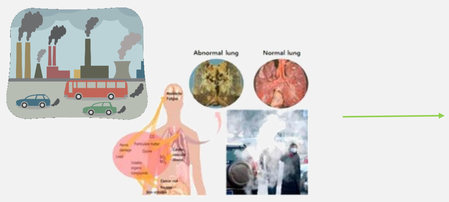
Atmospheric fate of prenol, a second-generation biofuel, in simulation chambers: Insights into kinetics and gaseous / particulate oxidation products formation

Reem AL MAWLA[1,2], Cécile CŒUR [1], Nicolas HOUZEL[1], Sylvain BILLET[2], Manolis N. Rommanias[3]

[1]Laboratoire de Physico-Chimie de l'Atmosphère (LPCA), Université du Littoral Côte d'Opale, Dunkerque, France
[2]Unité de Chimie Environnementale et Interactions sur le Vivant (UCEIV), Université du Littoral Côte d'Opale, Dunkerque, France
[3]IMT Nord Europe, Institut Mines-Télécom, Univ. Lille, Centre for Energy and Environment, F-59000 Lille, France

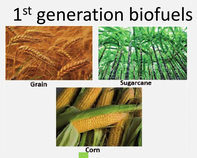
Introduction



Combustion of fossil fuels contribute to air pollution and climate change

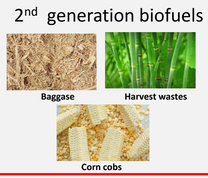
Find alternative green fuels

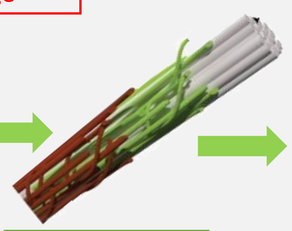
1st generation biofuels



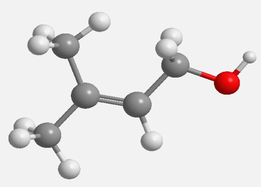
Ethanol

2nd generation biofuels



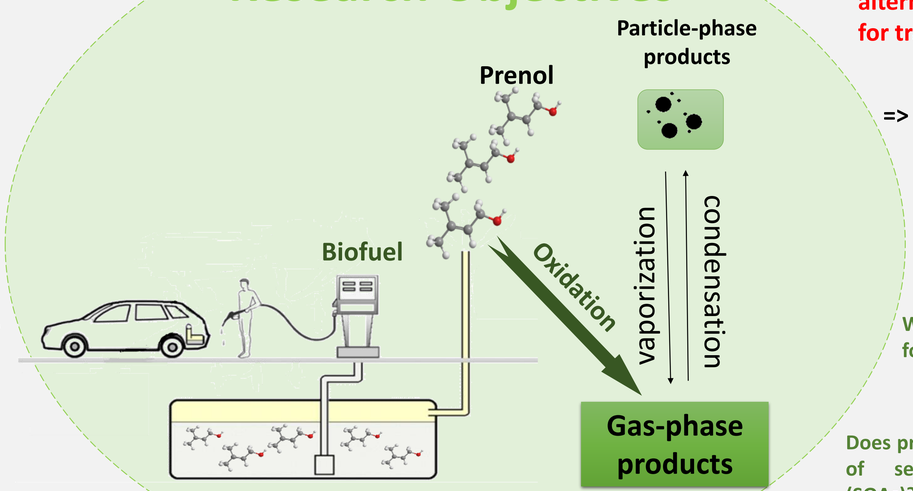


Lignocellulose



Prenol

Research Objectives



Question: Can prenol be a good alternative to the use of fossil fuels for transports?

Prenol emissions => Atmospheric reactivity with main atmospheric oxidants (OH, O_3, NO_3)??

Prenol lifetime in the atmosphere?

What are the gas-phase products formed from its reactivity?

Does prenol contribute to the formation of secondary organique aerosols (SOAs)?

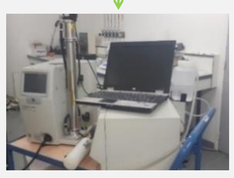
Experimental Part

Study the Reactivity of Prenol in Atmospheric Simulation Chambers

CHARME characteristics	
Localization	LPCA (Dunkerque- France)
Material	Stainless steel 304 L (electropolished)
Shape	Cylindrical
Temperature	(293 ± 2) K
Volume	9.2 m^3
Pressure	0.1 mbar - $P_{atmospheric}$

Analytical Techniques

Particle-phase products



SMPS coupled to CHARME

Determination of the aerosol size distribution and mass concentration

Gas-phase products

Coupled to CHARME

PTR-ToF-MS

VOC concentration monitoring

TD-GC-EI-MS

Oxidation products identification

Coupled to THALAMOS

SIFT-MS

VOC concentration monitoring

THALAMOS characteristics	
Localization	IMT Nord Europe (Douai- France)
Material	Teflon
Shape	Cuboid
Temperature	(231-453) K
Volume	0.6 m^3
Pressure	$P_{atmospheric}$

Results

Kinetic Studies

Oxidant	OH	O_3	NO_3
Rate coefficient (cm^3 $molecule^{-1}$ s^{-1})	$(1.48 \pm 0.10) \times 10^{-10}$	$(3.30 \pm 0.14) \times 10^{-16}$	$(3.20 \pm 0.1) \times 10^{-12}$
Lifetime (hours)	1[a]	0.3[b]	0.4[c]

[a]Calculated using $[OH] = 2 \times 10^6$ molecule.cm^{-3} (Hein et al., 1997).

