
	Experiment	Numerical	Experiment	Numerical
Fuels flow rate (slpm)	0.24	0.24	0.12	0.10
Air flow rate (slpm)	3.3	2.5	1.8	2.5
Flame length (mm)	60	64	27	18

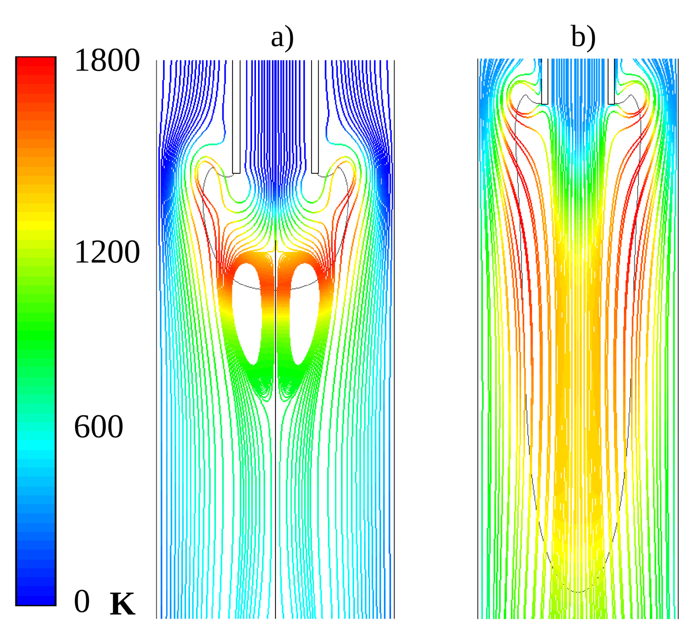


Figure 5: *Path-lines colored by* ***static temperature*** *for a) Inverted Flame with recirculation and b) Inverted Flame without recirculation.*

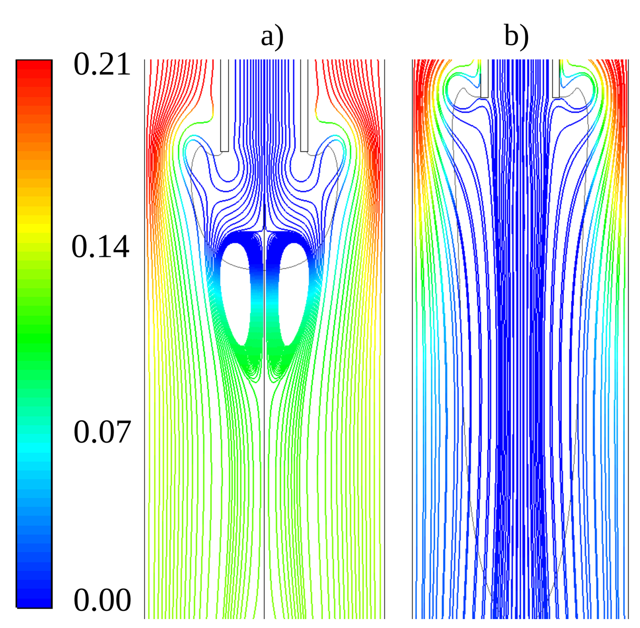


Figure 6: *Path-lines colored by* ***mole fraction of O_2*** *for a) Inverted Flame with recirculation and b) Inverted Flame without recirculation.*

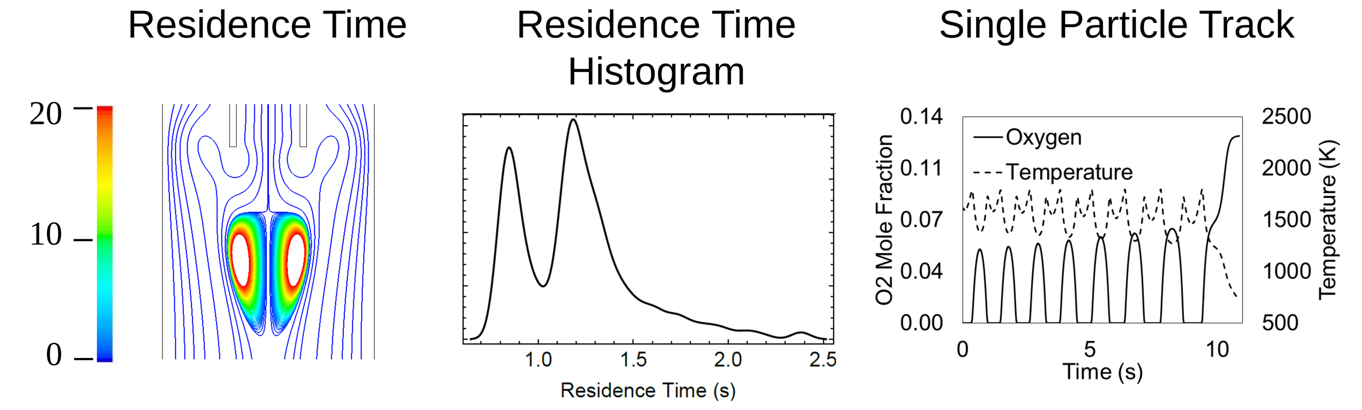


Figure 7*. Left: CFD showing recirculating path-lines and resulting residence time. Particles in the entrainment have residence times up 20 seconds. Middle: Probability distribution of residence times. Right: The surrounding oxygen and temperature of a single particle entrained for 10 seconds inside the recirculation region. The particle oscillates between rich and lean regions of the reactor.*

