EHLCATHOL

Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions

WP6: Measurements and modeling of fuel combustion and emission

Oxidation of guaiacol in a Jet-stirred reactor

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement no 101006744

http://ehlcathol.eu/

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Presentation outline

I. State of the art

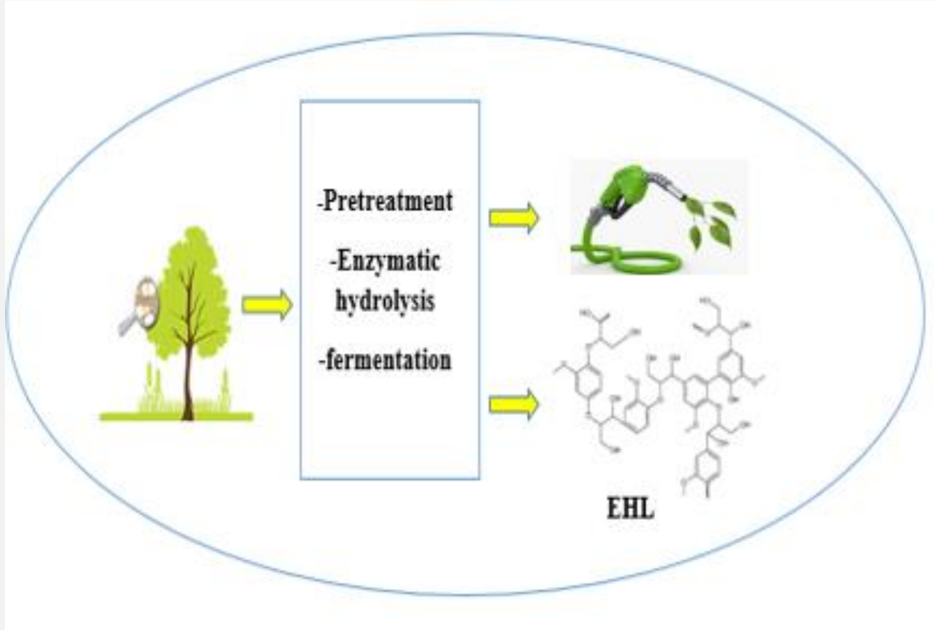
II. Experimental study of Guaiacol oxidation:

