Experimental and modelling study of acetone combustion

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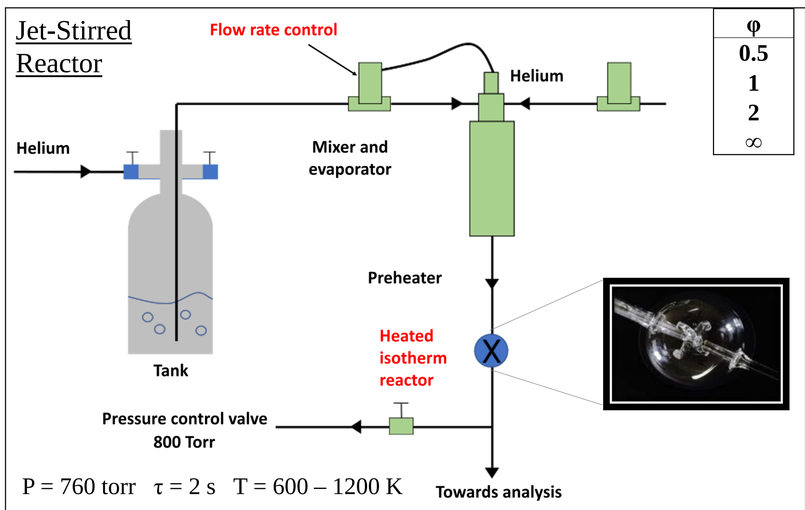
Context

Acetone is a key chemical species in various fields of science so its chemical mechanism is essential. This component is used as a solvent in processes[1]. It is present in upper troposphere[2] and promotes NO_x formation in atmosphere[3] what fasten global warming. Because of its absorption and fluorescence feature, acetone is used in spectroscopic and optic systems[4]. Thanks to its thermodynamic properties, it is an alternative fuel[5] and is a major intermediate in traditional fuel combustion. Its high volatility and affordability also make acetone a wildly used product for domestic tasks. The kinetics of acetone is studied using various apparatus allowing to improve knowledge on its pyrolysis consumption, its oxidation mechanism and also its ignition delay time and its burning velocities as global kinetic properties. A detailed kinetic model has been developed.

