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A. Cuoci, A. Frassoldati, T. Faravelli and E. Ranzi

Numerical modeling of auto-ignition of isolated fuel droplets in microgravity

35th International Symposium on Combustion

August 3-8, 2014 – San Francisco, California (USA)

Modeling of auto-ignition of isolated fuel droplets

isolated fuel droplets

no interactions between the different droplets of a spray

+

microgravity

the droplet and the flame are spherical

g μg g μg

spherical symmetry = 1D model

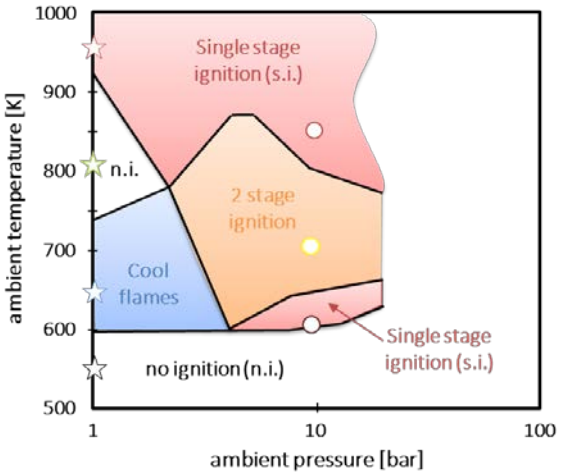
Numerical modeling with detailed kinetics

✓Phenomenological understanding of major burning features of droplet combustion

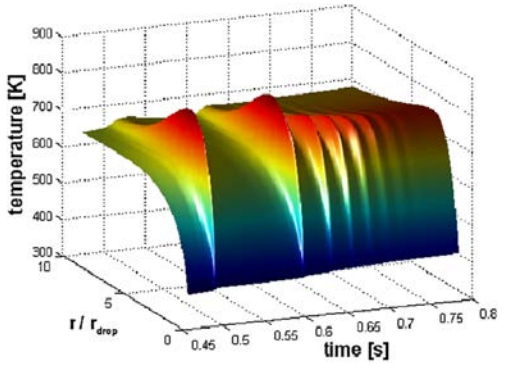
✓Kinetic analyses

✓Pollutant formation (soot, NOx, SOx …)

1. Auto-ignition regimes of n-alkanes droplets



2. "Anomalous" evaporation of nC10 droplets



Outline

1. Numerical modeling of isolated fuel droplets
   - ✓ Governing equations
   - ✓ Numerical methodology
   - ✓ Detailed kinetic mechanisms (low- and high-temperature)
2. Auto-ignition regimes of hydrocarbon fuel droplets
   - ✓ Auto-ignition regimes
   - ✓ Numerical simulations and analysis of results
   - ✓ Comparison with experimental data
3. "Anomalous" evaporation of n-decane ($C_{10}H_{22}$) droplets
   - ✓ Comparison with experiments
   - ✓ Analysis of numerical results
4. Conclusions

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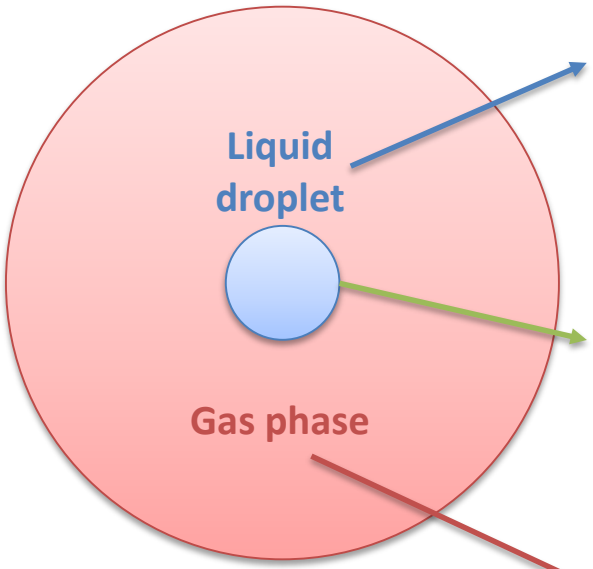
Mathematical model



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

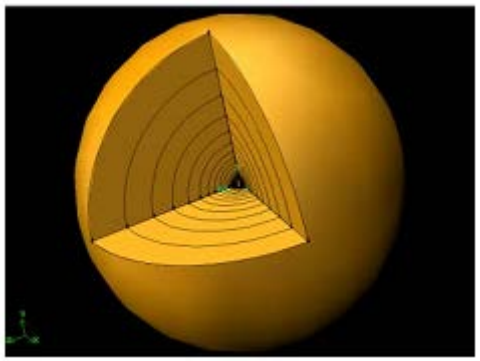
Interface (liquid/gas)

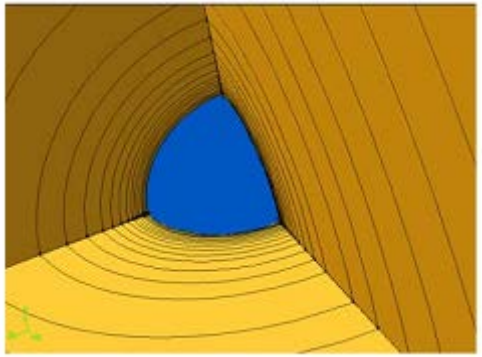
- ✓ Thermodynamic equilibrium
- ✓ Conservation of fluxes

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

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

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





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

Boundary and initial conditions

Center of the droplet

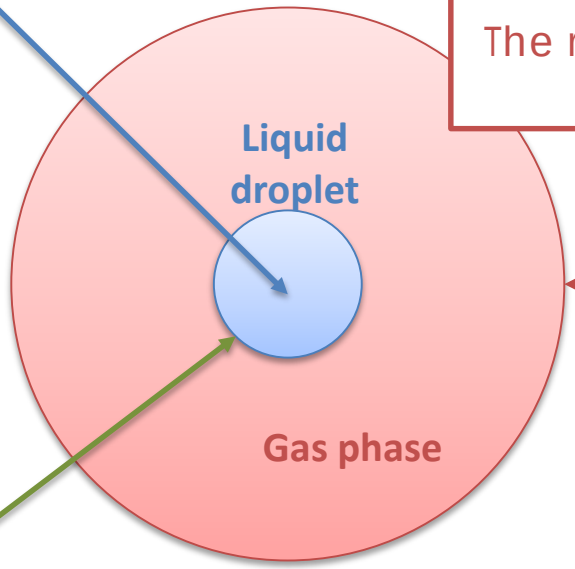
$$\frac{\partial \omega_i^L}{\partial r} = 0 \qquad \frac{\partial T_L}{\partial r} = 0 \qquad v_L = 0$$

Symmetry conditions

Outer border

$$\frac{\partial \omega_i^G}{\partial r} = 0 \qquad T_G = T_G^0 \qquad v_L = 0$$

The results are not sensitive to these BCS



Interface

Continuity of fluxes of mass and energy

$$\dot{m}_{G,i} = \dot{m}_{L,i} \qquad \dot{e}_G = \dot{e}_L$$

Thermodynamic equilibrium

$$f_{G,i} = f_{L,i}$$

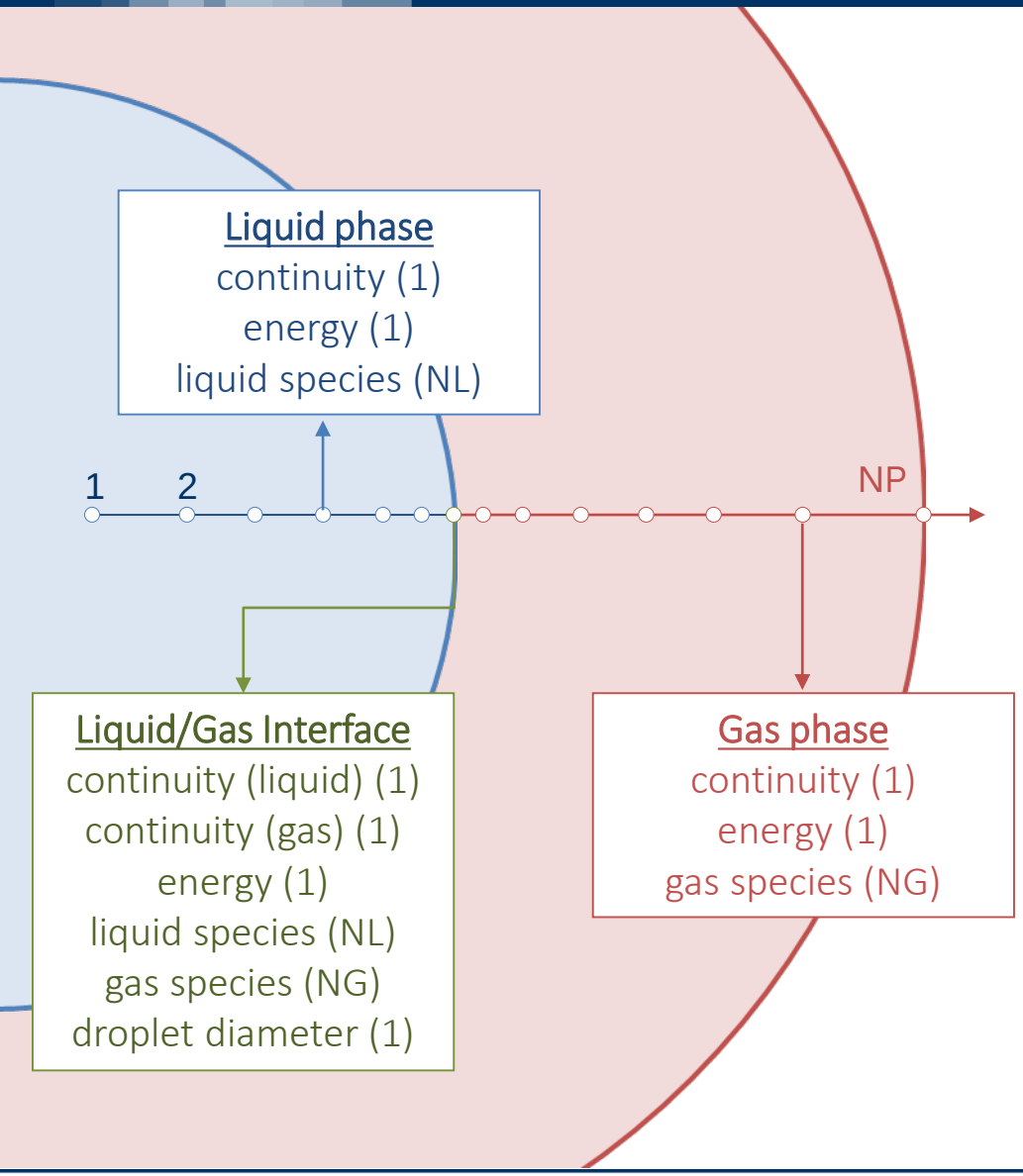
Continuity of temperatures

$$T_G = T_L$$

Initial conditions

Auto-ignition: the droplet is placed into an environment with high, uniform temperature

Numerical methodology (I)



finite difference in space

Differential-Algebraic Equations (DAE)

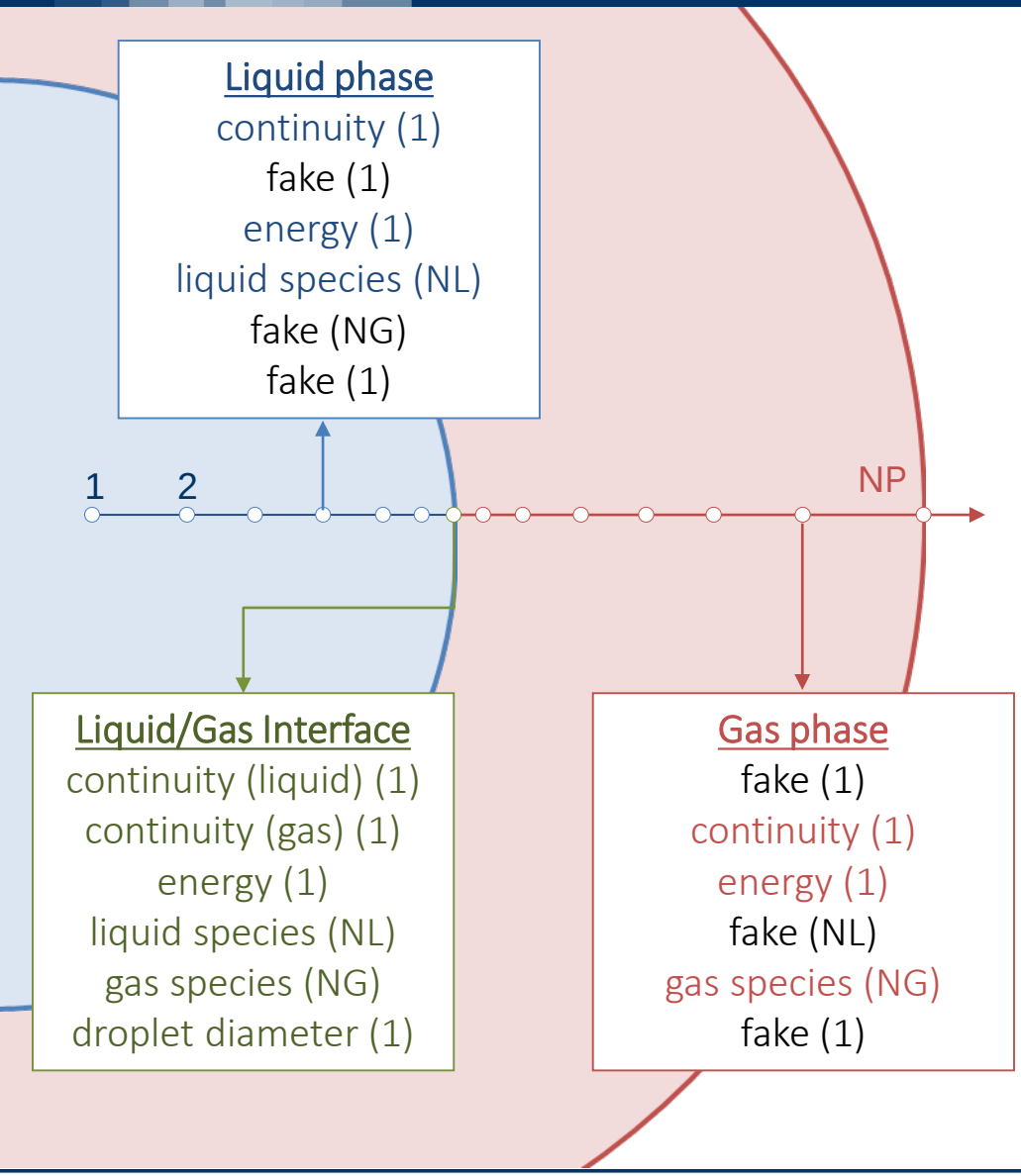
Algebraic equations:
Boundary conditions
+
Continuity equation