- experimental setup
- results

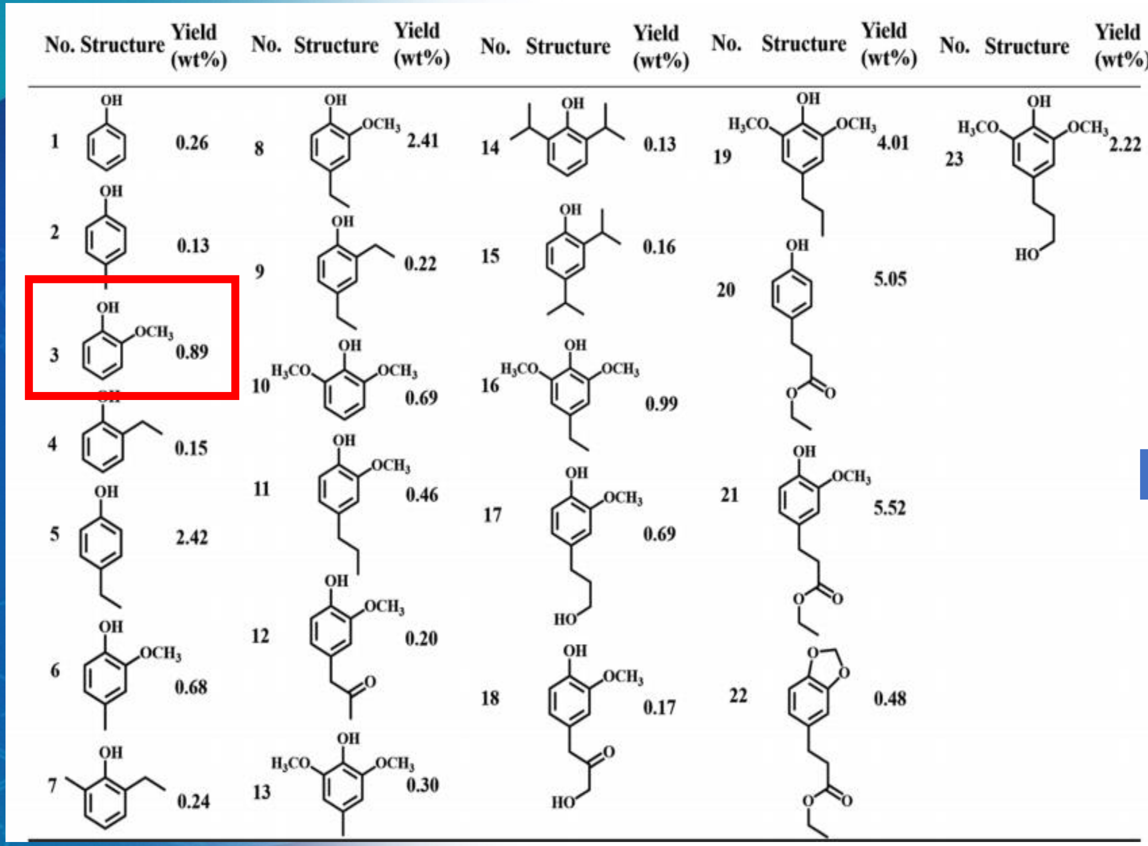
III. Conclusion and perspectives

1. State of the art

- EHLCATHOL project ⟶ **WP6:** Measurements and modelling of fuel combustion and emission (LRGP).
- Bioethanol production process ⟶ Enzymatic hydrolysis lignin.

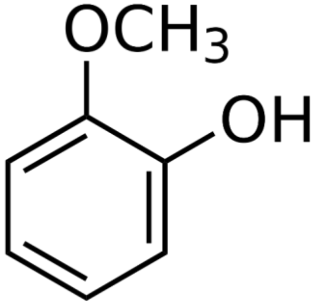


1. State of the art



Sang, Y., et al. 2020. Catalytic Depolymerization of EHL into Monomers over an Unsupported Nickel Catalyst in Supercritical Ethanol. Industrial & Engineering Chemistry Research.

Mainly oxygenated aromatics



Chemical structure of Guaiacol.

	Pyrolysis	Oxidation
Flow reactor	Klein et al., 1980 Ceylan et al., 1982	–
Jet-Stirred reactor	Nowakowska et al., 2018	Nowakowska et al., 2018

