



Experimental Study on Pollutant Formation in low-pressure Flames of Furanic Biofuels

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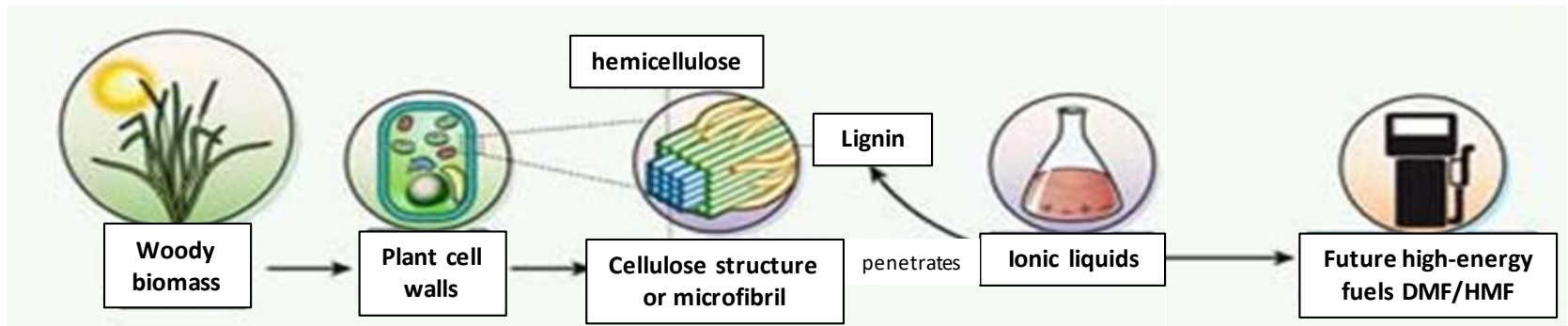
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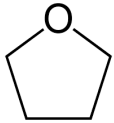
PhD Thesis financed by *Region Hauts-de-France* and *Université de Lille*

Motivation

Biofuels are seen as an interesting and promising alternative to fossil fuels.



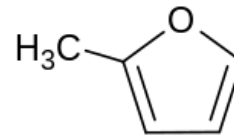
Furan family



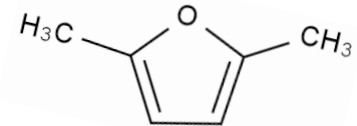
Tetrahydrofuran (THF)



Furan (F)



2-Methylfuran (MF)



2,5-Dimethylfuran (DMF)

- from **ligno-cellulosic biomass**
- **oxygenated fuels** comparable to commercial fuels
- What is **their impact on the formation of pollutant** emissions?

“Furan family” in literature...

➤ Oxidation in laboratory condition:

❖ Shock Tube

(Ignition delay time)

- SOMERS, K., et al." Proc. Combust. Inst., 34, (2013) **MF**
- XU, N., et al. Energy Fuels 29. (2015) **DMF, F, MF.**
- ...

❖ Premixed Laminar Flame

(Kinetics at High T)

- LIU, D., et al. Combust. Flame, 161, (2014) **F**
- TIAN, Z. et al. Combust. Flame ,158, (2011) **F**
- TRAN, L., et al. Combust. Flame, 162, (2015) **THF**
- TOGBÉ,C., et al.. Combust. Flame ,161, (2014) **DMF**
- ...

❖ Isothermal quartz flow reactor

(Kinetics at High T)

- ALEXANDRINO, K., et al., Proc. Combust. Inst ,35,(2015) **DMF**
- ...

➤ Oxidation in real condition:

❖ Rapid Compression Machine

(Kinetics at Low T - Ignition delay time)

- VANHOVE, G., et al. Energy Fuels 29 (2015) **THF**
- FENARD, Y. et al., Combust. Flame, 178 (2017) **MTHF**
- ...

➤ Nitrogen Oxides:

- ALEXANDRINO, K., et al. Energy Fuels, 28, (2014) **DMF, NO**

Nitrogen Oxides

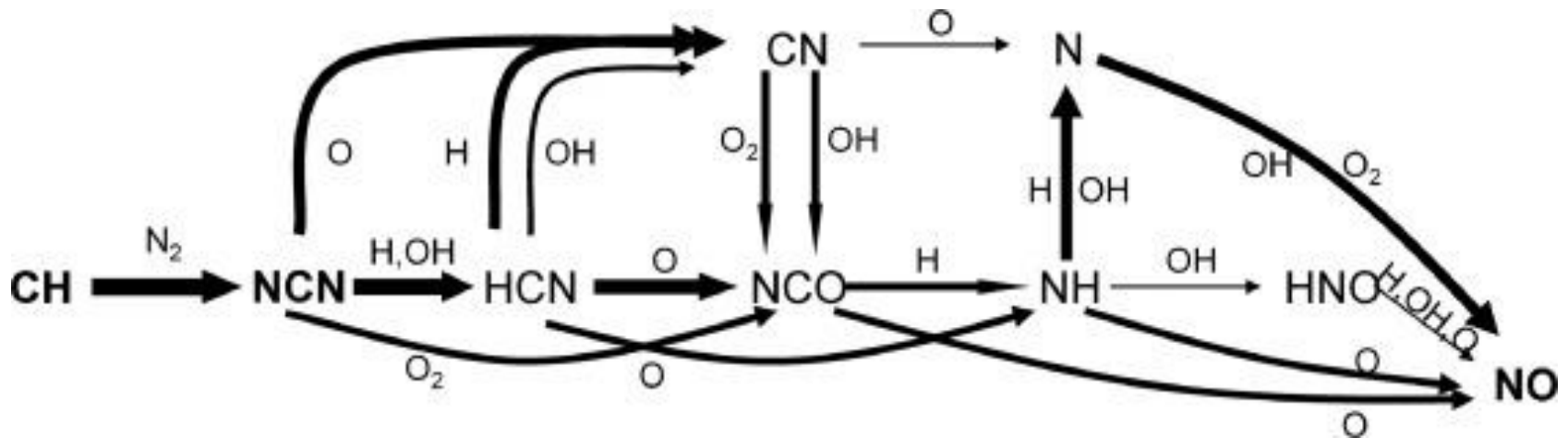
NO is one of the regulated pollutants formed during combustion. It is produced according to different, more or less well-known, pathways :

