PAH FORMATION CHARACTERISTICS OF HYDROGEN-ENRICHED METHANE DIFFUSION FLAMES

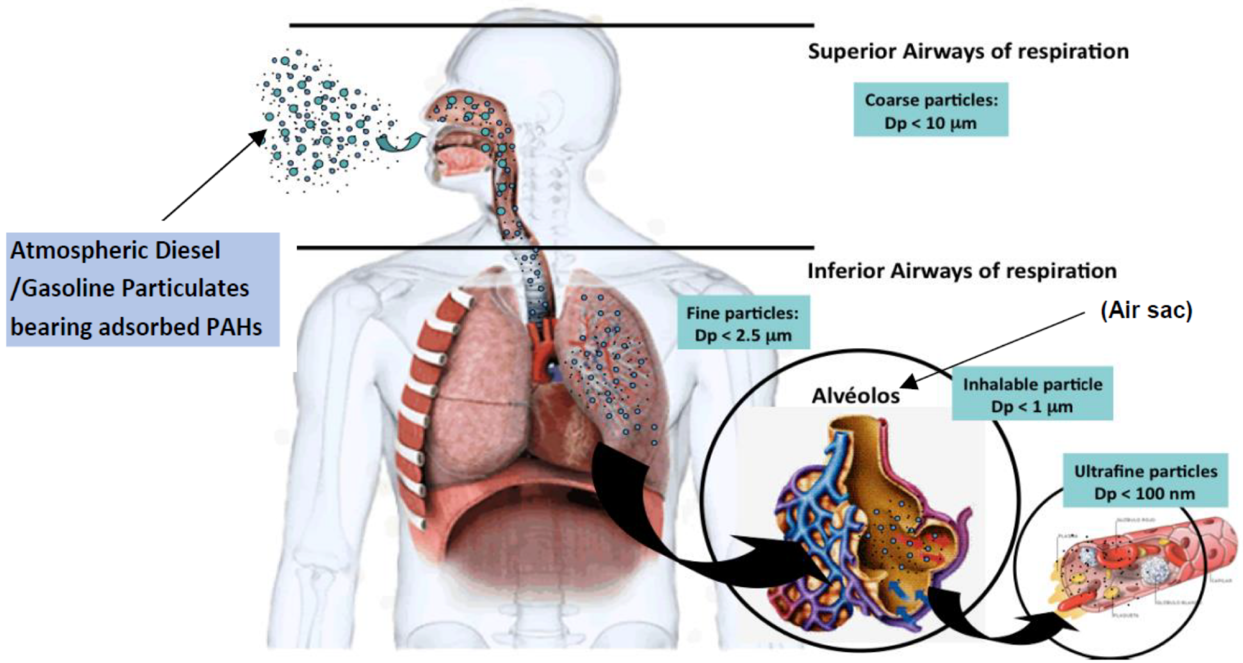
BY

CHINONSO EZENWAJIAKU, MIDHAT TALIBI, NAK DOAN, NEDUNCHEZHIAN SWAMINATHAN, RAMA BALACHANDRAN

ucemcee@ucl.ac.uk
Department of Mechanical Engineering, Torrington Place
University College London

SIG MEETING, 09 APRIL, 2019

WHY DO WE BOTHER ABOUT PAHS ?



- PAHs are **hydrocarbons** with 2 or more fused benzene rings and acts as **precursors** to **soot formation**
- PAHs are of sizes ranging from a few nanometres to micrometres (< 2µm)
- PAHs result from natural and/or anthropogenic sources

- Long-range transport almost non-degraded

- Toxic
- Mutagenic
- Carcinogenic

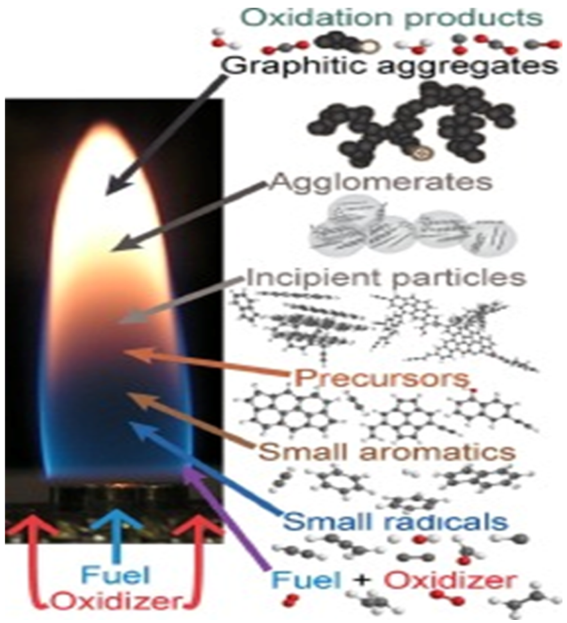
SOURCES OF PAH

Credit: Ted Christian

http://farm1.static.flickr.com/216/499969453_44089c6c1d.jpg

https://www.machinerylubrication.com/Read/30771/choose-right-lubricant

http://www.sfgate.com/blogs/images/sfgate/green/2009/06/03/diesel-smoke.jpg



H.A. Michelsen, Proceedings of the Combustion Institute Volume 36, Issue 1, 2017, Pages 717-735

https://envirochem.co.uk/blog/2018/01/26/construction-sites-contributing-towards-air-pollution-in-cities/