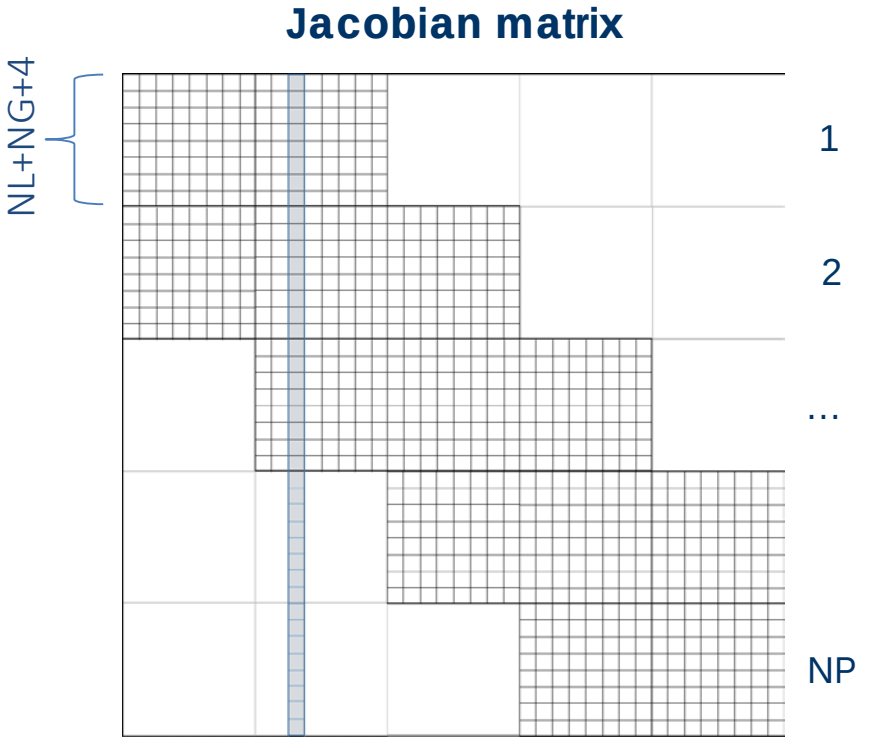
NP = total number of grid points
NL = number of liquid components
NG = number of gas species

Example:
2-component droplet + 100 gas species

Liquid phase: 4 eqs (per point)
Interface: 106 eqs
Gas phase: 102 eqs (per point)

Numerical methodology (II)

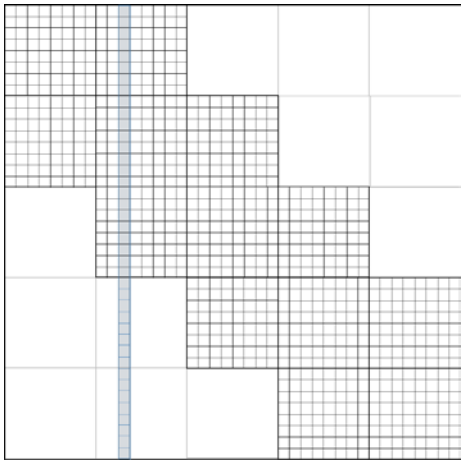




Introduction of **fake variables** and equations in the liquid and gas phase to have a (quasi) **block-tridiagonal** Jacobian matrix

Numerical methodology (III)

The associated Jacobian matrix is structured as a (quasi) block tridiagonal matrix with square and dense sub-matrices whose dimensions depend on the number of chemical species included in the kinetic scheme



Example:

200 points x 400 species ~ 80,000 fully-coupled equations

strong non linearity of reaction rates and transport properties

strong coupling among the equations

detailed kinetic mechanisms

→ The resulting DAE system is very stiff

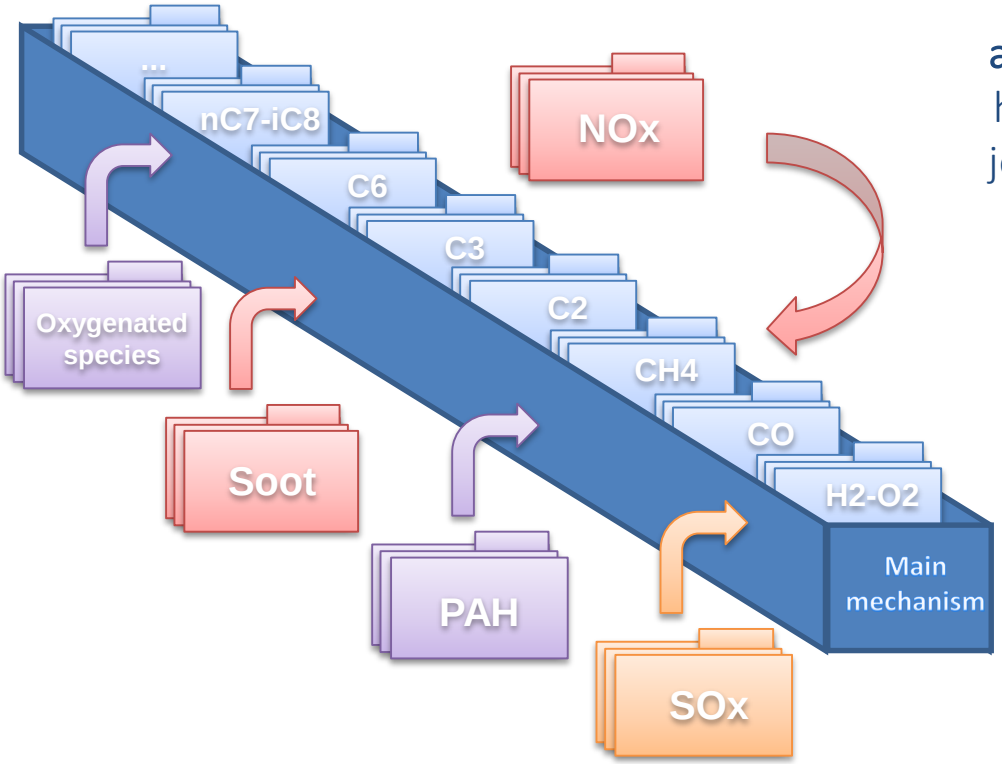
Fully-coupled approach

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)

Detailed kinetic mechanism (I)



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

Hierarchy

Modularity

Generality

~ 482 species

~ 19,072 reactions

http://creckmodeling.chem.polimi.it

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

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

Ranzi, E. at al., International Journal of Chemical Kinetics 46(9) (2014), pp. 512-542

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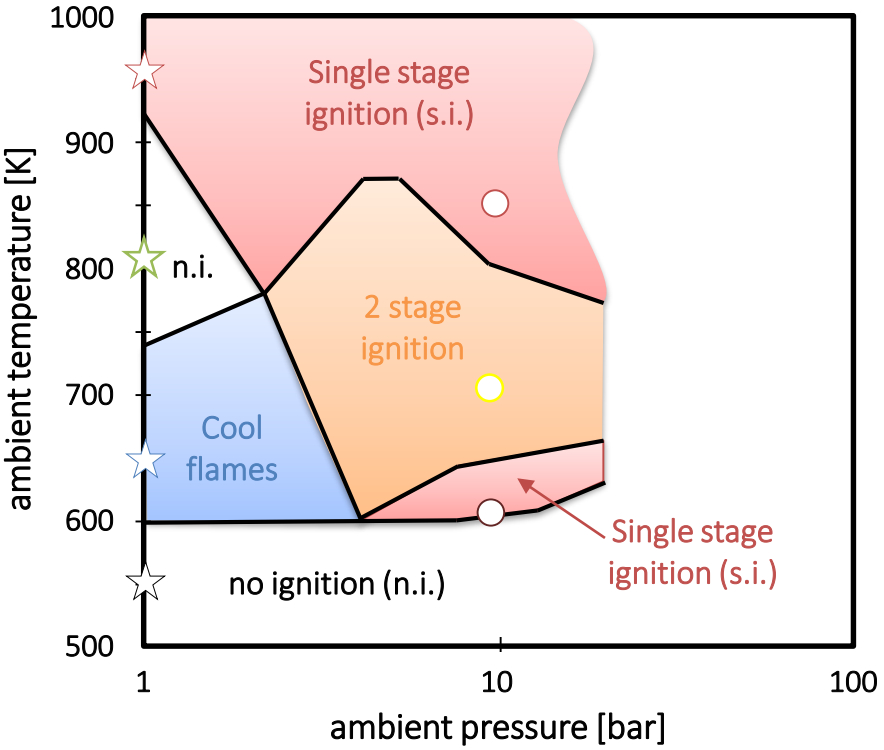
Auto-ignition experiments of n-alkanes droplets

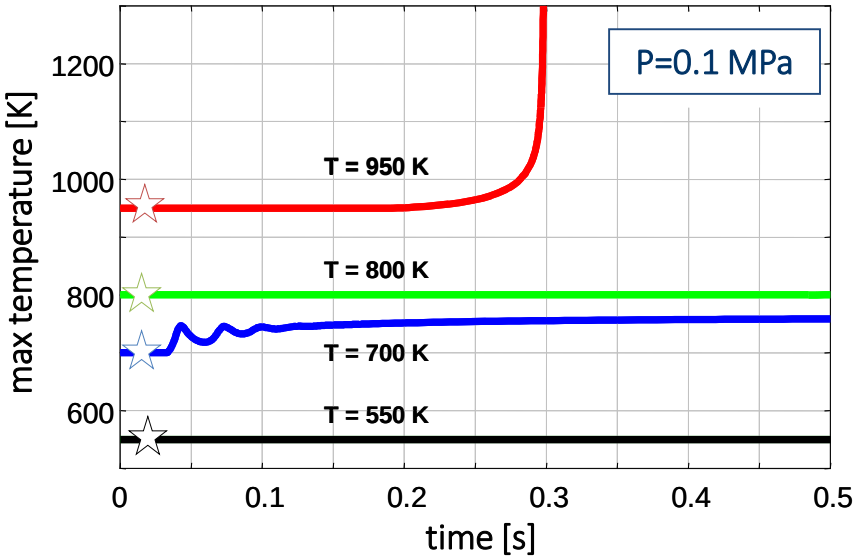
Auto-ignition experiments

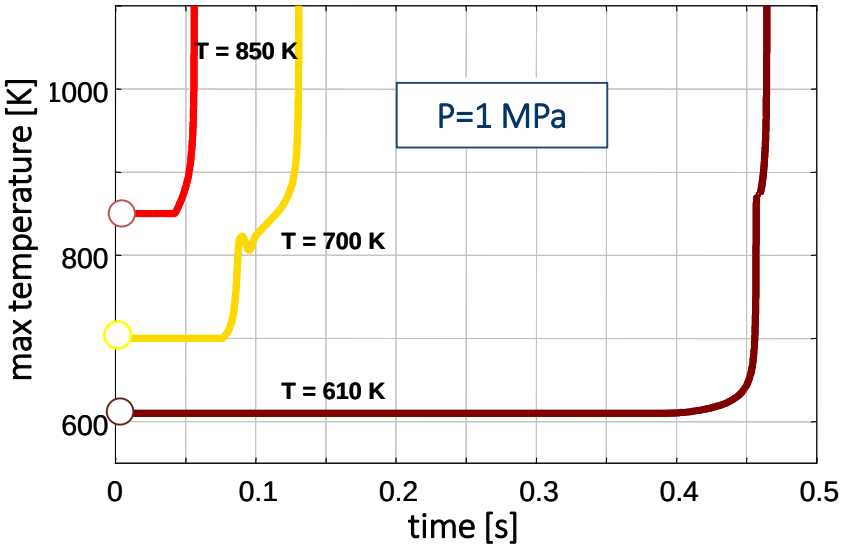
n-heptane droplets in air (d_0=0.70-0.80 mm)



