Department of Chemistry, Materials, and Chemical Engineering

Politecnico di Milano (Italy)

POLITECNICO DI MILANO





Alberto Cuoci

Cool flames in microgravity droplet combustion

20th March 2014
Université Libre de Bruxelles

The CRECK Modeling Group

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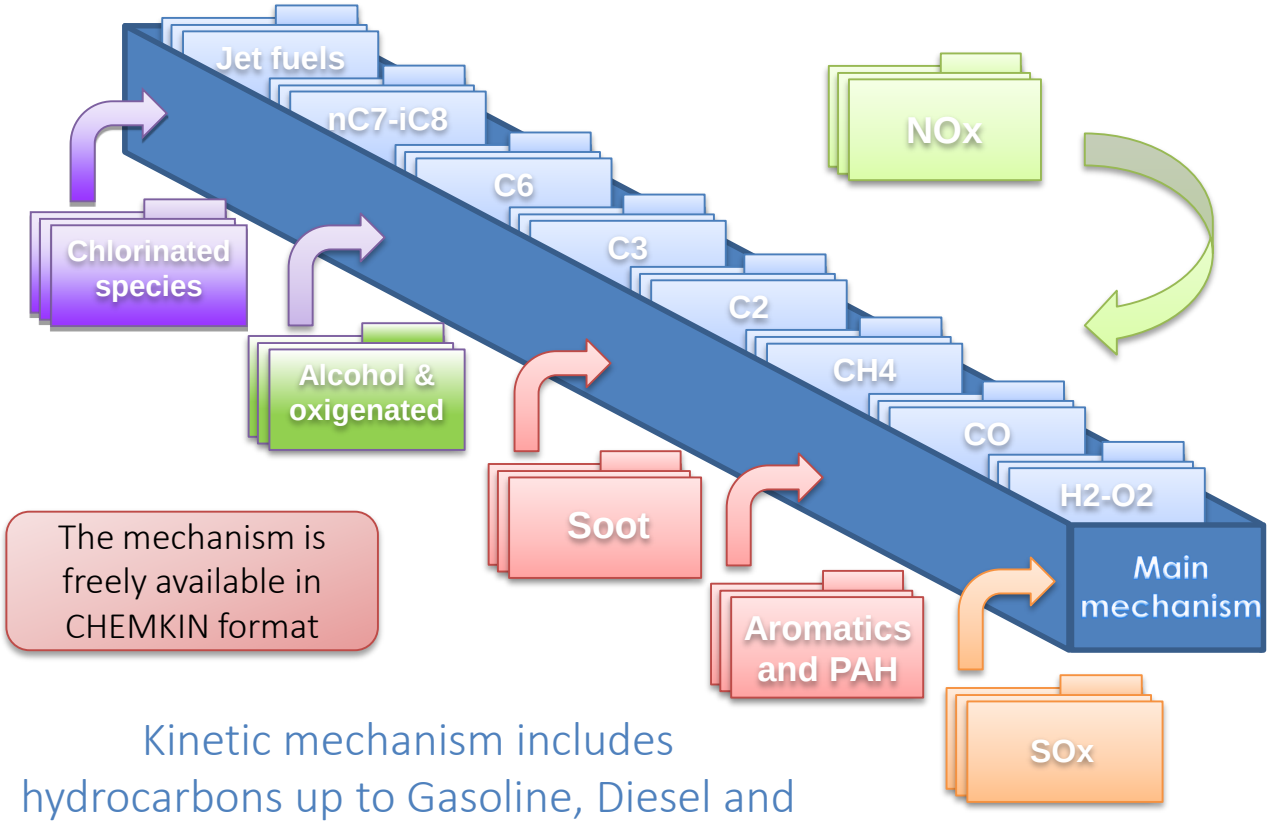
Dipartimento di Chimica, Materiali e Ingegneria Chimica *"Giulio Natta"*
Politecnico di Milano

http://creckmodeling.chem.polimi.it/

Detailed kinetic mechanism



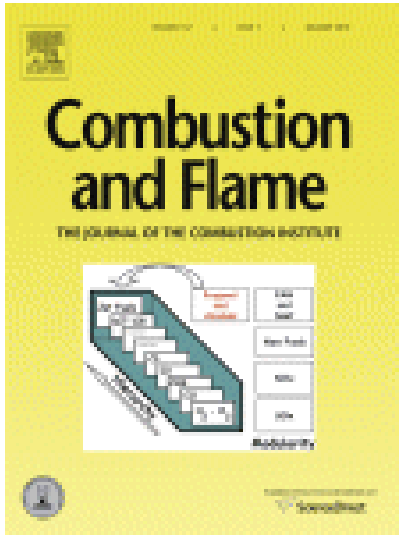
The mechanism is freely available in CHEMKIN format

Kinetic mechanism includes hydrocarbons up to Gasoline, Diesel and jet fuels, as well as several pollutants

- Hierarchy
- Modularity
- Generality

~ 500 species

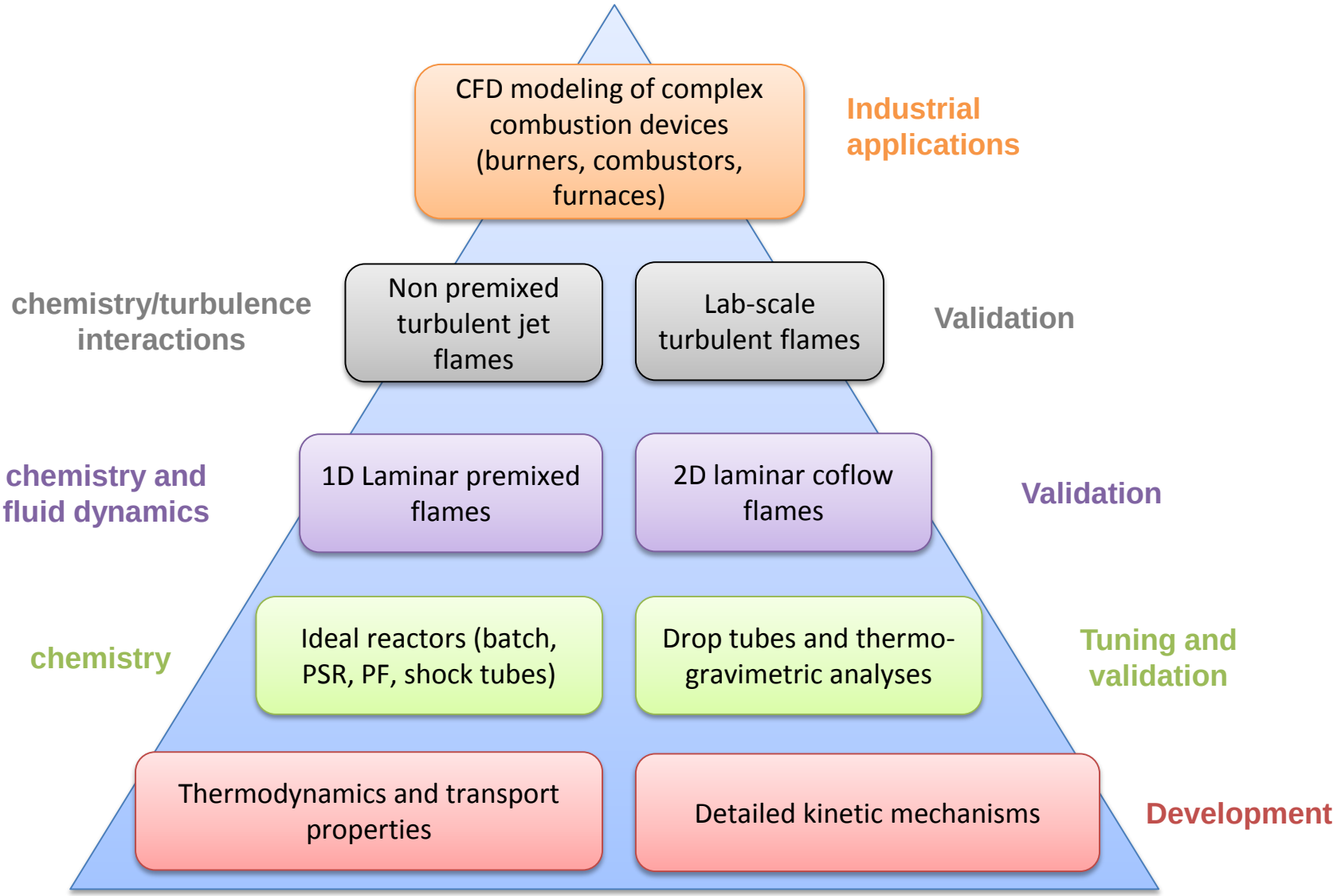
~ 15,000 reactions



A. Frassoldati, A. Cuoci, Faravelli T., Niemann U., Ranzi E., Seiser K., Seshadri K., Combustion and Flame 157(1), 2-16 (2010)

Ranzi, E., Frassoldati, A., Grana, R., Cuoci, A., Faravelli, T., Kelley, A.P., Law, C.K, Progress in Energy and Combustion Science, 38 (4), pp. 468-501 (2012)

From molecules to furnaces

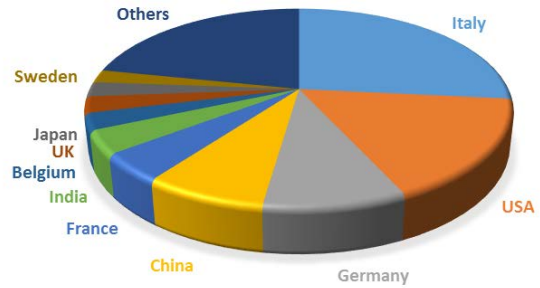


The CRECK Modeling Group on the web

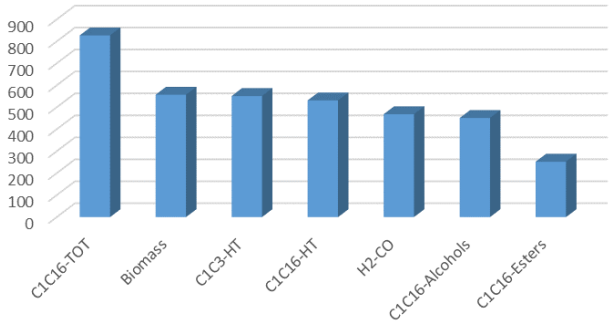
The kinetic schemes can be freely downloaded in CHEMKIN format from our web site:

http://creckmodeling.chem.polimi.it/

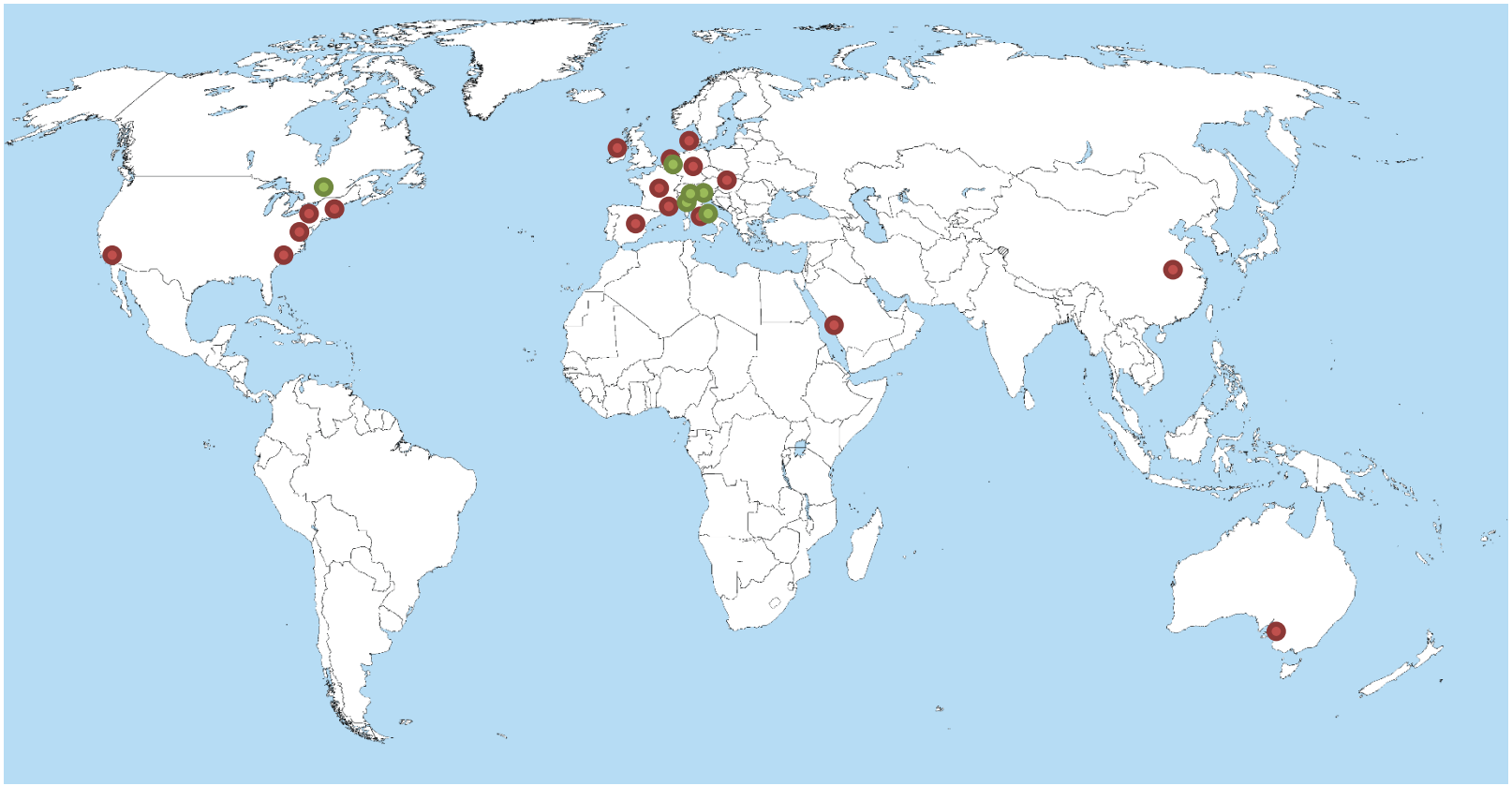
Statistics since January 2013
Unique visitors: 9,600
Visits: 12,000 (~28 per day)
Visits from 97 countries



The kinetic schemes were downloaded more than 3,600 times since Jan 2013



Academic and Industrial Collaborations



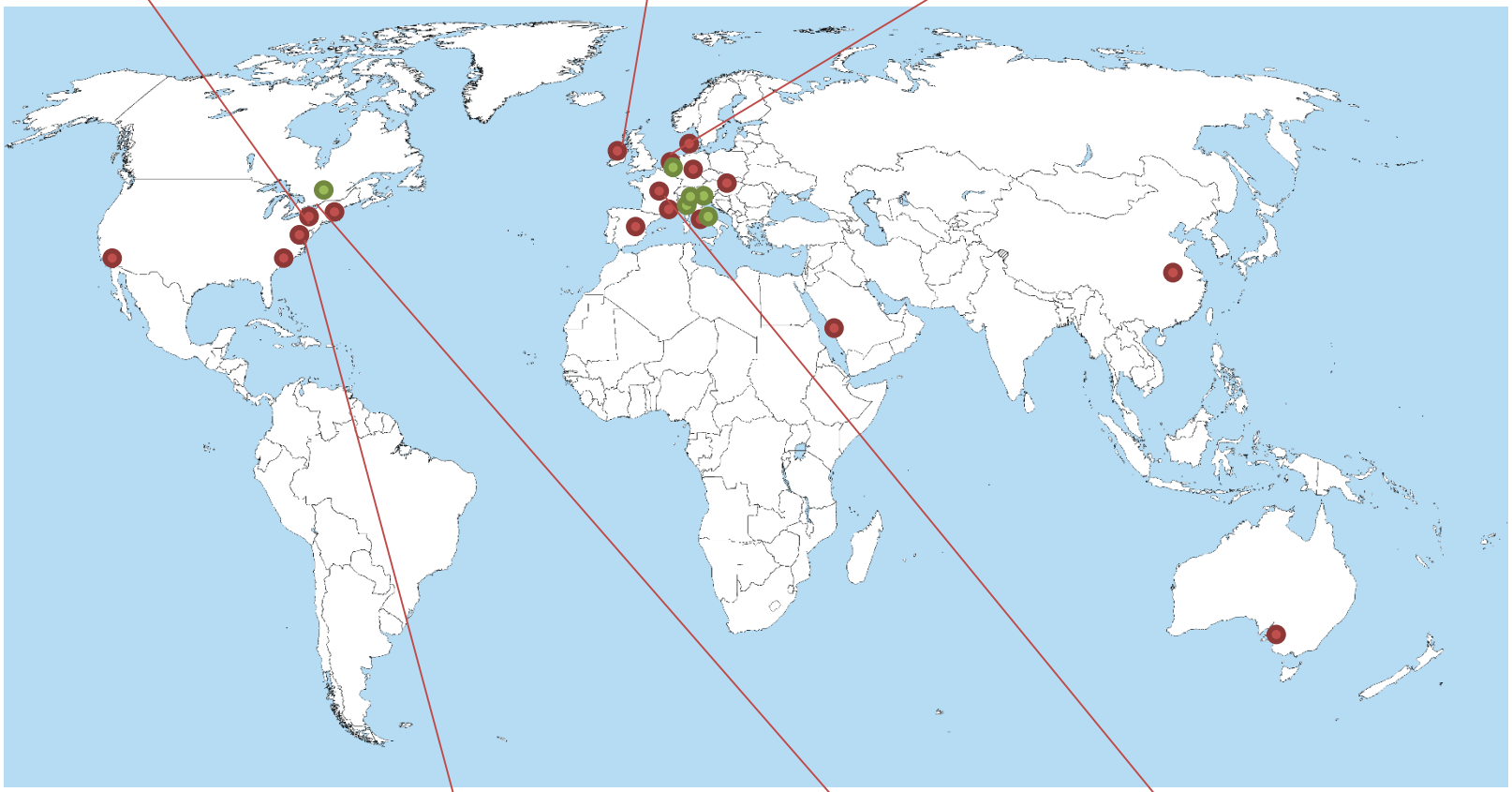
Academic Industrial

Academic collaborations (I)

Rensselaer Polytechnic Institute
M. Oehlschlaeger
Decalin ignition

University of Galway
H. Curran
Oxygenated fuels

Université Libre de Bruxelles
A. Parente
Reduction of kinetic mechanisms



University of Yale
S. Gomez
Kinetics of real fuels

Northeastern University
Y.A. Levendis
Coal

CNRS Orléans
P. Dagaut
Large fuels

Academic collaborations (II)

University of San Diego
K. Seshadri, F.A. Williams
Kinetics of real fuels
Droplet combustion

North Carolina University
P. Westmoreland
Alcohol kinetics

DTU
P. Glarborg
Kinetics of bromine and chlorine

University of Princeton
C.K. Law
Flame speeds

Cornell University
B. Fischer
Biomass kinetics

University of Zaragoza
M. Alzueta
Soot

Academic collaborations (III)