Thermal - NO

Prompt - NO

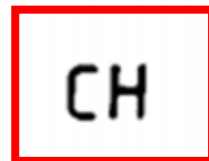
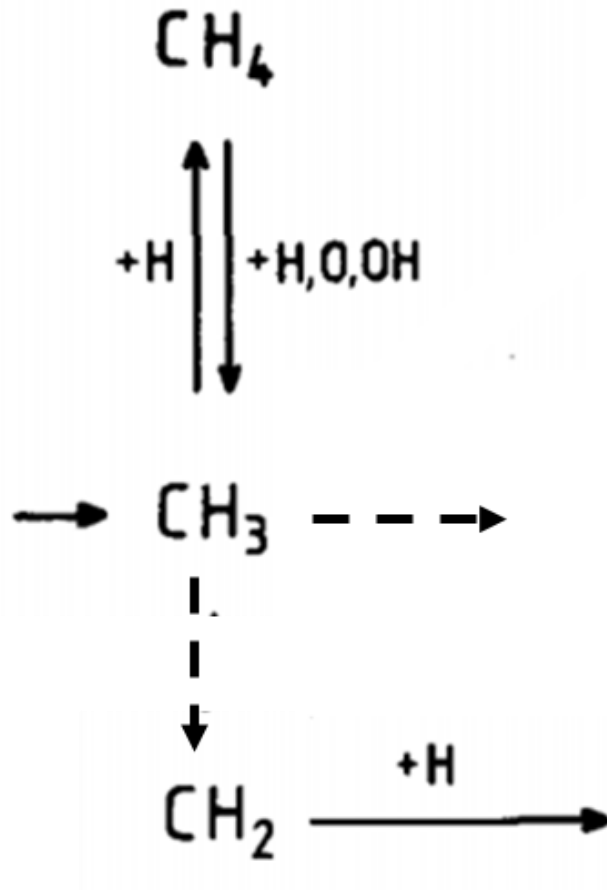
Fuel - NO

It involves intermediate hydrocarbon fragments, particularly CH, reacting with N_2 under fuel rich conditions.

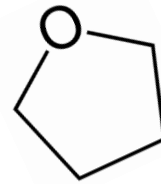


Fuel Oxidation

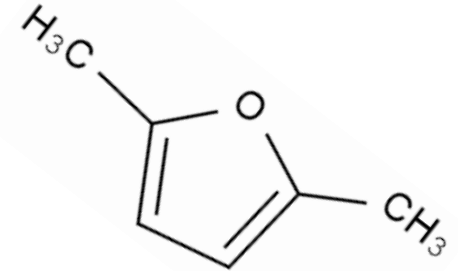
Methane oxidation



↓
NO

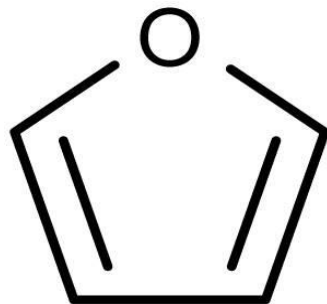


**Biofuel
Oxidation**

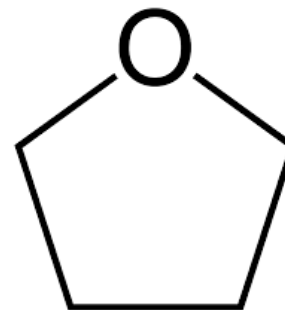


Objectives

Considered fuels :



Furan



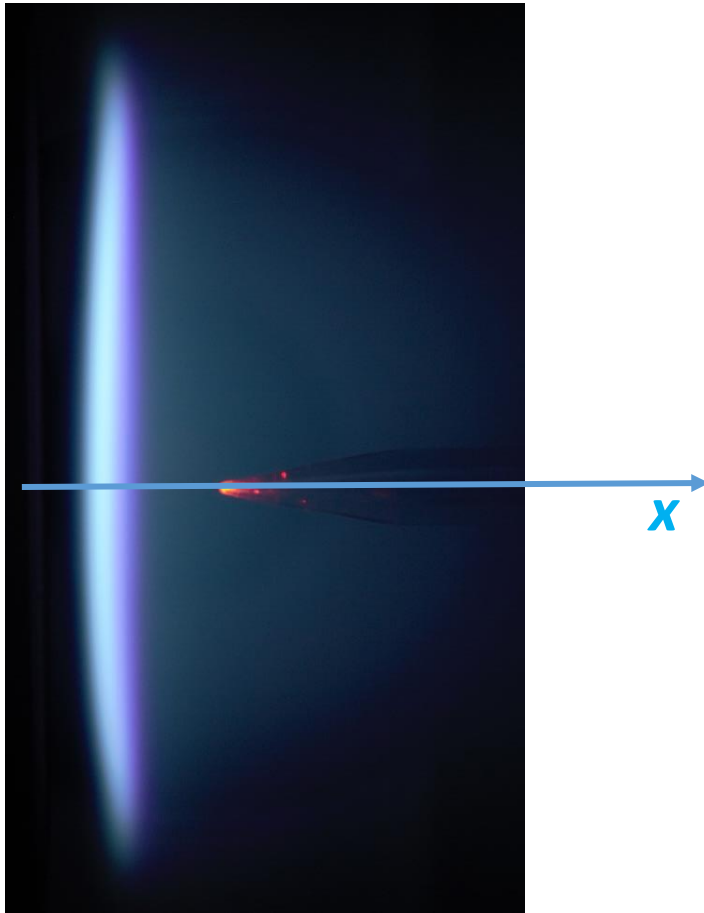
Tetrahydrofuran (THF)

