Co-formation of oxygenated and non-oxygenated aromatics in the flames of biofuel and fuel mixtures

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Biofuels and other biomass-derived chemicals are now considered as a vital part of sustainable energy portfolio, where they promise to contribute to our society's energy security [1]. Despite the undeniable interest presented by these biofuels, their combustion processes are likely to modify the formation of PAHs and OPAHs [2] that may profoundly modify the properties of formed soot particles.

In this work, five laminar premixed flames of anisole (a surrogate for lignin-based biofuels) and hydrocarbon fuel blends have been investigated using advanced gas chromatography which is equipped with a pre-concentration device to trap sufficient material in order to allow detection of PAHs and OPAHs at ppb levels. Employing this sample enrichment technique has enabled us to spot around 100 aromatic species in chromatographic analysis. An example of a part of a representative chromatogram and OPAH/PAH profiles has been shown in *Fig. 1*. Besides PAHs, several oxygenated aromatics (phenol, cresols, benzofurans, xanthones, etc.) were detected which highlights their significant co-formation. Moreover, anisole addition in flames is found to increase the formation of polyaromatic compounds. These species would allow us to link several primary reactions with the formation of pollutants and potential soot particles formed during the combustion of biofuels. The present results build a solid database for analysing OPAH/PAH co-formation during the combustion of lignin-based biofuels. Moreover, the impact of the biofuel composition on soot formation is envisioned to be studied in this project.

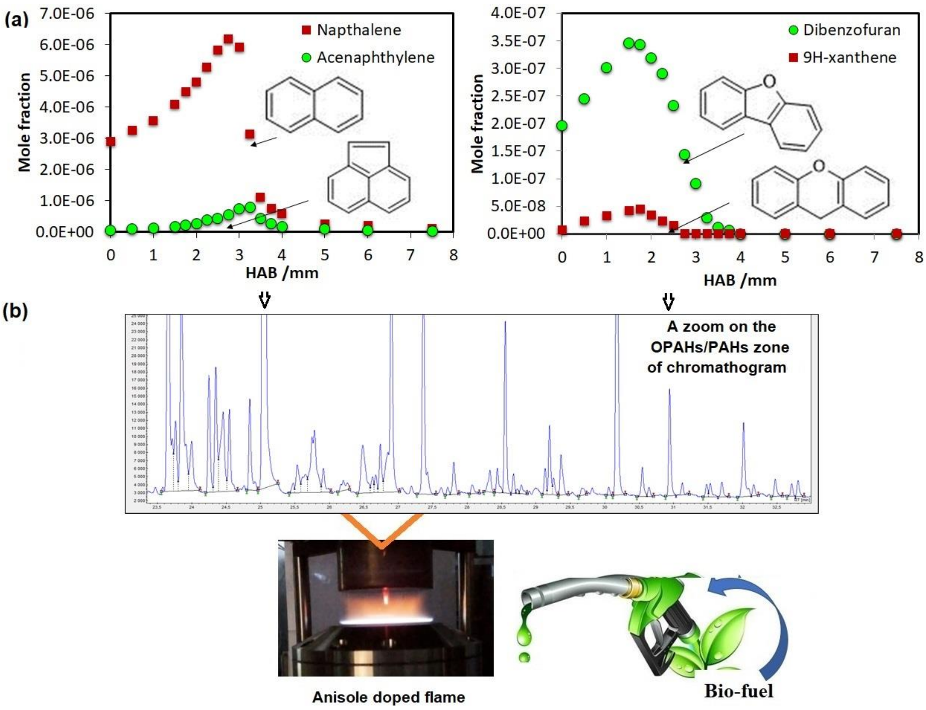

Fig. 1. Examples of OPAH/PAH profiles (a) and chromatogram for an anisole doped flame (b)

References

[1] W. Leitner, J. Klankermayer, S. Pischinger, et al., *Angew Chem-Int Edit*, 56, 5412-5452 (2017).

[2] C. Guan, C.S. Cheung, X. Li, Z. Huang, *Atmospheric Pollution Research*, 8, 209-220 (2017).

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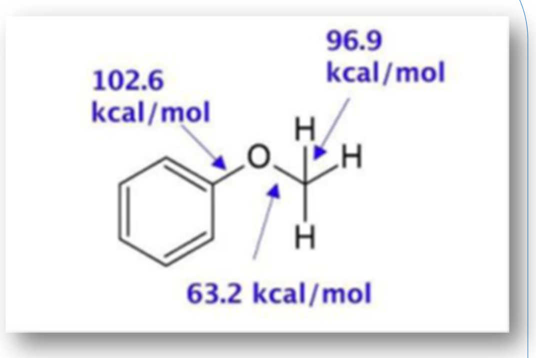
Context

- ~80% energy production from the combustion of fossil fuels. Research interests have shifted towards exploring environment friendly alternative fuels with the intercontinental awareness and recognition of energy and environmental concerns.



