Collaborative Tasks:

Alternative Fuels in Combustion

Studies on reaction kinetics of combustion and emission formation : Neat oxygenated compounds

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Methylal Study

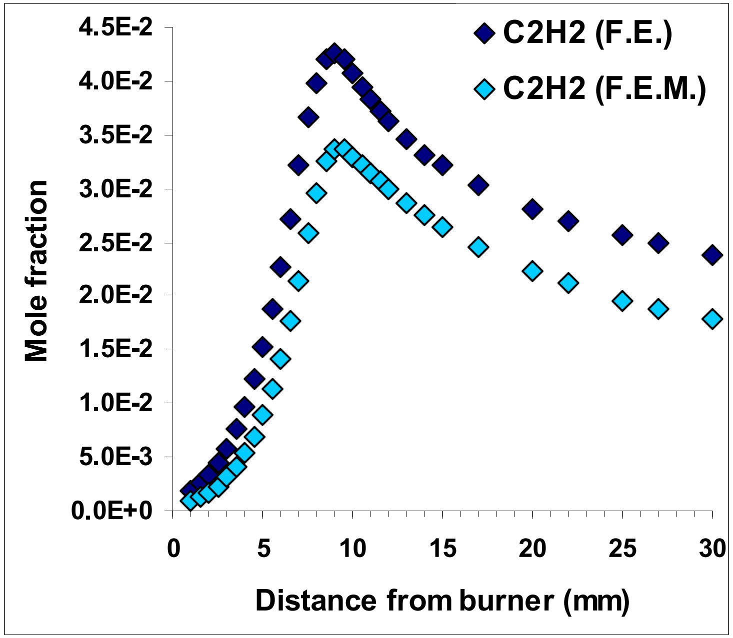
Dimethoxymethane ($C_3H_8O_2$), also called methylal and DMM, is a diether of interest because it has a potential as a neat or blended diesel fuel:

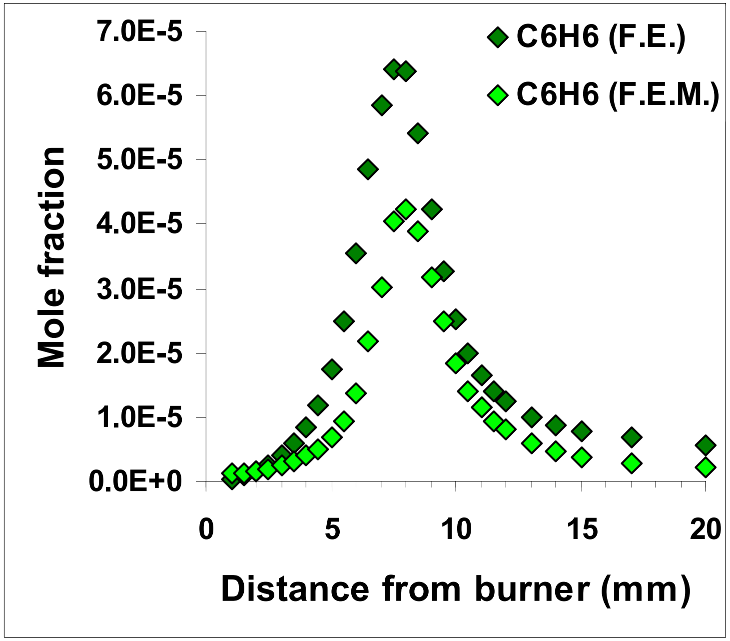
$$CH_3\text{-}O\text{-}CH_2\text{-}O\text{-}CH_3$$

Naegeli (1992) Dodge et al. (1994)	Caterpillar diesel engine	20 % methylal blend in diesel fuel	reduction of smoke opacity by about 50 % at start-up and high idle
Sirman et al. (1998).	Daimler-Benz turbodiesel	15 % methylal blend in ultra-low sulfur diesel	52 % lower particulate matter emission 4 % lower oxides of nitrogen emission
Vertin et al. (1999).	unmodified turbocharged diesel engine	10 % to 30 % blends of methylal in diesel fuel	substantial reduction of particulate matter emission
Cheng et al. (2001)	diesel engine	methylal-in-diesel blends	reduction of the total particle mass concentration, as well as the particle number density and the mean particle diameter

Methylal Study

The addition of dimethoxymethane to rich ethylene flames showed a large decrease of the concentrations of soot precursors (Renard et al., 2002).





However, modeling of this rich flame is difficult due to the lack of thermodynamic and kinetic data on DMM and related species.