Guaiacol oxidation

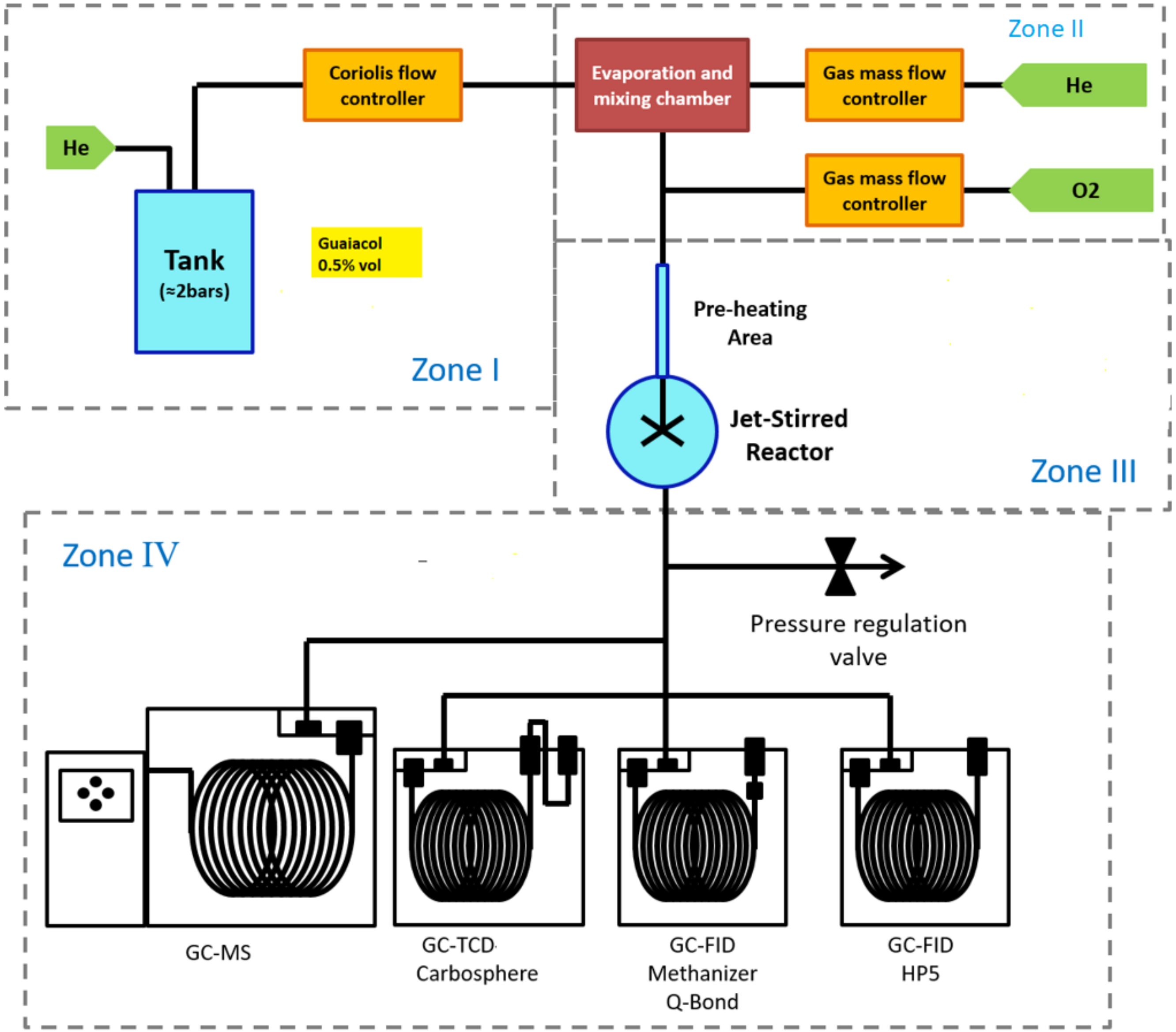
Jet-stirred reactor

2. Experimental setup

Complete oxidation reaction:

$$C_7H_8O_2 + 8\,O_2 = 7\,CO_2 + 4\,H_2O$$

Temperature (τ)	**600-950 K**
Residence time (τ)	**2s**
Pressure (P)	**1.07 bar**
Equivalence ratio (φ)	**1**



3. Analytical devices

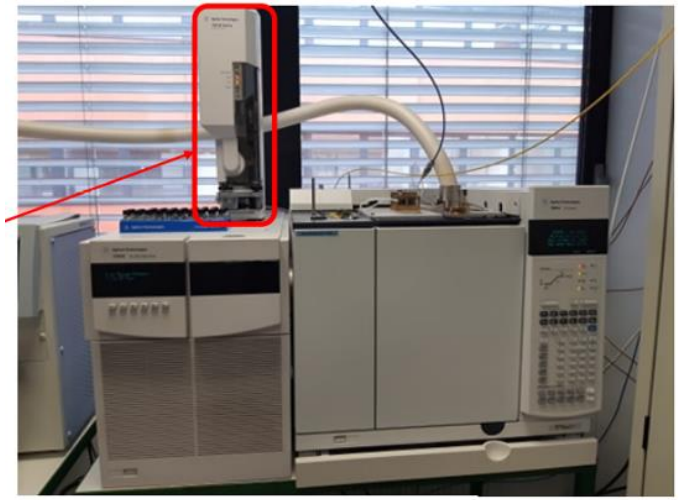
- **Quantification**

GC-1D

- **TCD:** Carbosphere packed column: light products (C_1-C_2)
- **FID** Q-Bond capillary column preceded by a methanizer : (C_1-C_6)