Aims of this study :

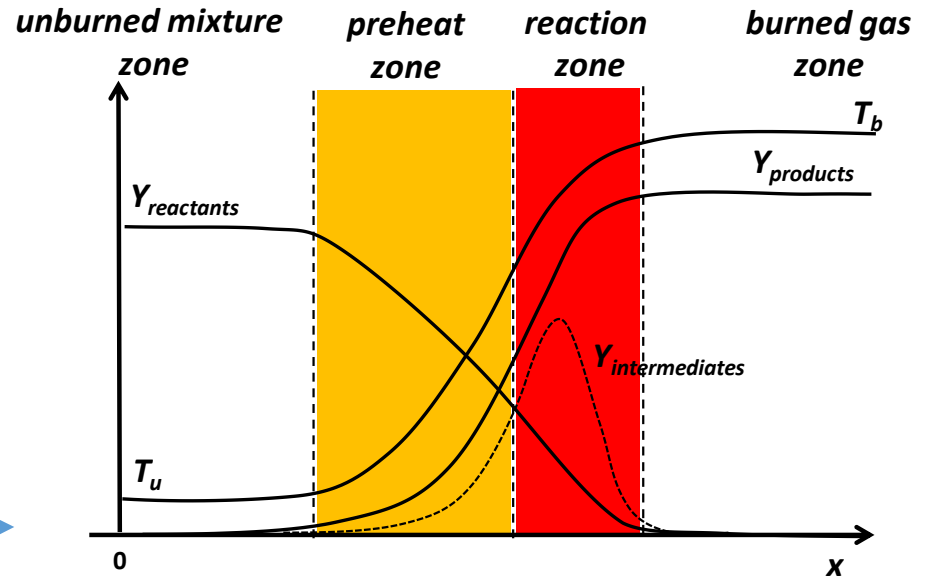
- **Experimental characterization** of NO formation during Furan and THF combustion
- **Development of a model** for NO formation during Furan and THF combustion
- Discussion on **NO formation routes**

Laminar Premixed Flame

Low pressure Flame



Flame structure



Species mole fraction
Temperature

→ $x = \text{HAB}$

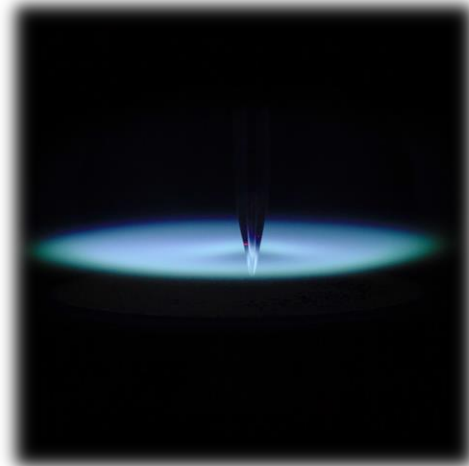
HAB = Height Above the Burner

Operating conditions

Flames	ϕ	*%CH ₄	*%F	*%THF
<i>M1.0</i>	1.0	100	0	0
<i>M1.2</i>	1.2	100	0	0
<i>FM1.0</i>	1.0	50	50	0
<i>FM1.2</i>	1.2	50	50	0
<i>THFM1.0</i>	1.0	50	0	50
<i>THFM1.2</i>	1.2	50	0	50