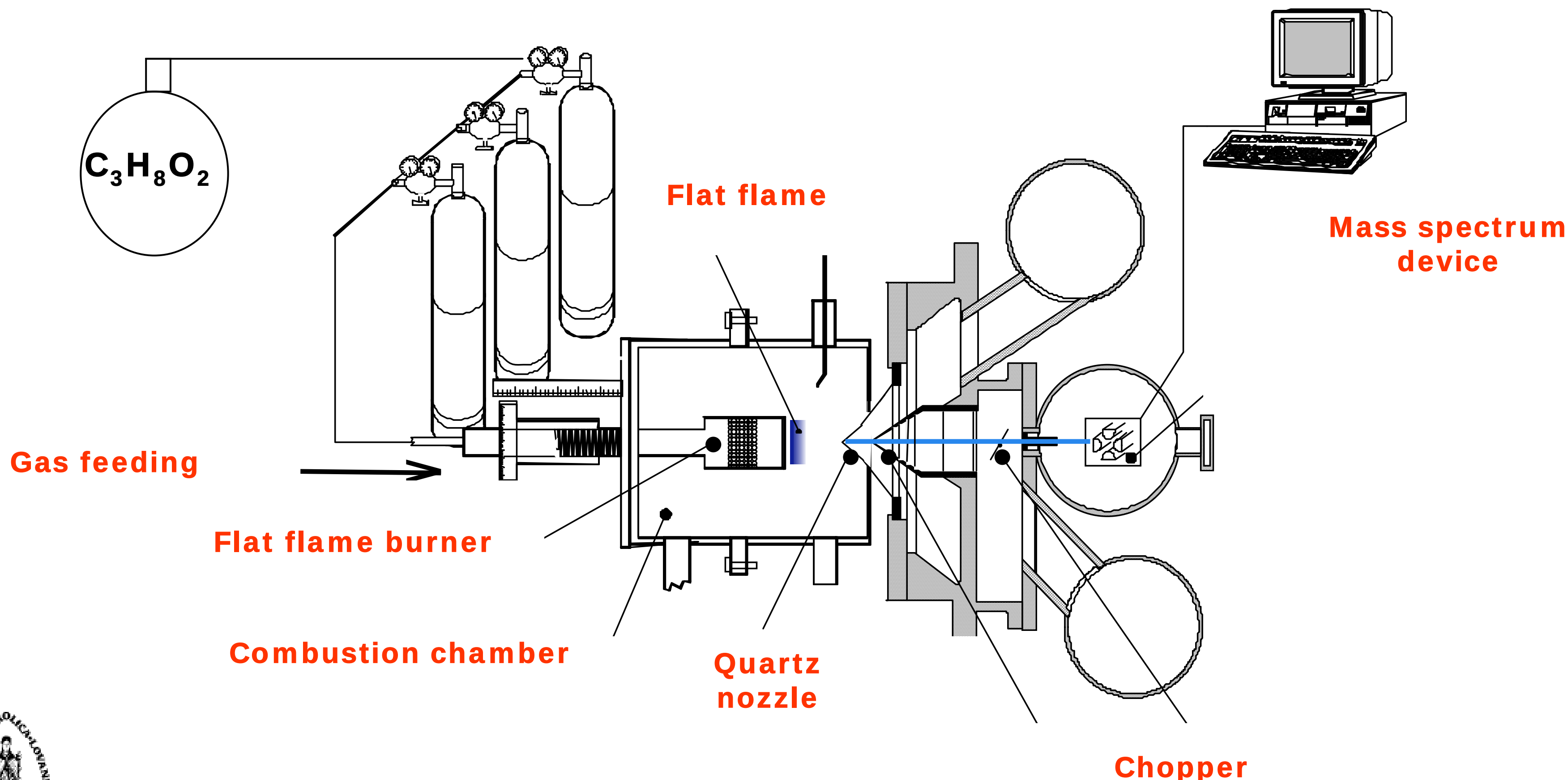
Renard C., Van Tiggelen P.J., Vandooren J., Proc. Combust. Inst., 29, 1277-1284 (2002)