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

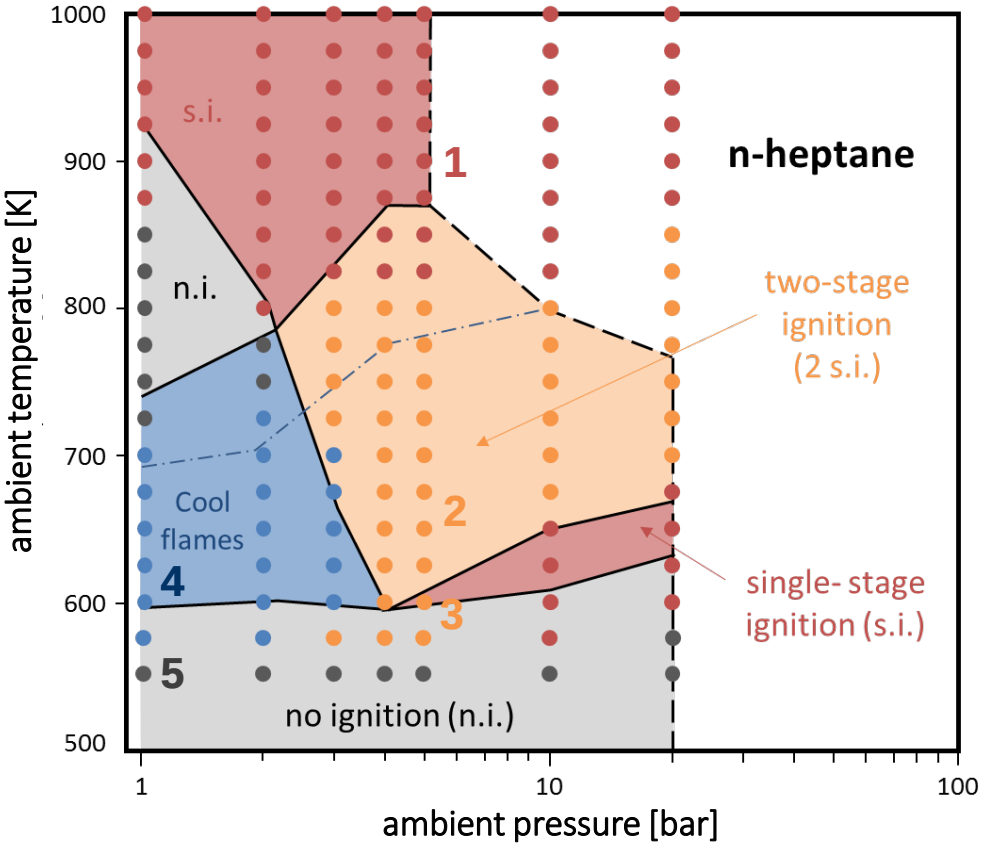
Moriue et al., 28th Symposium (International) on Combustion (2000) 969-975.



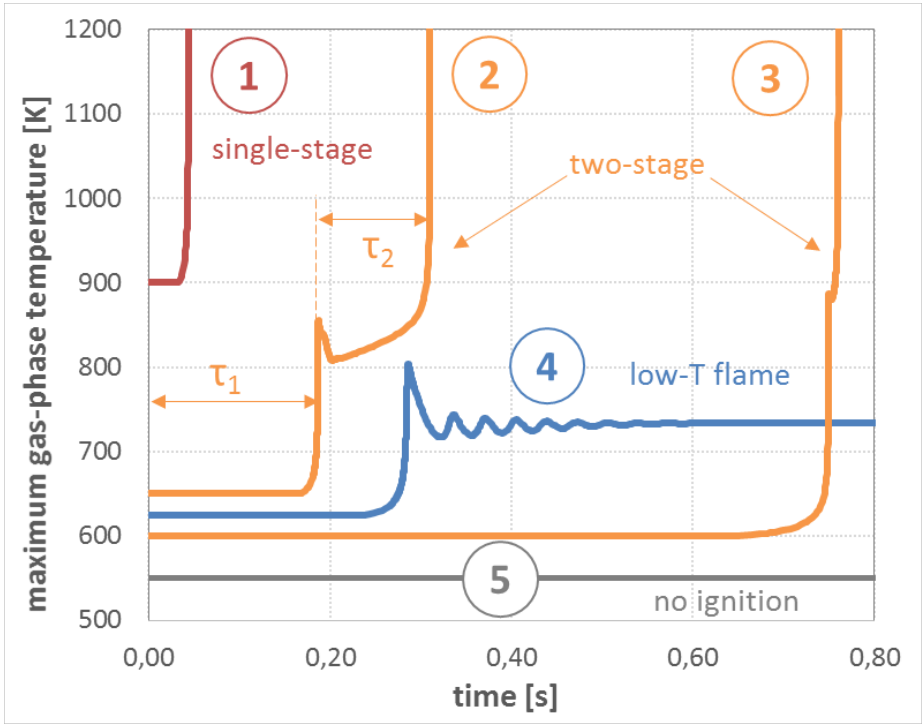


Ignition regions of n-heptane in air

Comparison between experiments (maps) and numerical predictions (points).



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

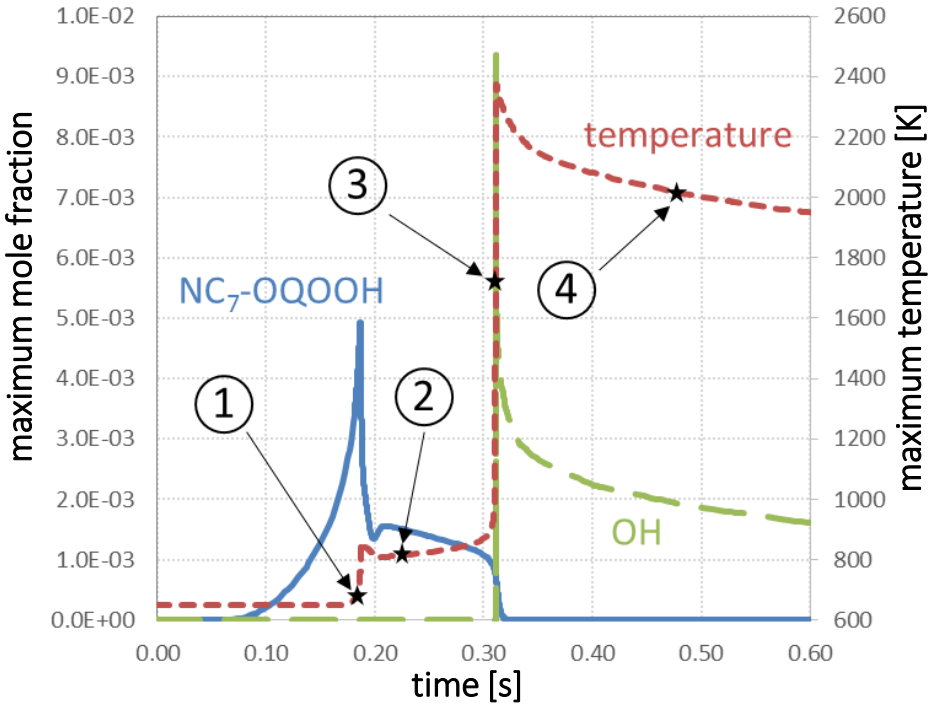


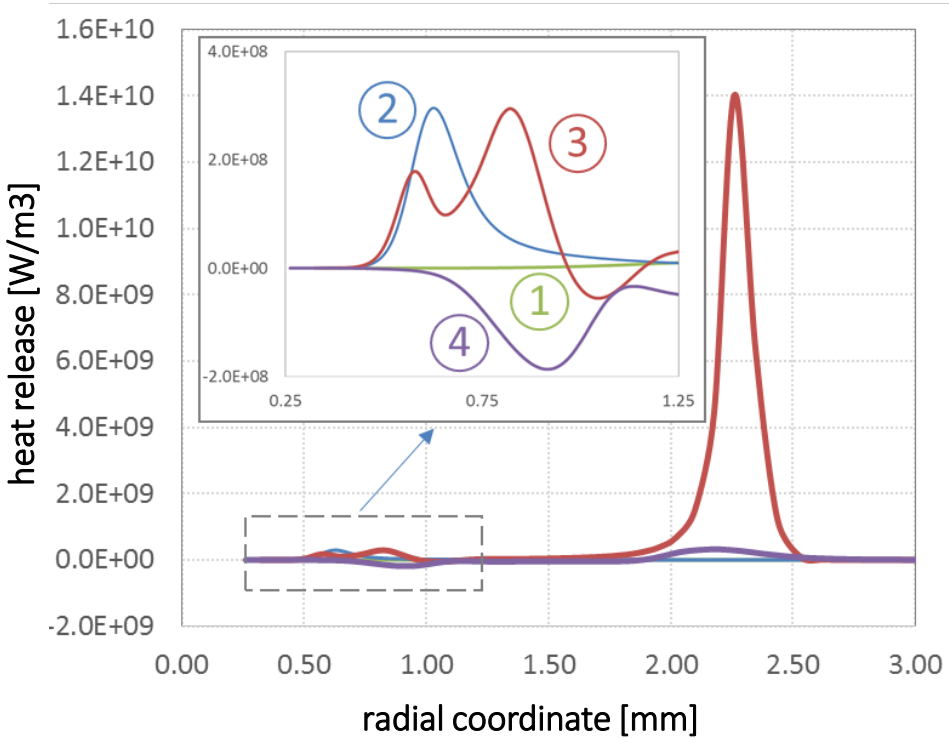
The total induction time τ_t is the sum of the first (τ_1) and the second (τ_2) induction times.

Two-stage ignition of n-heptane droplets (I)

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

The first ignition occurs when the concentration of the NC7-OQOOH becomes sufficiently large to promote the LT ignition