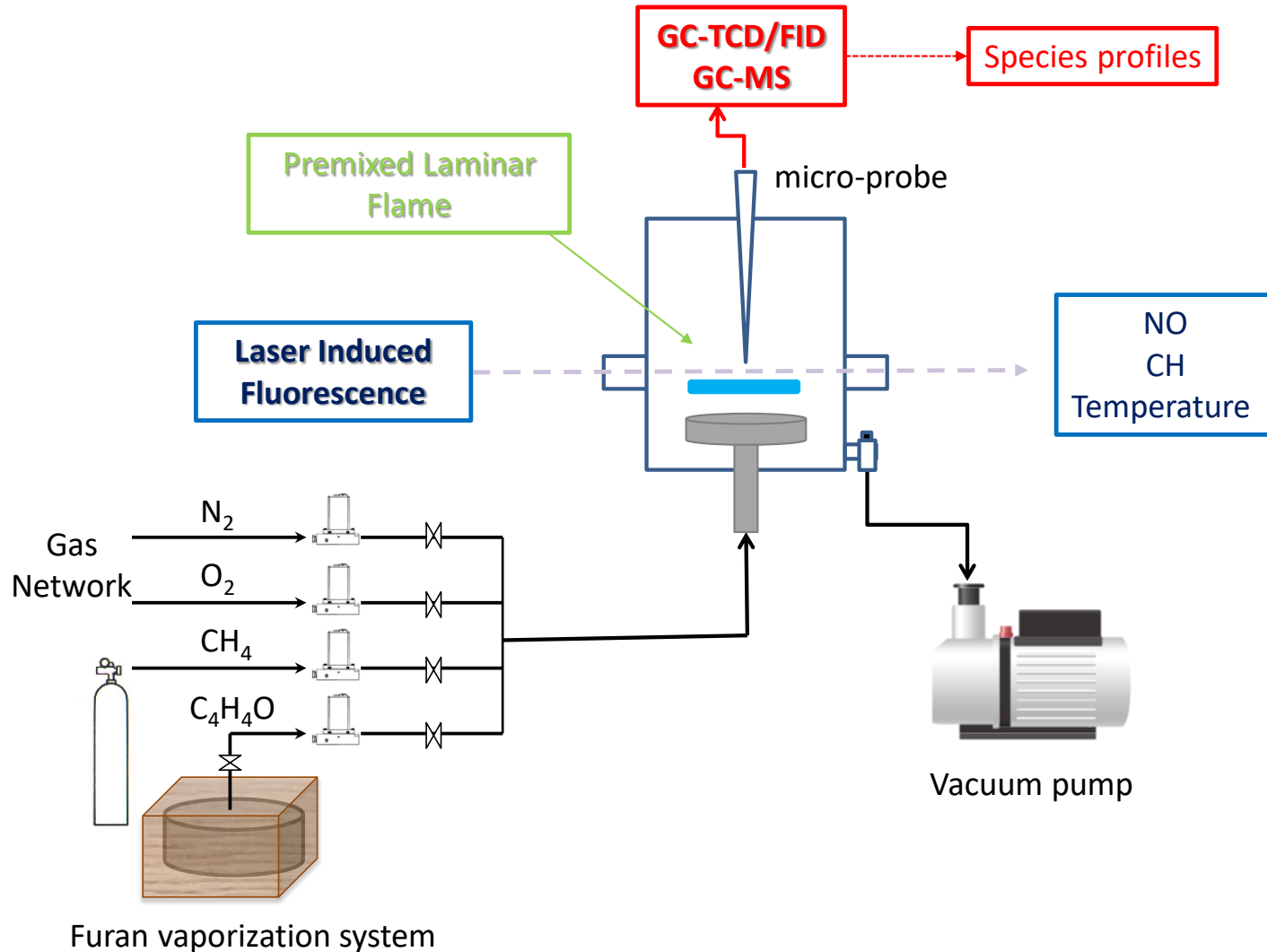
* Fuel composition

Pressure
5.3 kPa



Total Flow
5 sL/min

Experimental set-up



Combustion products and stable intermediates

Gas-Chromatography Results

➤ 6 flames analyzed by gas chromatography equipped with:

- **MS detector**
- **FID detector** coupled with methanizer
- **TCD detector**

➤ 63 species have been detected globally:

❖ *14 in Methane flames*

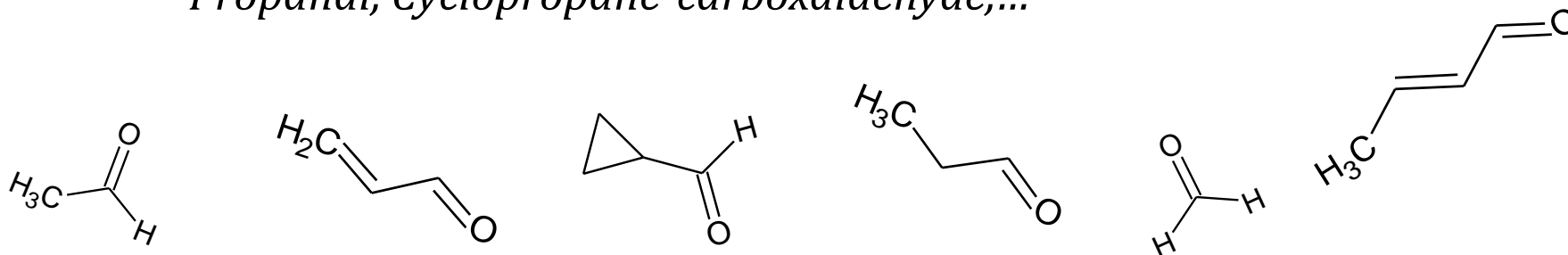
❖ *47 in Furan doped flames*

❖ *49 in THF doped flames*

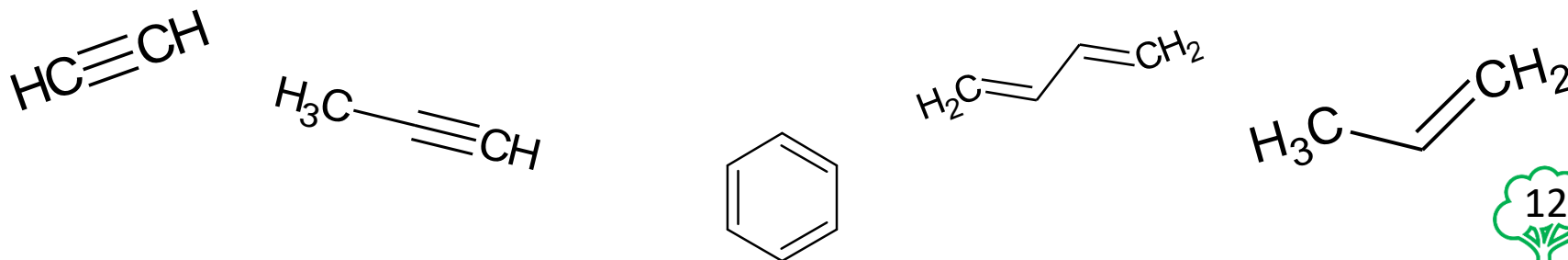
Gas-Chromatography Results

Different pollutants found in Furan and THF flames :