Methylal Study

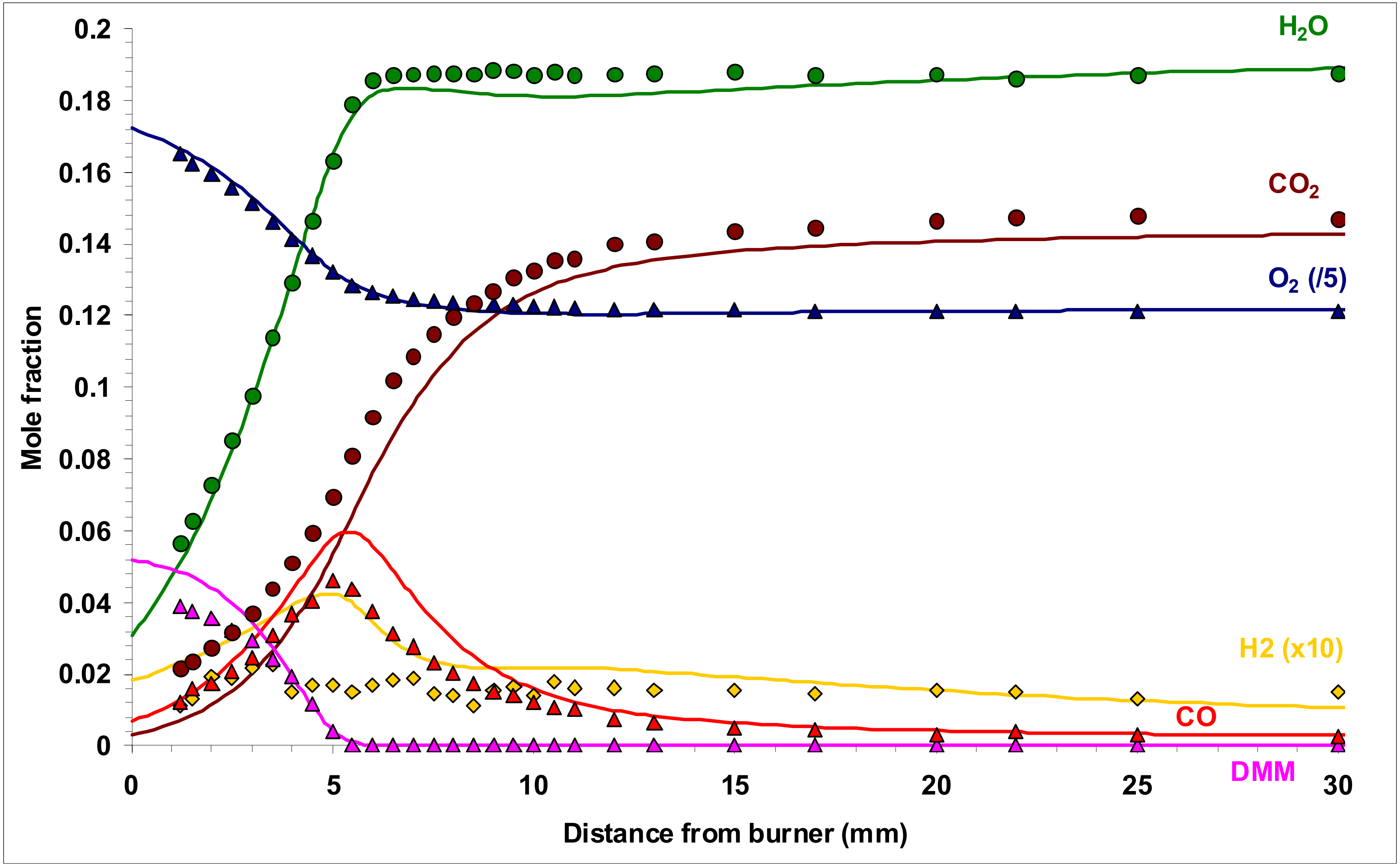
The knowledge of the structure of a lean and a rich DMM flames ($C_3H_8O_2/O_2/Ar$) will help:

- determine the main oxidation routes of this compound and its degradation products