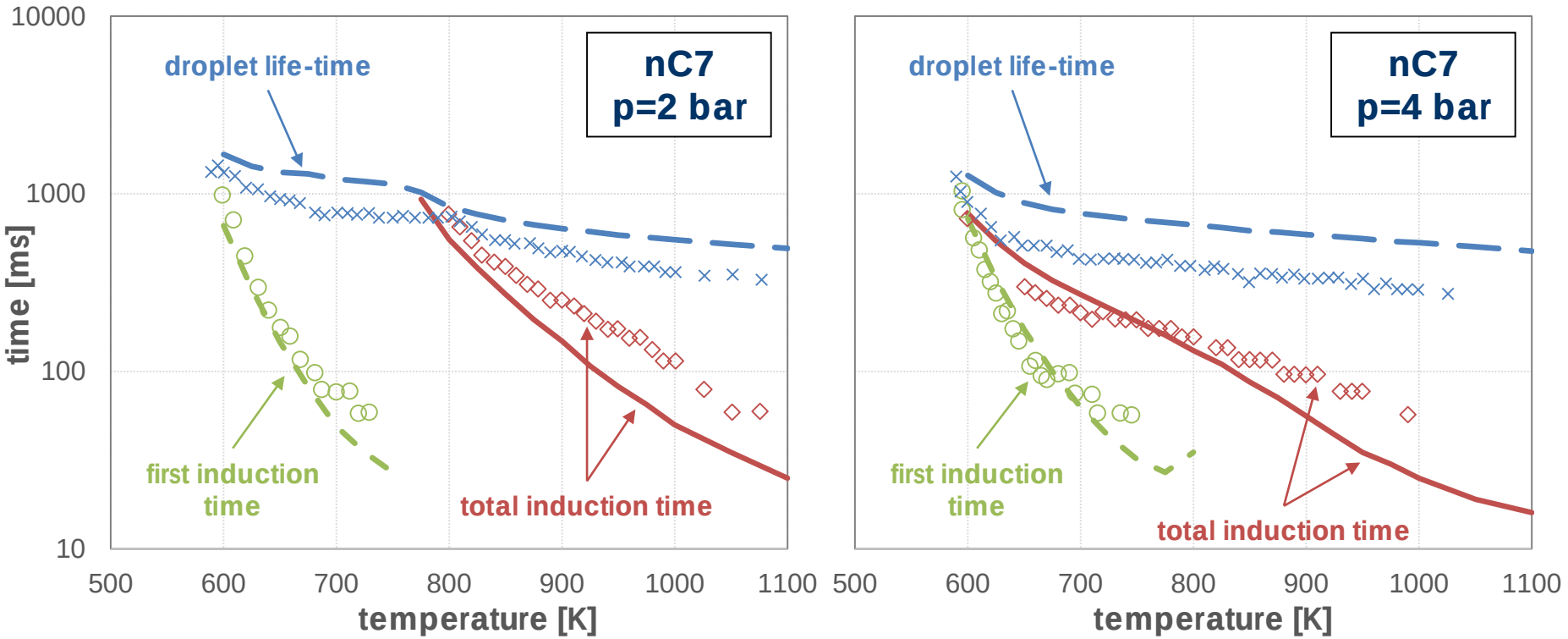




Radial profiles of heat release at the four different times

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

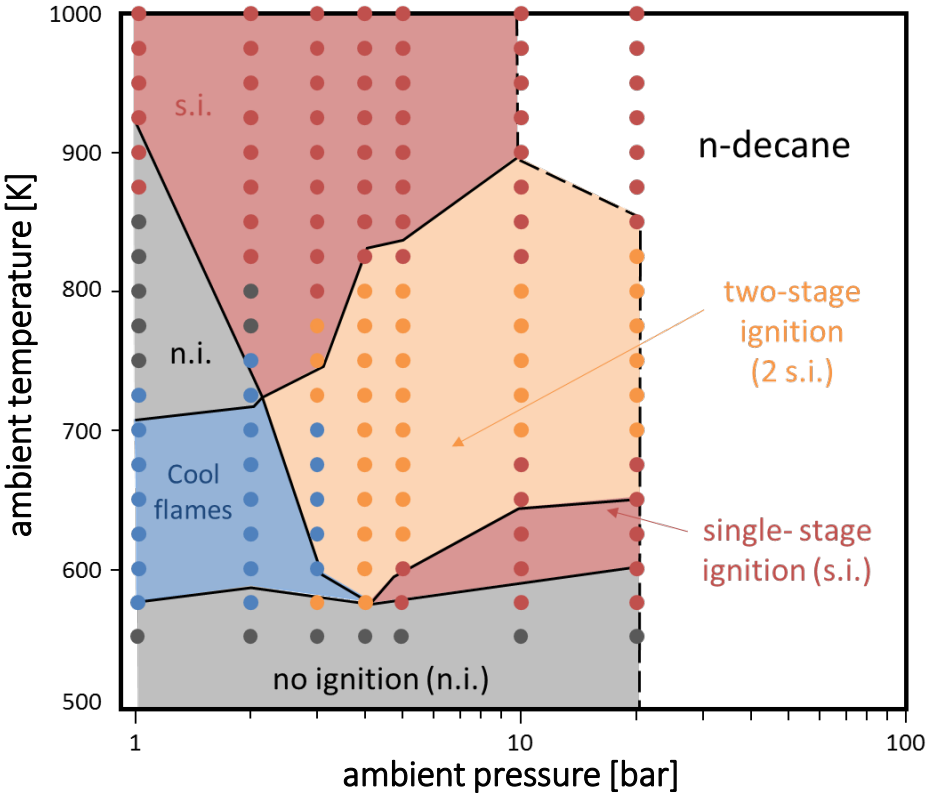
Ignition delay times



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

Ignition regions of nC10 and nC12

Comparison between experiments (maps) and numerical predictions (points).



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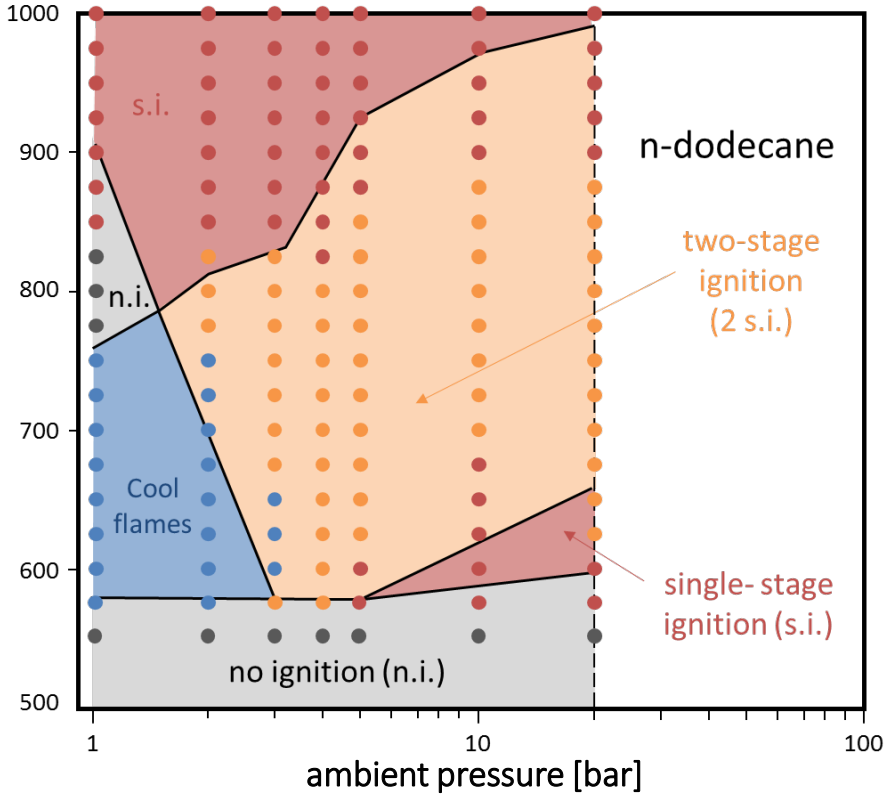

Moriue et al., 28th Symposium (International) on Combustion (2000) 969-975.

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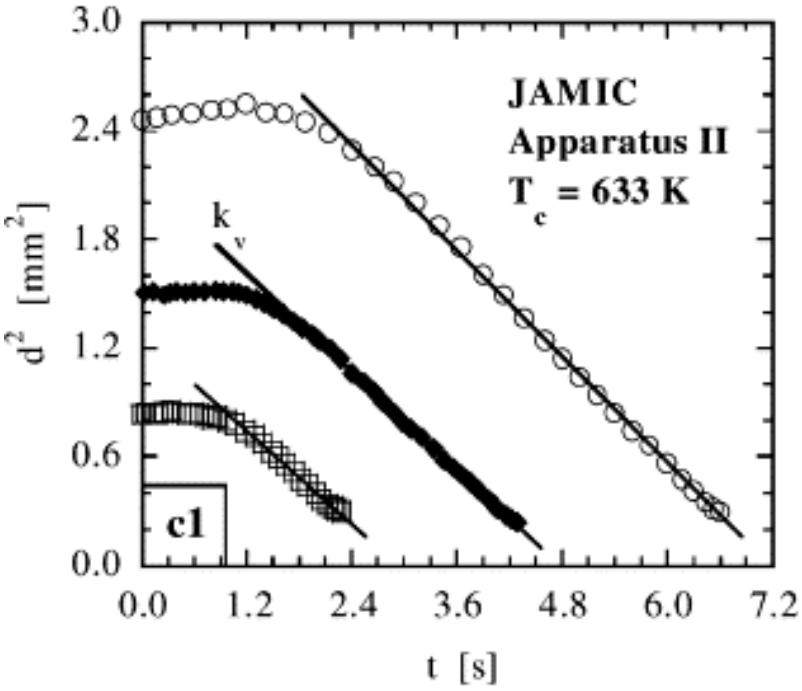
“Anomalous” evaporation of n-decane droplets

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)
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)

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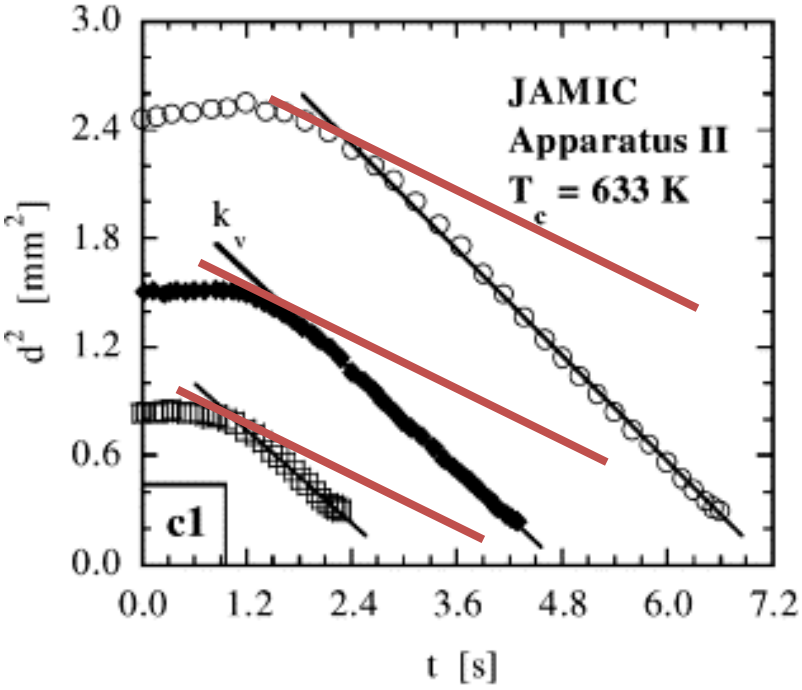

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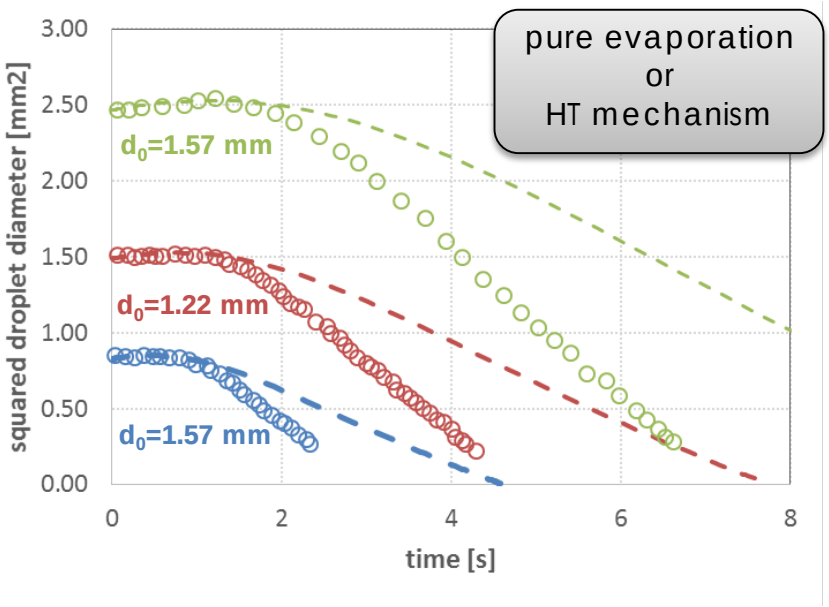
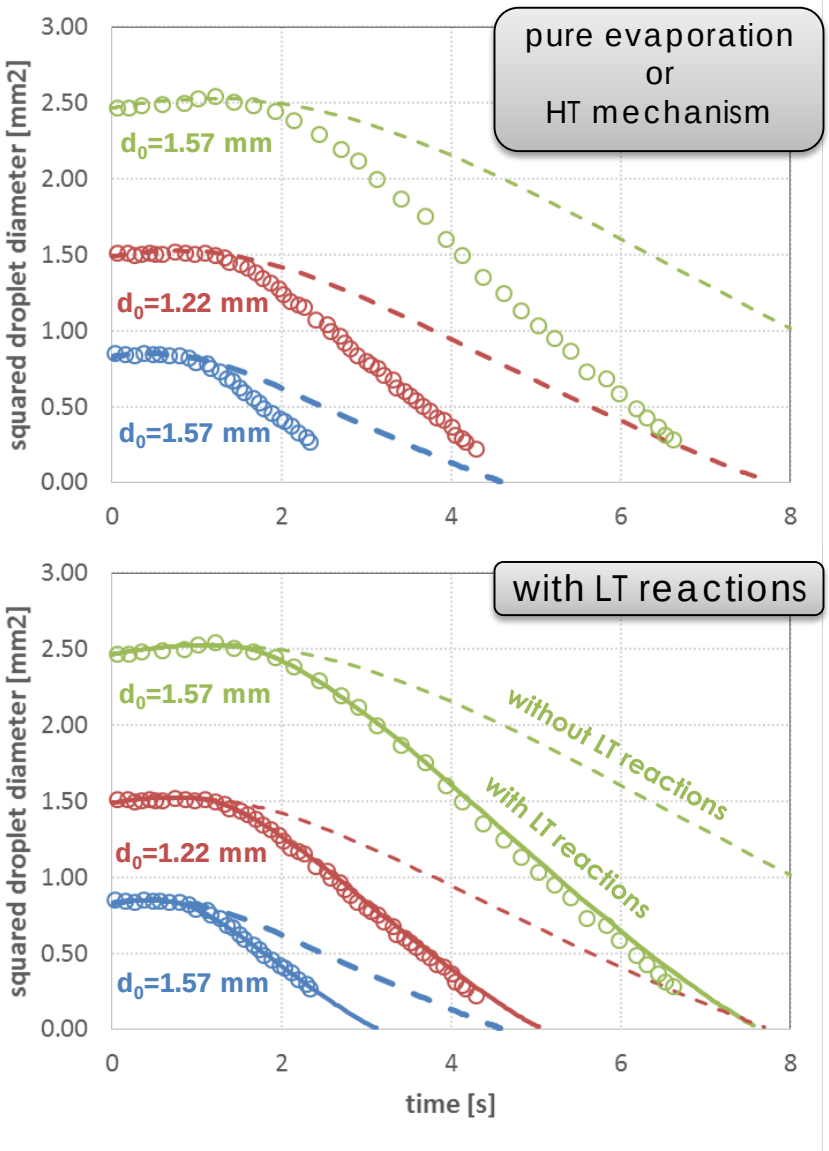
Numerical simulations