GAPS AND KEY OBJECTIVES

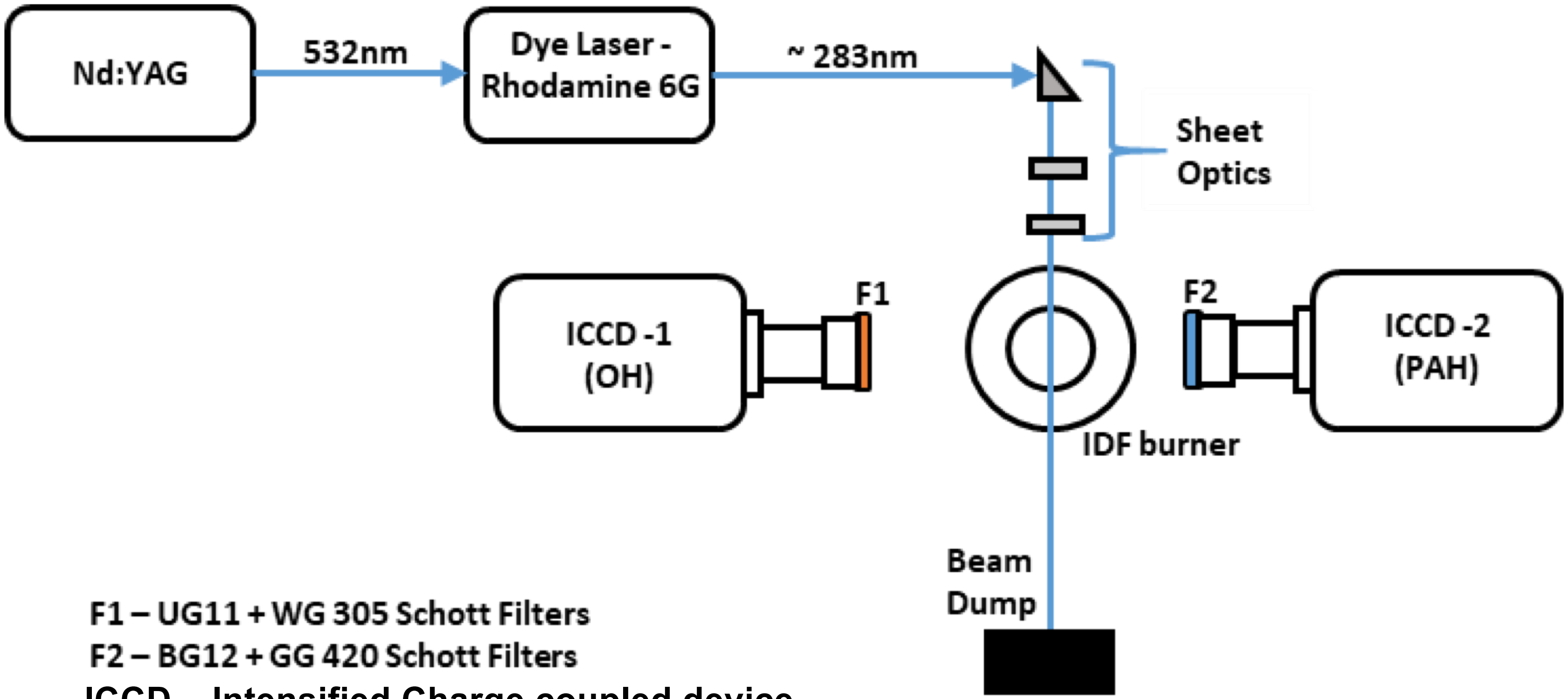
MOTIVATION

- To develop effective soot reduction measures, understanding PAH formation processes is imperative.
- Though most soot formation mechanisms are replete with significant role of H-atom in soot production, experimental campaigns on the effects of hydrogen addition on PAH formation are scant.

KEY OBJECTIVES

- Systematically investigate PAH formation characteristics in methane-air diffusion flames
- Understand the effects of hydrogen addition on PAH formation characteristics in methane-air diffusion flames
- Compare the experimental results with 1-D flame simulations utilising detailed chemical mechanisms.

EXPERIMENTAL SET-UP



F1 – UG11 + WG 305 Schott Filters
F2 – BG12 + GG 420 Schott Filters
ICCD – Intensified Charge coupled device

***1-D Flame Calculation**

- CANTERA coupled with ABF-gas phase mechanism

- **Detection wavelength for OH is ~ 310 nm**
- **Detection wavelength range for PAHs is 420nm – 480 nm (for 3-5 rings)**