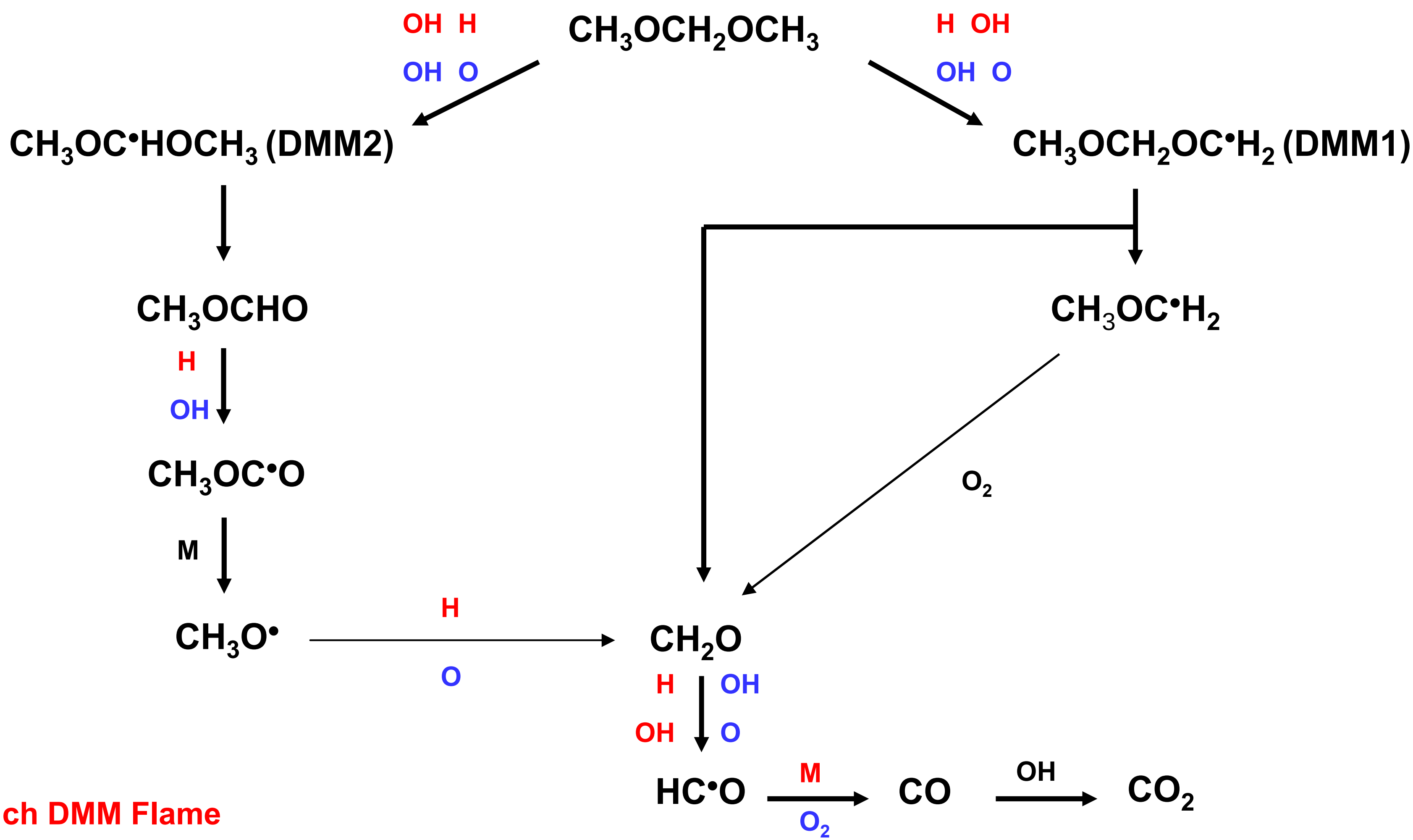
- elaborate and validate a kinetic model.