University of Bielefeld
K. Kohse-Höinghaus
Alcohols kinetics

University of Ostrava
V. Nevrly
Pulsating flames

University of Hefei
F. Qi
Laminar, coflow flames

University of Nancy
F. Battin-Leclerc
Kinetics of large methyl-esters

KAUST University
M. Sarathy
PRIME Project

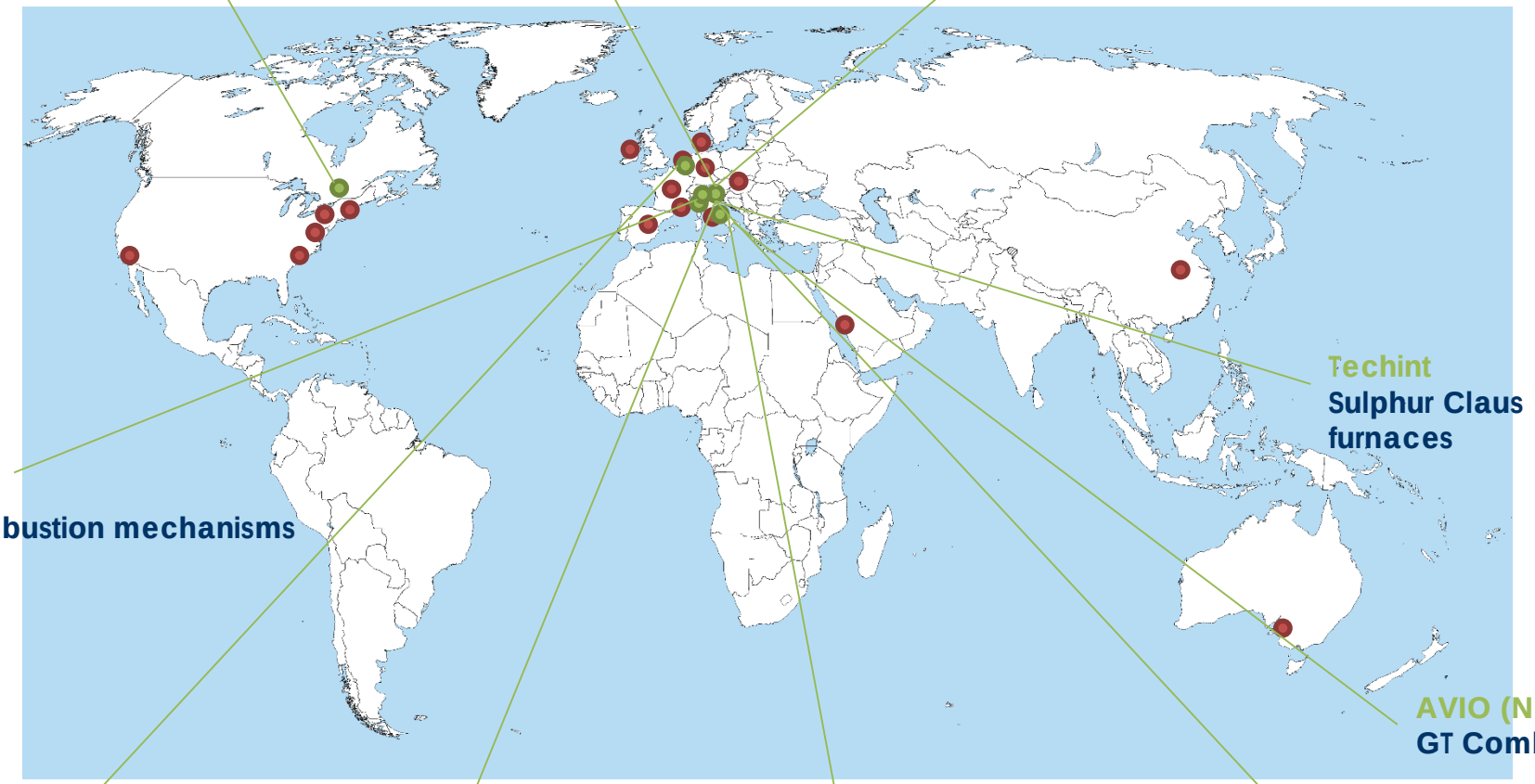
University of Adelaide
P. Medwell
MILD combustion

Industrial collaborations

Rolls-Royce Canada
NOx modeling

Danieli
Industrial burners (flameless)

MORE
Oxy-combustion burners and NOx



Techint
Sulphur Claus furnaces

CSM
Combustion mechanisms

AVIO (Napoli)
GT Combustors

Technip
NOX from furnaces

Agusta-Westland
NOX from helicopters

Riello
Domestic burners

ENGITEC
Oxy-combustion

Outline

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   - ✓ Cool flames
   - ✓ Low-temperature mechanism
2. Numerical modeling of isolated fuel droplets
   - ✓ Governing equations and numerical methodology
   - ✓ Detailed kinetic mechanism
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4. Auto-ignited n-decane ($C_{10}H_{22}$) droplets
   - ✓ Comparison with experiments
   - ✓ Structure of the cool flame
5. Hot-wire ignited n-heptane (NC_7H_{16}) droplets
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   - ✓ Kinetic analysis
6. Conclusions and future works

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   - ✓ **Low-temperature mechanism**

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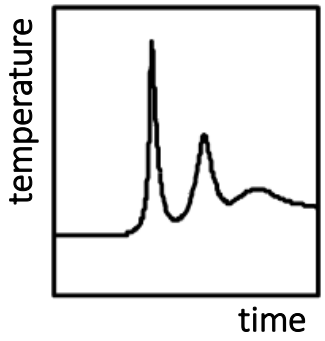
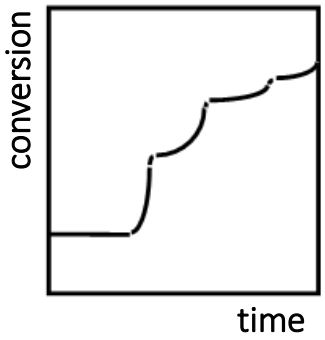
6. Conclusions and future works

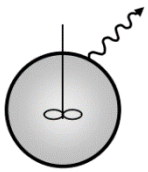
Cool flames

Closed, non-adiabatic systems

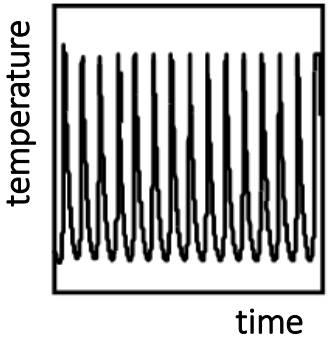


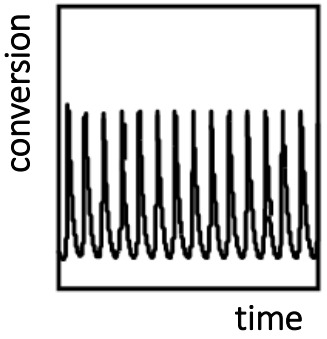


internal combustion engines, batch reactors, etc

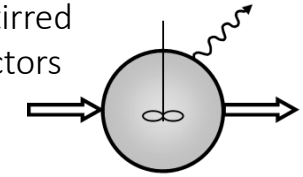


Open, non-adiabatic systems





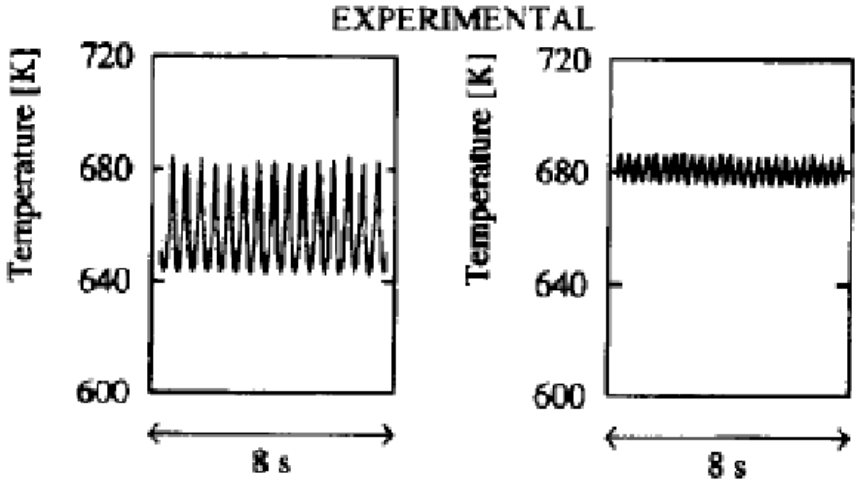
jet stirred reactors



Ordinary, visible flames burn at a high temperature between 1500K and 2000K.

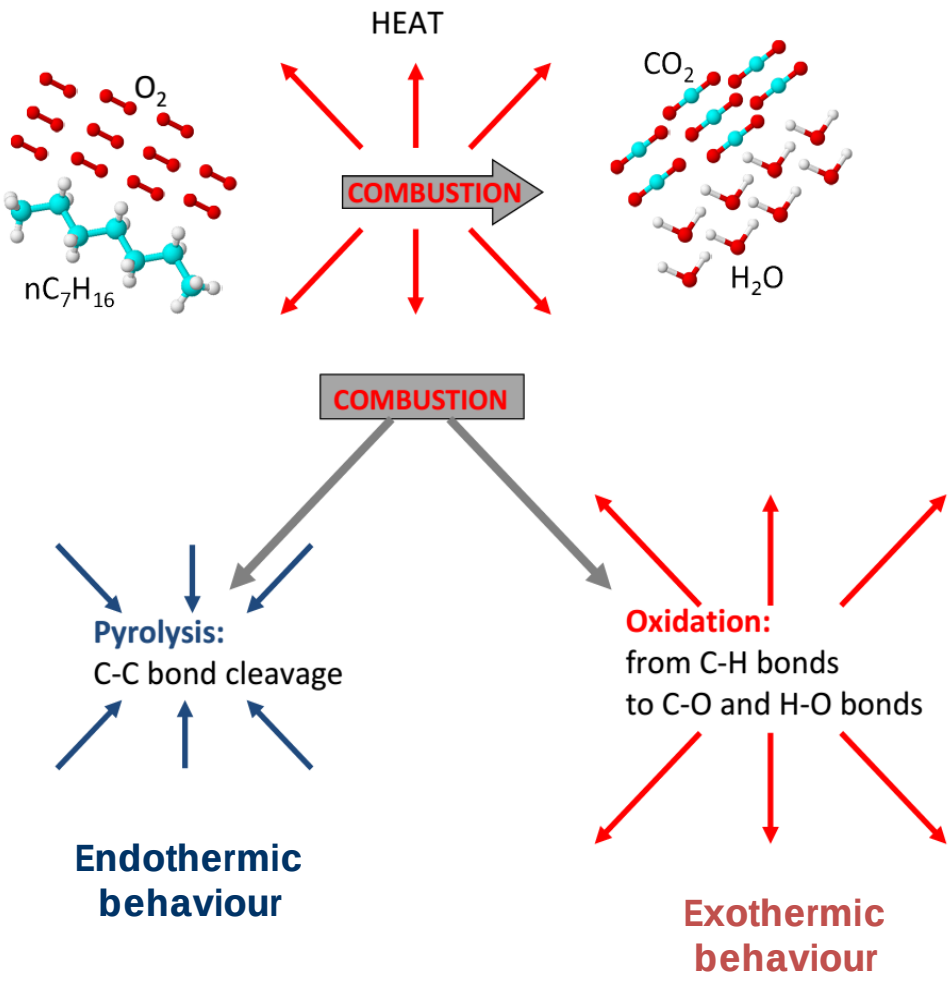
Cool flames burn at the relatively low temperature of 500K to 800K, and their chemistry is completely different. Normal flames produce soot, CO_2 and water. Cool flames produce CO and CH_2O.

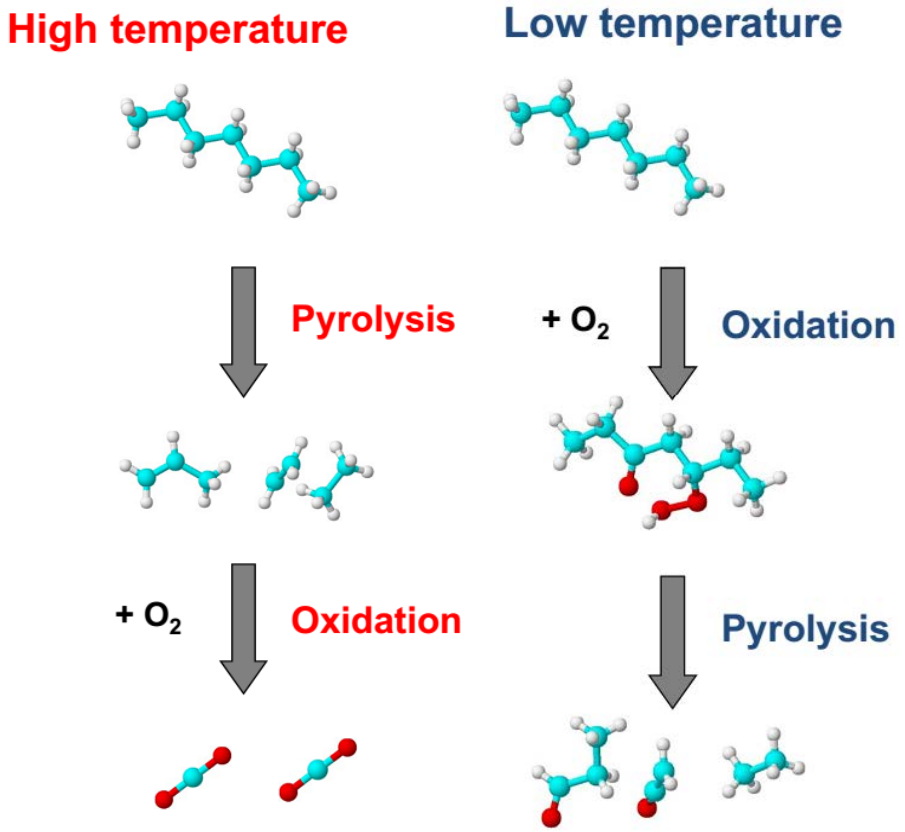
Jet Stirred Reactor: i-octane/air at 7 bar



Ranzi E., Faravelli T., Gaffuri P., Sogaro A., D'Anna A., Combustion and Flame 108, p. 24-42 (1997)

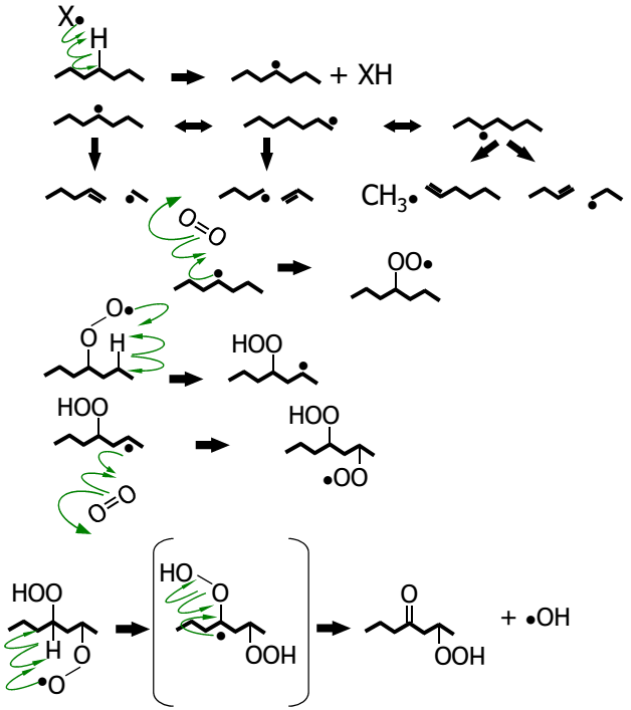
Complexity of Combustion Chemistry



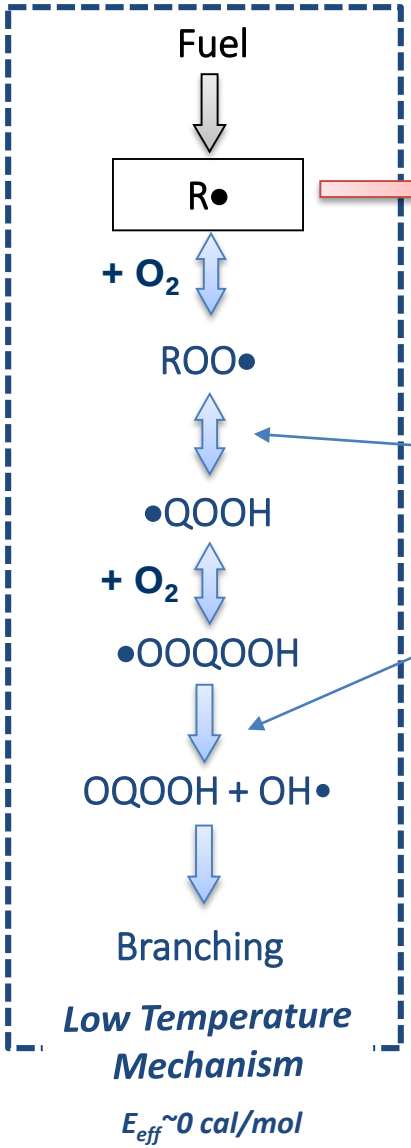


Combustion of alkanes (I)

H-atom abstraction primarily by OH and HO2, and to a lesser extent by H, CH3,and O2



Combustion of alkanes (II)



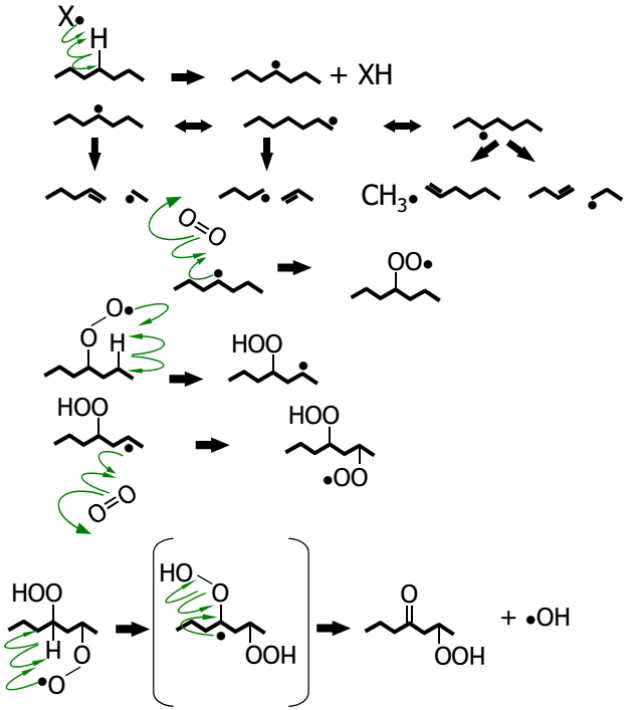
High Temperature Mechanism

β-Decomposition Products

E_{eff}~30,000 cal/mol

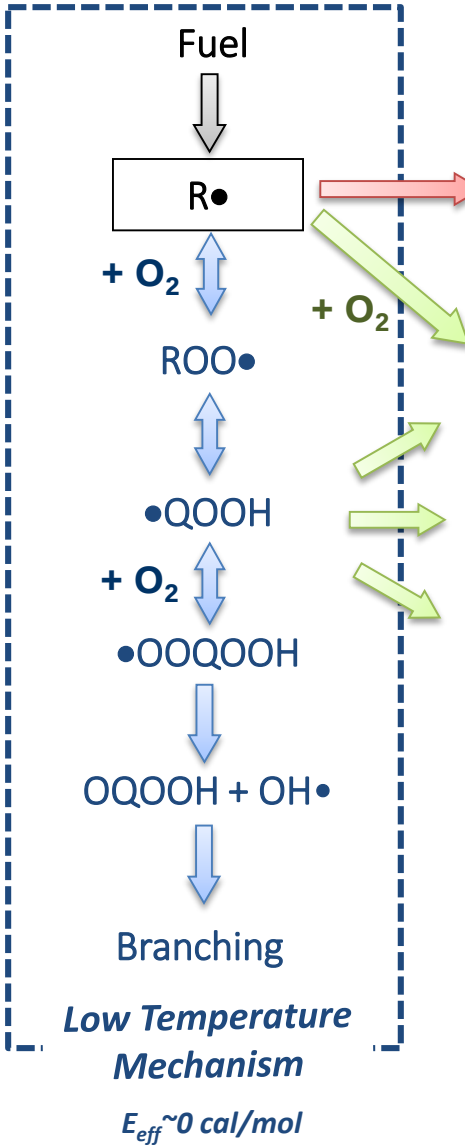
internal isomerization

isomerization-decomposition



R• = alkyl-radical (e.g. C_7H_{15})
ROO• = peroxy radical
•QOOH = hydroperoxy-alkyl rad.
•OOQOOH = alkyl-hydroperoxy rad.
OQOOH = ketohydroperoxyde

Combustion of alkanes (II)



