Experimental and numerical study of laminar burning velocity of neat oxygenated aromatics

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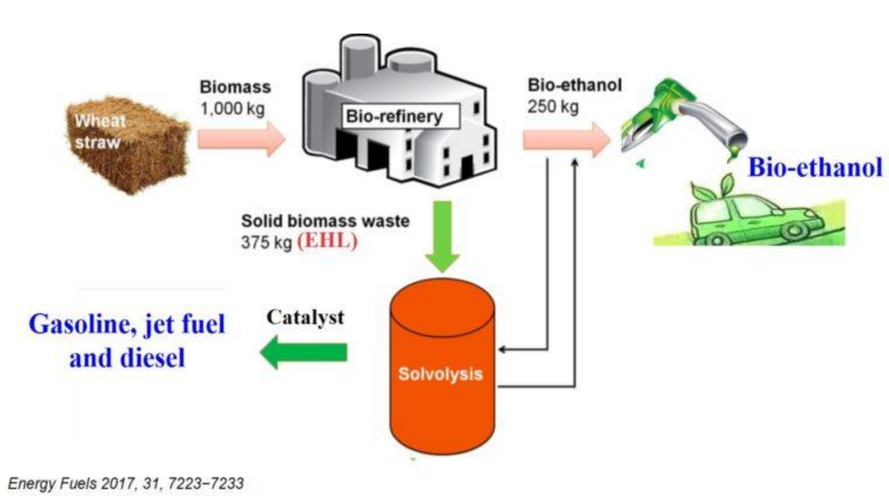
Context

The European project EHLCATHOL [1] aims to develop a new kind of Second Generation (2G) biofuel derived from enzymatic hydrolysis lignin, a waste product of 2G bio-ethanol refineries. The expected chemical composition is a mixture of arenes and oxygenated aromatics [2], these last ones are very scarcely studied in kinetics.

The Laminar Burning Velocity (LBV) is a global indicator of fuels performance. As surrogate compounds of oxygenated aromatics, benzaldehyde, benzylalcohol, 2-phenylethanol (2-PE), anisole, phenol, o-guaiacol and the 3 cresol isomers were studied. A new detailed kinetic model named COLIBRI, containing the chemistry for arenes and oxygenated aromatics, was developed to model and analyze the experimental results obtained in flame as well as all experimental data found in literature for those reactants..

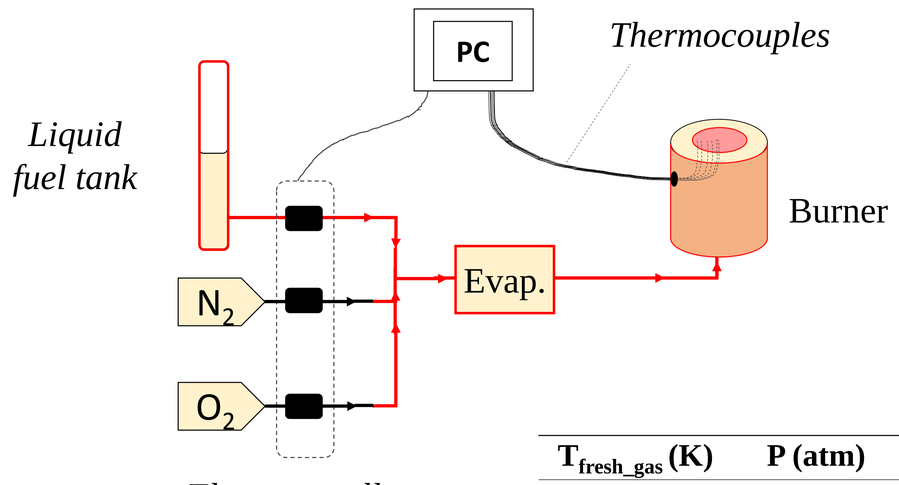


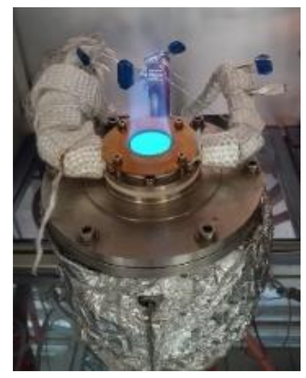
Detailed kinetic model: COLIBRI

Based on the existing models of :