Methylal Study : lean flame



Methylal Study



Rich DMM Flame

Lean DMM Flame

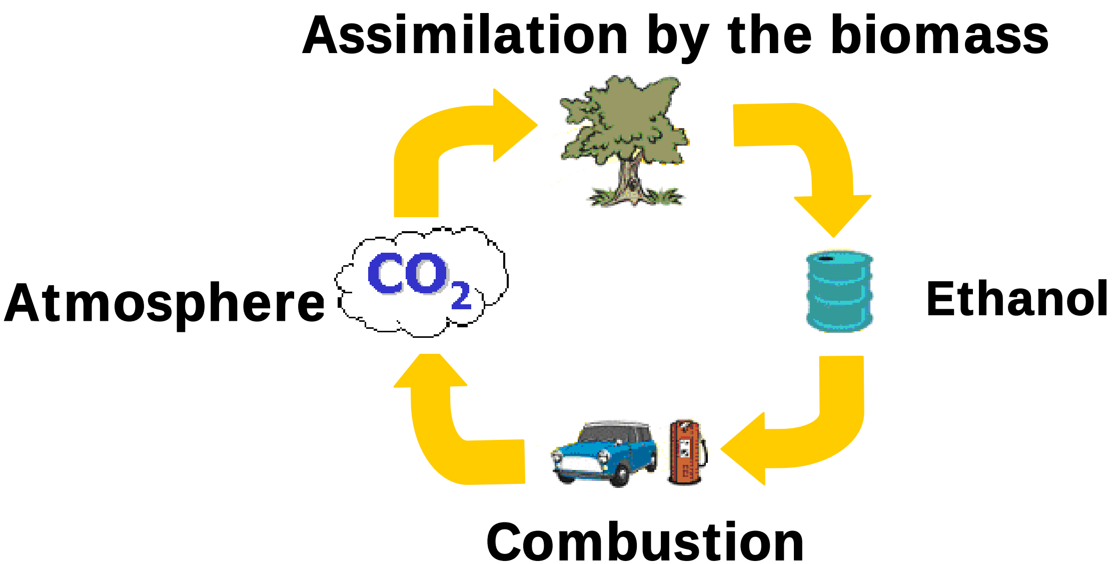
Methylal Study

Future work consists in completing this model with the sub-mechanism for diethoxymethane combustion ($C_5H_{12}O_2$, also called ethylal), and testing it on neat diethoxymethane flames.

$\Rightarrow$ Other ethers/diethers, or esters can also be studied

Ethanol, acetaldehyde, acetic acid study

- Produced from renewable source
- Easily used as fuel or fuel extender
- Environmental benefits

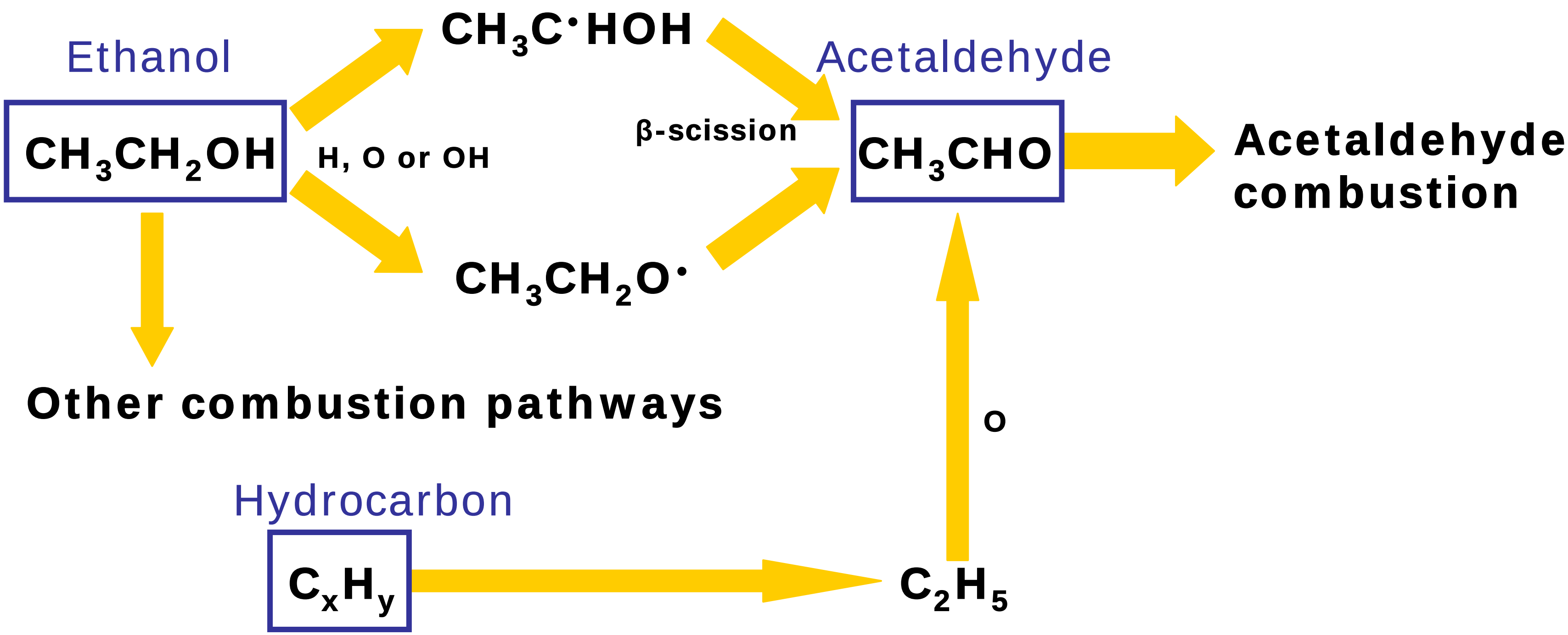


- Environmental damage due to an intensive agriculture
- Diminution of food supply
- High production cost

Ethanol, acetaldehyde, acetic acid study

Why study acetaldehyde combustion?