- **Identification**

- **GC-MS-FID**



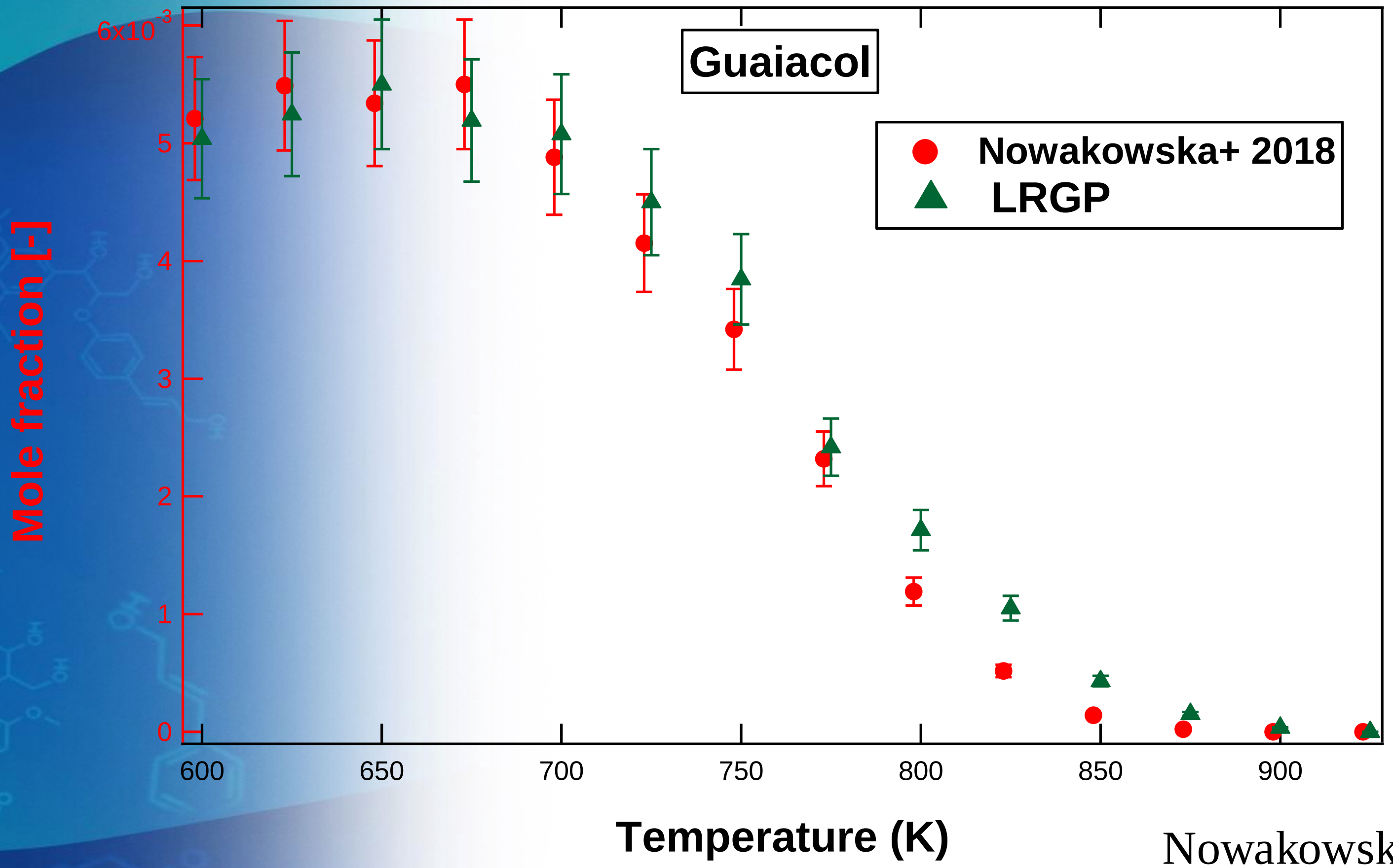
- **2D-GC (improved separation)**

4. Analysis of heavy species

Trap at liquid nitrogen temperature

- ✓Preparation of samples
- ✓100 μL standard solution (*n*-octane)
- ✓5 mL of acetone

5. Guaiacol reactivity