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

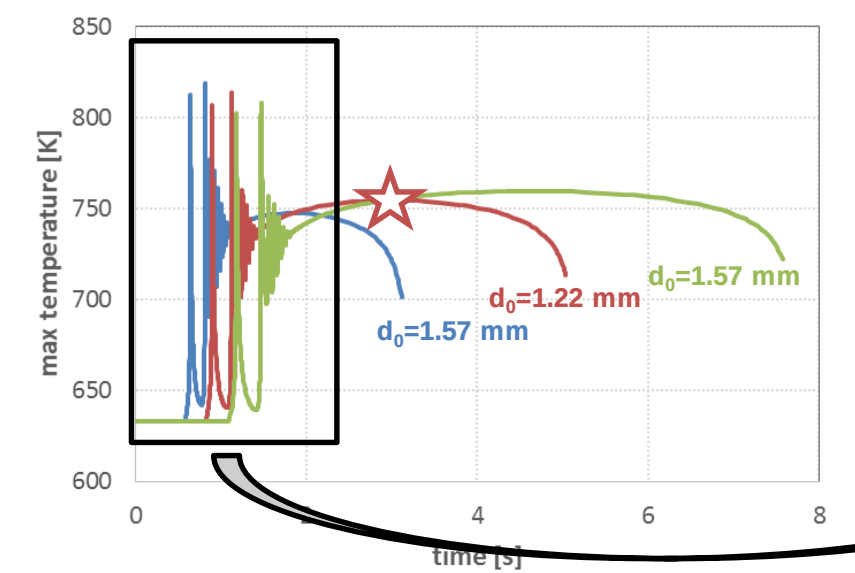
Numerical simulations

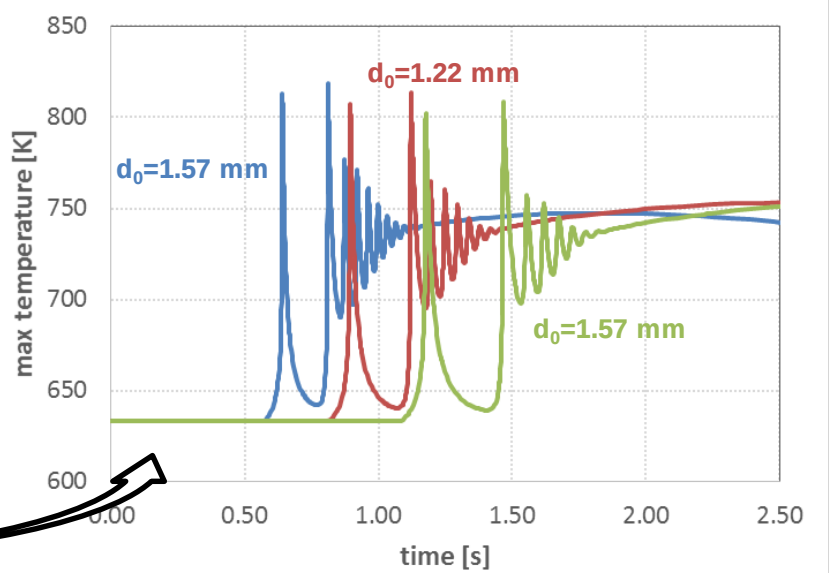


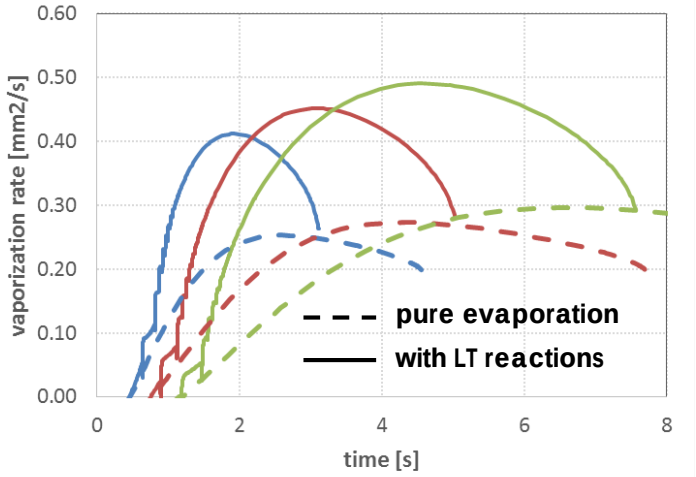
If the simulations are performed without considering any reactions in the gas phase, the calculated vaporization rate is smaller than the experimental value

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

Dumped cool flames







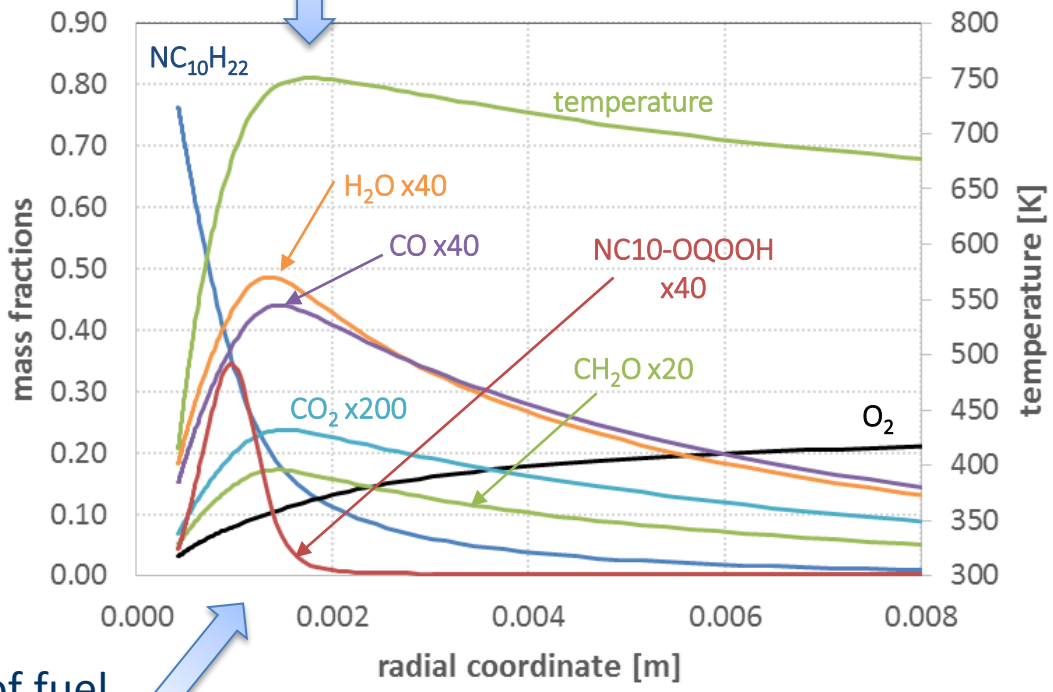
- ✓ initial damped cool flame and a successive more stable temperature profile at ~750 K.
- ✓ once the first flame ignites, fuel is consumed and only partially replaced by the vaporization.
- ✓ the successive cool flames exhibit a higher frequency, produce less heat and gradually move the system from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

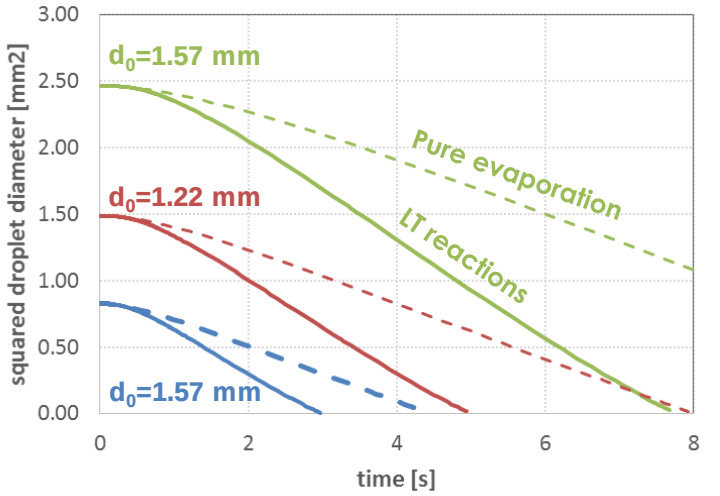


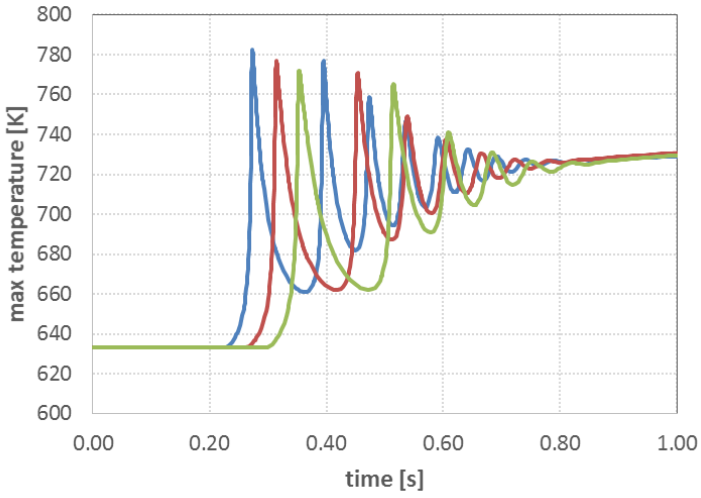
Co-existence of fuel ($C_{10}H_{22}$) and oxidizer (O_2)

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

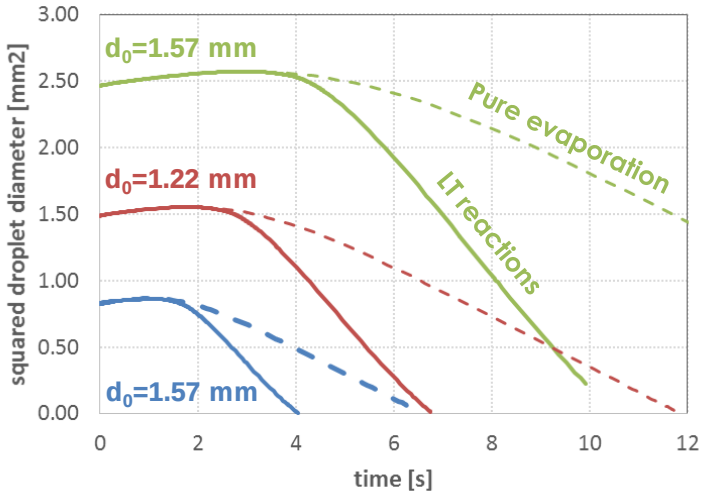
Extension to nC7 and nC12

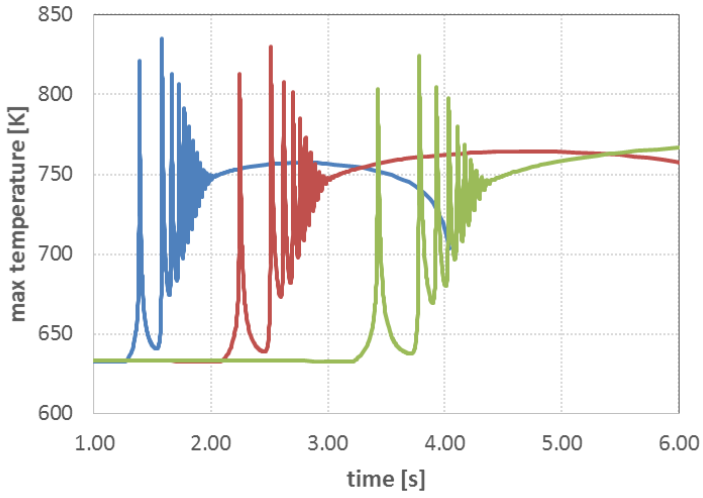
n-heptane





n-dodecane





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Conclusions

- ✓ the auto-ignition of isolated fuel droplets of nC7, nC10, and nC12 was numerically investigated using a detailed kinetic mechanism in a wide range of operating conditions (500-1000 K and 1-20 bar ranges)
- ✓ satisfactory agreement with experimental data was obtained
- ✓ the application to real and complex fuels (diesel or jet fuels) could make this numerical model a powerful tool for investigations about droplet ignition
- ✓ the low-temperature chemistry plays a fundamental role when the ambient temperature is not sufficiently high to promote the hot-temperature combustion reactions

low-temperature chemistry in hot-wire ignition

Nayagam, V., et al., Combustion and Flame, 159(12): p. 3583-3588 (2012)
Farouk T.I. and Dryer F.L., 8th US National Combustion Meeting of the Combustion Institute (2013)
Cuoci A. et al., 36th Meeting of the Italian Section of The Combustion Institute (2013)
Farouk T.I. and Dryer F.L., Combustion and Flame, 161(2), p. 565-581 (2014)
Farouk T.I. et al., (4D05), 35th International Symposium on Combustion, San Francisco (2014)

Acknowledgments

The authors acknowledge **Prof. Forman A. Williams** (University of San Diego, USA) and **Dr. Daniel L. Dietrich** (NASA Glenn Research Center, Cleveland, USA) for the useful discussions and suggestions about the analysis of experimental data.