Acetaldehyde is a main intermediate species appearing in the first step of ethanol combustion



Acetaldehyde combustion is a zoom on a part of the ethanol (and other hydrocarbon) reaction pathway

Ethanol, acetaldehyde, acetic acid study

Acetic acid (CH_3COOH) is a pollutant emitted in small quantity in flames, contributing to acid rains. There is thus an interest to know how this species is consumed.

Flame compositions:

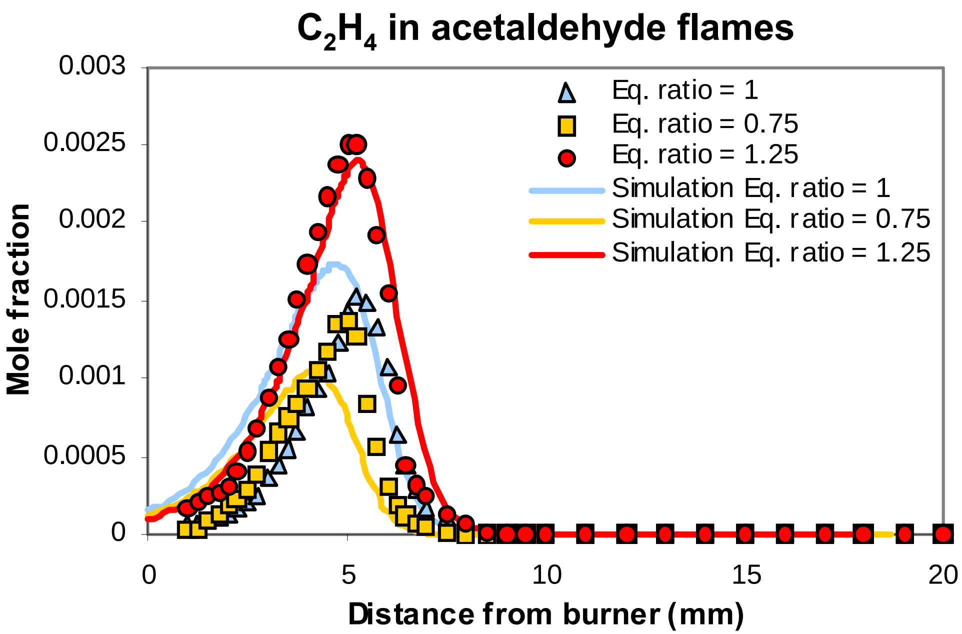
	Fuel	**O_2**	**Ar**	**Flow rate (l/min)**	**Equivalence ratio**
Ethanol 1.0	0.069	0.206	0.725	8.39	1.00
Ethanol 0.75	0.069	0.275	0.657	8.39	0.75
Ethanol 1.25	0.085	0.206	0.709	8.39	1.25
Acetaldehyde 1.0	0.075	0.187	0.738	6.71	1.00
Acetaldehyde 0.75	0.075	0.249	0.666	6.71	0.75
Acetaldehyde 1.25	0.090	0.181	0.729	6.71	1.25
Acetic acid 0.90	0.117	0.260	0.623	4.57	0.90
Acetic acid 0.77	0.095	0.245	0.660	4.84	0.77
Acetic acid 1.10	0.128	0.232	0.640	4.45	1.10

Ethanol, acetaldehyde, acetic acid study

Detected species in these 9 flames:
H_2, CH_3, CH_4, OH, H_2O, C_2H_2, C_2H_4, CO, CH_2O, O_2, Ar, CO_2, CH_2CO, CH_3CHO and C_2H_5OH

⇒ A complete kinetic model for these three oxygenated compounds is in progress…

Example:



Perspectives

Present studies of neat oxygenated species :

$C_3H_8O_2$, $C_5H_{12}O_2$, C_2H_5OH, CH_3CHO, CH_3COOH

CH_2O (important intermediate in oxygenated species)

NH_3 (to bypass such difficulties in hydrogen combustion : storage and transport need specific techniques)

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Elaboration of kinetic model to understand emission formation:

Conversion of reactants, formation of pollutants, effects of additives, etc

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Reduction of the kinetic model according to initial conditions

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Use of reduced mechanisms in industrial processes (engines, furnaces, boilers, …) to define the best operation conditions