Residence time (tau)	**2s**
Pressure (P)	**1.07 bar**
Inlet concentration	**0.5% (vol)**

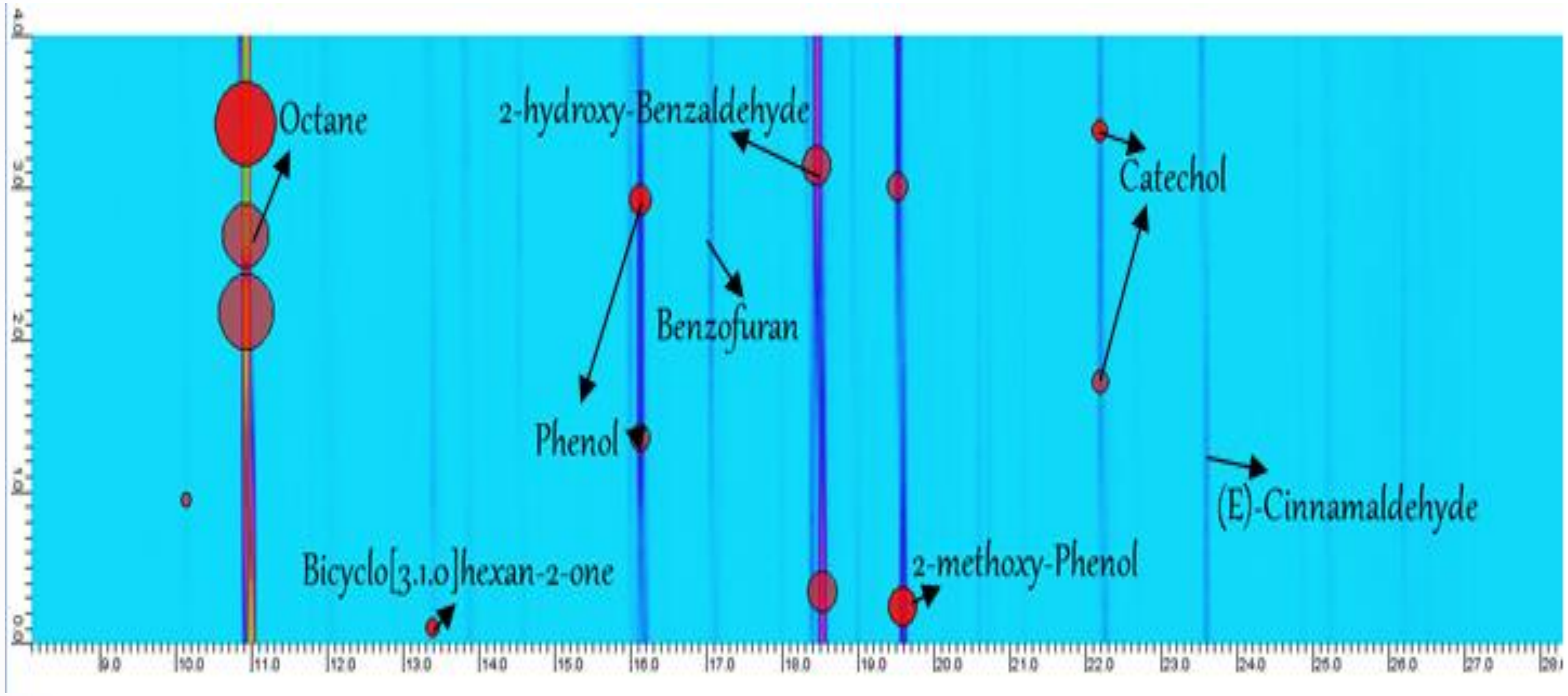
Nowakowska, M., Herbinet, O., Dufour, A., Glaude, P.-A. 2018. *Kinetic Study of the Pyrolysis and Oxidation of Guaiacol. The Journal of Physical Chemistry A.*