FLOW CONDITIONS

Q_{CH4} = 10 lpm, Q_{air} = 1.5 lpm

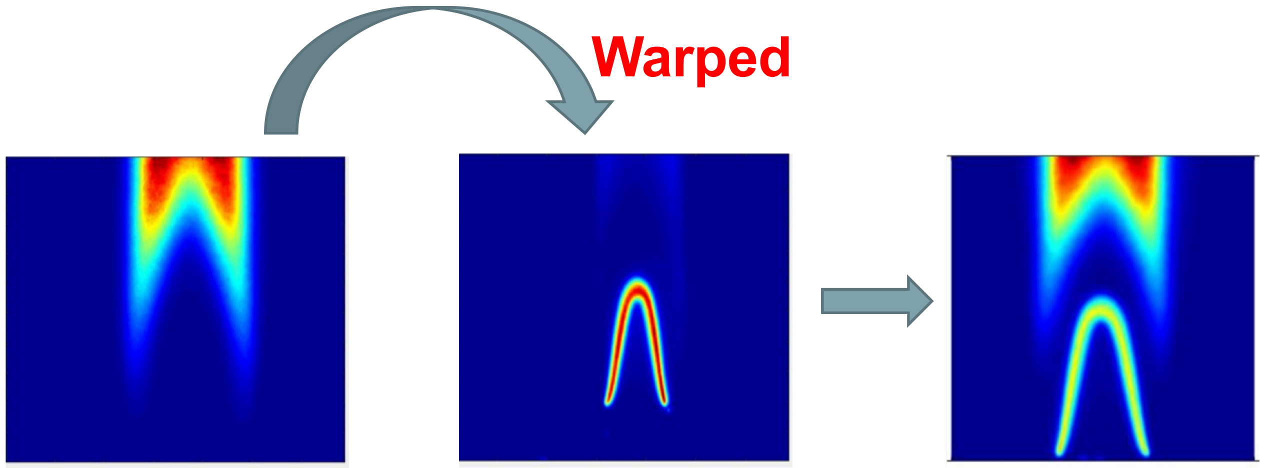
H_2 ADDITION (lpm)	% H_2 ADDITION	T at $[PAH]_{max}$ (K)	T_{max} (K)
0	0	1520	2152
0.2	2	1530	2159
0.4	4	1540	2165
0.6	6	1550	2171
0.8	8	1520	2178
1.0	10	1540	2184
1.2	12	1550	2190
1.4	14	1560	2196
1.6	16	1530	2202
1.8	18	1540	2208
2.0	20	1550	2213

DATA PROCESSING

200 Images Accumulated →

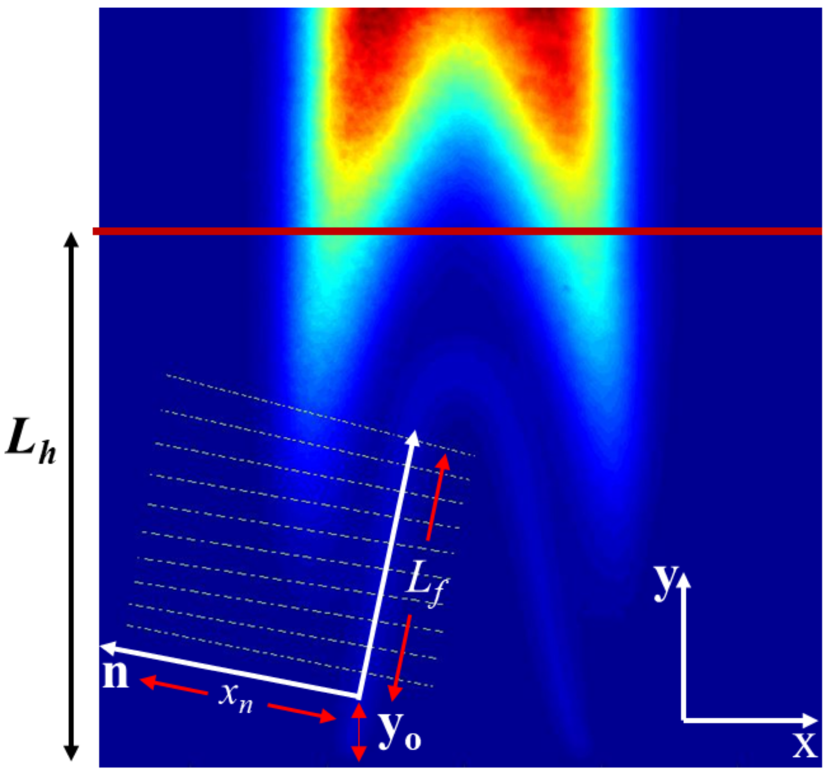
- **Background correction**
- **Averaging**
- **Filtering**
- **Transposed**