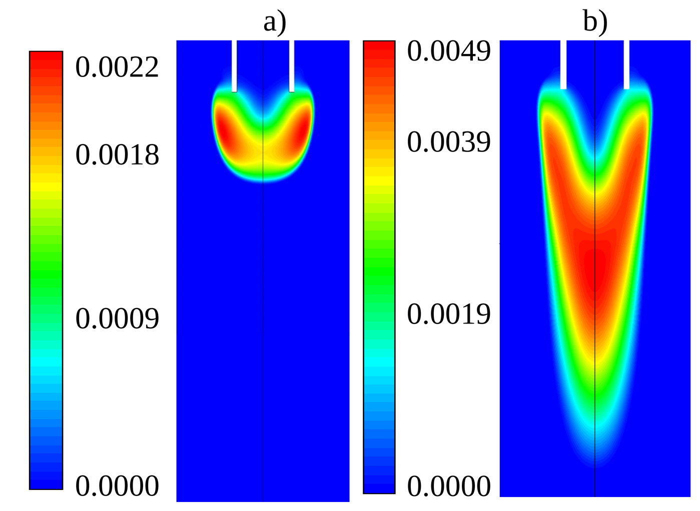


Figure 8: *Contours of* ***mole fraction of C_2H_2*** *for: a) Inverted Flame with recirculation and b) Inverted Flame without recirculation*

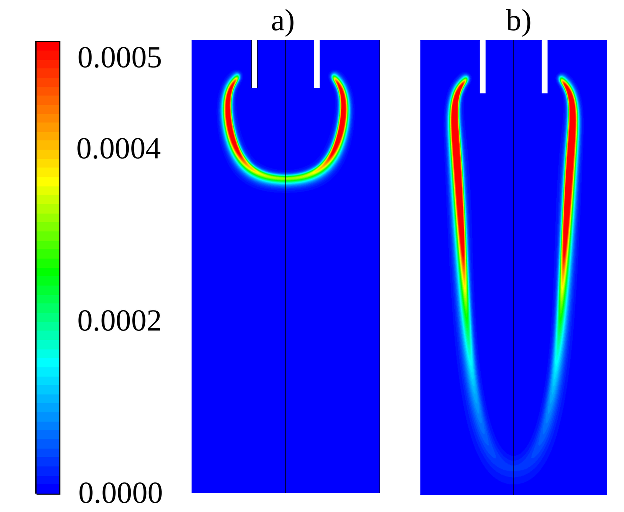


Figure 9: *Contours of* ***mole fraction of H radical*** *for: a) Inverted Flame with recirculation and b) Inverted Flame without recirculation*

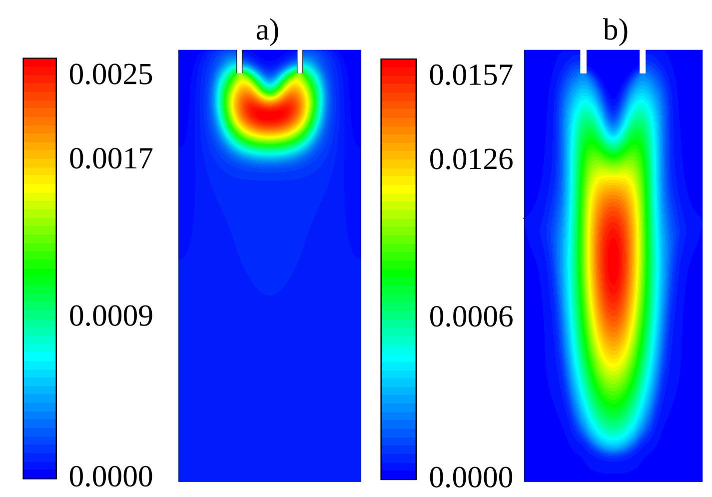


Figure 10: *Contours of* ***mass fraction of soot*** *for: a) Inverted Flame with recirculation and b) Inverted Flame without recirculation*

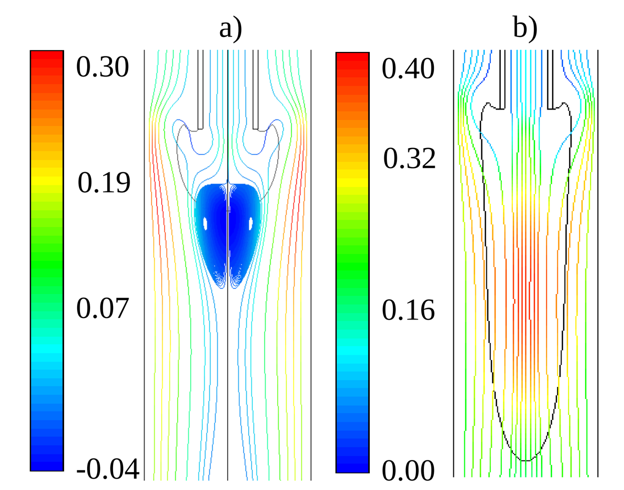


Figure 11: *Pathlines colored by axial velocity (m/s) for: a) Inverted Flame with recirculation and b) Inverted Flame without recirculation*

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.

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[2] "GRI-Mech Home Page." [Online]. Available: http://combustion.berkeley.edu/gri-mech/. [Accessed: 13-Oct-2017].