High Temperature Mechanism

β-Decomposition Products

E_{eff}~30,000 cal/mol

E_{eff}~19,000 cal/mol

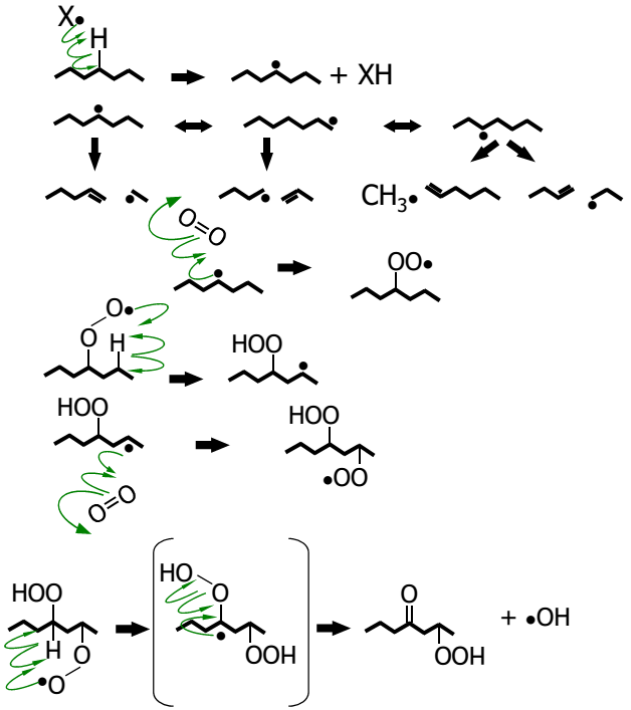
+ O_2

HO_2• + alkenes

OH• + Cyclic Ethers

OH• + aldehydes + alkanes

Intermediate Temperature Mechanism



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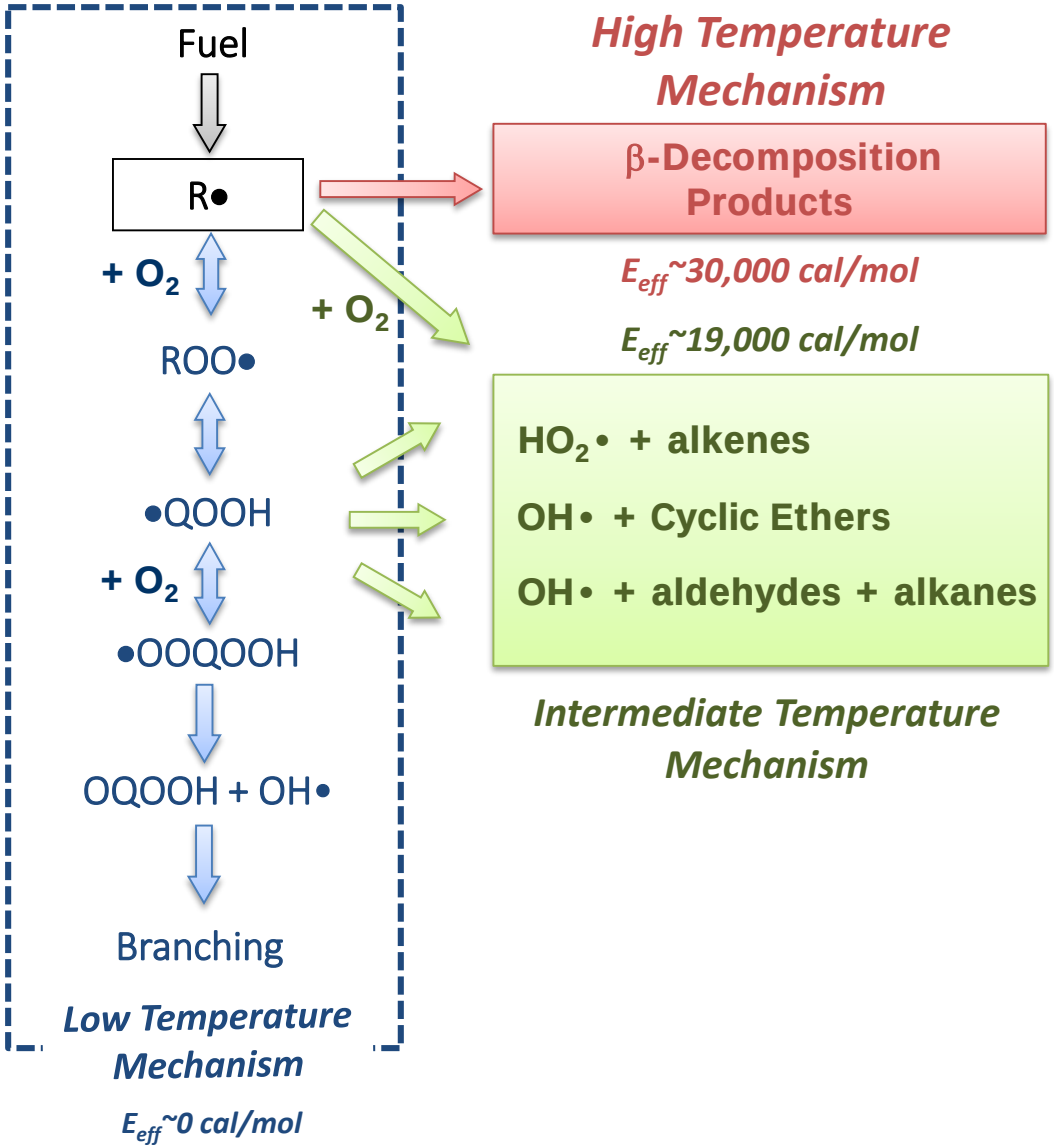
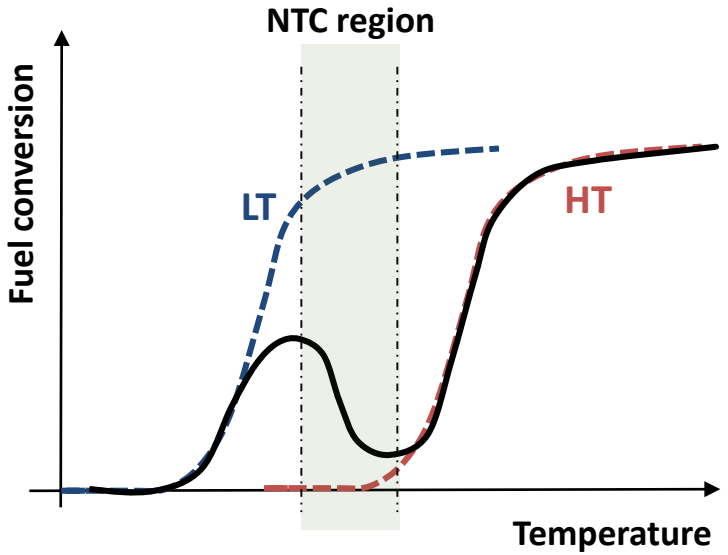
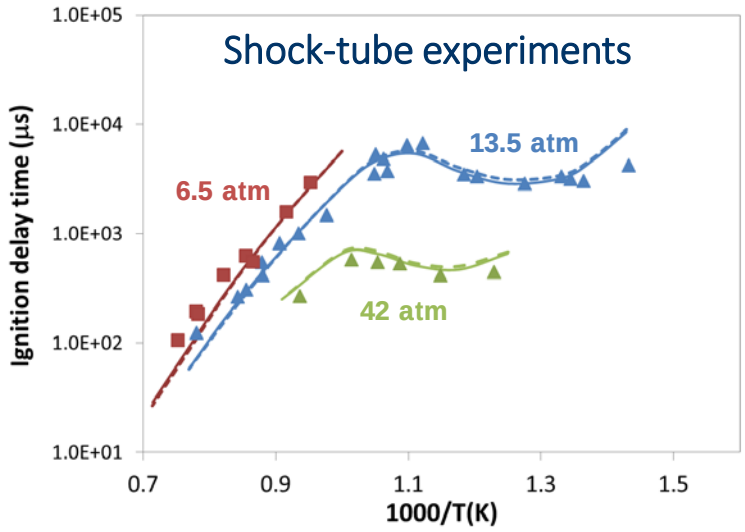
Negative Temperature Region (NTC)







Competition between mechanisms (I)

Transition from the LT to the HT mechanism ruled by the decomposition of peroxy radicals

$R\bullet + O2 \leftrightarrows ROO\bullet$

$k_{add} = 10^{9}$ [l/mol/s]

$k_{dec} = 10^{13} \exp(-28000/RT)$ [1/s]

Competitive pathways: at high temperatures alkyl radicals are favored over the peroxy radicals, or pyrolysis is favored over oxidation.

Ceiling Temperature is the transition temperature from one mechanism to the other

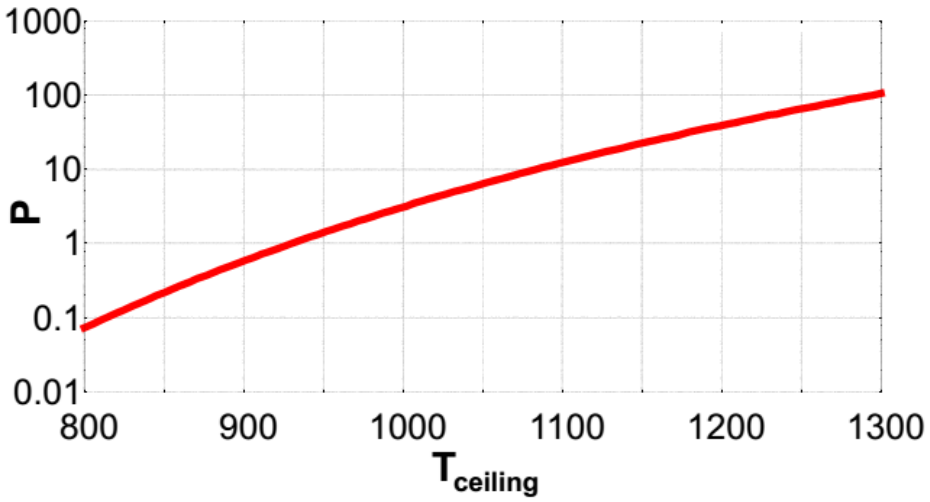
At the equilibrium the addition (forward) and the decomposition (reverse) reaction rates are equal:

$r_{add} = r_{dec} \Rightarrow k_{add}[R\bullet][O2] = k_{dec}[ROO\bullet]$

Competition between mechanisms (II)

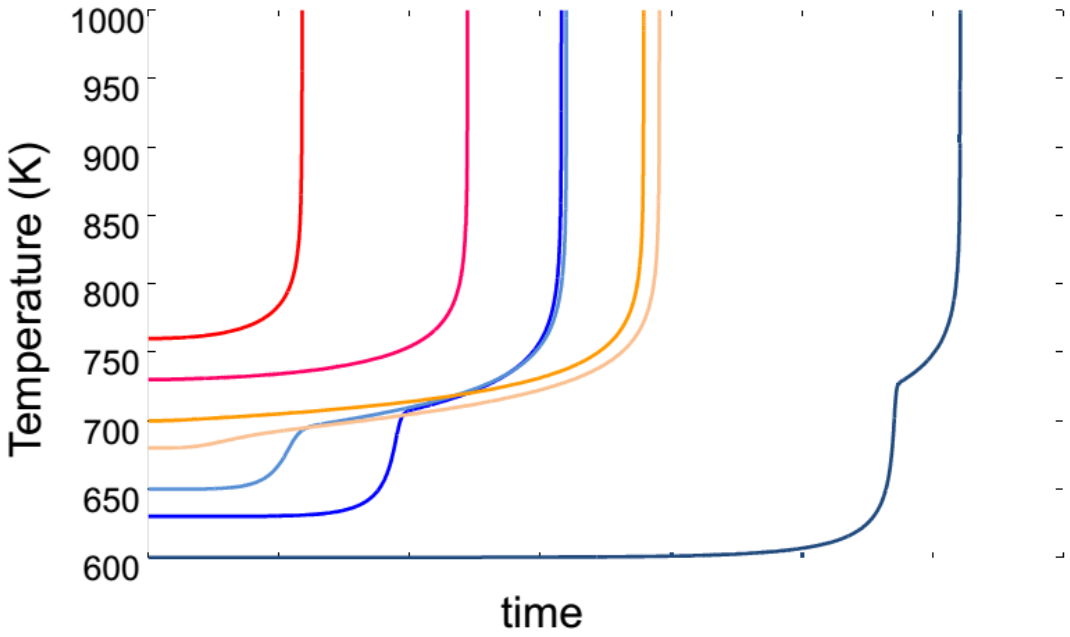
$$\frac{[R\bullet]}{[ROO\bullet]} = \frac{k_{dec}}{k_{add}[O_2]} \cong \frac{10^{13}\exp(-\frac{28000}{RT})}{10^9 \frac{P}{RT} x_{O_2}}$$

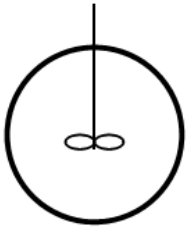
$$P \cong \frac{RT}{x_{O_2}} \frac{10^{13}\exp(-\frac{28000}{RT})}{10^9}$$



Ceiling temperature increases with the pressure: higher oxygen concentration favors direct reaction of peroxy radical formation: NTC region moves toward higher temperatures

Ignition of C3H8 in closed, non-adiabatic systems





No heat exchange
No mass exchange

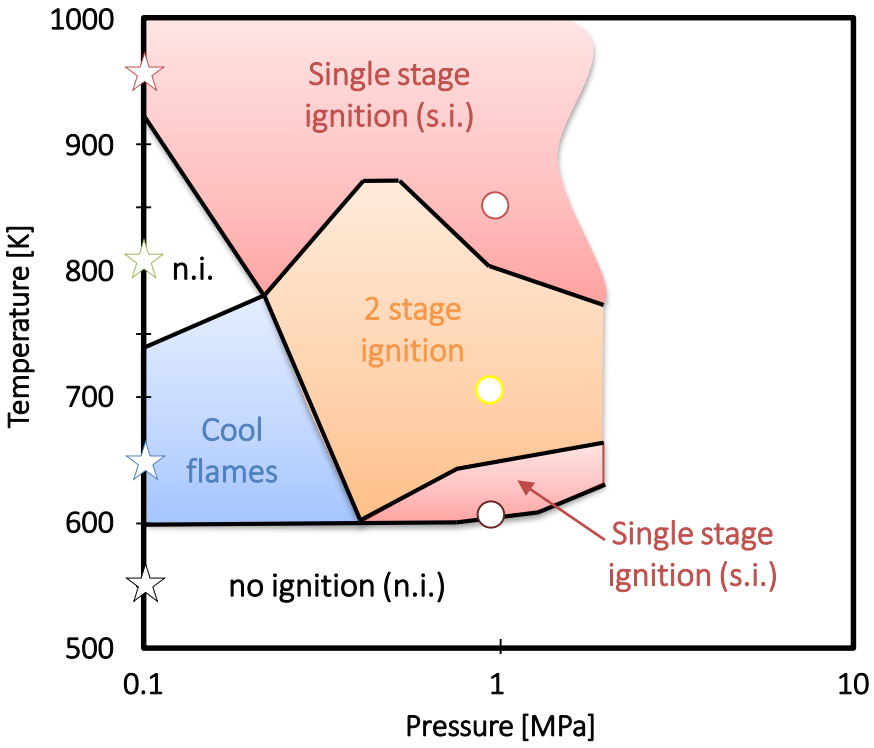
- One or two stage ignition.

- NTC between 650-700 K

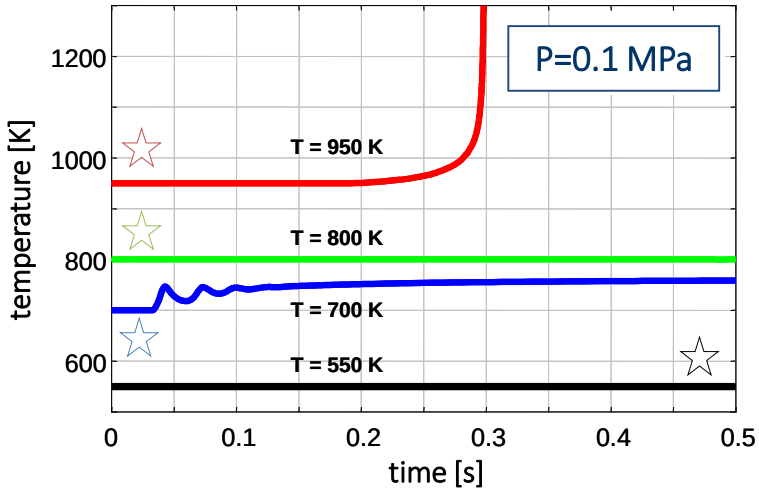
Cool flames in droplet combustion (I)

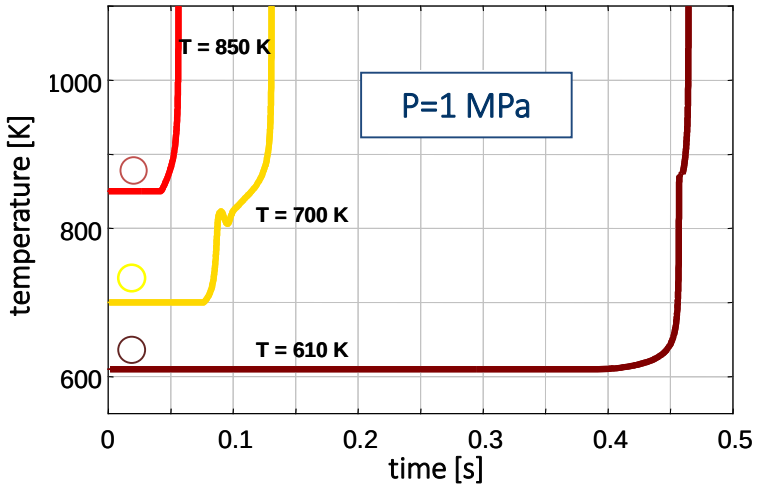
Auto-ignition experiments

n-heptane droplets in air (d_0=0.70 mm)



Adapted from: **Tanabe et al.**, 26th Symposium (International) on Combustion, p. 1637-1643 (1996)





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6. Conclusions and future works

Why studying isolated fuel droplets?

