

Collaborative Tasks: Alternative Fuels in Combustion

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

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Objectives

The combustion of different oxygenated compounds considered as alternative fuel are studied in laminar premixed flat flames, at low pressure to evaluate pollutants concentration during their combustion.

Measurements of concentrations of chemical species throughout the flame front of premixed flammable mixtures are performed experimentally by molecular beam mass spectrometry or by gas chromatography. The aim of the work is to build a reaction mechanism taking into account the formation and the consumption of species detected in these flames.

The interest of understanding these combustion mechanisms lies in the possibility of predicting from initial experimental conditions, the formation and the composition of burned gases as well as the evolution of the concentrations of initial fuels and the intermediate species.

We so obtain precious information on the degrees and the rates of conversion of the reactants, the formation of pollutants, the effects of additives, etc...



Projects

Present and future experimental studies of neat oxygenated species:

$\text{C}_3\text{H}_8\text{O}_2$, $\text{C}_5\text{H}_{12}\text{O}_2$, $\text{C}_2\text{H}_5\text{OH}$, 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)

Triacetine ($\text{C}_9\text{H}_{14}\text{O}_6$), **Tripropionine** ($\text{C}_{12}\text{H}_{20}\text{O}_6$), **Tributyrine** ($\text{C}_{15}\text{H}_{26}\text{O}_6$):

Triglycerides obtained by esterification between glycerin and volatile fatty acid



Elaboration of kinetic model to understand emission formation:

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

Reduction of the kinetic model according to initial conditions



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



Milestone Chart

Present and future experimental studies of neat oxygenated species:

C₃H₈O₂: From now to August 2010

C₅H₁₂O₂: From now to September 2010

C₂H₅OH, CH₃CHO, CH₃COOH: From now to October 2010

CH₂O: September 2010 – June 2011

NH₃: From now to January 2011

Tributyrine (C₁₅H₂₆O₆): September 2010 – October 2011

Triacetine (C₉H₁₄O₆), **Tripropionine** (C₁₂H₂₀O₆): Starting October 2011



We are available to study some others oxygenated species from common projects in the Collaborative Task.

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