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

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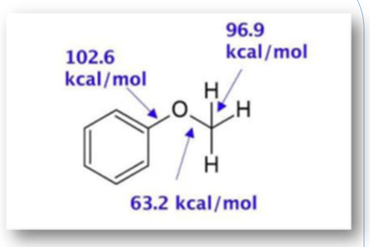
Context

- ~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.

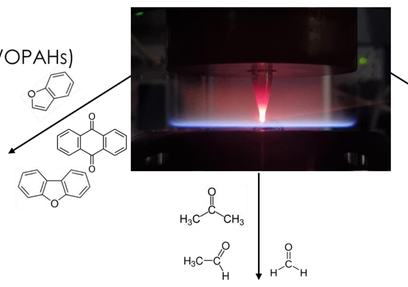
Fuel	Formula	Molar mass (g/mol)	Boiling Point (°C)	LHV[a] (MJ/L)	Viscosity (cP[a])	RON[a]
Anisole	C_7H_8O	108.14	154	33	1.00	103
Ethanol	C_2H_5OH	46.07	78	27	1.1	107
iso-Octane	C_8H_{18}	114.23	99	44	0.50	100

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

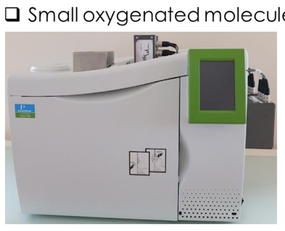
Methodology

Premixed Flame at atmospheric pressure

GC-SCION (1-D)
- ❑ SPT ~ 1 ppb! (PAHs/OPAHs)
- ❑ detectors TCD/FID



GC-Perkin (1-D)
- ❑ FID with methanizer
- ❑ Small oxygenated molecules



GC-MS Agilent (1-D)
- ❑ Identification of PAHs/OPAHs and small molecules

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

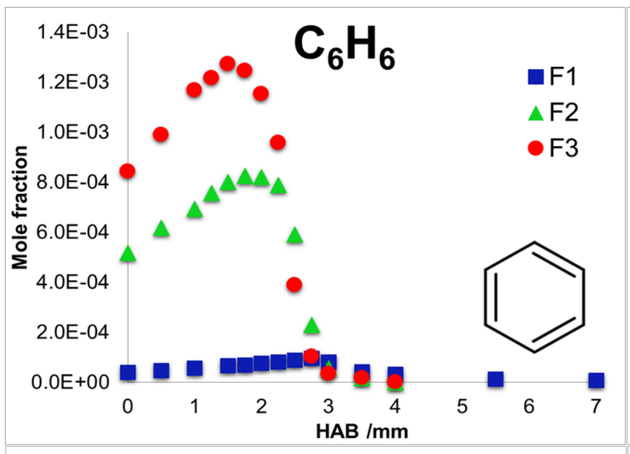
Selected Flames

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)

References

1. Zhou et al. *Fuel*, vol. 115, pp. 469–478, Jan. 2014, doi: 10.1016/j.fuel.2013.07.047.

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

Acknowledgments

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