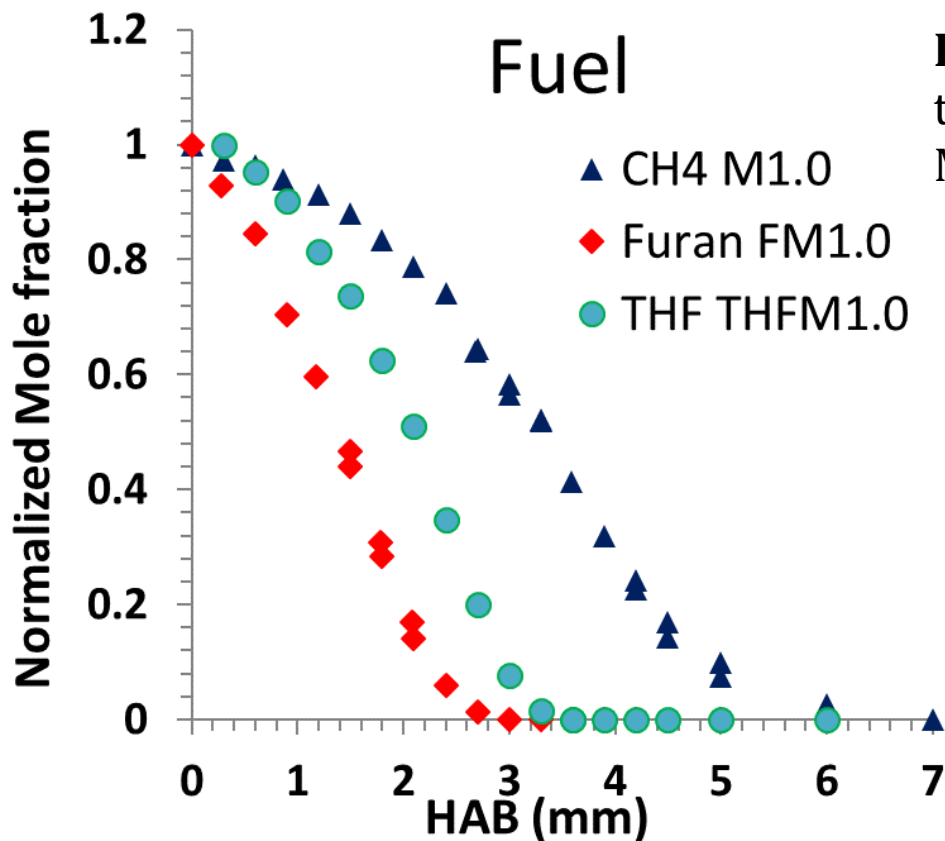
- **Aldehydes** : *Formaldehyde, Acetaldehyde, Acrolein, 2-Butenal, Propanal, Cyclopropane-carboxaldehyde,...*



- **PAH Precursors** : *Acetylene, Propene, Propyne, Allene, 1,3Butadiene, Cyclopentadiene, Benzene,...*



Species profiles



Biofuels flames are stabilized closer to the burner surface with respect to Methane flames

Furan is consumed faster than THF

Burning velocity

$P=101\text{kPa}$ $T=298\text{K}$ $\phi=1$

CH_4^{a} : $S_{u\text{CH}_4} = 36.3 \text{ cm.s}^{-1}$

THF^{b} : $S_{u\text{THF}} = 41.4 \text{ cm.s}^{-1}$

Furan^{c} : $S_{u\text{Furan}} = 62.5 \text{ cm.s}^{-1}$

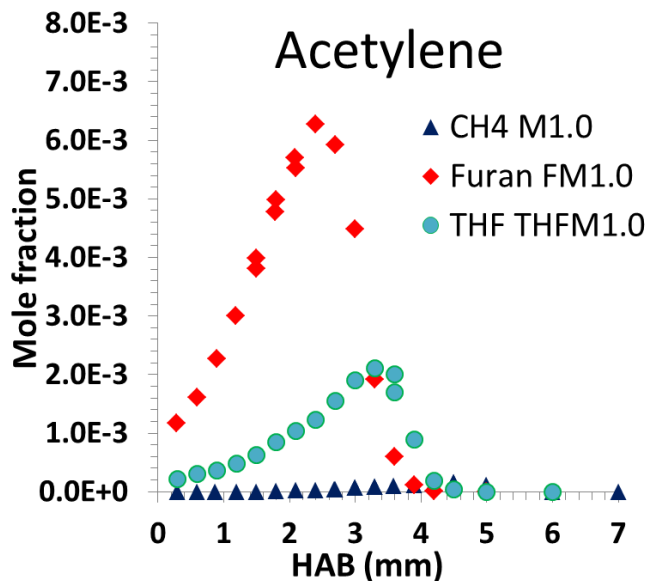
$$S_{u\text{Furan}} > S_{u\text{THF}}$$

^aDirrenberger et al., Energy Fuel, 25 (2011) 3875-3884

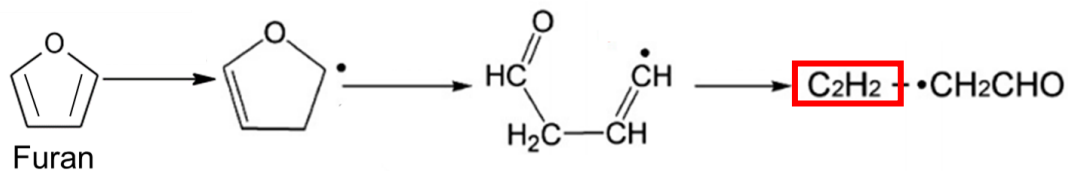
^bTran et al., Combustion and Flame, 162 (2015), 1899-1918