Combustion of liquid fuels
- -industrial burners
- -Diesel engines
- -…

complex **chemistry** due to the combustion reactions in the gaseous phase

- -heating
- -evaporation
- -radiative heat transfer
- -ignition delay times
- -…

strong **interactions** between the different droplets of a spray

Isolated fuel droplets

microgravity

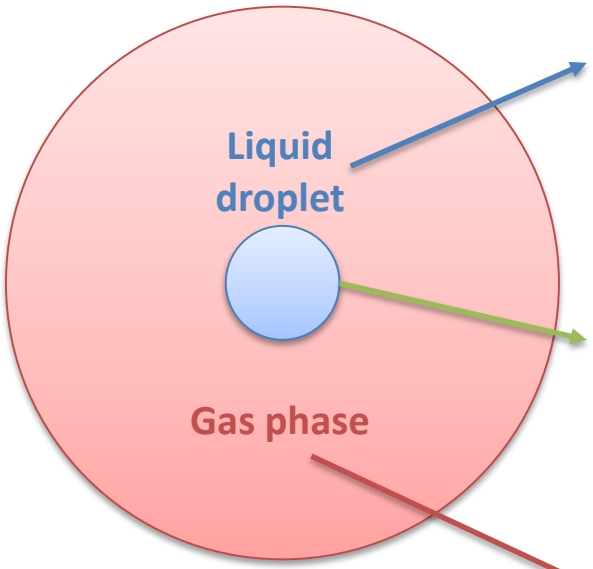
the droplet and the flame are spherical

μg μg

natural convection is absent

- Phenomenological understanding of major burning features of droplet combustion
- Detailed kinetic analyses
- Pollutant formation (soot, NOx, SOx …)

Mathematical model



- ✓ Continuity equation
- ✓ Energy equation
- ✓ Species equations

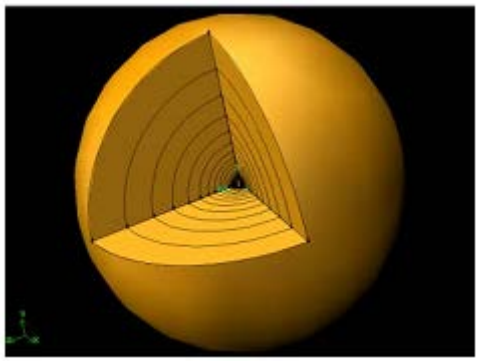
Interface (liquid/gas)

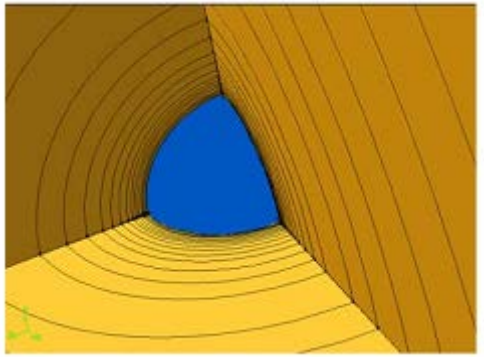
- ✓ Thermodynamic equilibrium
- ✓ Conservation of fluxes

- ✓ Continuity equation
- ✓ Energy equation
- ✓ Species equations

Cuoci et al., Combustion and Flame 143, p. 211-226 (2005)

- ✓ Spherical symmetry
- ✓ 1D equations
- ✓ Stretched grid





Kazakov A., Conley J., Dryer F.L., Combustion and Flame 134, p. 301-314 (2003)

Ratio between gas and liquid radii: ~120

Equation of state (gas phase): ideal gas

Radiative heat transfer (gas phase): from Kazakov et al. (2003)

Dufour effect: neglected

Soret effect: accounted for

Governing equations

The governing equations are the usual conservation equation for mass, species and energy, both for the gas and the liquid phase

Continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho r^2 v\right) = 0$$

Species equations

$$\rho\left(\frac{\partial \omega_i}{\partial t} + v\frac{\partial \omega_i}{\partial r}\right) = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 j_i\right) + \dot{\Omega}_i$$

Mass diffusion flux

Formation rates due to chemical reactions

Energy equation

$$\rho C_P\left(\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial r}\right) = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q\right) - \frac{\partial ln\rho}{\partial lnT}\frac{Dp}{Dt} - \sum_{i=1}^{N} j_i\frac{\partial H_i}{\partial r} + Q_R + \mu\Phi_v$$

Heat flux

Heat release due to chemical reactions

Enthalpyfluxes associated to mass diffusion

Viscous dissipation term

Mass diffusion fluxes

Fick's Law (mixture averaged formulation)

Thermophoretic effect (only for carbonaceous particles)

$$j_i = \omega_i V_i = -\Gamma_{i,mix}\frac{\partial \omega_i}{\partial r} + \Gamma_{i,mix}\theta_k \frac{M_i}{M}\frac{1}{T}\frac{\partial T}{\partial r} + \omega_i V_i^{Th} + \omega_i V_C$$

Soret effect (thermal diffusion)

Correction velocity (to ensure conservation of mass)

In the evaluation of the soot transport properties, the thermophoretic effect is also considered [Gomez and Rosner (1993)]. The thermophoretic velocities are expressed as:

$$V_i^{Th} = \alpha \frac{\mu}{\rho T}\frac{\partial T}{\partial r}$$

Since the equations are solved using a fully coupled algorithms it is very important to ensure that the sum of mass diffusion fluxes is equal to zero

$$\sum_{i=1}^{N} \omega_i V_i = 0$$

$$V_C = \sum_{i=1}^{N} \Gamma_{i,mix}\frac{\partial \omega_i}{\partial r} - \frac{1}{T}\frac{\partial T}{\partial r}\sum_{i=1}^{N}\Gamma_{i,mix}\theta_k \frac{M_i}{M} - \sum_{i=1}^{N}\omega_i V_i^{Th}$$

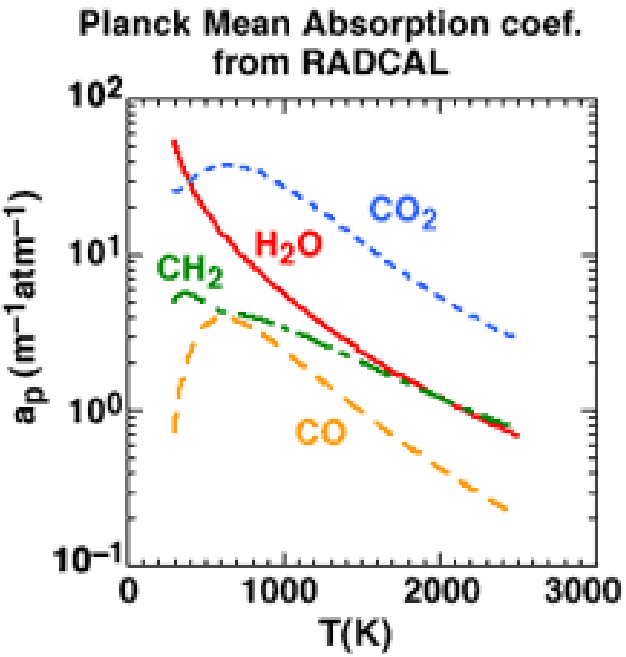
Heat fluxes

Fourier's Law (thermal conductivity)

$$q_{cond} = -k_G \frac{\partial T}{\partial r}$$

Radiative heat transfer

$$q = q_{cond} + q_{rad}$$



Analitical solution proposed by Kazakov *et al.* (2003): absorbing gas phase between two concentric spheres

$$\frac{\partial q_{rad}}{\partial t} = 2\sigma_B K_P T_s^4 \left[2\tilde{T}(r) - g_1 - g_2\right]$$

Planck mean absorption coefficients

$$K_P = p_{CO} a_P^{CO} + p_{CO2} a_P^{CO2} + p_{H2O} a_P^{H2O} + \beta f_V T$$

Gas phase species

Soot particles

Boundary and initial conditions

- Center of the droplet:

$$\frac{\partial \omega_i^L}{\partial r} = 0 \qquad \frac{\partial T_L}{\partial r} = 0 \qquad v_L = 0$$

- Droplet/gas phase interface:

$$\vec{n}_i^L = \vec{n}_i^G \qquad \bar{f}_i^L\left(T, p, \underline{X}_L\right) = \bar{f}_i^G\left(T, p, \underline{X}_G\right)$$

$$\vec{e}^L = \vec{e}^G \qquad T_L = T_G \qquad \sum_{i=1}^{NCG} \omega_i^G = 1$$

- Outer border:

$$\omega_i^G = \omega_i^{G,0} \qquad T_G = T_G^0$$

- Initial conditions

$$r \le R_d^0: \quad \omega_j^L = \omega_j^{L,0} \qquad T_L = T_L^0 \qquad v_L = v_L^0$$

$$r > R_d^0: \quad \omega_j^G = \omega_j^{G,0} \qquad T_G = T_G^0 \qquad v_G = v_G^0$$

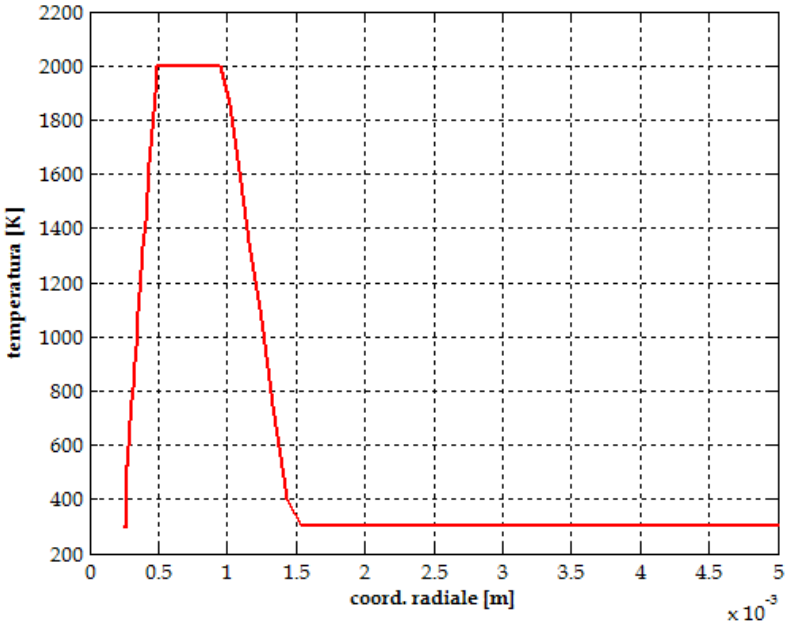
Initial conditions

1. autoignition experiments: the droplet is injected into an environment with high ambient temperature

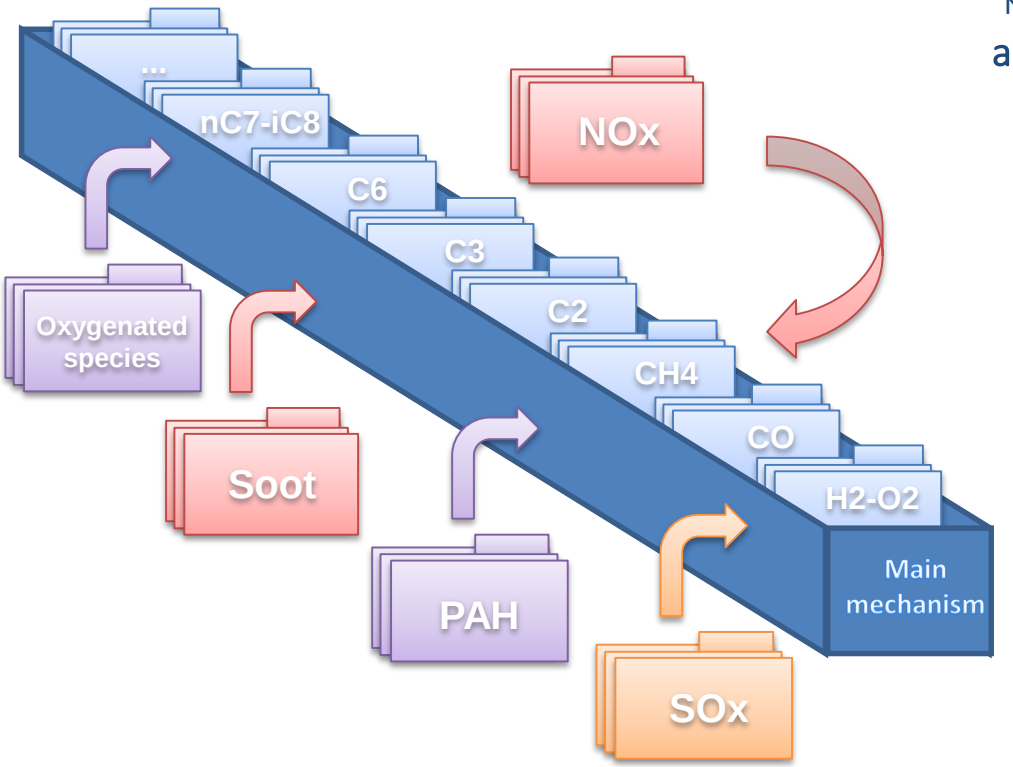
2. spark ignition experiments: the deployement of the droplet into a cold environment is usually followed by the local application of a transient external ignition source (sparks or hot wires)

a) a short period of pure evaporation at ambient temperature, followed by a non-uniform temperature radial profile peaking at 2000 K

b) addition of a generation term in the gas phase energy balance for a time which accounts for the typical duration of an electrically generated spark (1 ms)



Detailed kinetic mechanism



Kinetic mechanism of **pyrolysis, oxidation and combustion** of small (C1-C3) and large hydrocarbons up to Diesel and jet fuels (C16) as well as several pollutants

Hierarchy

Modularity

Generality

~ 435 chemical species

~ 13,495 reactions

http://creckmodeling.chem.polimi.it

The kinetic mechanism is freely available in CHEMKIN format at this web address

Frassoldati, A. et al., Combustion and Flame 157(2010), pp. 2-16

Ranzi, E. at al., Progress in Energy and Combustion Science 38 (2012), pp. 468-501

Numerical methodology

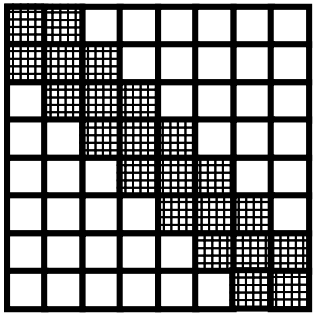
finite differences in space ⇒ Ordinary DAE system

large dimensions of the problem
non linearity of reaction rates and transport properties
⇒ Numerical difficulties in solving the resulting very stiff DAE system

The DAE system is structured as a (quasi) tridiagonal block matrix with square and dense submatrices whose dimensions depend on the number of chemical species included in the kinetic scheme

Example

200 points x 435 species ~ 90,000 equations ⇒ ~24 h of CPU time



Jacobian matrix of the global system

BzzDAEBloTri, a specifically conceived numerical solver, allows to efficiently treat the structured sparsity of the Jacobian matrix as well as the stiffness of the DAE system.

http://www.chem.polimi.it/homes/gbuzzi

Buzzi-Ferraris G., Manca D., Computers and Chemical Engineering, 22(11), p. 1595-1621 (1998)

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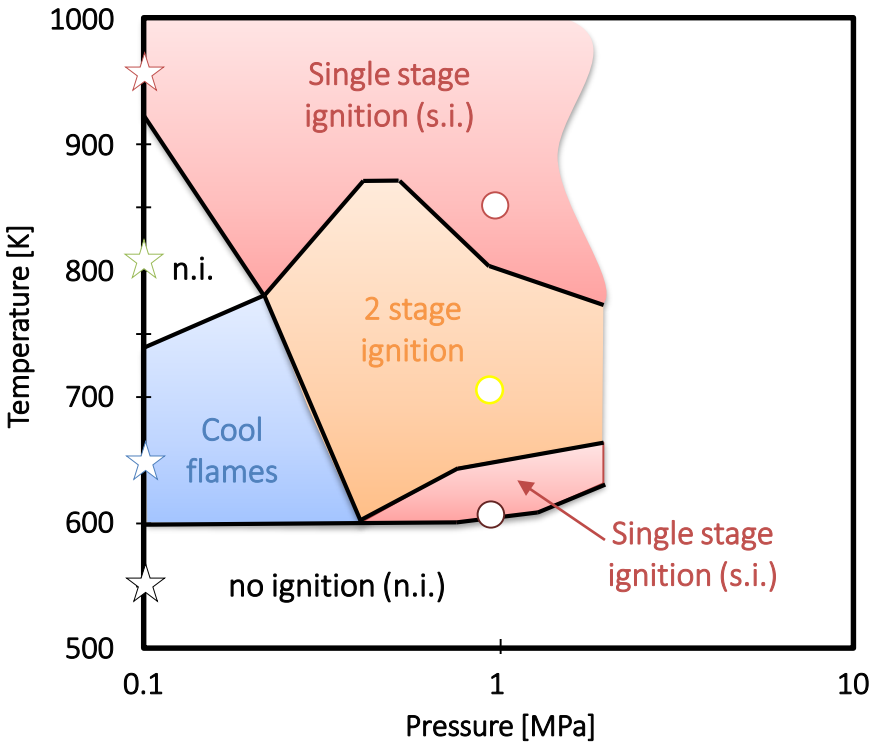
   - ✓ Kinetic analysis

6. Conclusions and future works

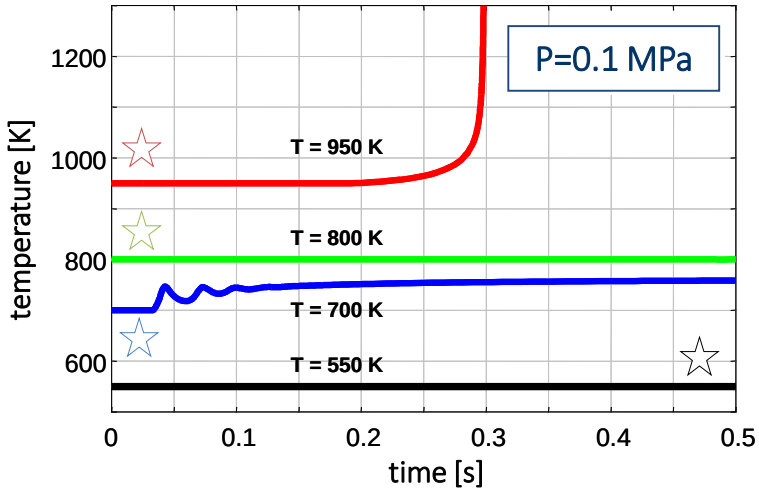
Autoignition experiments of Tanabe et al.

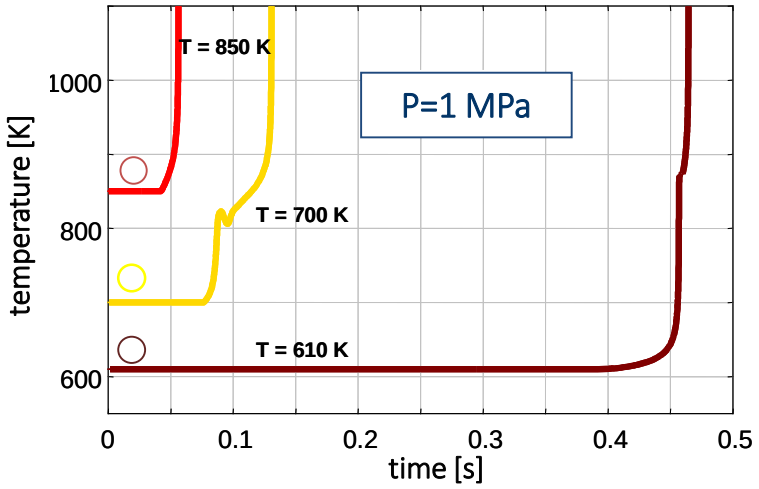
Auto-ignition experiments

n-heptane droplets in air (d_0=0.70 mm)



Adapted from: **Tanabe et al.**, 26th Symposium (International) on Combustion, p. 1637-1643 (1996)





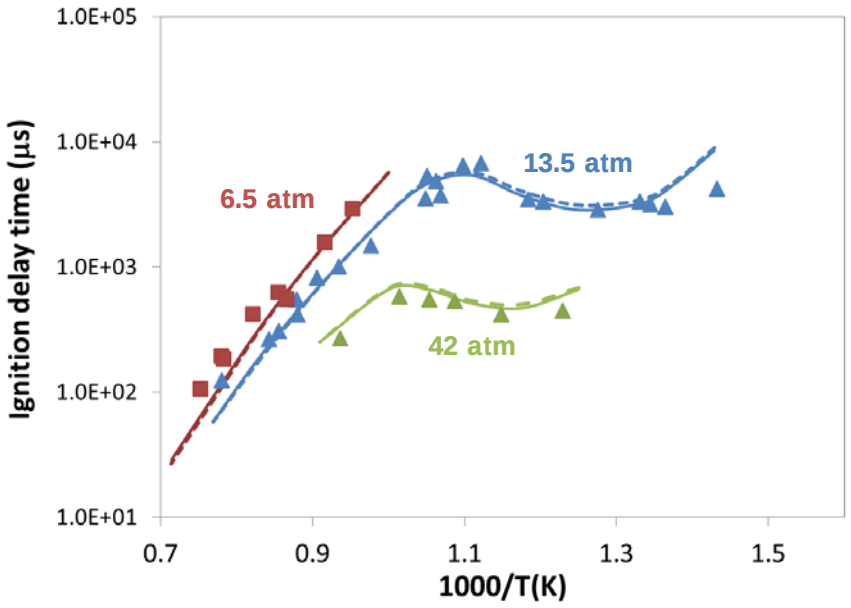
Validation of the kinetic mechanism: n-heptane

——— Original mechanism (435 species)

- - - - - Reduced mechanism (100 species)