6. Main products

The main products	
Light products	Heavy products
CO, CO_2 , CH_4, C_2H_4, C_2H_4, C_2H_6, C_3H_6, C_3H_4,	2-Hydroxy-benzaldehyde; Phenol; Pyrocatechol; Cinnamaldehyde; Benzofuran; 1,3-Benzodioxol-2-one; Cresol.

7. Improved separation by 2D-GC

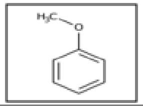
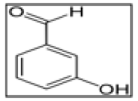
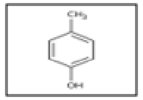
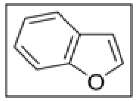
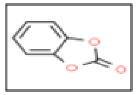
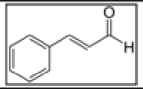
Octane is not a product ; it is the standard used for the quantification

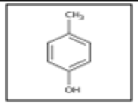
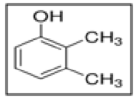
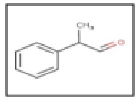
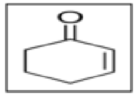
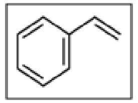
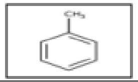


First Retention time

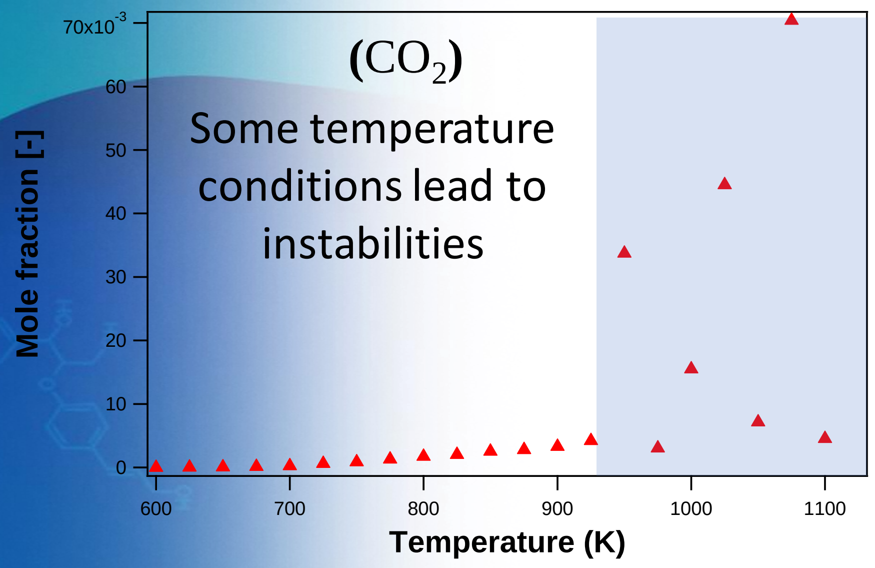
Second Retention time

8. Comparaison between 1D-GC and 2D-GC products

Molecules	GC-1D	GC-2D
Anisole 	✓	✓
2-hydroxybenzaldehyde 	✓	✓
2,3-dimethylphenol 	✓	✓
Benzofurane 	✓	✓
1,3-benzodioxol-2-one 	✓	✓
(E)-Cinnamaldehyde 	✓	✓