^cGibbs and Calcotte, J. Chem. Eng. Data, 4 (1959), 226-237

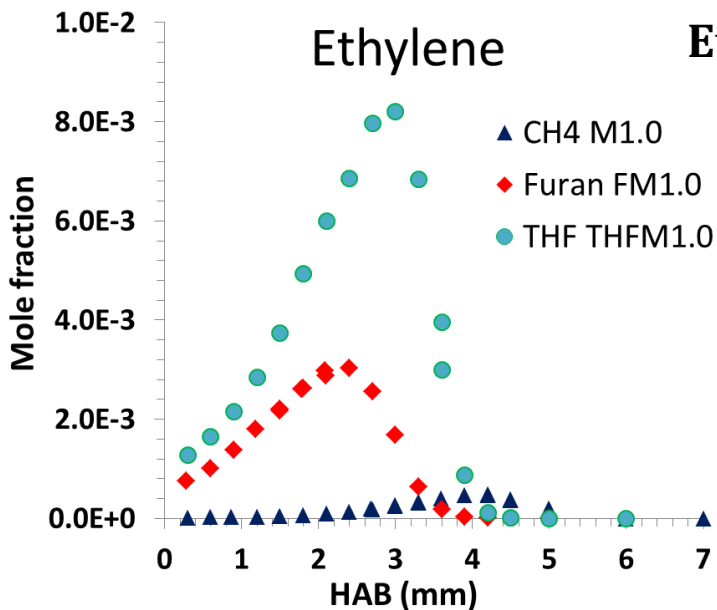
Species profiles



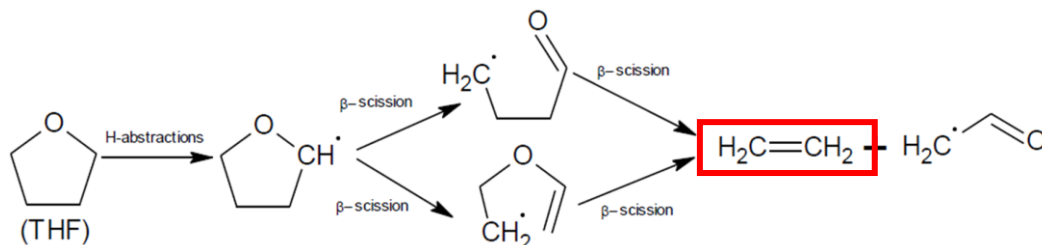
Acetylene formation is enhanced in furan oxidation



Liu et al., Combust. Flame, 61, (2014) 748-7651



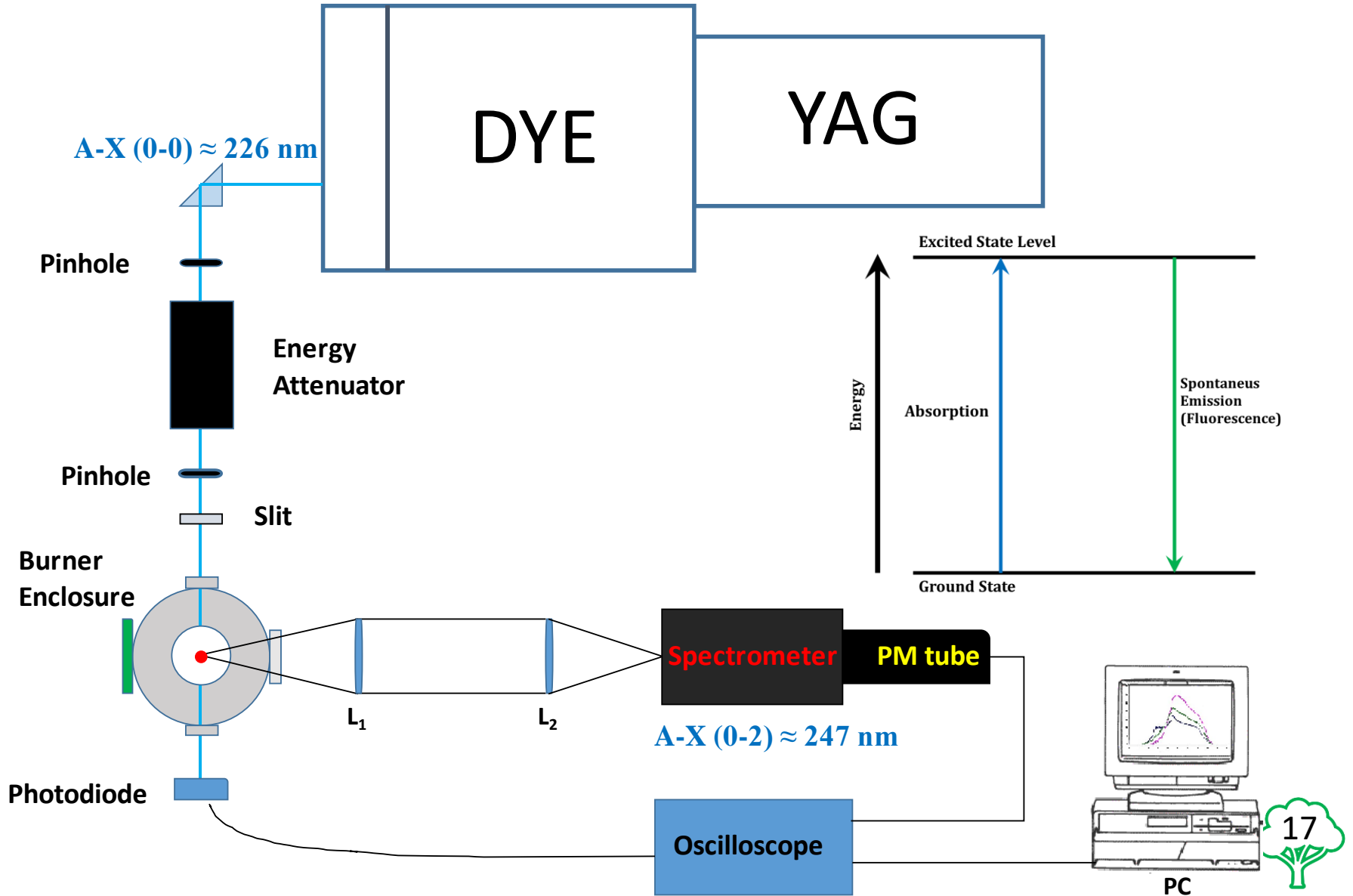
Ethylene formation is enhanced in THF oxidation