→ **Processed Image ready for Analysis**

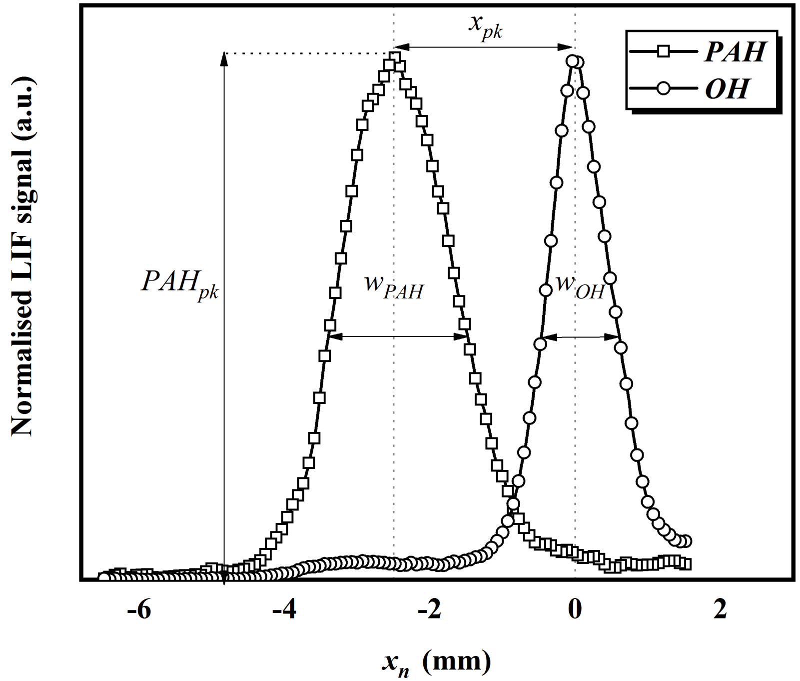


Transposed image with resolution of 25 $\mu m/pixel$

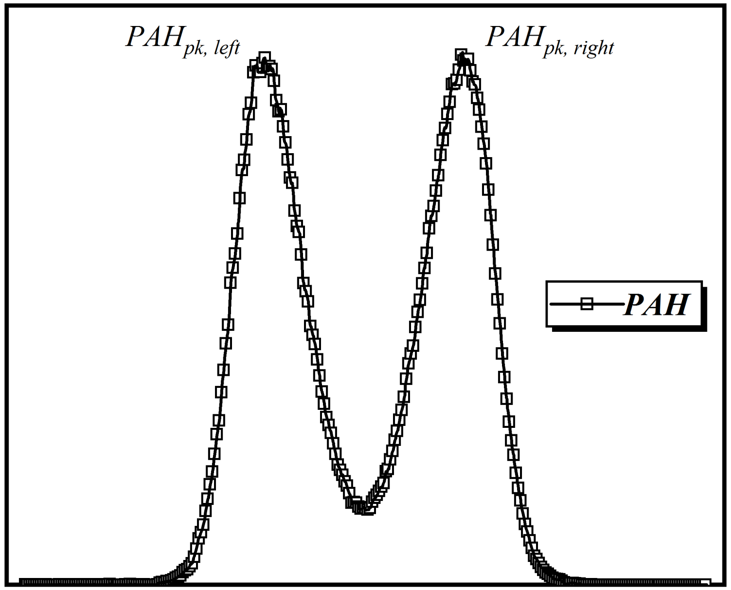
DATA ANALYSIS



Case A

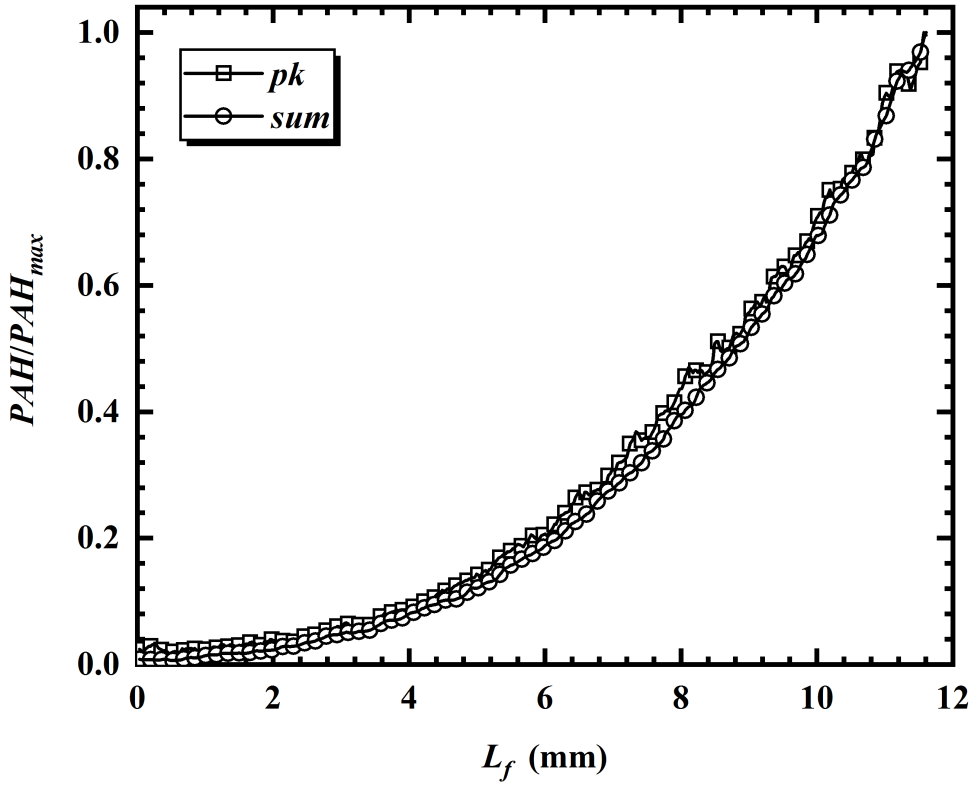


Case B

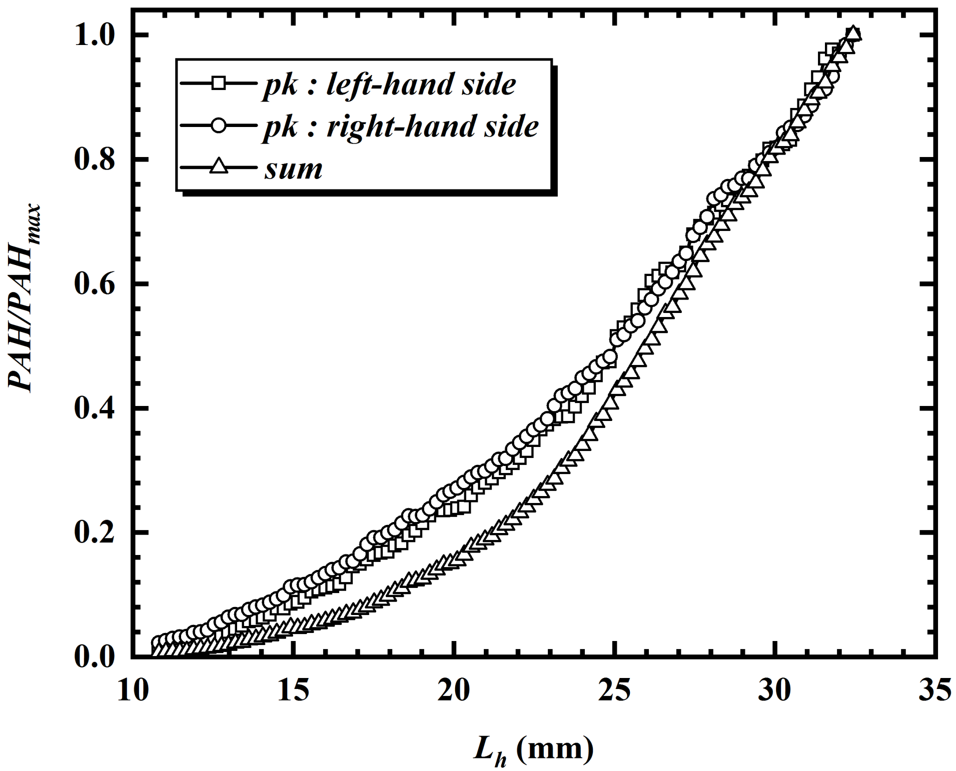


- **Case A – PAH change w.r.t. flame normal statistics**
- **Case B – PAH change w.r.t. to vertical height above burner (HAB)**