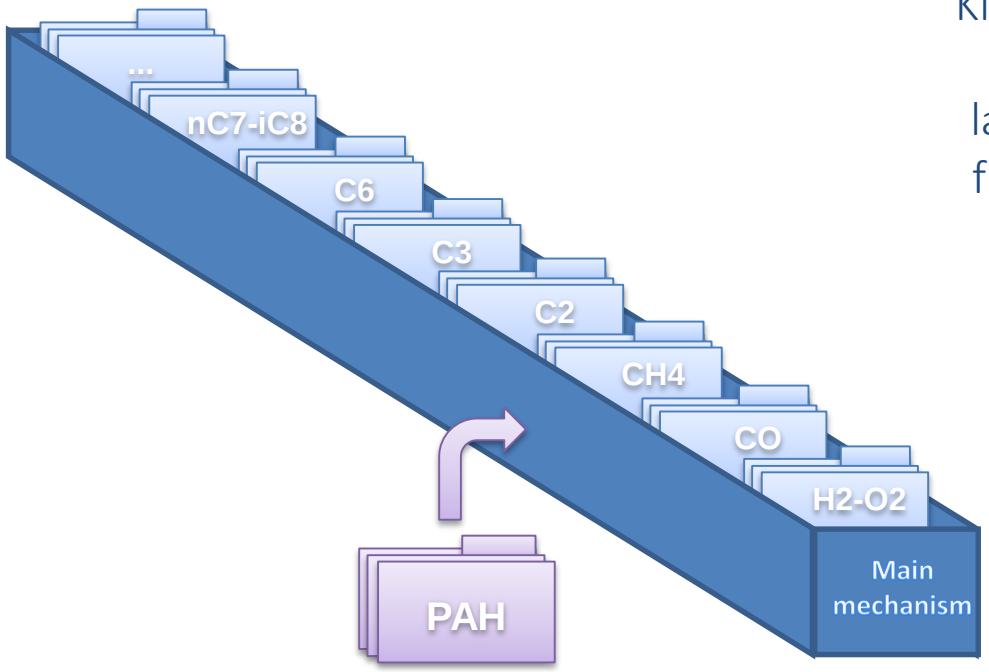
The authors also acknowledge **Alessandro Stagni** (Politecnico di Milano) for providing the validation of the kinetic mechanism.

The **Italian MSE and CNR-DIITET** are acknowledged for their financial support (Project Number D44G12000040001).

Additional slides

- governing equations
- validation of n-heptane kinetic mechanism
- hot-wire ignition experiments (n-heptane): exp vs simulations
- hot-wire ignition experiments (n-heptane): skeletal mechanisms
- auto-ignition maps for nC12: comparison between mechanisms
- auto-ignition times for n-heptane (comparison with exp)
- Xu experiments (nC7): comparison between mechanisms
- Xu experiments (nC12): comparison between mechanisms

Detailed kinetic mechanism (II)



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POLIMI_PRF_PAH_RFUELS_LT_1407
Kinetic Mechanism up to Real Transportation Fuels

http://creckmodeling.chem.polimi.it

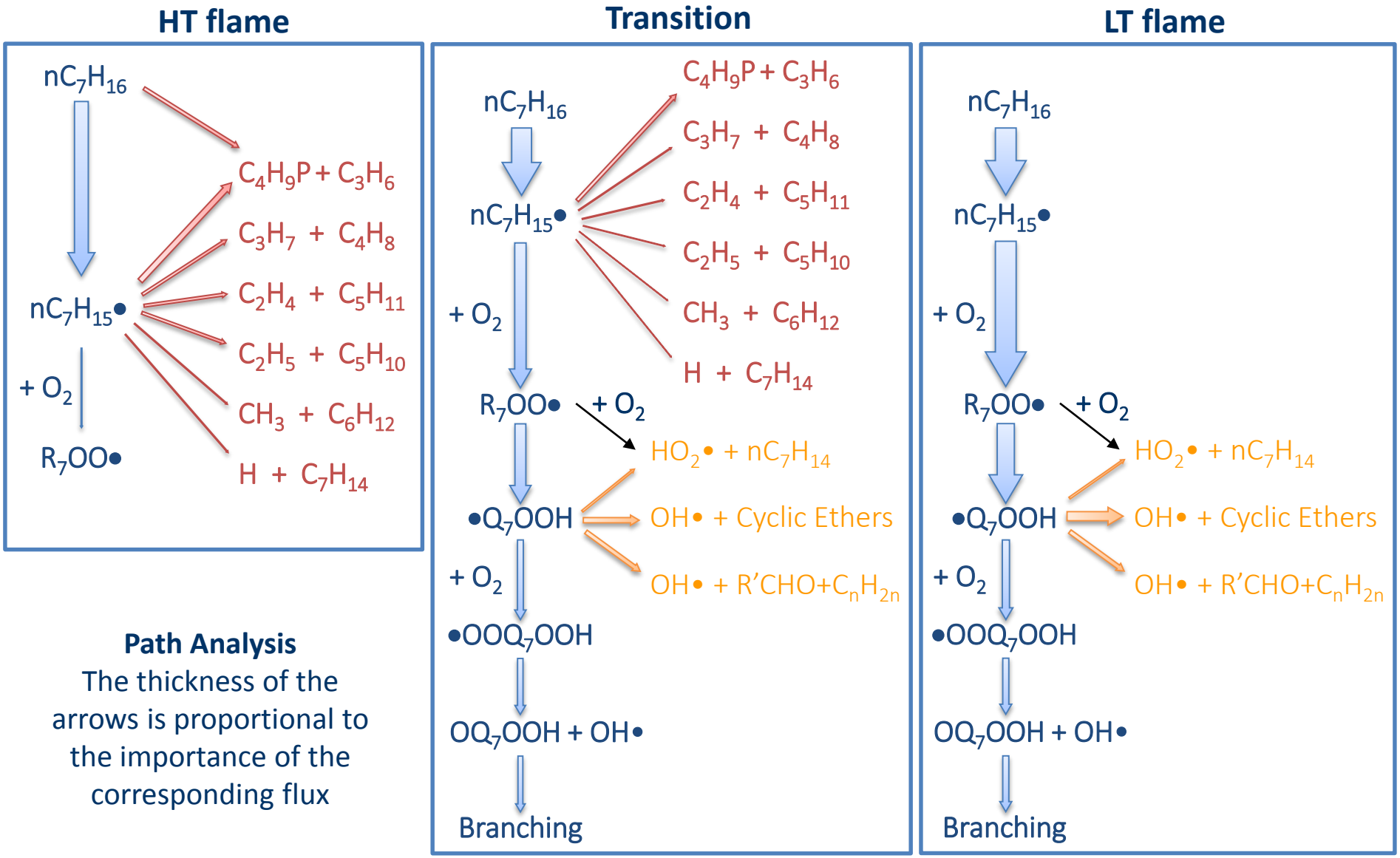
~ 352 chemical species

~ 13,166 reactions

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

Ranzi, E. at al., International Journal of Chemical Kinetics 46(9) (2014), pp. 512-542

Two-stage ignition of n-heptane droplets (II)



Path Analysis

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

Governing equations

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

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

Species equations

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

Mass diffusion flux

Formation rates

Energy equation

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

Enthalpy fluxes associated to mass diffusion

Heat flux

Heat release

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)

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

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

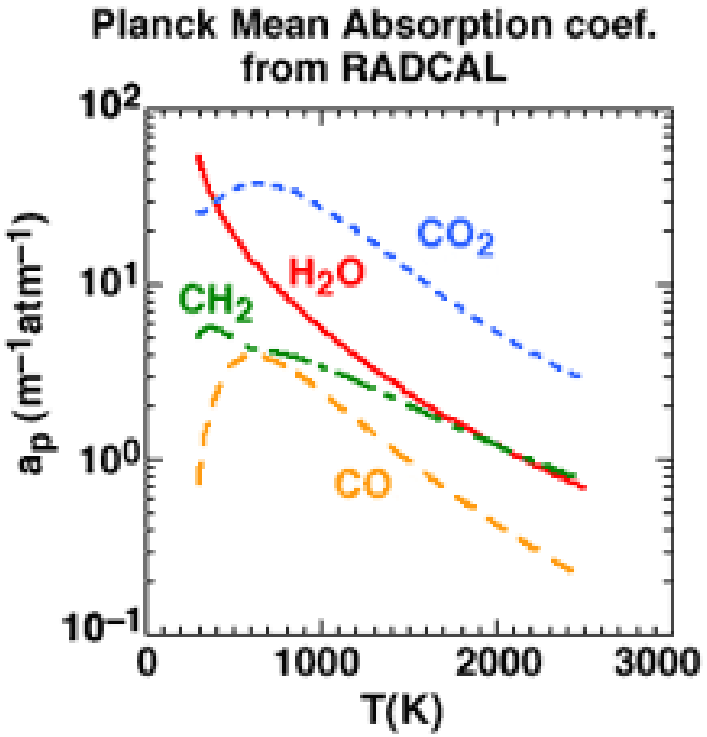
$$V_C = \sum_{i=1}^{N} \Gamma_{i,mix}\frac{\partial \omega_i}{\partial r} - \frac{1}{T}\frac{\partial T}{\partial r}\sum_{i=1}^{N} \Gamma_{i,mix}\theta_k \frac{M_i}{M} - \sum_{i=1}^{N} \omega_i V_i^{Th}$$

Heat flux

Fourier's Law (thermal conductivity)

Radiative heat transfer

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



http://www.sandia.gov/TNF/radiation.html

Analytical 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

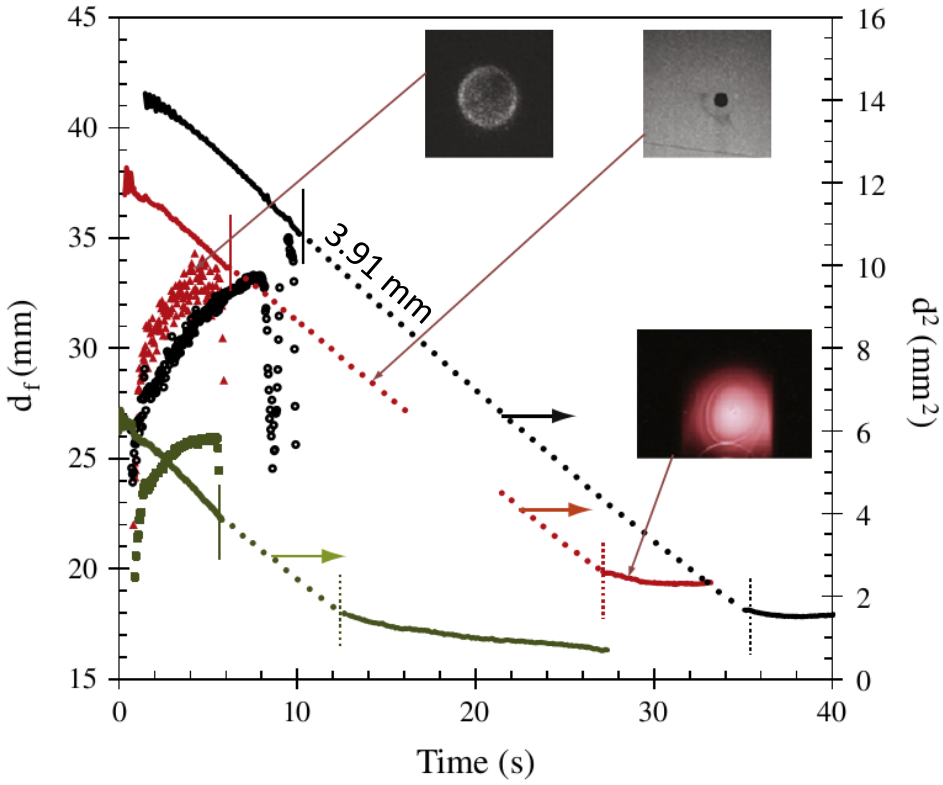
Hot-wire ignition experiments (cool flames)

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)