Tran et al., Combustion and Flame, 162 (2015), 1899-1918

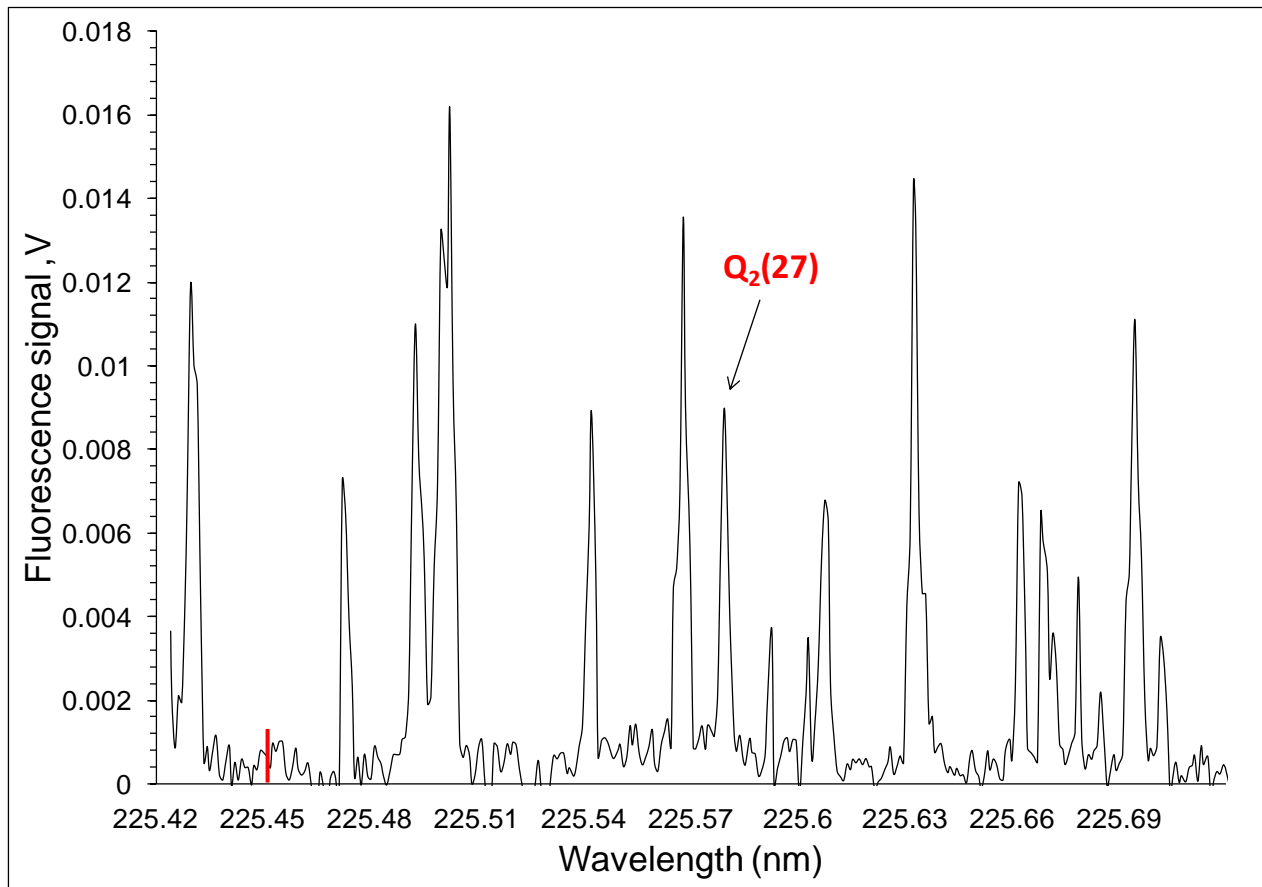
NO measurements

Laser Setup



Excitation-Detection scheme

Experimental NO LIF excitation spectra.