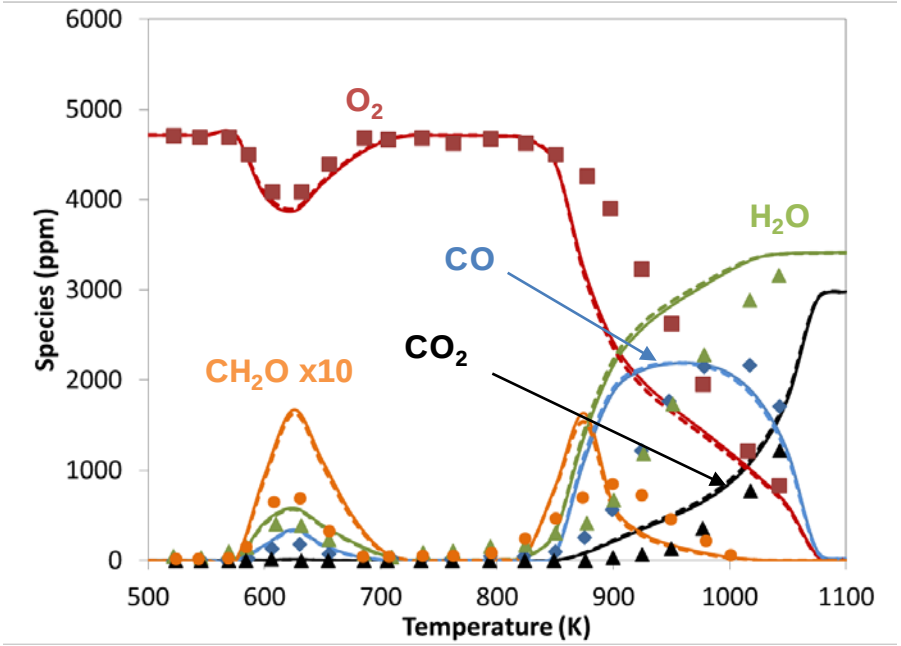
Polimi C1C16TOT

Shock-tube experiments



Experimental data from:
Ciezki H.K. and Adomeit G., Combustion and Flame 93 p. 421–433 (1993)

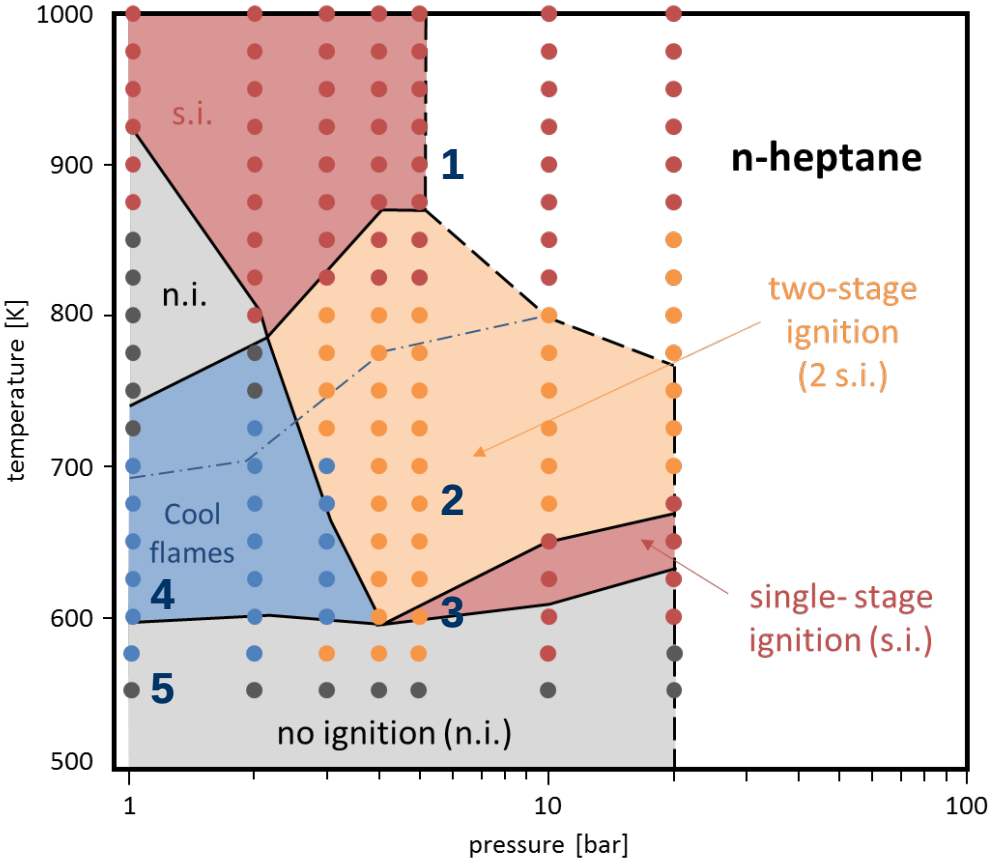
Princeton Variable Pressure Flow Reactor at temperatures of 500-1000 K and at a pressure of 8 atm



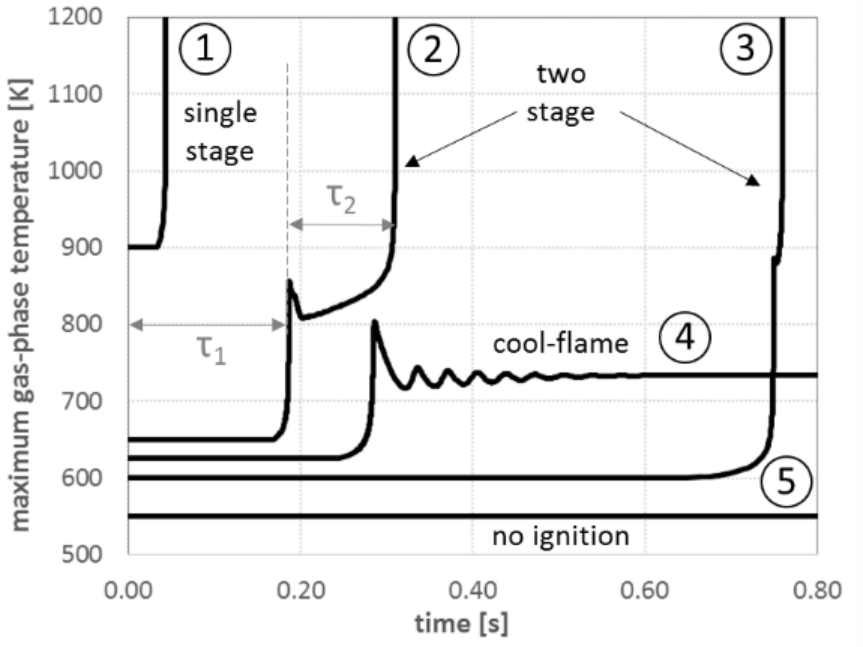
Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)

Ignition regions of n-heptane in air (I)

Comparison between experiments (maps, d0=0.7-0.8 mm) and numerical predictions (points, d0=0.7 mm).



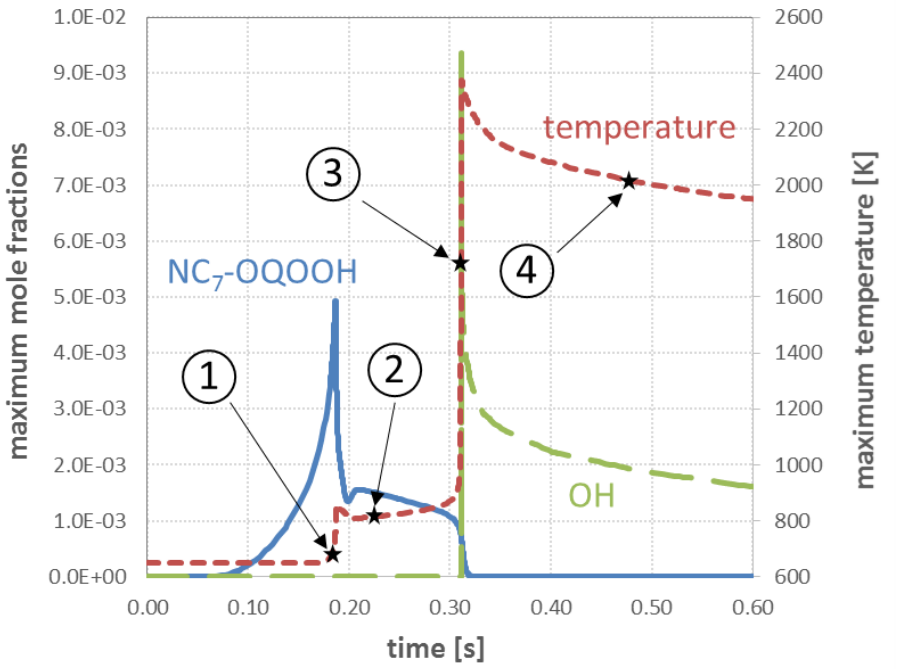
Maximum gas-phase temperature versus time for n-heptane droplets (numerical simulations).



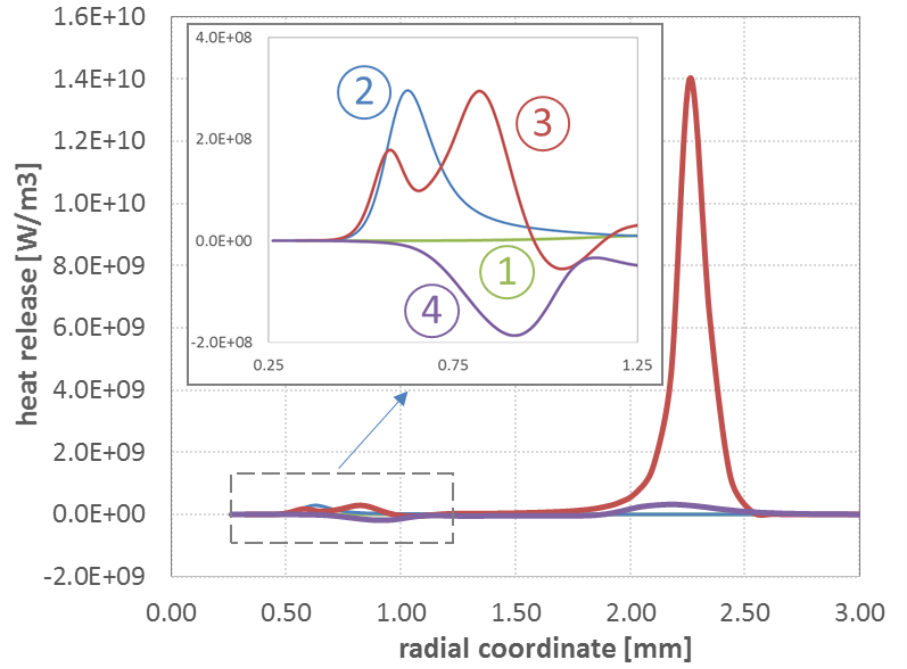
The total induction time τt is the sum of the first (τ1) and the second (τ2) induction times.

Ignition regions of n-heptane in air (II)

Maximum values of mole fractions of NC7-OQOOH and OH and temperature vs time.



Radial profiles of heat release at the four different times, reported on the left panel.

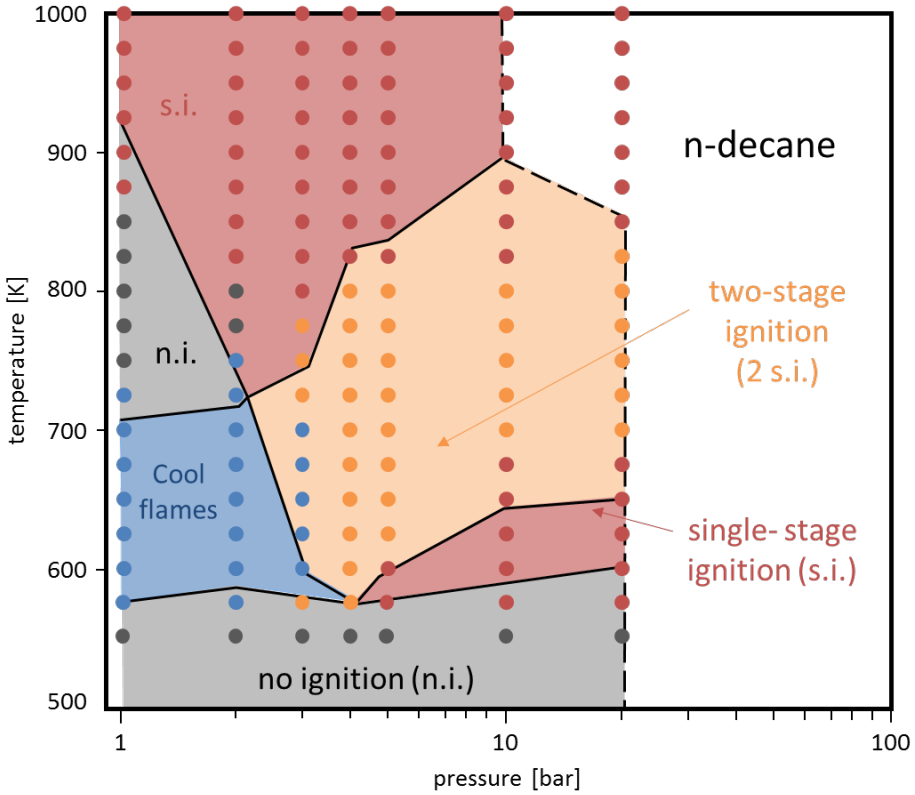


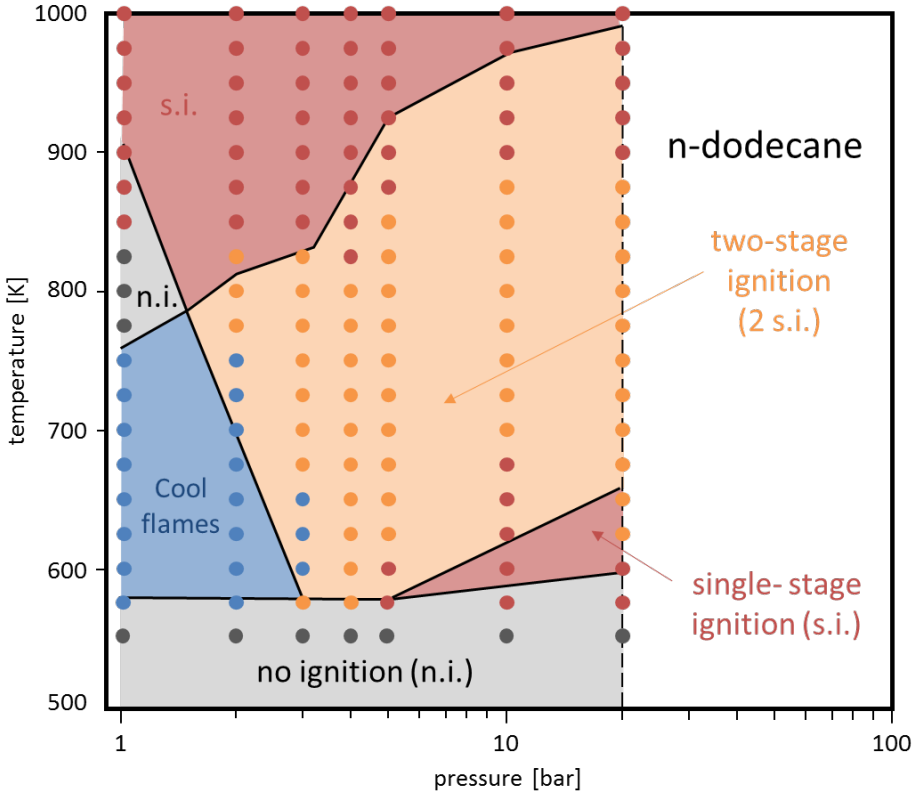
The first ignition occurs after 180 ms, when the concentration of the ketohydroperoxides NC7-OQOOH becomes sufficiently large to promote the low-temperature ignition

The cool flame (curve 2) is weakly exothermic, if compared to the HRR during the ignition (curve 3). The negative values of the HRR for the hot-flame (curve 4) is due to the endothermic reactions of fuel pyrolysis.

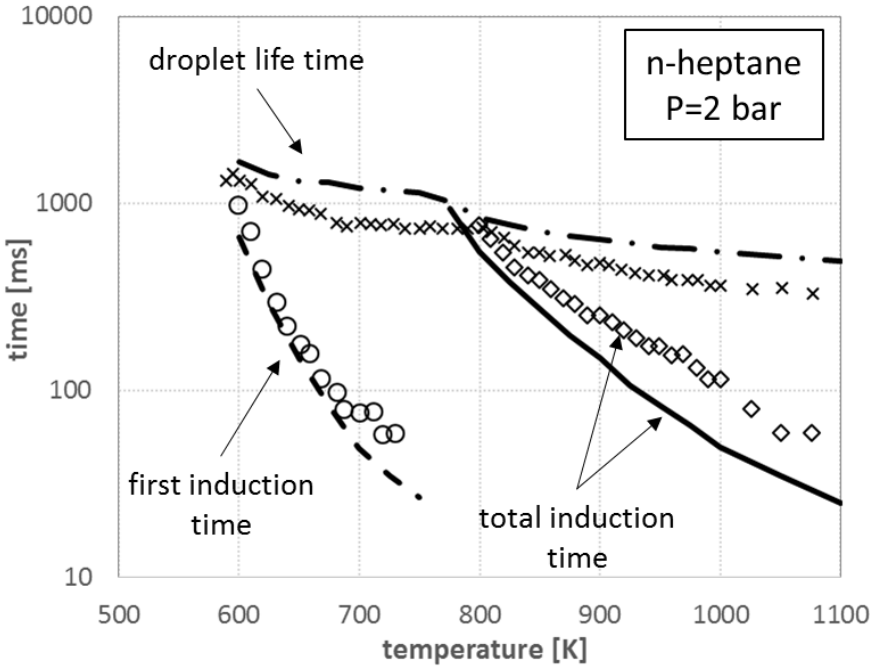
Ignition regions of n-C10 and n-C12

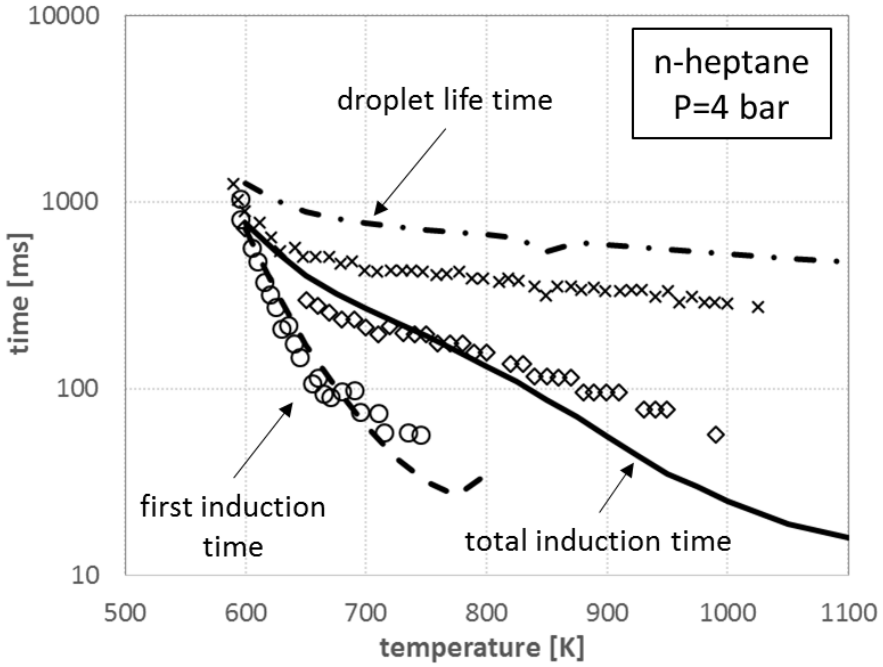
Comparison between experiments (maps, d0=0.7-0.8 mm) and numerical predictions (points, d0=0.7 mm).