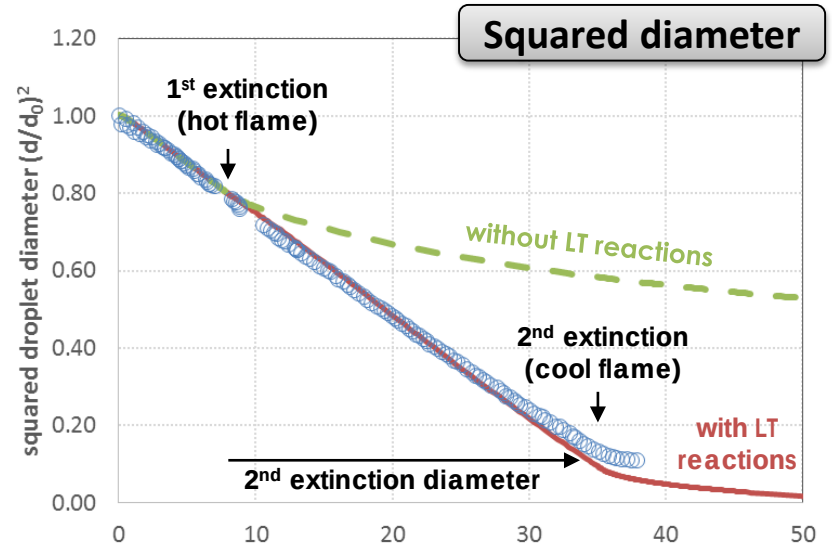
Fuel: n-heptane (NC_7H_{16})
Initial diameter: 3.91 mm
Pressure: 1 atm
Initial temperature: 300 K
Gas phase composition: air
Negligible soot formation
Droplet tethered by a fine silicon carbide filament

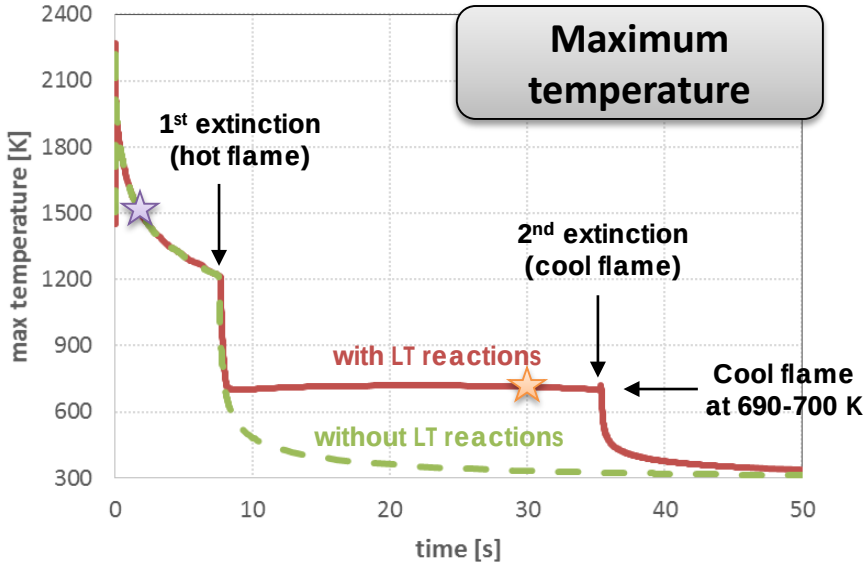
Adapted from Nayagam et al. (2012)



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)

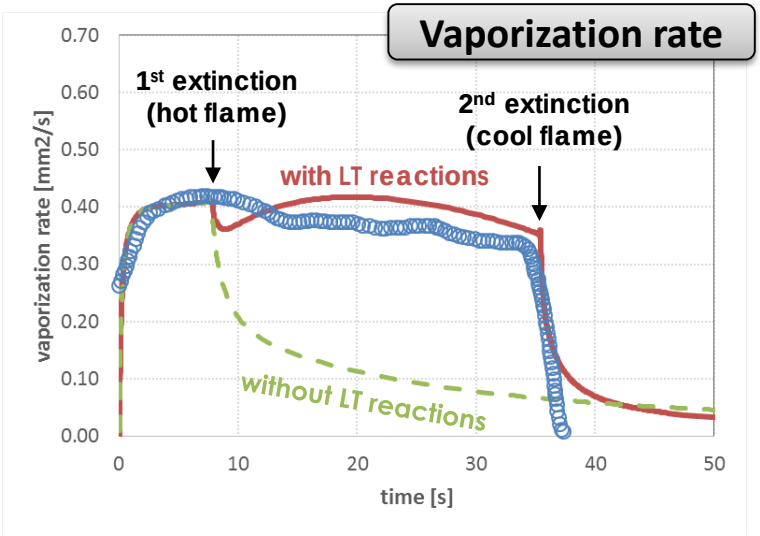
Numerical results





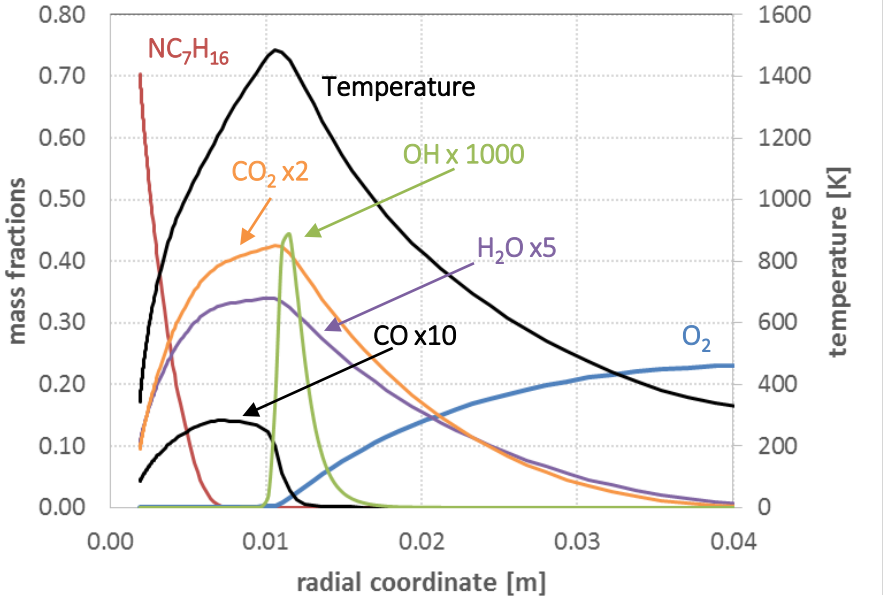
The agreement with the experiments is satisfactory if the LT mechanism is accounted for.