METHANE-AIR FORMATION CHARACTERISTICS



Case A

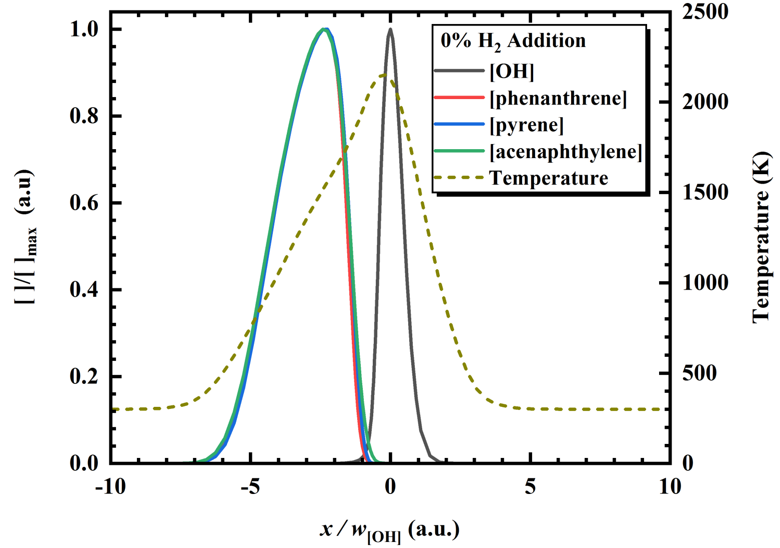


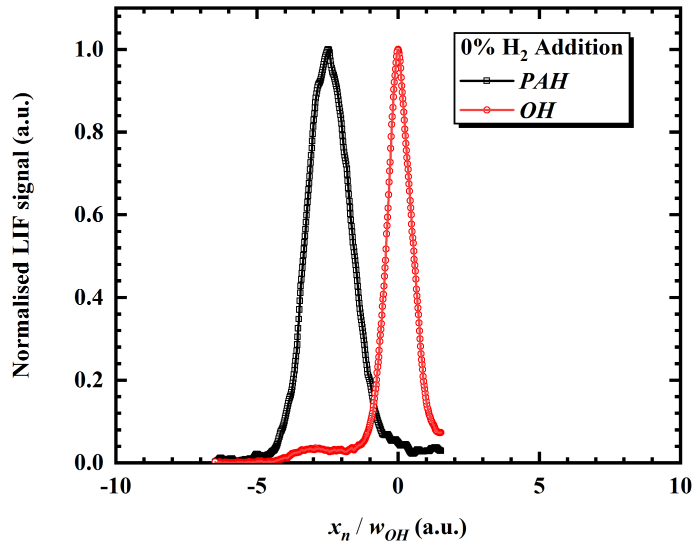
Case B

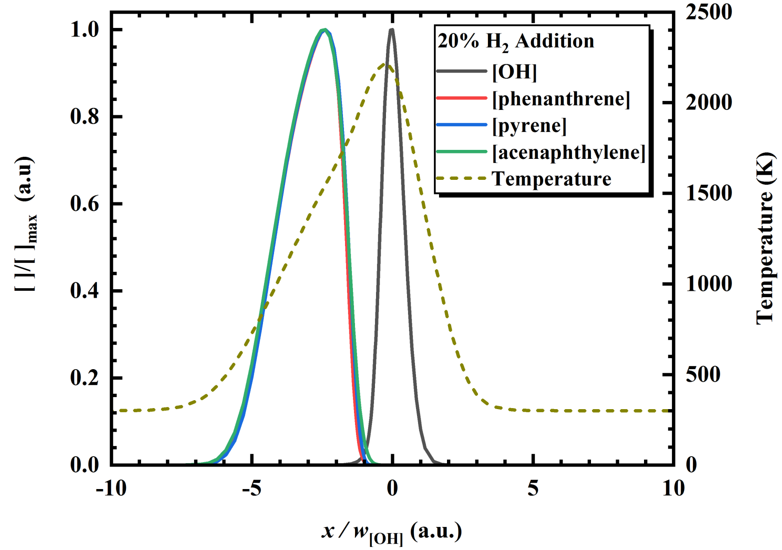
COMPARING OH-PAH PROFILES

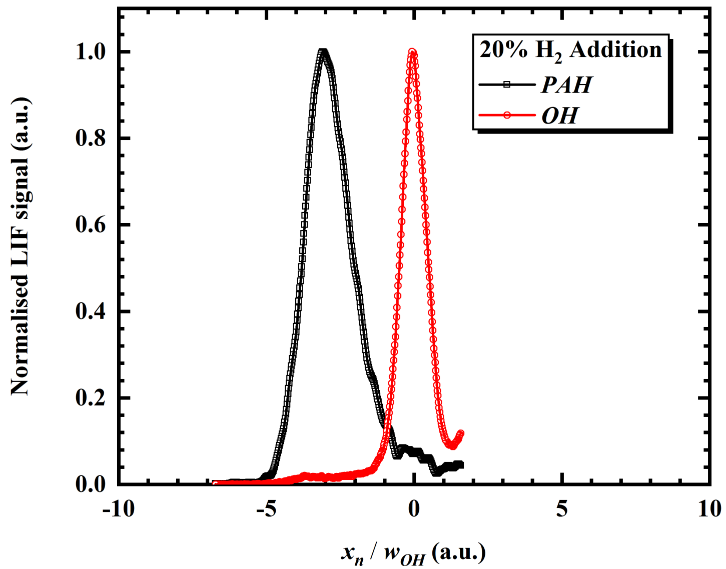
NUM.

EXPT.