NO molecules are excited by using the $Q_2(27)$ transition of the $A-X(0,0)$ at 225.58 nm

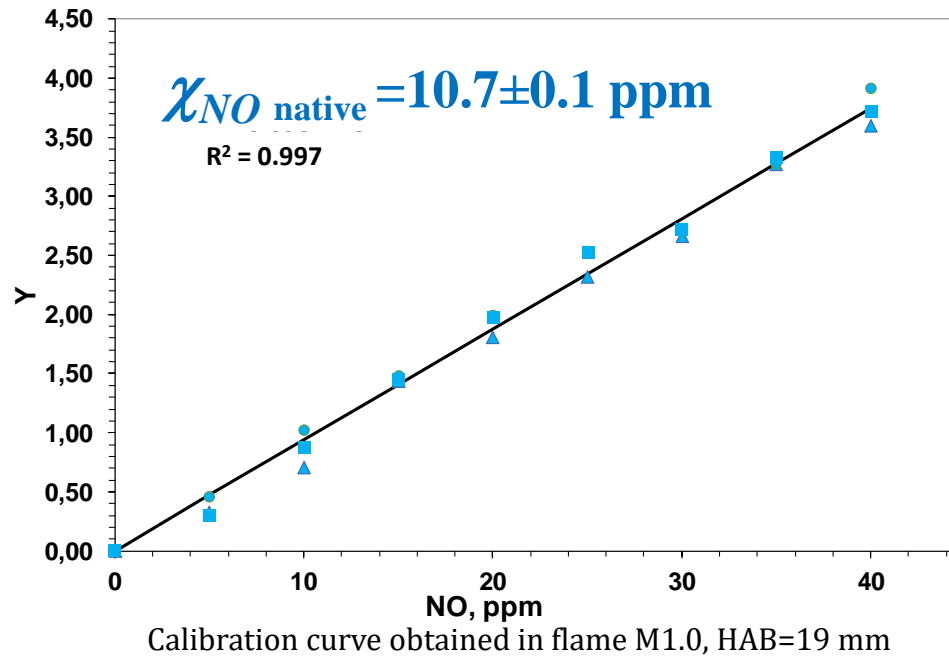
NO LIF signal profile

➤ NO LIF relative profile

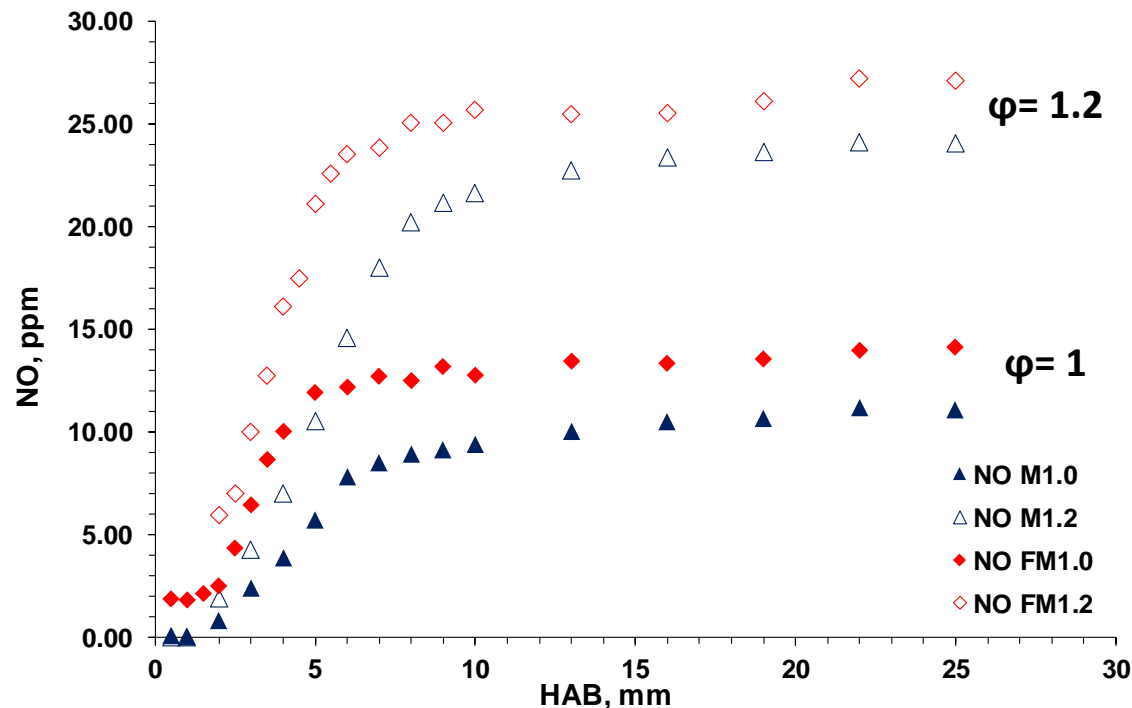
$$\Phi(t) = \frac{GV\Omega}{4\pi} N_{tot} f_b(J'', v'', T) B_{12} U_\nu \frac{A_{21}}{A_{21} + Q_{21}}$$

Concentration of NO molecules

➤ NO doping calibration method in flame M1.0



NO mole fraction profiles



➤ NO formation is enhanced in **fuel-rich conditions**

➤ NO formation is enhanced in **Furan flames** :

+27% at $\phi=1$ and +11% at $\phi=1.2$

(with respect to Methane flames in same operating conditions)

Perspectives....

- Measurement of the NO in THF flames and CH profiles in flames by LIF
- Measurement of the temperature profiles in the flames by NO-LIF thermometry
- Detailed chemical kinetic modeling helps the interpretation of the data

BioFuel oxidation
mechanism

available in literature



NO mechanism
NOMecha2.0*

developed in PC2A
laboratory



Thanks for the attention