Ignition delay times





- the first and total induction times tend to decrease with increasing the ambient temperature, since the vaporization of the fuel droplet is enhanced
- the total induction time decreases with increasing the pressure, because of the higher reactivity of the system
- since the ambient pressure reduces the vaporization rate, the first induction time, significantly influenced by the physical processes, increases with increasing the pressure

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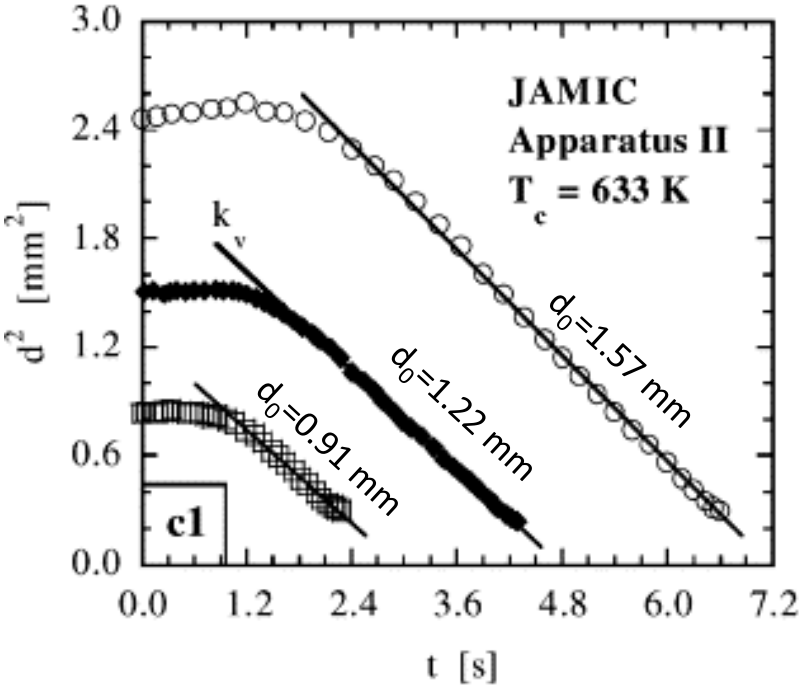
6. Conclusions and future works

Description of the experiments

Autoignition experiments
Experiments performed in either the Japan Microgravity Center (JAMIC) or the NASA Glenn Research Center

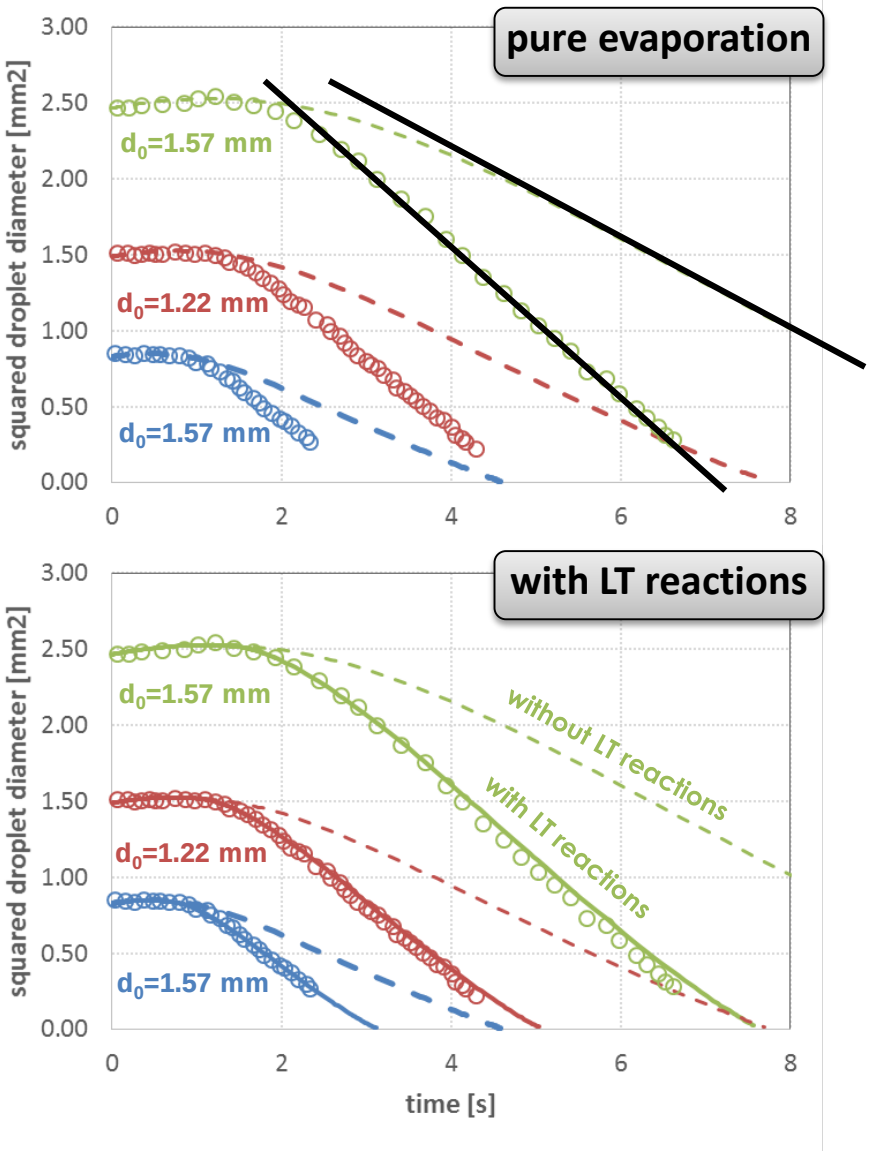
Fuel: **n-decane (NC10H22)**
Initial diameters: 0.91, 1.22 and 1.57 mm
Pressure: 1 atm
Droplet temperature: 300 K
Gas phase temperature: 633 K
Gas phase composition: air (21% O2, 79% N2)
Negligible soot formation
Droplet was suspended using a quartz fiber

Adapted from Xu et al. (2003)



Xu G., Ikegami M., Honma S., Ikeda K., Ma X., Nagaishi H., Dietrich D.L., Struk P.M., *Inverse influence of initial diameter on droplet burning rate in cold and hot ambiences: a thermal action of flame in balance with heat loss*, International Journal of heat and mass transfer, 46, p. 1155-1169 (2003)

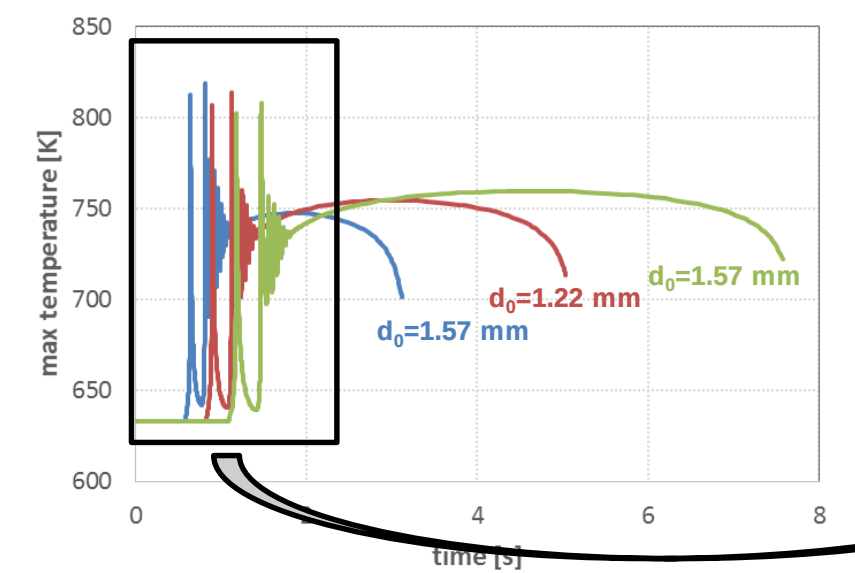
Numerical simulations

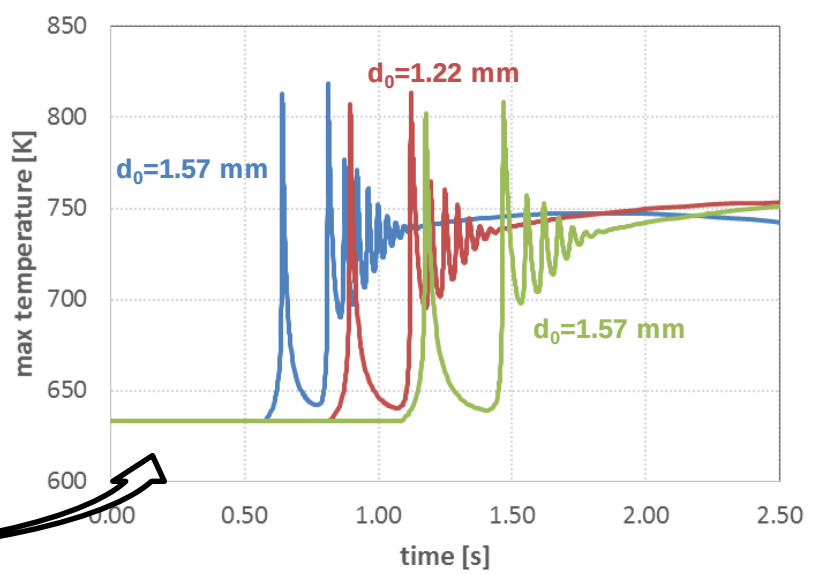


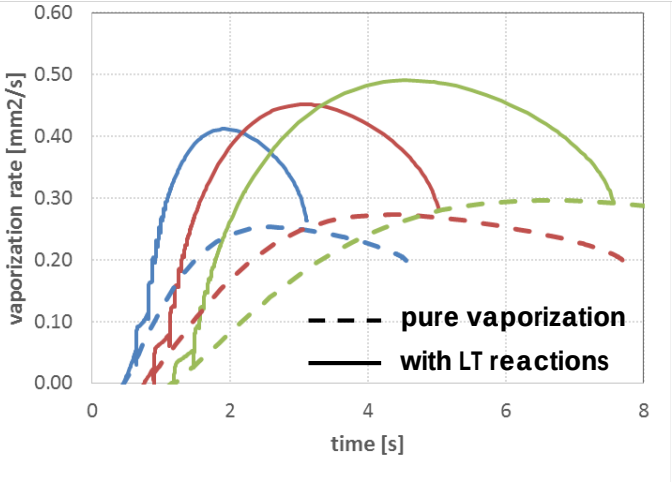
If the simulations are performed without considering any reactions in the gas phase, the calculated vaporization rate is smaller the experimental value

Only with the inclusion of low temperature (LT) reactions the numerical simulations are able to correctly reproduce the experimental data

Dumped cool flames







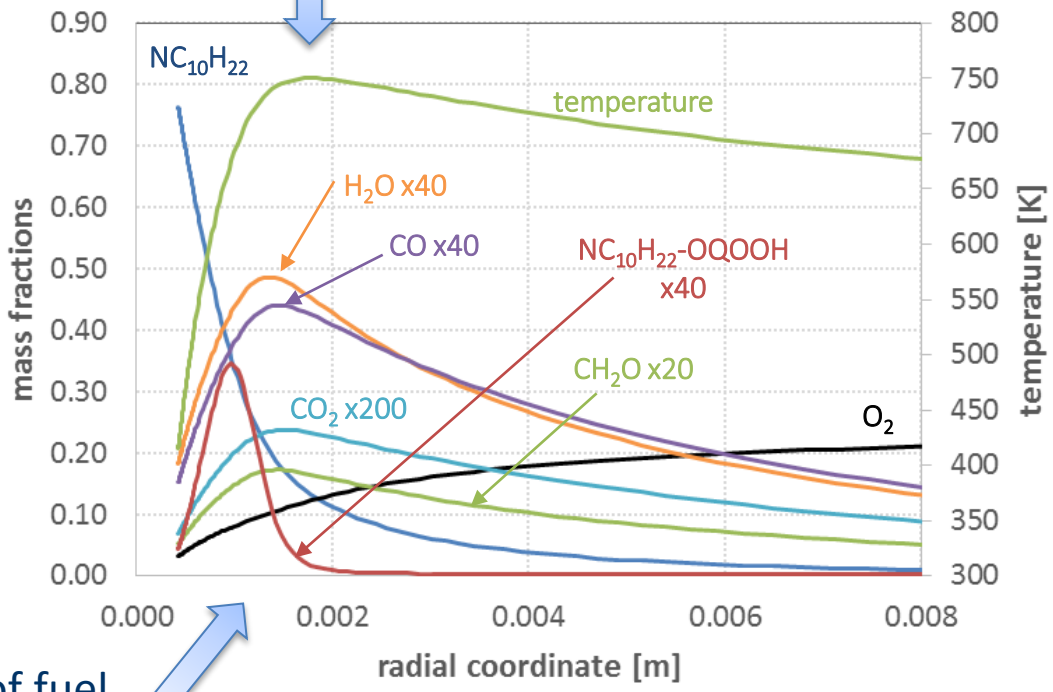
- ✓ initial dumped cool flame and a successive more stable temperature profile at ~750 K.
- ✓ once the first flame ignites, fuel is consumed and only partially replaced by the vaporization.
- ✓ the successive cool flames exihibit a higher frequency, produce less heat and gradually move the system from the cool flame to the slow combustion regime.

Cool flame structure

Small amounts of H_2O and CO_2 with respect to conventional flames
No OH radicals

Peak temperature ~750K

d_0=1.22 mm
Time = 3 s

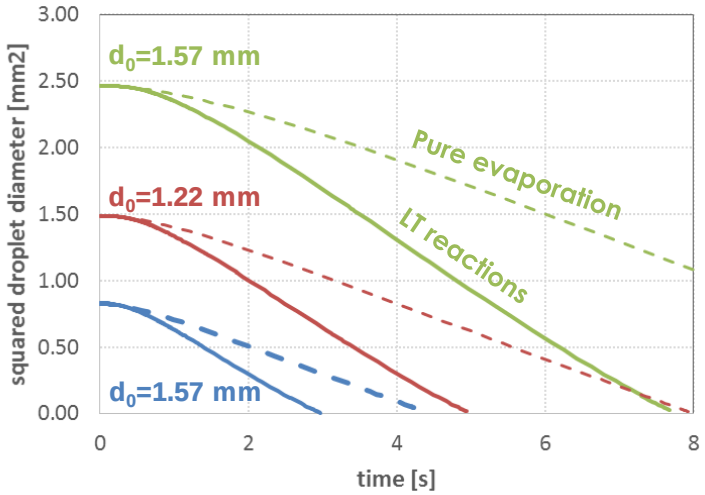


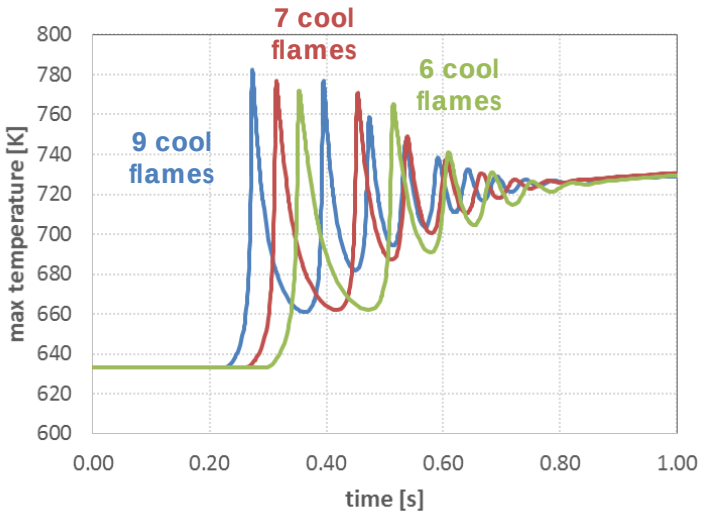
Co-existence of fuel ($C_{10}H_{22}$) and oxidizer (O_2)

Large amounts of ketohydroperoxides (e.g. $NC_{10}H_{22}$-OQOOH)

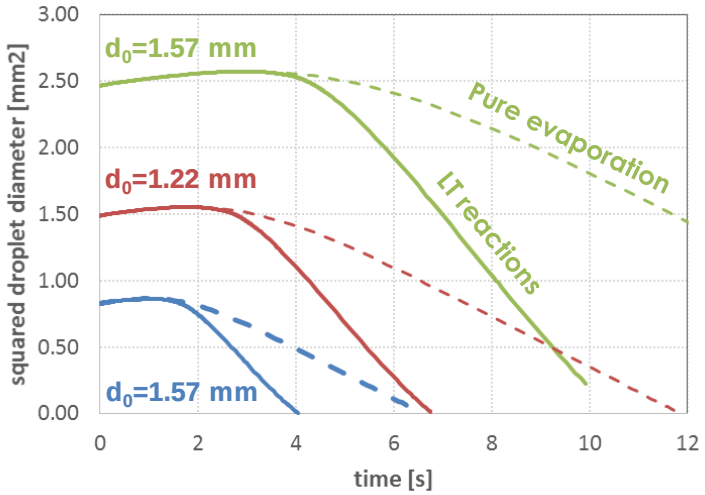
Extension to n-heptane and n-dodecane

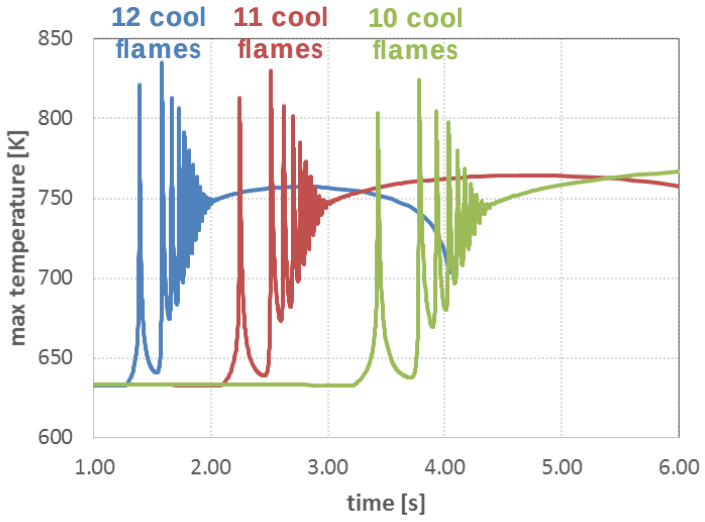
n-heptane





n-dodecane





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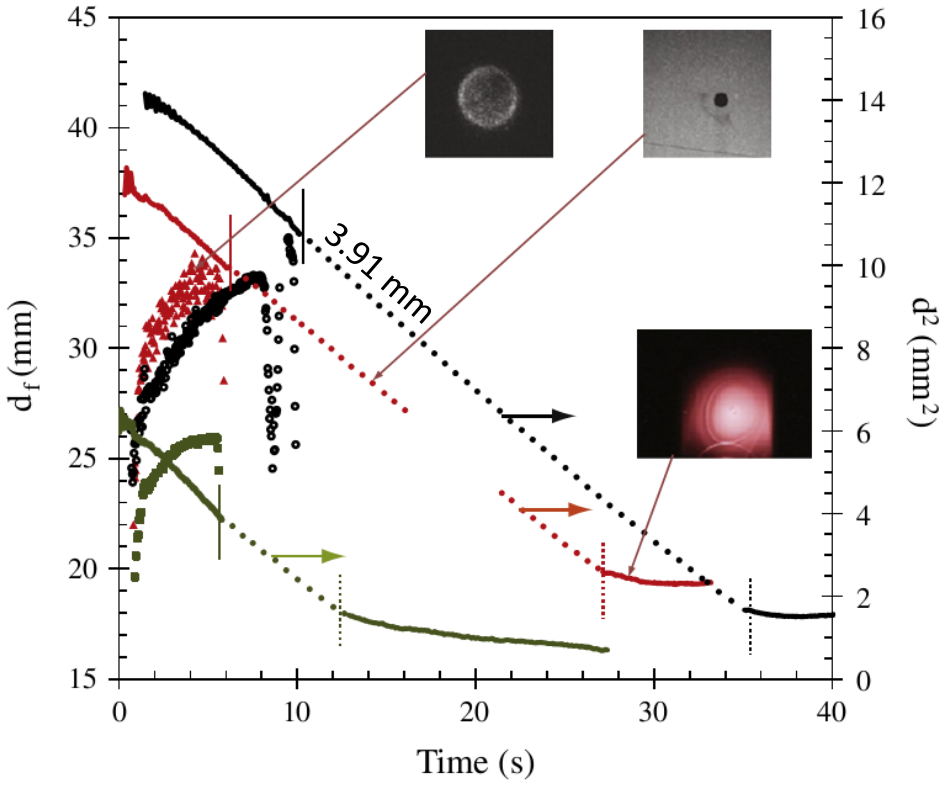
6. Conclusions and future works