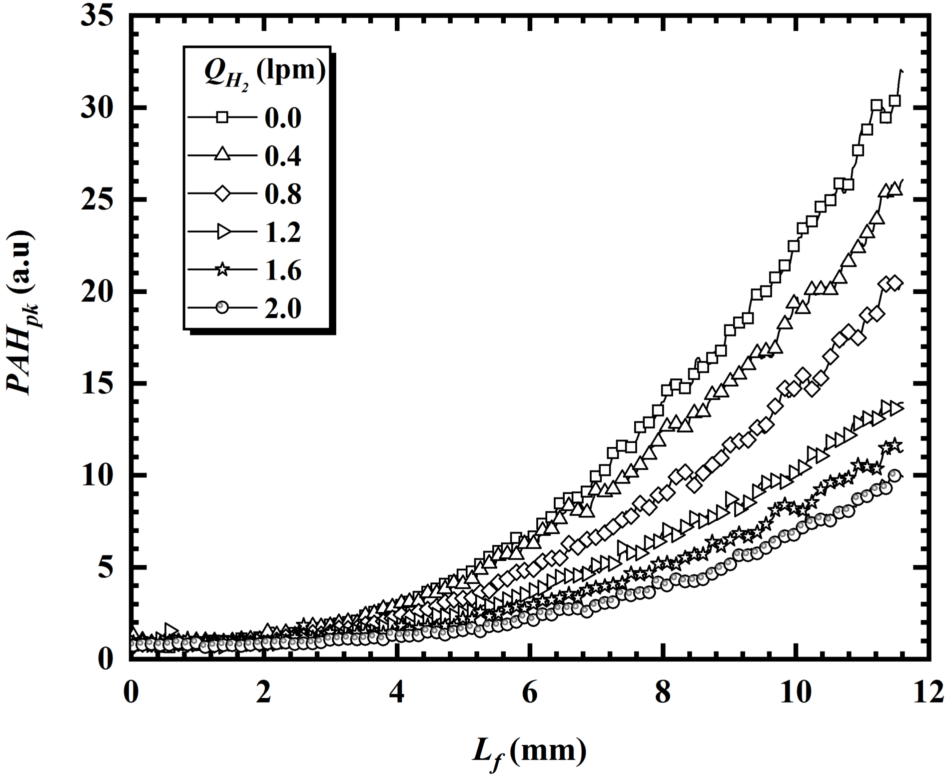


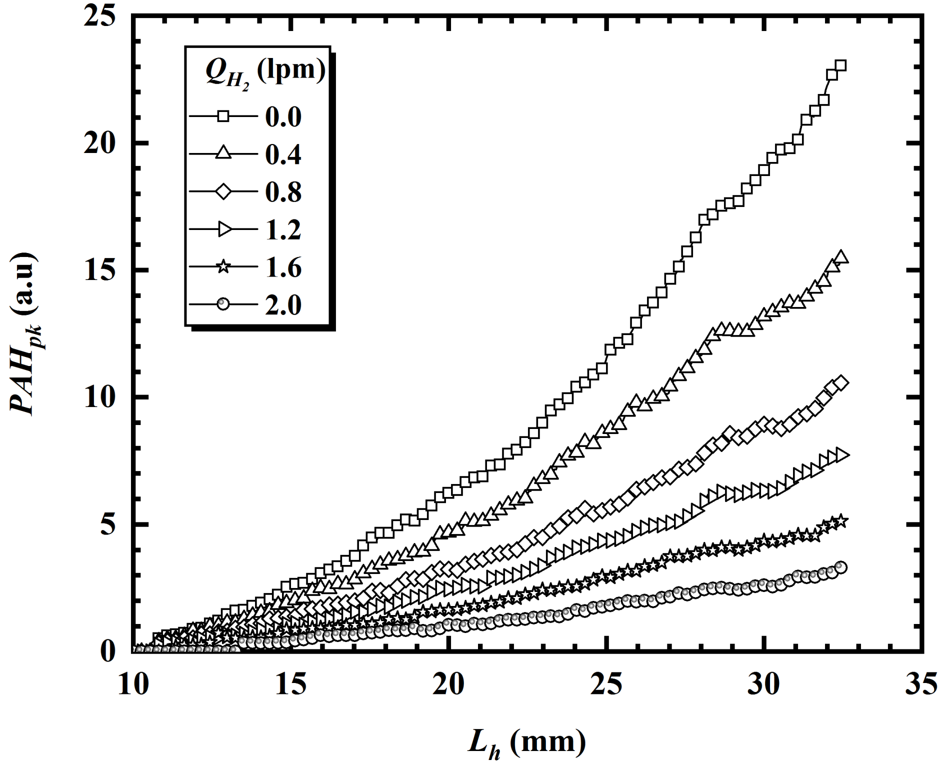






EFFECT OF HYDROGEN ADDITON