Molecules	GC-1D	GC-2D
P-cresol 	✗	✓
2,3-dimethylphenol 	✗	✓
2-phenylpropenal 	✗	✓
2-cyclohexan-1-one 	✗	✓
Styrène 	✗	✓
Toluène 	✗	✓

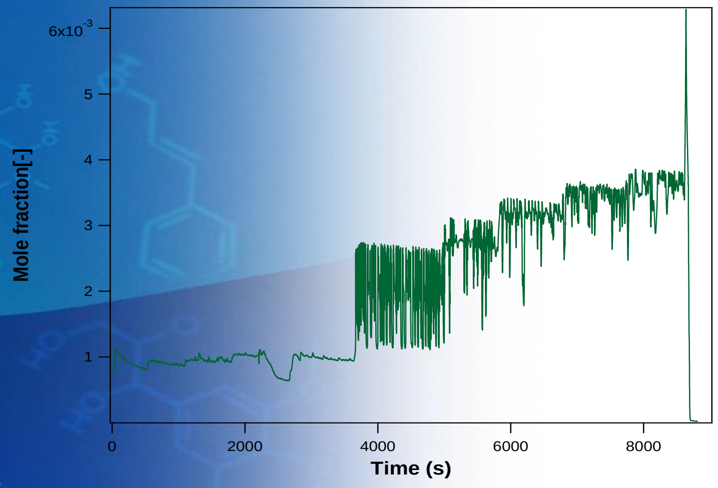
9. High temperature oscillations behaviour (CO_2)

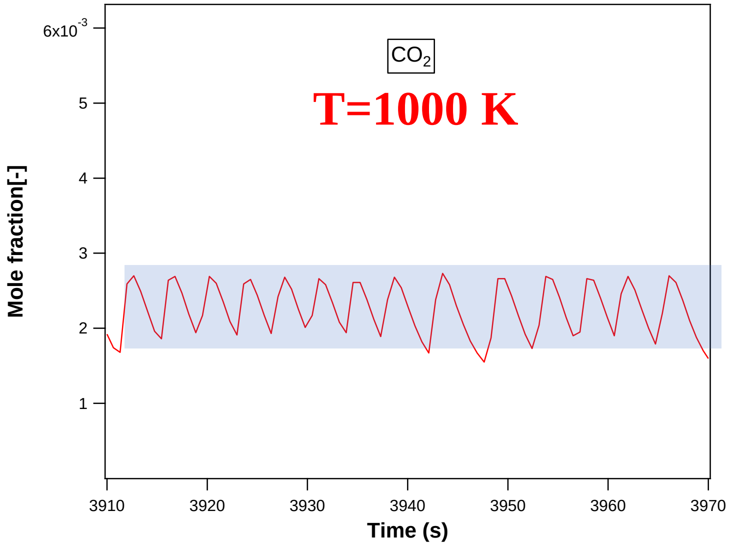


Lubrano Lavadera, M., et al. (2018). Oscillatory Behavior in Methane Combustion: Influence of the Operating Parameters. Energy & Fuels.

Stagni, A., et al. (2019). The role of chemistry in the oscillating combustion of hydrocarbons: an experimental and theoretical study. Chemical Engineering Journal, 123401.

Quantification using online MS





Conclusion

- Same guaiacol conversion observed between our study and literature.
- The same reactivity of heavy and light species.
- 2D-GC: improved separation of the species.

Perspectives for Guaiacol

- Study of guaiacol oxidation in fuel-lean (Φ=0.5) and fuel-rich (Φ=2.0) environments,
- Continue the study of oscillations for the heavy species (>C_5), the identification of conditions (amplitude, temperature range)
- Identification of the structures of new compounds detected by GC-2D,
- Development of a detailed kinetic model for the oxidation of Guaiacol

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