Experimental set-up

Jet-Stirred Reactor



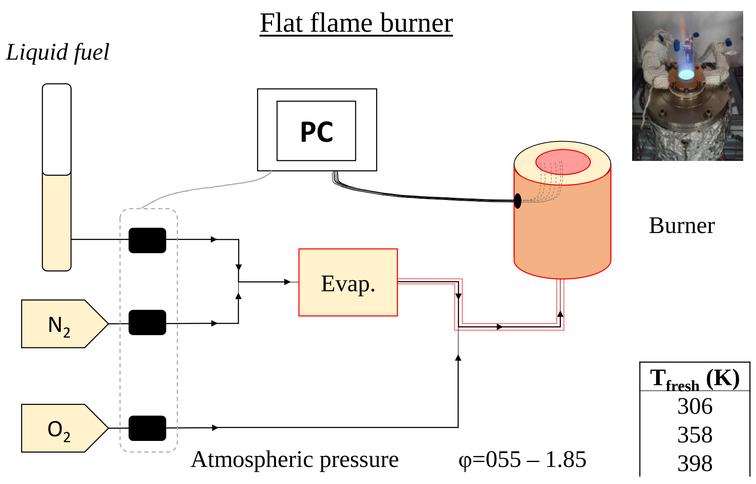
φ
0.5
1
2
∞

P = 760 torr τ = 2 s T = 600 – 1200 K

Rapid Compression Machine

φ = 1 T = 850 – 1100 K **P = 20 & 40 bar**

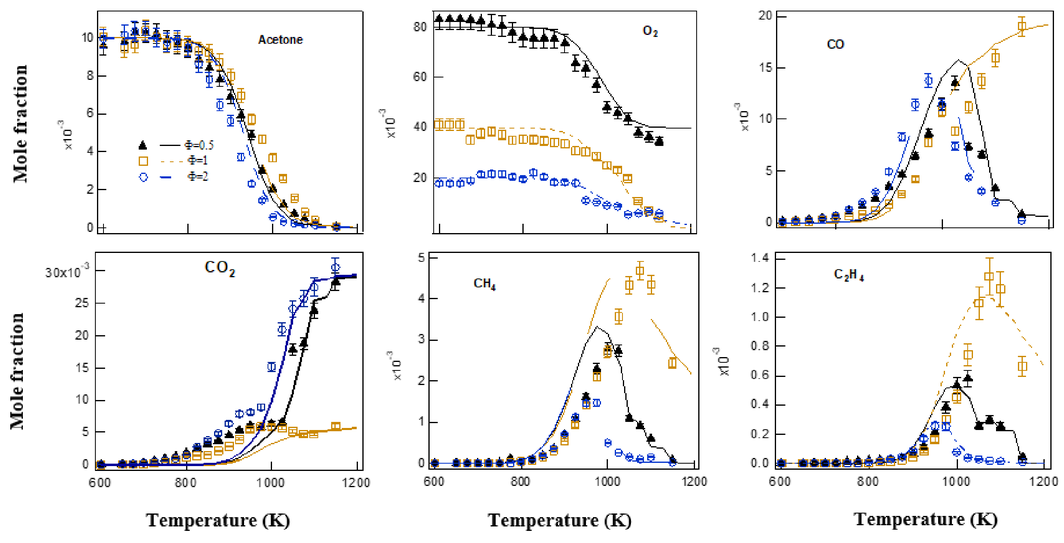
Flat flame burner



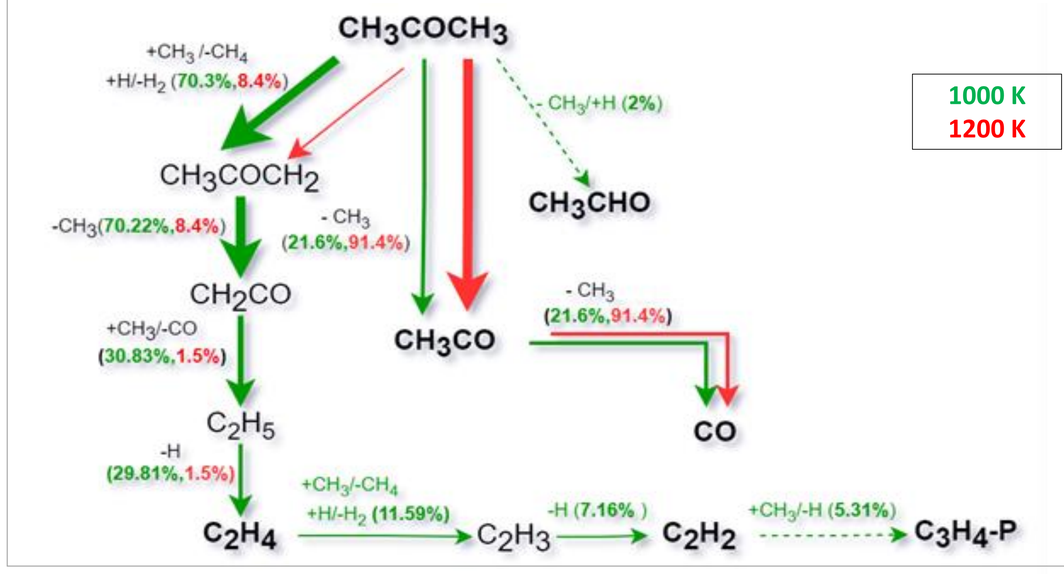
T_{fresh} (K)
306
358
398

Results

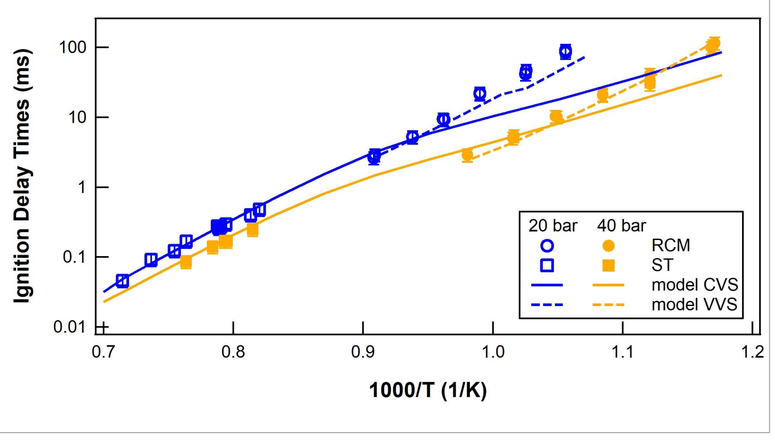
Species profiles during acetone oxidation in JSR



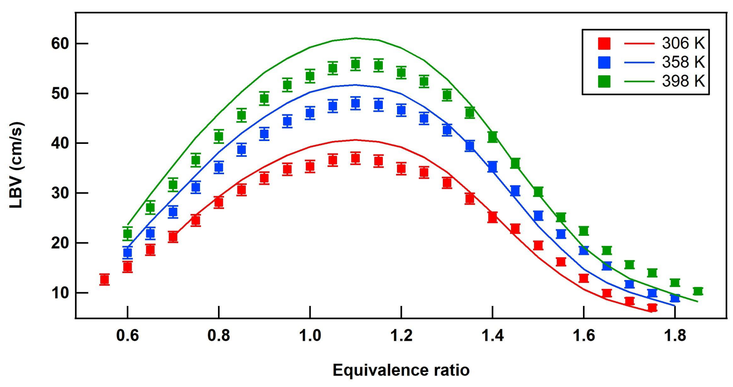
Rate of consumption analysis during pyrolysis



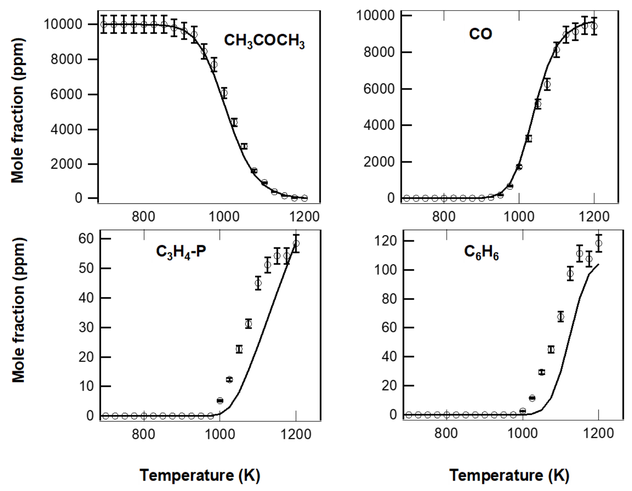
Ignition delay times under stoichiometric conditions



Laminar Burning Velocities for various fresh gas temperatures



Species profiles during acetone pyrolysis in the JSR



Analysis:

- The model predicts very well the ignition delay times and major species in JSR experiments
- LBVs are slightly overestimated around an equivalence ratio of 1.1
- During pyrolysis, acetone is mainly consumed by metathesis at low temperatures and by unimolecular reaction at higher temperatures
- It would be interesting to investigate the mechanism of acetaldehyde, an intermediate species involved in many combustion systems

[1] Energy Conversion and Management. 49 (2008) 3498–3504
[2] Nature. 410 (2001) 1078–1081
[3] Journal of Geophysical Research: Atmospheres. 107 (2002) ACH 5-1-ACH 5-17
[4] Experiments in Fluids. 17 (1994) 330–336
[5] Fuel. 210 (2017) 133–144

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