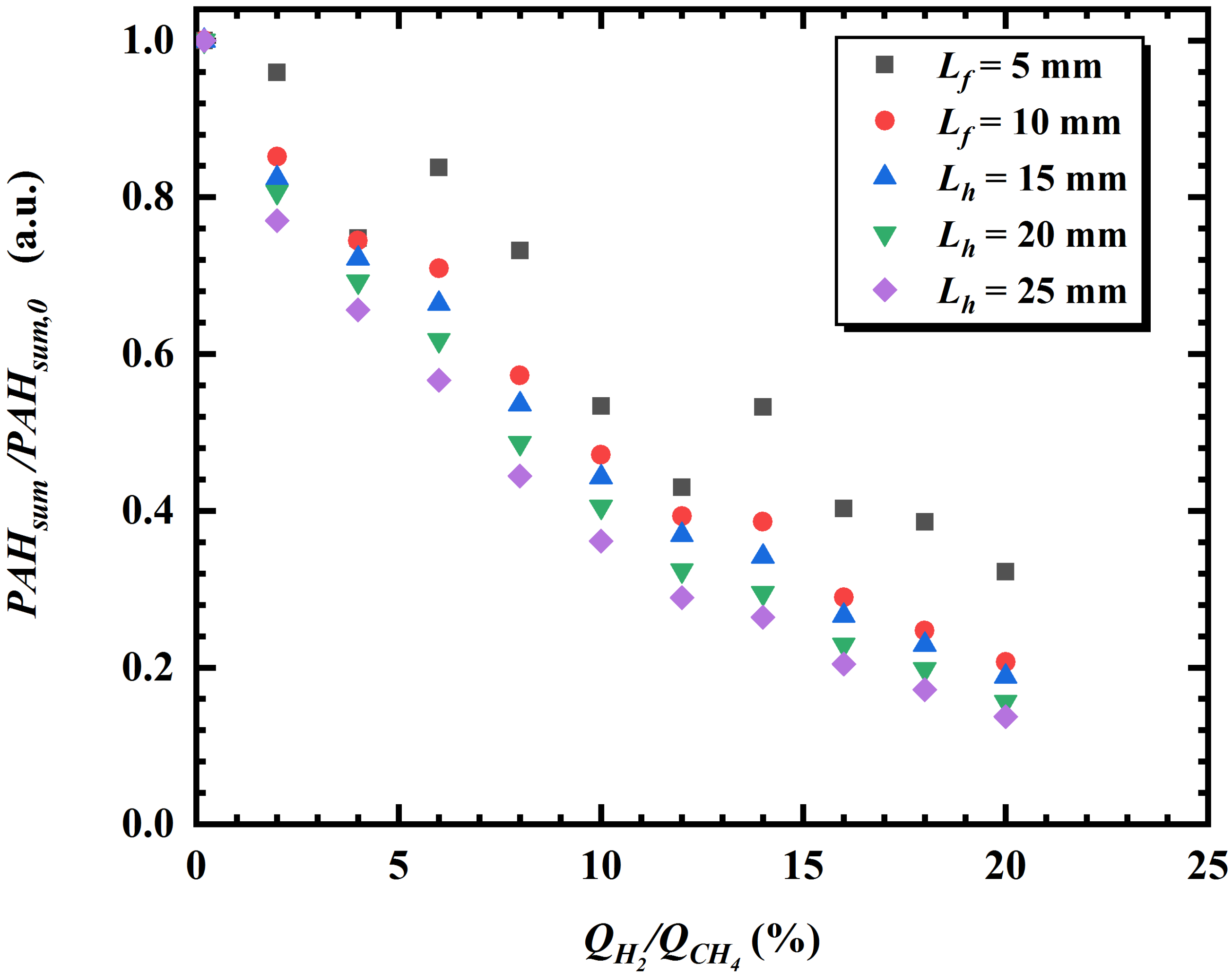




PAH CONCENTRATION INCREASES WITH INCREASING HEIGHT (L_f OR L_h)