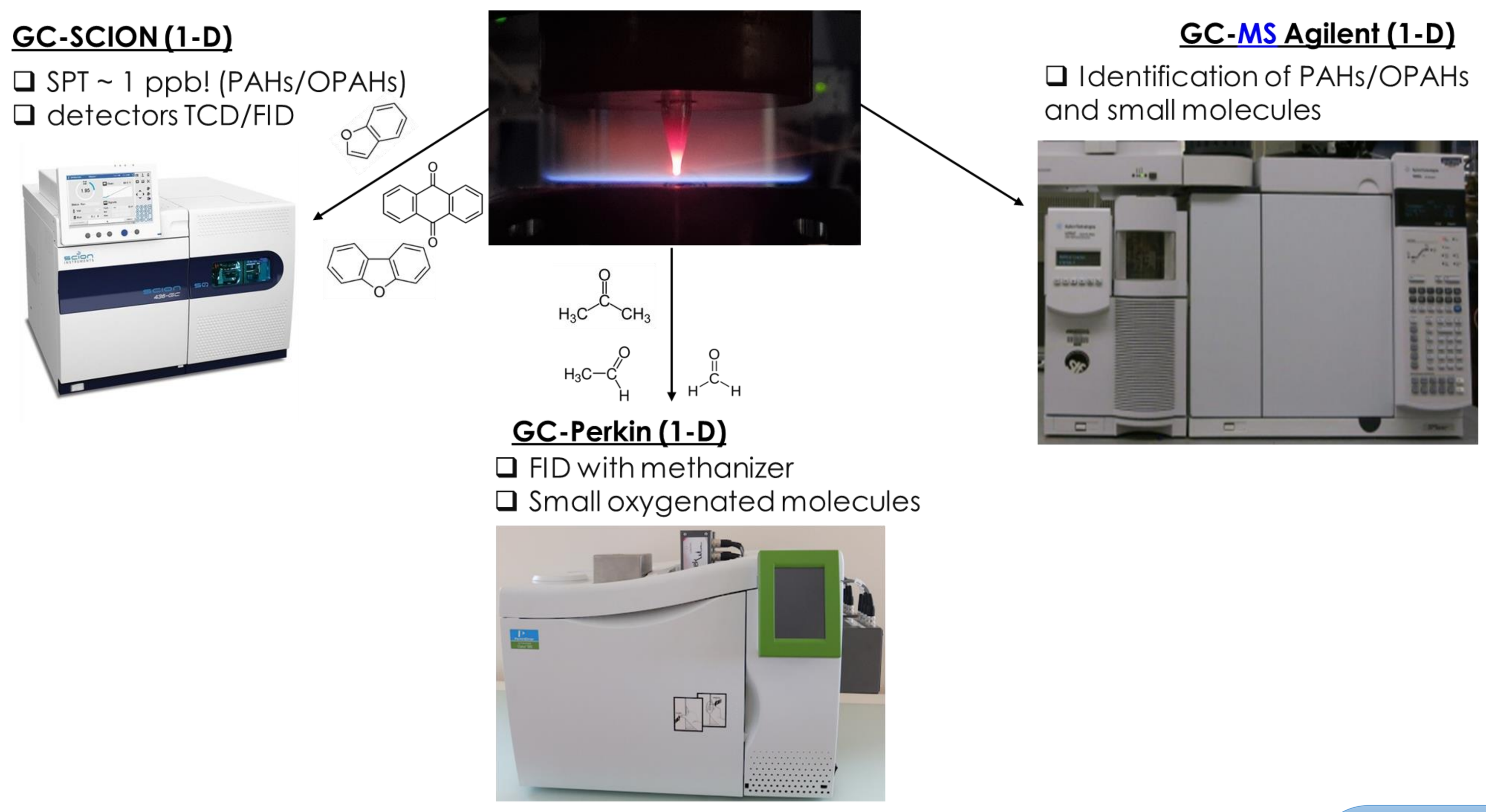
- Anisole has been chosen as an effortless model compound for lignin-based biofuels. It is also a worthy biofuel candidate owing to its suitable properties, for instance, its high octane number and a superior net heating value than ethanol [1], [2]. Development and validation of kinetic mechanisms need reliable experiments.