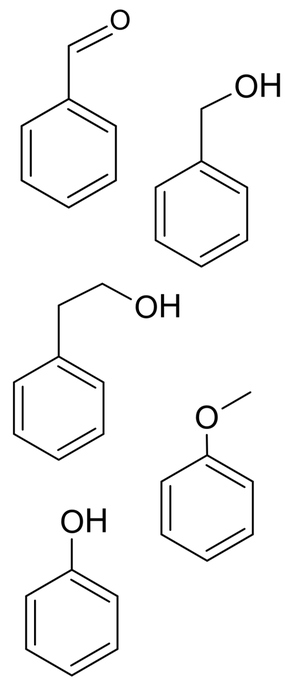
- Burke [3] for C_0-C_3 species,
- Yuan [4] for toluene and PAH mechanisms including many monoaromatic compounds,
- Kukkadapu [5] for xylenes kinetics,
- Büttgen [6] for anisole submechanism completed by that of Wagnon [7] for methylanisole and ethylphenol,
- Nowakowska [8] for guaiacol block.

Experimental facility: flat flame burner with the heat flux method [9]

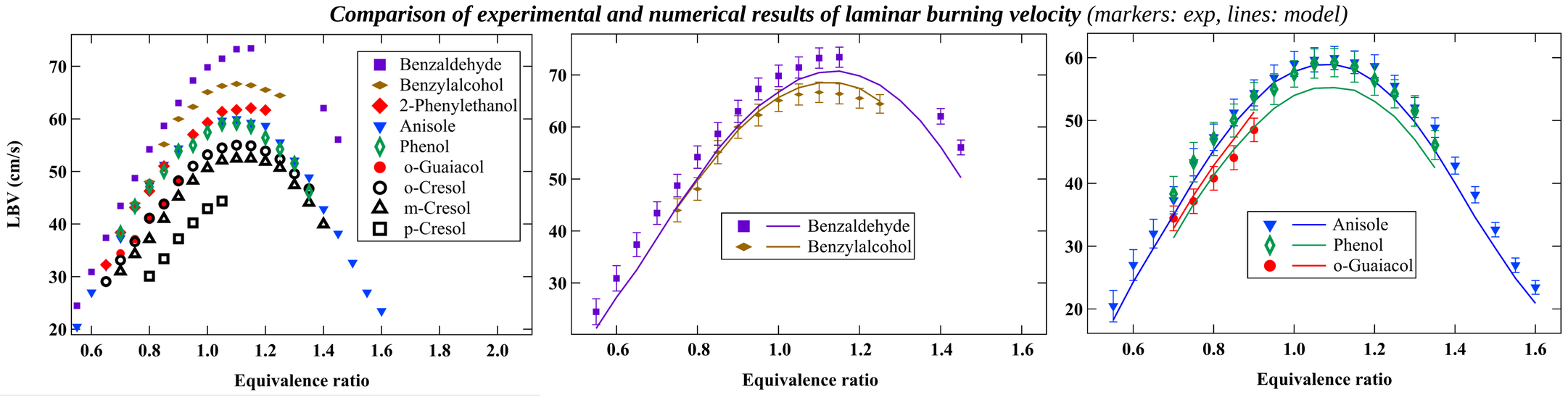


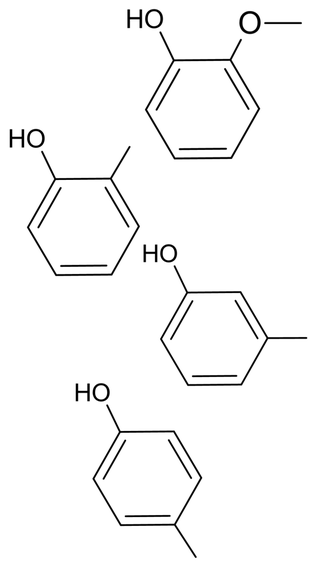


T_{fresh_gas} (K)	P (atm)	Φ
398	1	0.55 – 1.6

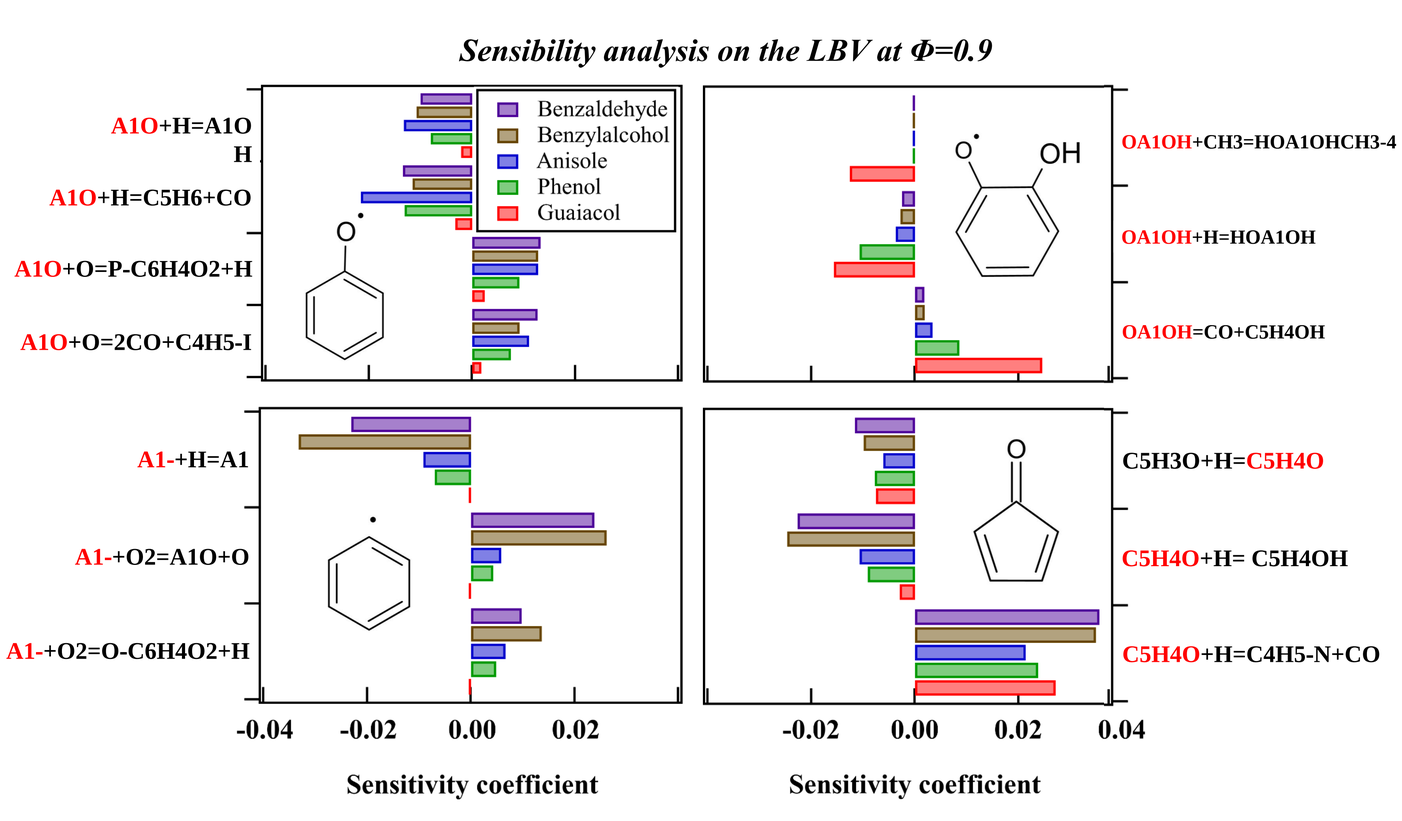


Comparison of experimental and numerical results of laminar burning velocity *(markers: exp, lines: model)*





Sensibility analysis on the LBV at Φ=0.9



Results and analyses:

- 2-PE, anisole and phenol have really close LBVs.
- O-guaiacol and o-cresol have almost the same LBVs.
- The LBV of p-cresol is clearly lower than that of other isomers.
- The sensibility analyses highlight the key role of resonantly stabilized radicals and cyclopentadienone.

Future works:

- Model development for 2-PE and differentiated cresol isomers.
- Experimental study of mixtures made of iso-octane / n-heptane / oxygenated aromatics.

[1] http://ehlcathol.eu/ . [2] F. Battin-Leclerc, Catalysis Today 408 (2022) 150-167. [3] U. Burke, Combust. Flame 165 (2016)125-136. [4] W. Yuan, Combust. Flame 162 (2015) 3-21. [5] G. Kukkadapu, Proc. Combust. Inst. 37 (2019) 521-529. [6] R.D. Büttgen, Fuel 269 (2020) 117190. [7] S. Wagnon, Combust. Flame 189 (2018) 325-336. [8] M. Nowakowska, J. Phys. Chem. A 122 (2018) 7894-7909. [9] K.J. Bosschaart, Combust. Flame, 136 (2004) 261-269.

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