[b]Calculated using $[O_3] = 2.46 \times 10^{12}$ molecule.cm^{-3} (100 ppbv; polluted area) (Lin et al., 2001).

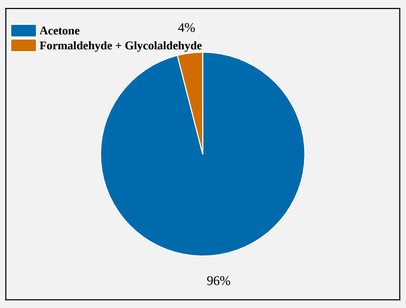
[c]Calculated using $[NO_3] = 2 \times 10^8$ molecule.cm^{-3} (Brown et al., Chem. Soc. Rev., 2012).

[e]Arrhenius equation in the range 273 – 353 K.

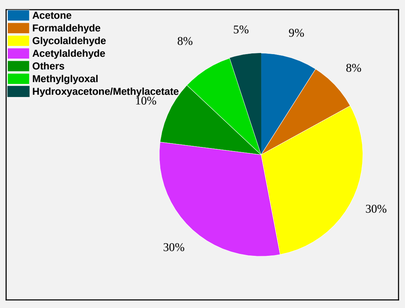
Arrhenius equation in the range 283 – 353 K.

Fast removal from the atmosphere!

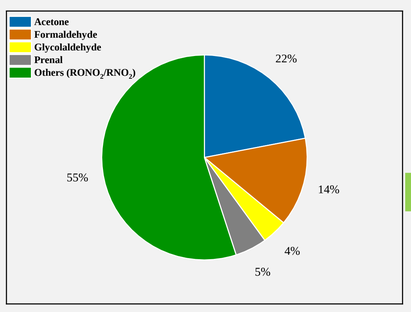
Yields of Identified Gaseous Oxidation Products



Prenol + OH

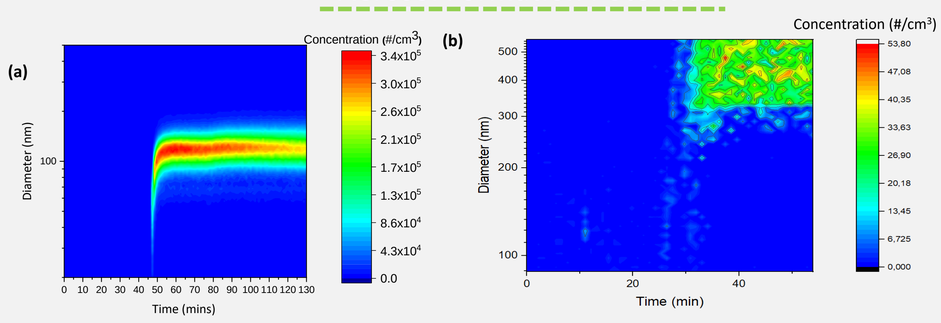


Prenol + O_3



Prenol + NO_3

Aerosol Formation Potential



Time Profile of the aerosol formation from the reaction prenol + O_3 (a) and prenol + NO_3 (b)

Maximum aerosol formation yields from the reaction prenol + O_3 is ≈ **3 %** and from prenol + NO_3 is ≈ **1 %**

These yields are much lower than those formed from the OH reaction of benzene and xylene and toluene (released from gasoline) with maximum SOA yields of ≈ 10 % , 17 % and 11 % respectively (Borrás et al., 2012; Zhang et al., 2019; Deepchandra et al., 2023)

Prenol is a good alternative to the use of fossil fuels with respect to its potential to form secondary organic aerosols

- Major products are **carbonyl compounds** which are directly removed from the atmosphere through photolysis and/or reaction with atmospheric oxidants such as OH radicals
- The use of fossil fuels is a source of benzene in the atmosphere which reacts with OH and leads to the formation of phenol, formic acid, and tropospheric ozone

Conclusion

- **Prenol is fastly removed from the atmosphere by oxidants (OH, O_3 and NO_3) during both night and day, with lifetimes between 0.3 and 1 hour**
- **Low aerosol formation yields in the atmosphere from prenol oxidation by O_3 (≈ 3 %) or NO_3 (≈ 1 %)**
- **Acetone, Formaldehyde and Glycolaldehyde common major products for the reaction between prenol and the different oxidants (OH, O_3 and NO_3) which are also fastly removed from the atmosphere**

Based on our results, prenol (a second generation biofuel) is a good alternative to the use of fossil fuels for transport !!!

Acknowledgement

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