Description of the experiments

Hot-wire ignition experiments
Experiments performed on board the International Space Station (ISS) using the multi-User Droplet Combustion Apparatus (MDCA) installed in the Combustion Integrated Rack (CIR) facility as a part of the Flame Extinguishment Experiments (FLEXs)

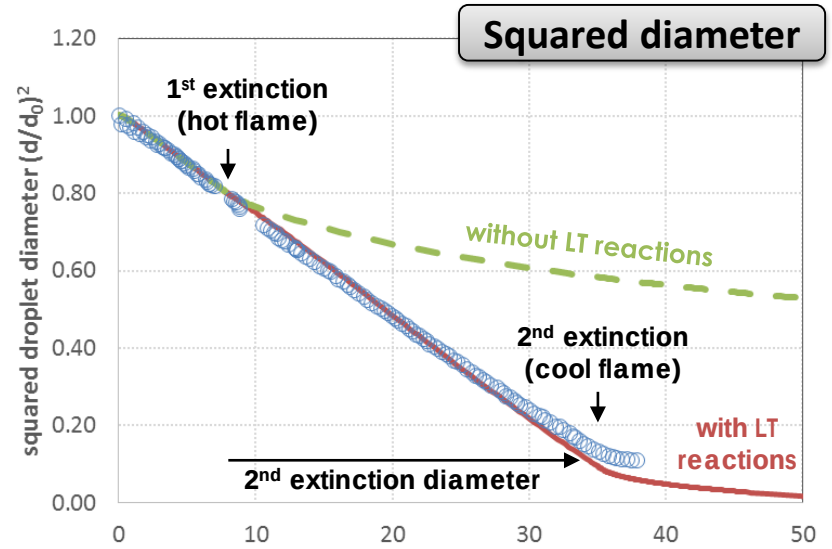
Fuel: n-heptane (NC_7H_{16})
Initial diameter: 3.91 mm
Pressure: 1 atm
Initial temperature: 300 K
Gas phase composition: air
Negligible soot formation
Droplet tethered by a fine silicon carbide filament

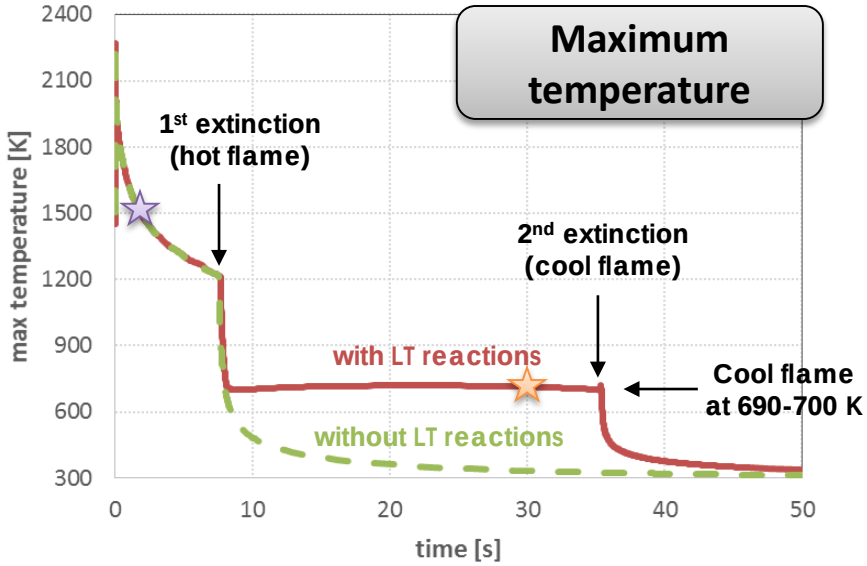
Adapted from Nayagam et al. (2012)



Nayagam V., Dietrich D.L., Ferkul P.V., Hicks M.C., Williams F.A., *Can cool flames support quasi-steady alkane droplet burning?*, Combustion and flame, 159, p. 3583-3588 (2012)

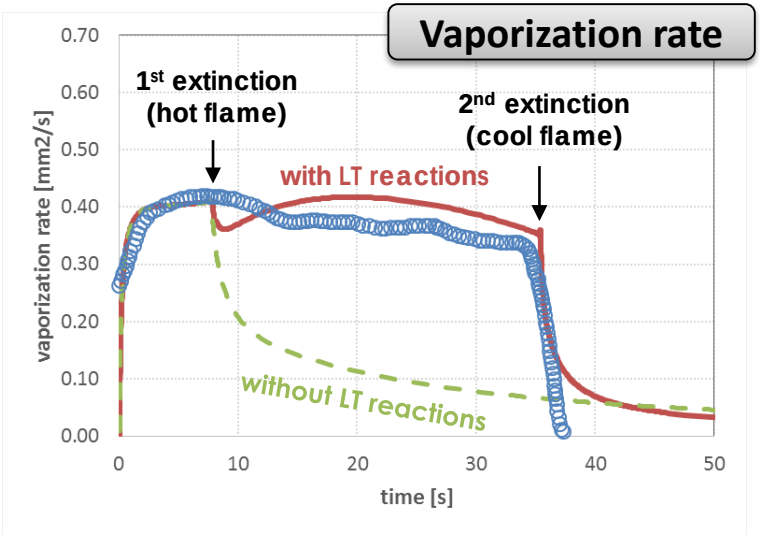
Numerical results





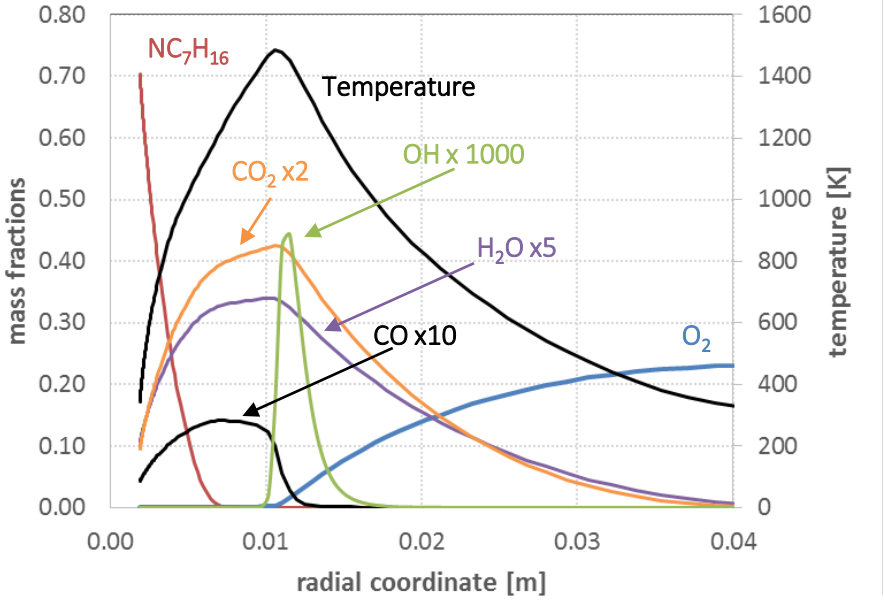
The agreement with the experiments is satisfactory if the LT mechanism is accounted for.

	Experiment	Simulation
1st extinction diameter [mm]	3.28	3.45
2nd extinction diameter [mm]	1.30	1.10
mean vaporization rate [mm2/s]	0.368	0.390

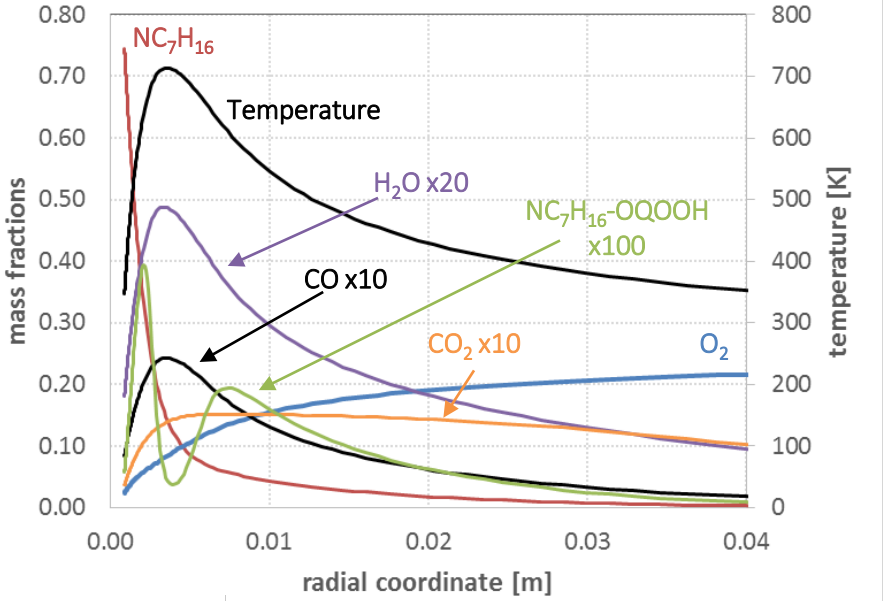


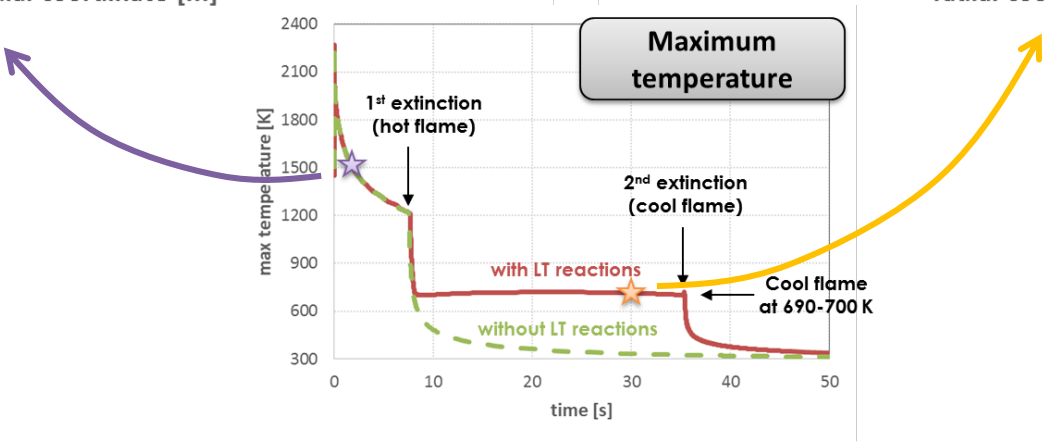
Flame structures

Hot flame @ 2 s



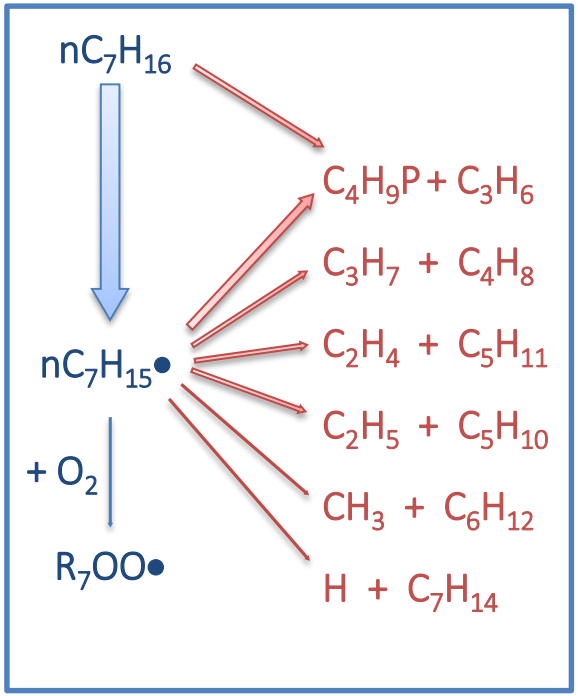
Cool flame @ 30 s





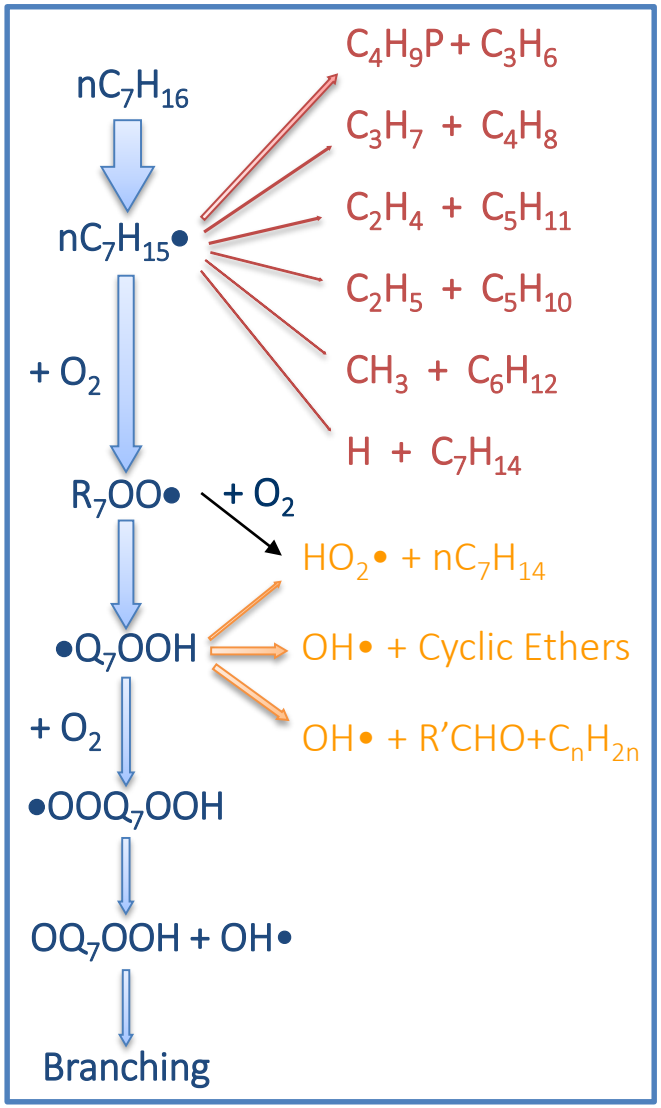
Path analysis

Hot flame @ 2 s

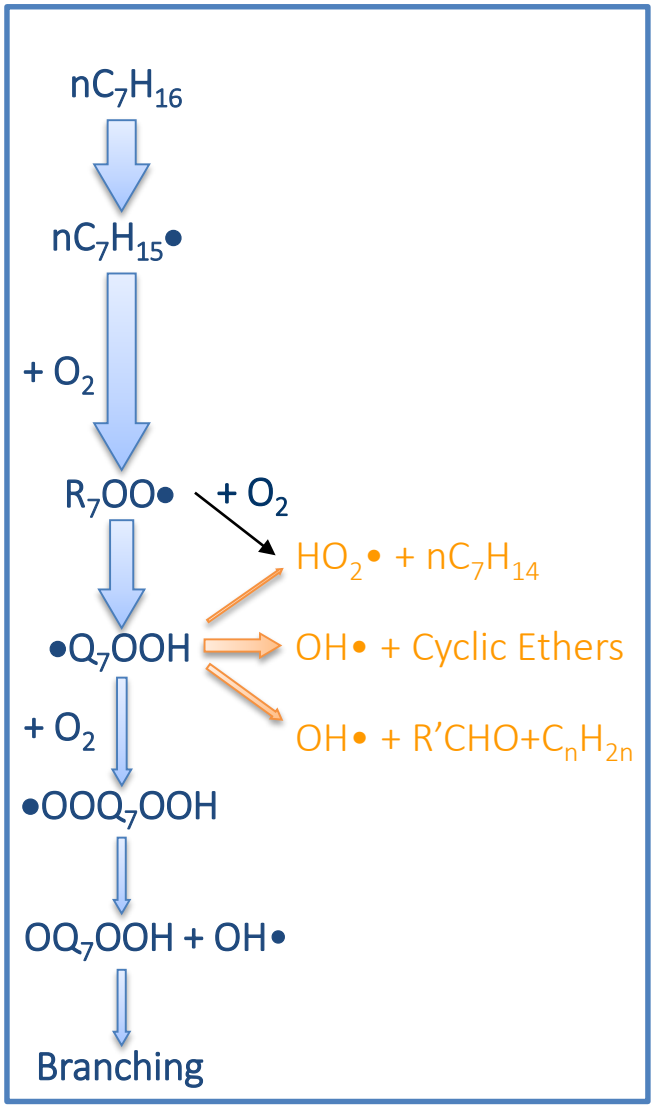


The thickness of the arrows is proportional to the importance of the corresponding flux

Transition @ 8 s

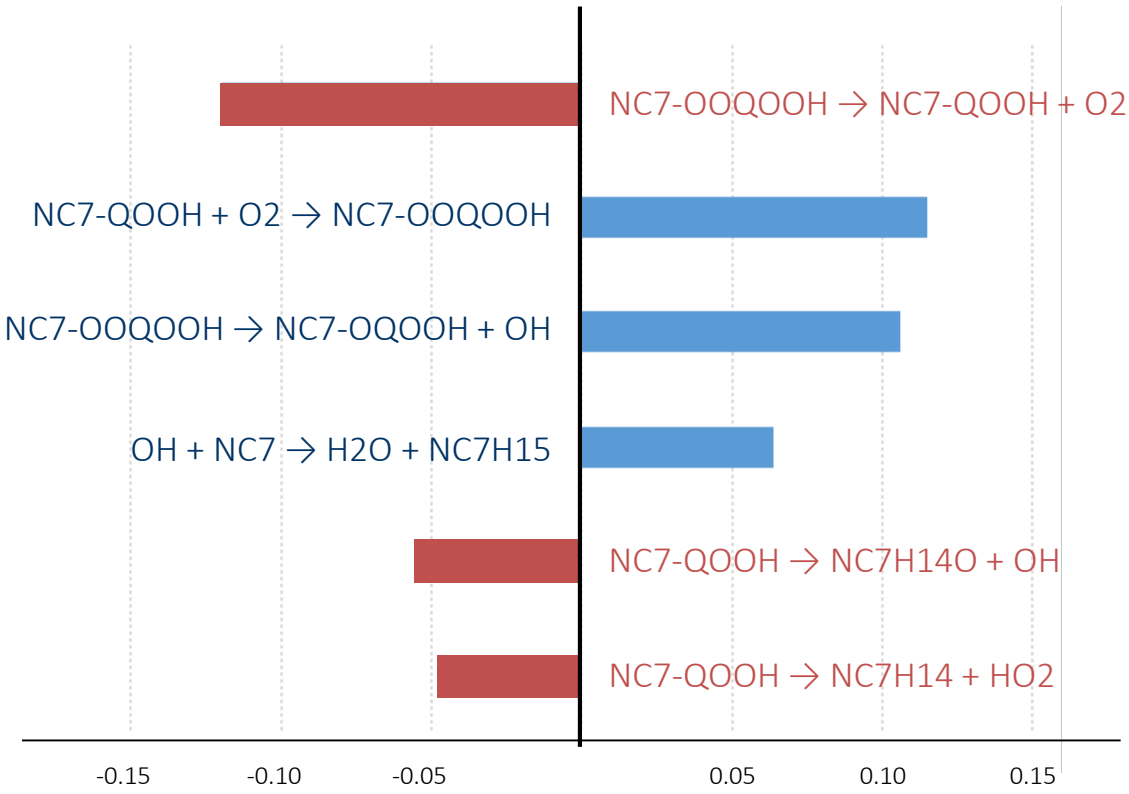


Cool flame @ 30 s

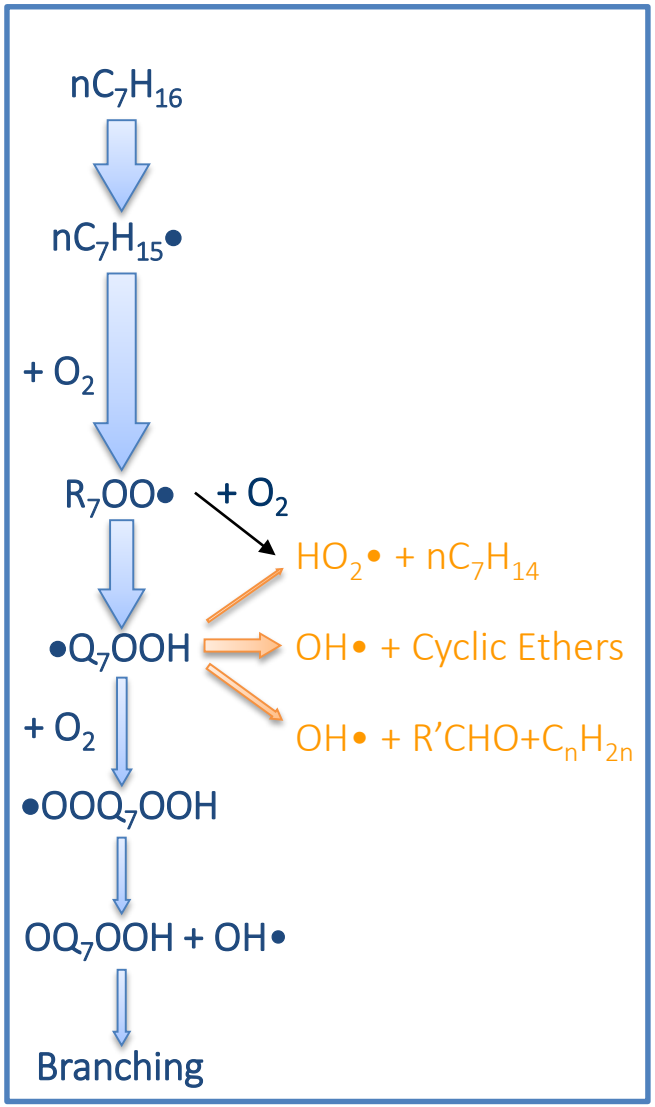


Sensitivity analysis

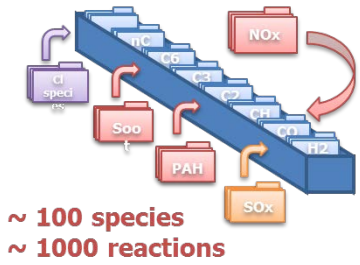
Global sensitivity coefficients of the vaporization rate during the LT combustion