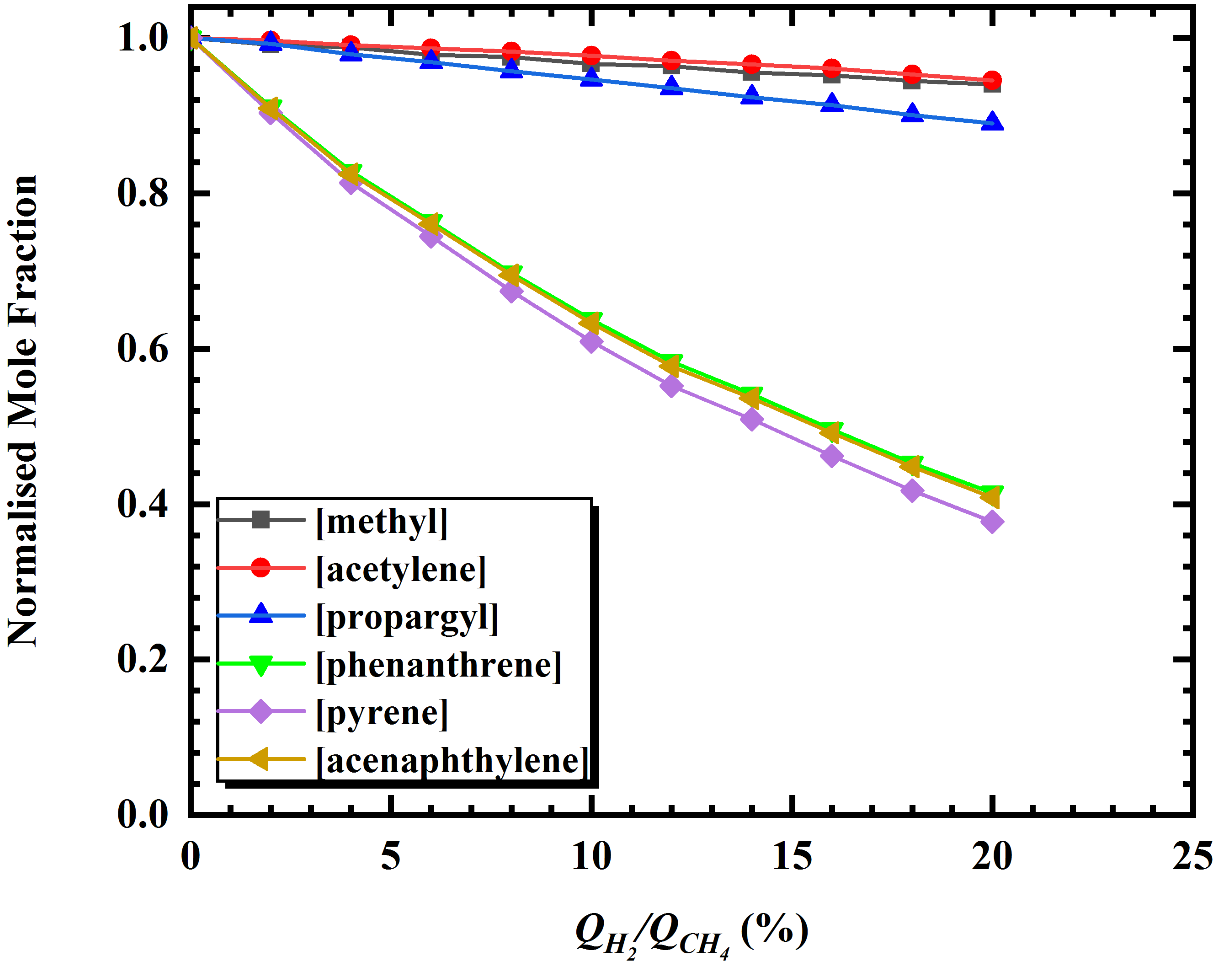
ADDITION OF HYDROGEN REDUCES PAH CONCENTRATION

EFFECT OF HYDROGEN AT VARIOUS HEIGHTS



- **PAH SPECIES REDUCED AT ALL HEIGHTS**
- **HIGHER PAH REDUCTION AT HIGHER HEIGHTS**

EFFECT OF HYDROGEN ON KEY SPECIES



- **HYDROGEN ADDITION IS EFFECTIVE FOR ALL ROUTES OF PAH/SOOT FORMATION**
- **SIMULATED PAH SPECIES COMPARES WELL WITH 5mm PROFILE FROM THE EXPERIMENTAL RESULTS**

CONCLUSIONS

- PAH increased with increasing height above burner attributed to both higher concentration of PAHs as well as formation of larger rings.

- Both experimental and numerical results showed similar PAH profile width with no significant change observed with hydrogen addition. However, the peak PAH location from experimental results were observed to shift slightly away from peak OH location (maximum temperature region).

- Similar PAH reduction observed at 5mm between experimental and numerical results. This is because 1D - flame simulations cannot capture resident time effects.

- Hydrogen addition effective in the reduction of PAH concentration notwithstanding the PAH/soot formation mechanism considered

THANK YOU FOR LISTENING!

EFFECT OF METHANE AND AIR FLOW RATES