Fuel	Formula	Molar mass (g/mol)	Boiling Point (°C)	LHV[a] (MJ/L)	Viscosity (cP[a])	RON[a]
Anisole	C_7H_8O	108.14	154	33	1.00	103
Ethanol	C_2H_5OH	46.07	78	27	1.1	107
iso-Octane	C_8H_{18}	114.23	99	44	0.50	100

[a]*LHV – Lower Heating Value/Net Calorific Value; RON-Research Octane Number; cP-centipoise*

Methodology

Premixed Flame at atmospheric pressure



Aim

Understand the co-formation of oxygenated and non-oxygenated aromatics in flames of biofuel and fuel mixtures at atmospheric pressure

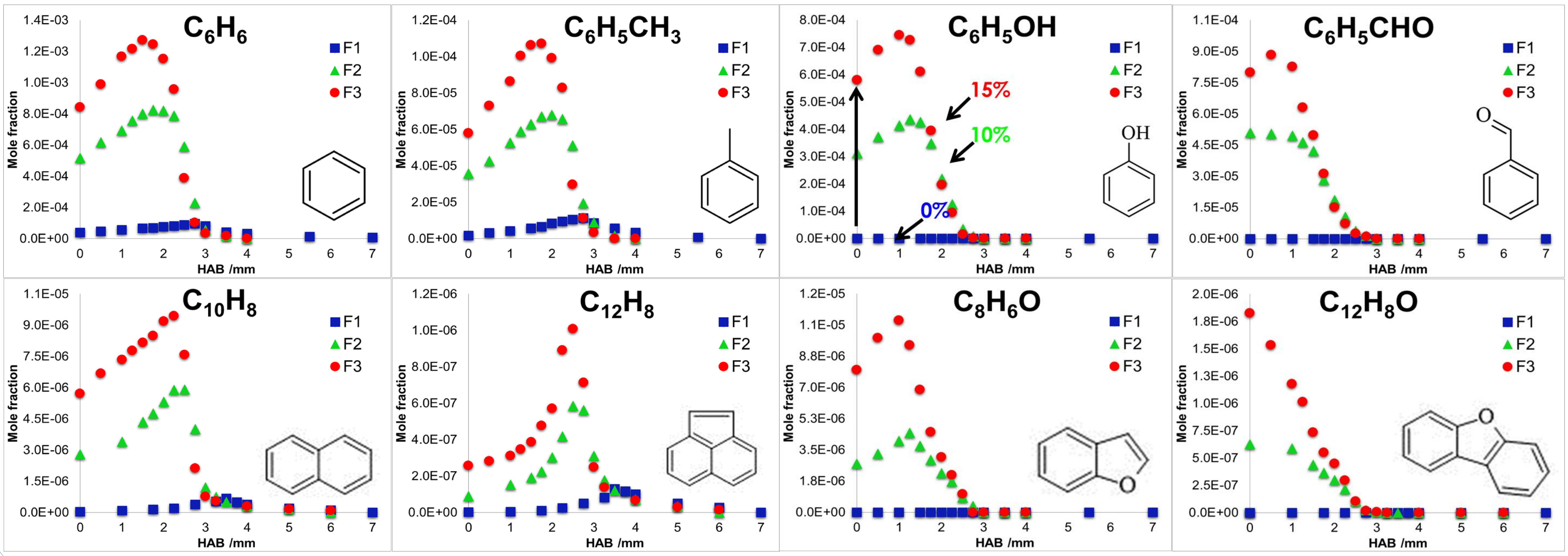
Results

- 5 laminar premixed flames were stabilized (3 selected flames are shown here)
- Some selected oxygenated and non-oxygenated aromatics have been shown here in selected flames
- Around 70 species have been identified and quantified
- Out of these, 30 species are aromatics
- Out of these 30 aromatics, 65% are oxygenated species
- Benzene is the major species amongst classical aromatic compounds while phenol being the major species amongst oxygenated aromatic compounds

Selected Flames

Equivalence Ratio-1.82 Anisole (%)-0 | *Equivalence Ratio-1.82 Anisole (%)-10* | *Equivalence Ratio-1.82 Anisole (%)-15*

Selected oxygenated and non-oxygenated aromatics



Conclusions and perspectives

- We have identified and quantified several aromatics and oxygenated aromatics that are formed during the combustion of anisole blends in flame conditions using advanced Gas Chromatography
- Temperature measurements have been performed using Thermometry in collaboration with Dr. X. Mercier and Dr. A. Faccinetto
- Soot size measurements using SMPS and laser diagnostics will be performed in collaboration with Dr. P. Desgroux and Dr. A. Faccinetto
- Simulations will be performed using the kinetic model being developped in our Laboratory (a modeling work in progress is being carried out simultaneously in the group which would allow a precise interpretation of the effects of the oxygenated additives to complete this work)

Acknowledgments

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2. McCormick et al. *Energy Fuels*, vol. 29, no. 4, pp. 2453–2461, Apr. 2015, doi: 10.1021/ef502893g.