Cool flame @ 30 s



Comparison with other kinetic mechanisms (I)



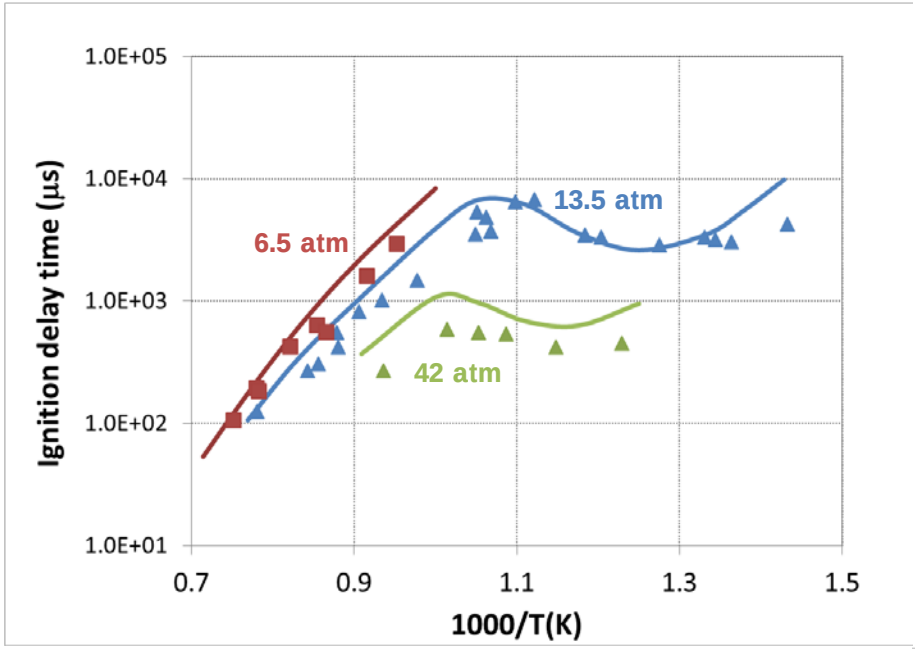
Several detailed kinetic mechanisms (with Low Temperature chemistry) were tested and compared

Polimi-C1C16TOT (version 1212)	**Species: 435 Reactions: 13,495**	**E. Ranzi, A. Frassoldati, R. Grana, A. Cuoci, T. Faravelli, A.P. Kelley, C.K. Law**, *Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels*, Progress in Energy and Combustion Science, 38 (4), pp. 468-501 (2012)
Lu-NC7	**Species: 188 Reactions: 939**	**C.S. Yoo, T.F. Lu, J.H. Chen, C.K. Law**, *Direct numerical simulations of ignition of a lean n-heptane/air mixture with temperature inhomogeneities at constant volume: Parametric study*, Combustion and Flame, 158(9), p.1727–1741 (2011)
LLNL-NC7	**Species: 658 Reactions: 2,827**	**Mehl M., W.J. Pitz, C.K. Westbrook, H.J. Curran,** *Kinetic Modeling of Gasoline Surrogate Components and Mixtures Under Engine Conditions*, Proceedings of the Combustion Institute33:193-200 (2011)

Validation of the kinetic mechanism: n-heptane

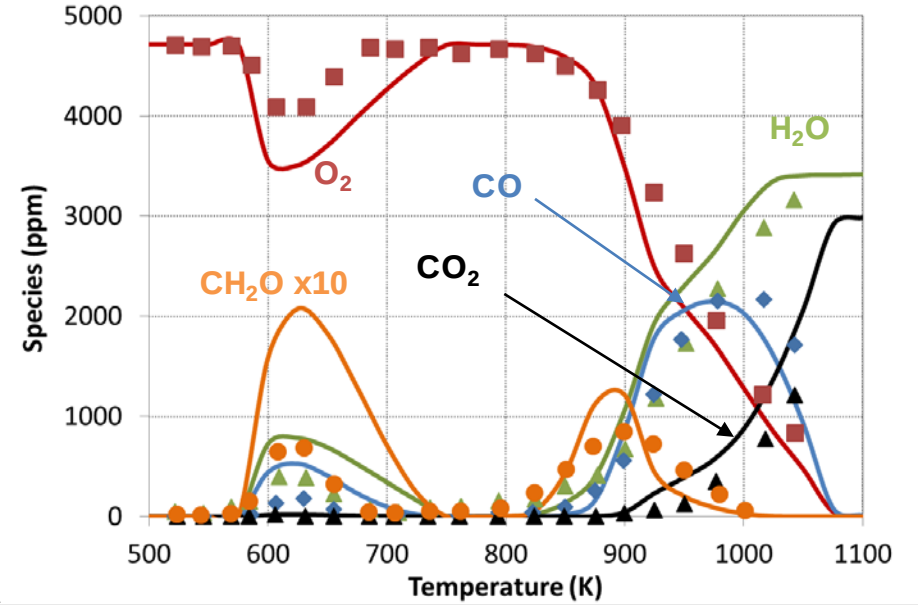
Lu NC7 (188 species)

Shock-tube experiments



Experimental data from:
Ciezki H.K. and Adomeit G., *Shock-tube investigation of self-ignition of n-heptane-air mixtures under engine relevant conitions*, Combustion and Flame 93 p. 421–433 (1993)

Princeton Variable Pressure Flow Reactor at temperatures of 500-1000 K and at a pressure of 8 atm

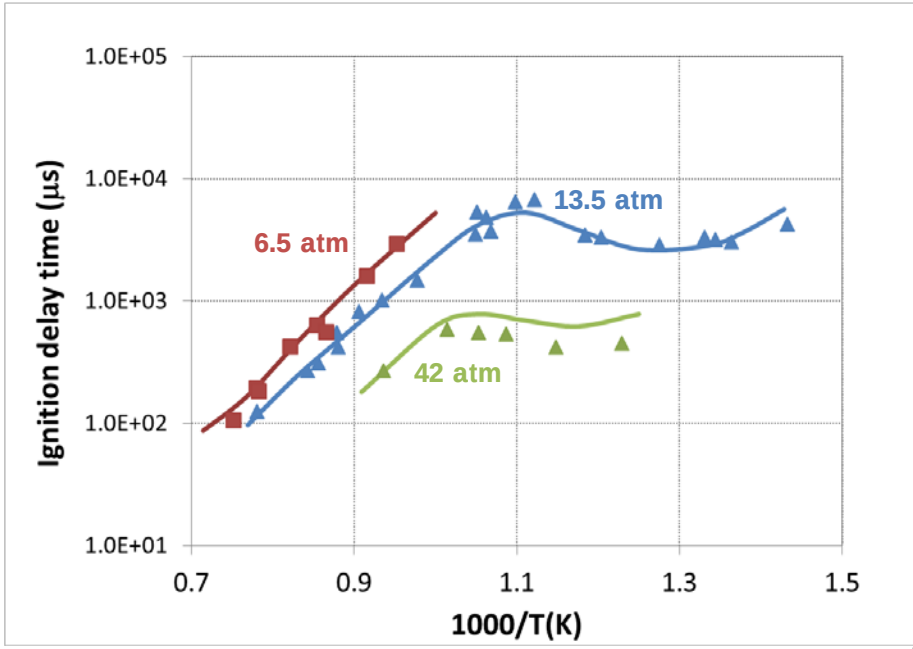


Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., *An experimental and kinetic modeling study of the two stage auto-ignition kinetic behavior of C7, C10, C12, and C14 n-alkanes*, Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)

Validation of the kinetic mechanism: n-heptane

LLNL NC7 (658 species)

Shock-tube experiments



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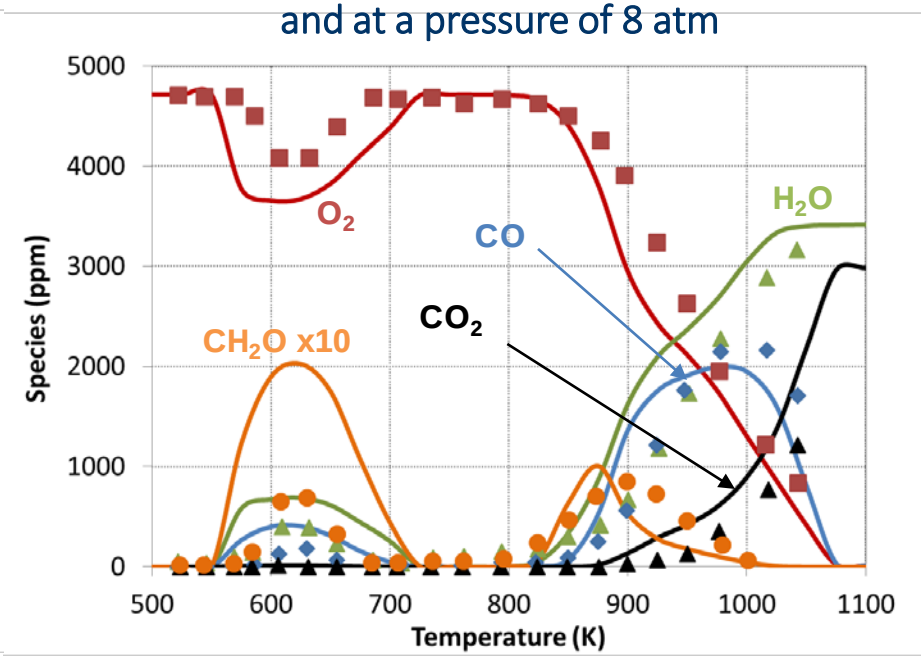

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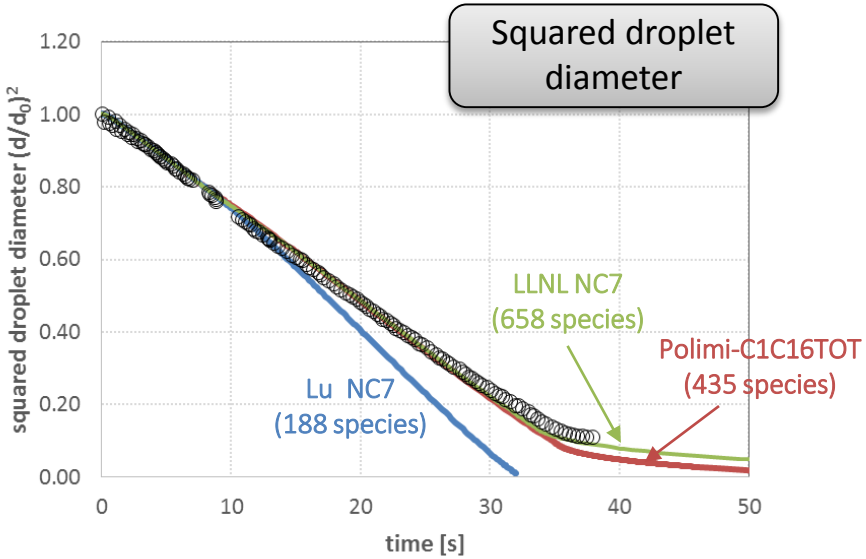
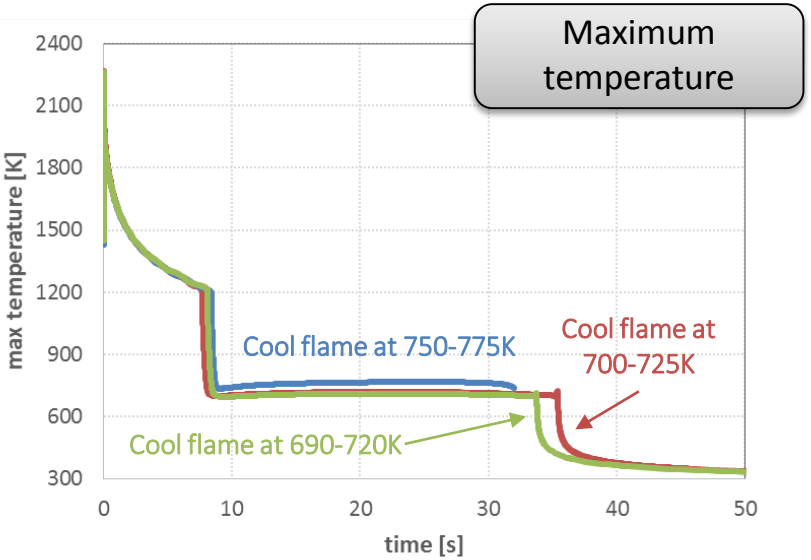
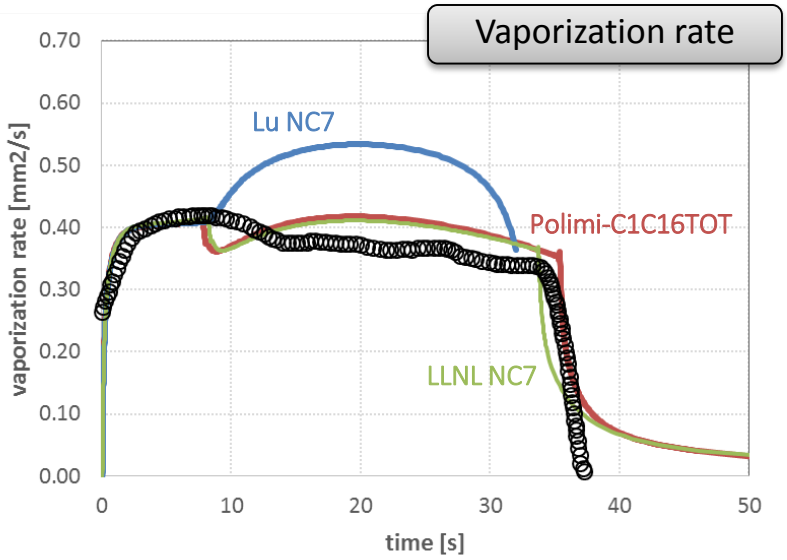
Comparison with other kinetic mechanisms (II)







The results are strongly affected by the ability of the **kinetic mechanism** to correctly capture the features of the cool flame (i.e. by the accuracy and the reliability of the low-temperature chemistry)

Outline

1. Introduction
   - ✓ Cool flames
   - ✓ Low-temperature mechanism
2. Numerical modeling of isolated fuel droplets
   - ✓ Governing equations and numerical methodology
   - ✓ Detailed kinetic mechanism
3. Auto-ignition regions of hydrocarbon fuel droplets
   - ✓ Auto-ignition regions
   - ✓ Ignition delay times
4. Auto-ignited n-decane ($C_{10}H_{22}$) droplets
   - ✓ Comparison with experiments
   - ✓ Structure of the cool flame
5. Hot-wire ignited n-heptane (NC_7H_{16}) droplets
   - ✓ Comparison with experiments
   - ✓ Kinetic analysis
6. **Conclusions and future works**

Conclusions

Numerical modeling of **auto-ignited** and **hot-wire ignited** isolated droplets in microgravity with **detailed kinetic mechanisms** were successfully performed

The formation of **cool flames**, both for **n-decane** and **n-heptane droplets**, was observed, explained and compared with experimental measurements

Auto-ignition of n-decane droplets (experiments performed by Xu et al.)

We demonstrated that the observed vaporization rates can be explained only by the presence of a cool flame around the droplet

Hot-wire ignited n-heptane droplets (experiments performed by Nayagam et al.)

We confirmed the hypothesis that after the first-stage extinction, the vaporization is sustained by a low-temperature, soot-free, ‘‘cool-flame’’ heat release.

Future work

Additional simulations of experiments of hot-wire ignition experiments on n-heptane droplets to check the formation of cool flames

Deeper investigations about the chemistry of cool flames

Improvements in the numerical model (radiative heat transfer, numerical methodology, etc.)

Modeling of soot formation through a detailed kinetic mechanism (based on the discrete sectional method)

Table 1
Experimental conditions, measured droplet initial diameter d_0, hot-flame extinction diameter d_{he}, and the second-stage extinction diameter d_{ce}.

Test #	P (atm)	O_2 (%)	CO_2 (%)	d_0 (mm)	d_{he} (mm)	d_{ce} (mm)	K (mm^2/s)	B
1	2	21	9	2.92	1.73	0.42	0.475	4.44
2	1	21	0	3.91	3.28	1.30	0.368	4.48
3	1	21	0	3.58	2.8	0.73	0.448	4.48
4	1	21	0	3.69	3.46	0.72	0.462	4.48
5	1	18	0	3.48	3.16	1.60	0.356	3.82
6	1	17.5	0	2.74	2.03	0.78	0.412	3.75
7	1	18	15	3.76	3.63	1.88	0.361	3.51
8	1	18	15	2.84	2.55	1.46	0.36	3.51
9	1	18	15	3.82	3.66	1.82	0.359	3.51
10	1	18	15	2.49	1.97	1.25	0.343	3.51
11	1	19	10	3.51	3.15	1.50	0.381	3.82
12	1	19	10	2.6	1.72	1.01	0.334	3.82
13	1	17	20	3.76	3.71	2.16	0.346	3.22
14	1	20	5	2.9	2.79	1.74	0.355	4.14
15	1	20	5	3.04	2.33	1.18	0.351	4.14
16	1	16	0	3.34	3.18	1.97	0.346	3.38
17	1	16	0	2.52	2.13	1.50	0.333	3.38
18	1	15	0	2.55	2.31	1.73	0.319	3.16
19	1	21	0	3.65	2.85	1.34	0.424	4.48
20	0.7	23.5	55.8	3.77	3.04	1.83	0.412	3.74
21	0.7	23	23	3.87	3.42	1.89	0.412	4.35
22	0.7	21	30	4.05	3.83	2.91	0.393	3.74
23	0.7	19.6	35	3.11	2.9	2.37	0.3649	3.43
24	0.7	18	40	2.68	2.49	2.16	0.3593	3.04
25	0.7	18	40	2.53	2.37	2.05	0.304	3.04
26	0.7	23	25	3.42	2.62	2.04	0.3542	4.21

Adapted from **Nayagam et al.,** Combustion and Flame, 159, p. 3583-3588 (2012)

Acknowledgments

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