	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

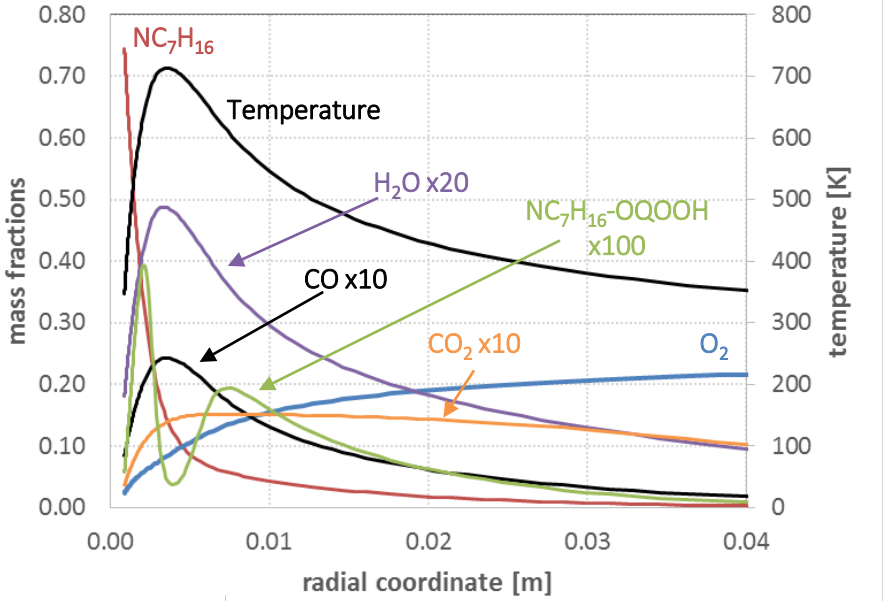


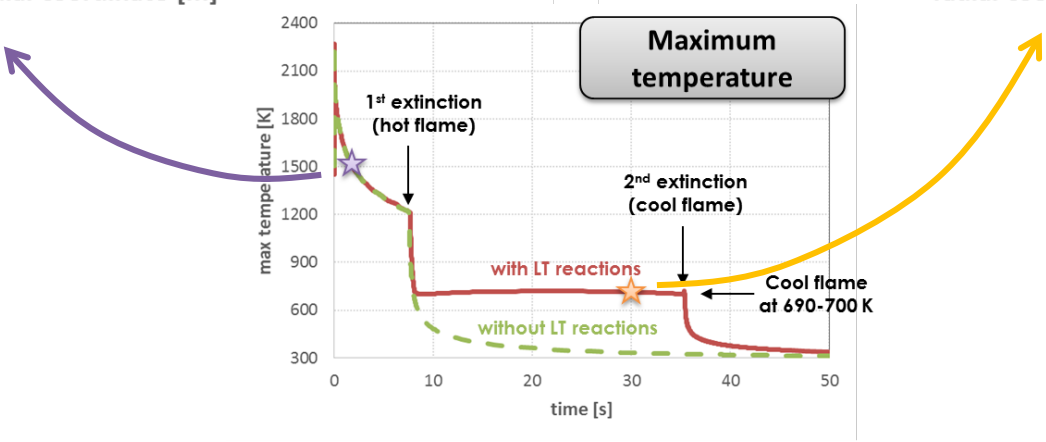
Flame structures

Hot flame @ 2 s



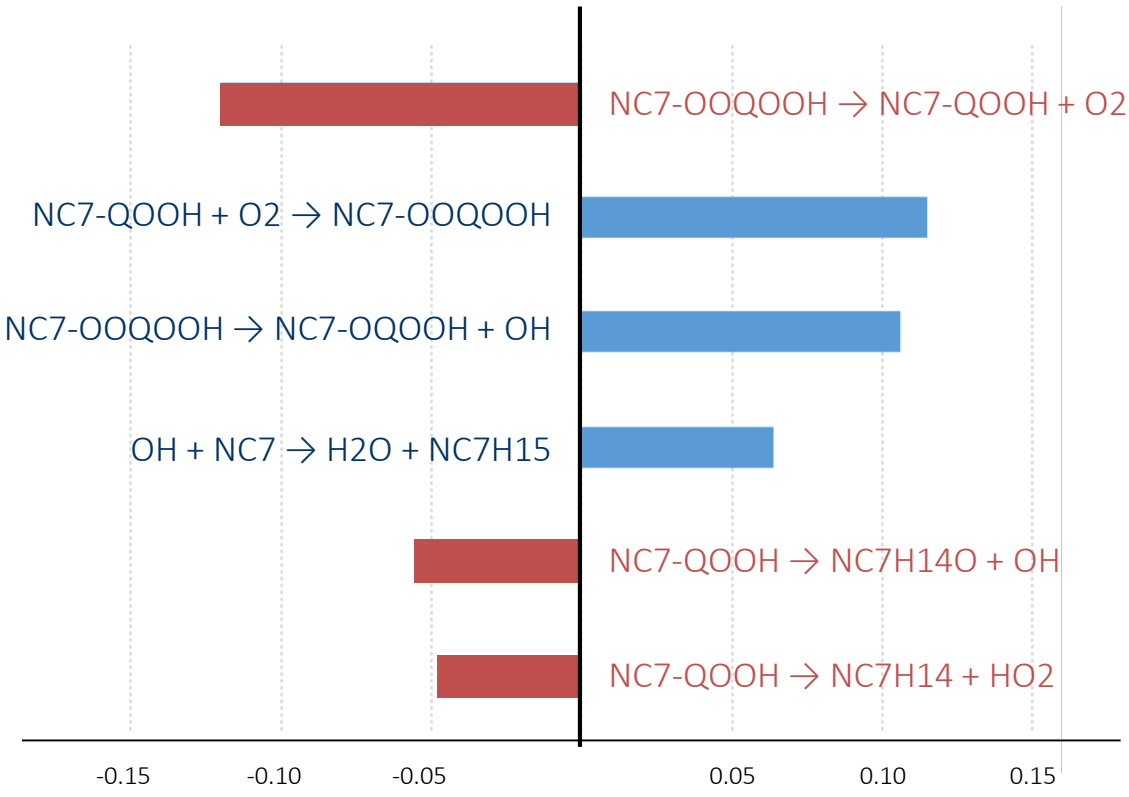
Cool flame @ 30 s



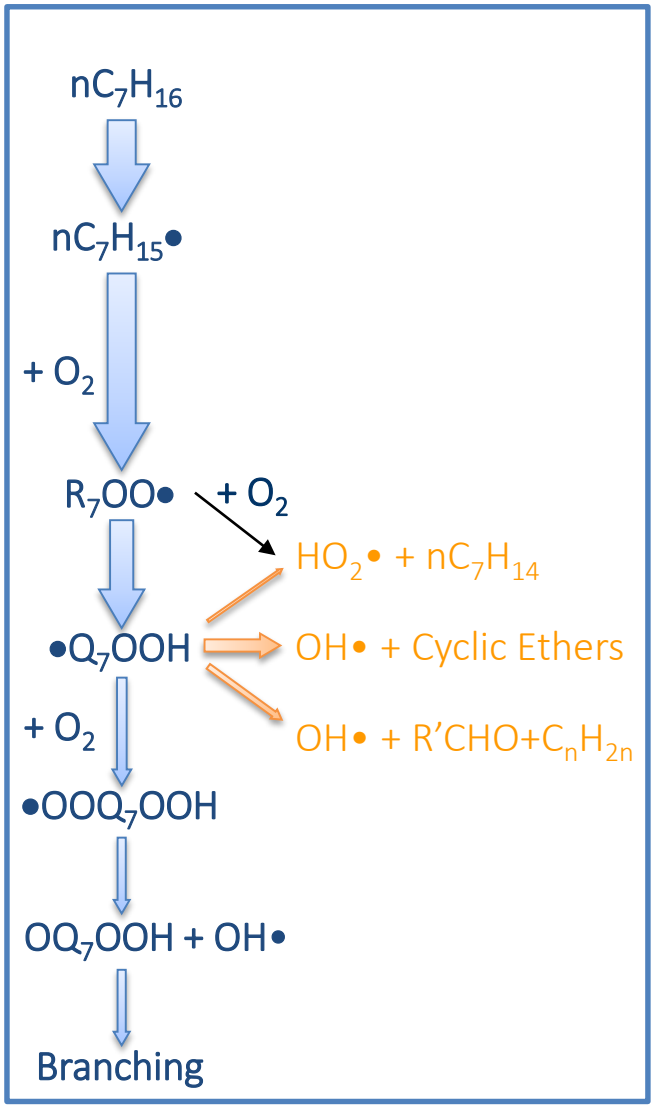


Sensitivity analysis

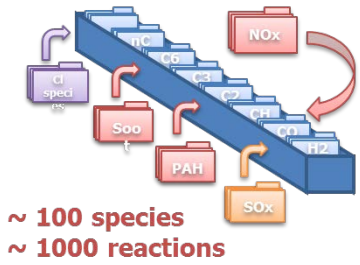
Global sensitivity coefficients of the vaporization rate during the LT combustion



Cool flame @ 30 s



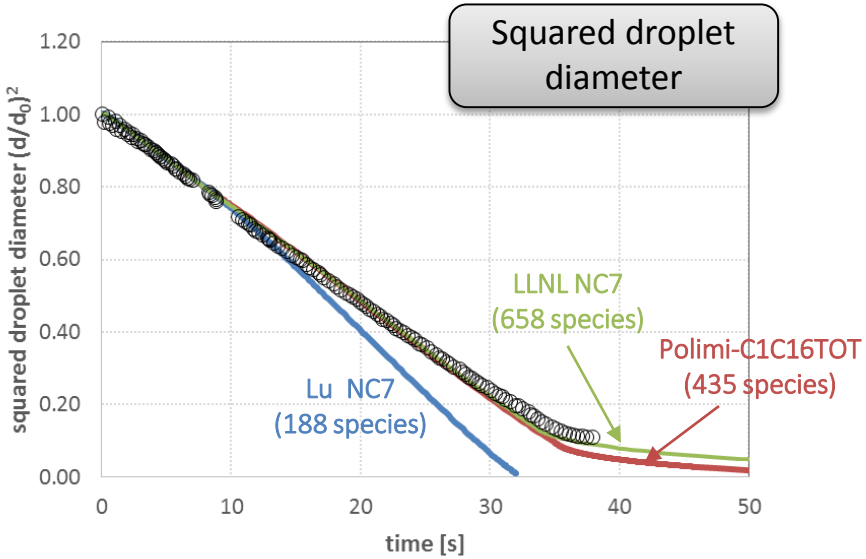
Comparison with other kinetic mechanisms (I)

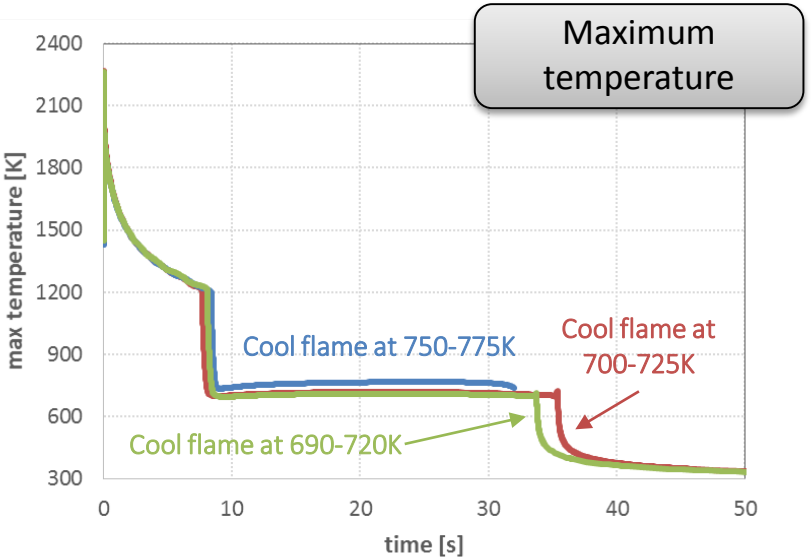


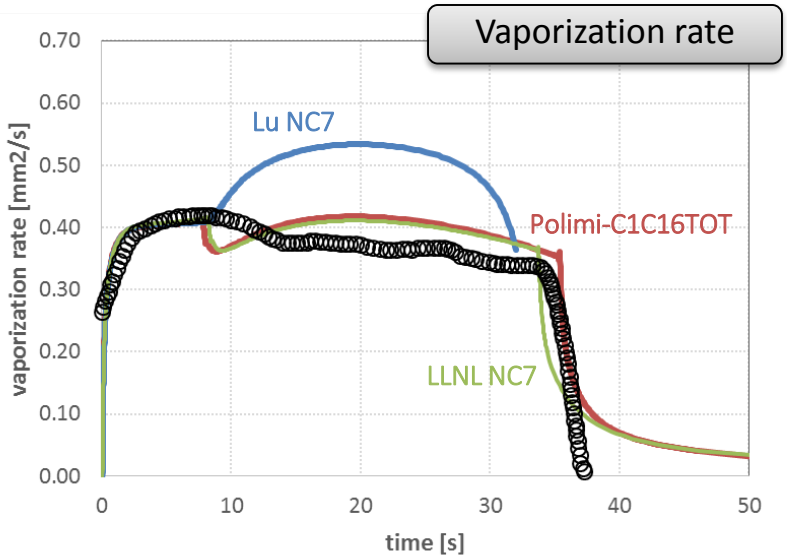
Several detailed kinetic mechanisms (with Low Temperature chemistry) were tested and compared

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)

Comparison with other kinetic mechanisms (II)







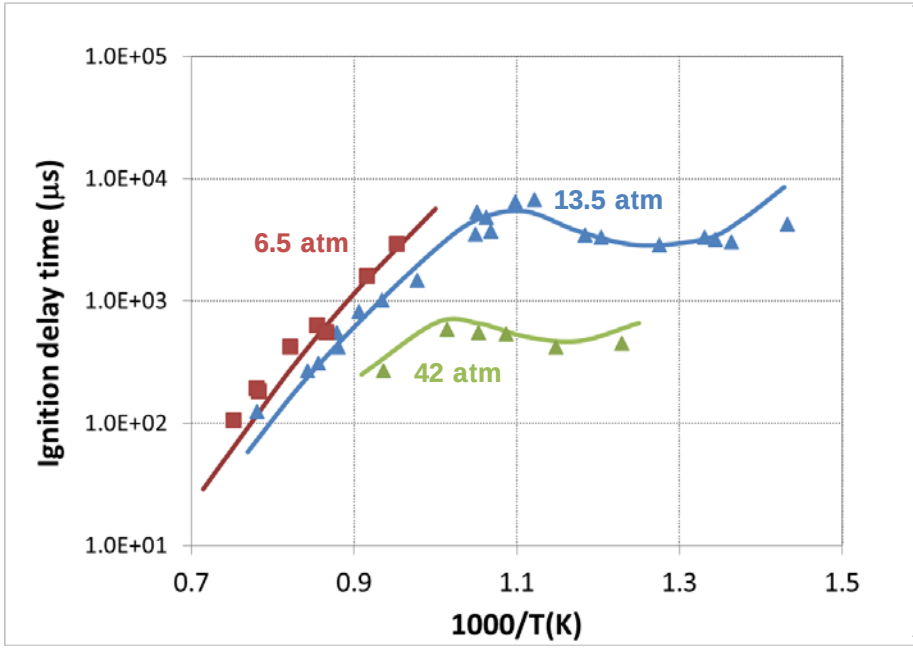
The results are strongly affected by the ability of the **kinetic mechanism** to correctly capture the features of the cool flame (i.e. by the accuracy and the reliability of the low-temperature chemistry)

Validation of n-heptane kinetic mechanism

Validation of the kinetic mechanism: n-heptane

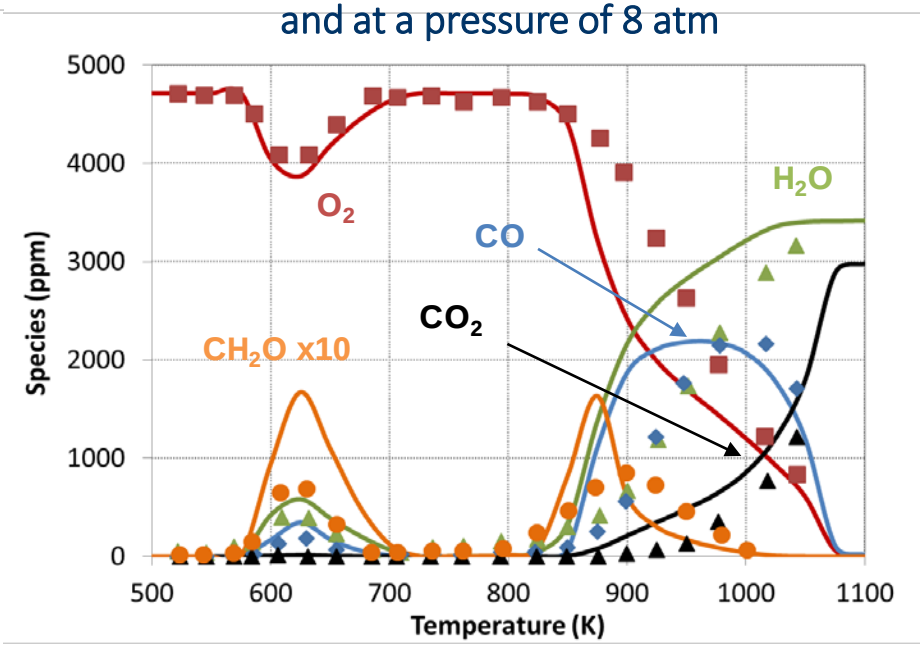
Polimi C1C16TOT (435 species)

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

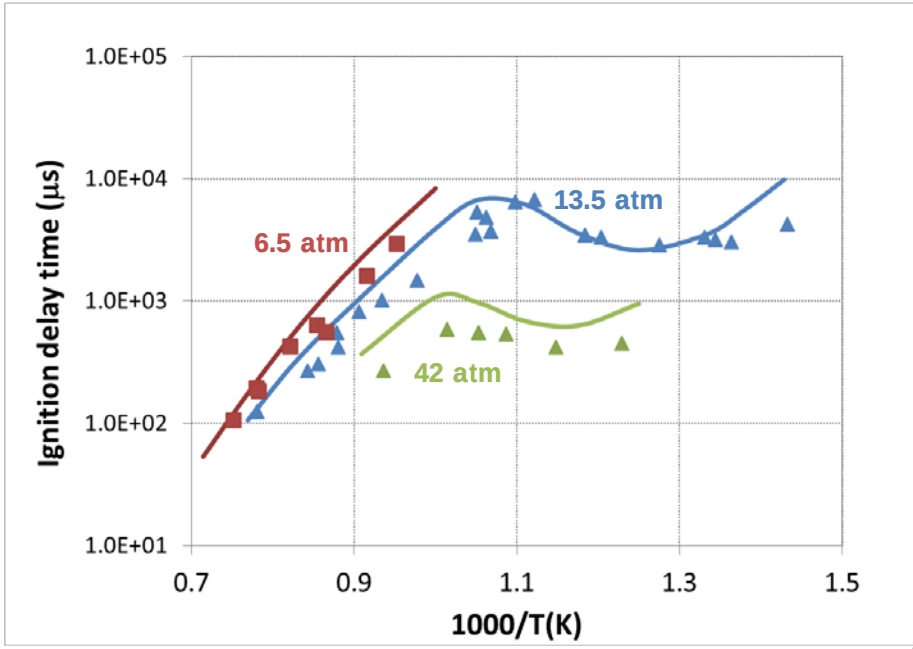


Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., *An experimental and kinetic modeling study of the two stage auto-ignition kinetic behavior of C7, C10, C12, and C14 n-alkanes*, Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)

Validation of the kinetic mechanism: n-heptane

Lu NC7 (188 species)

Shock-tube experiments



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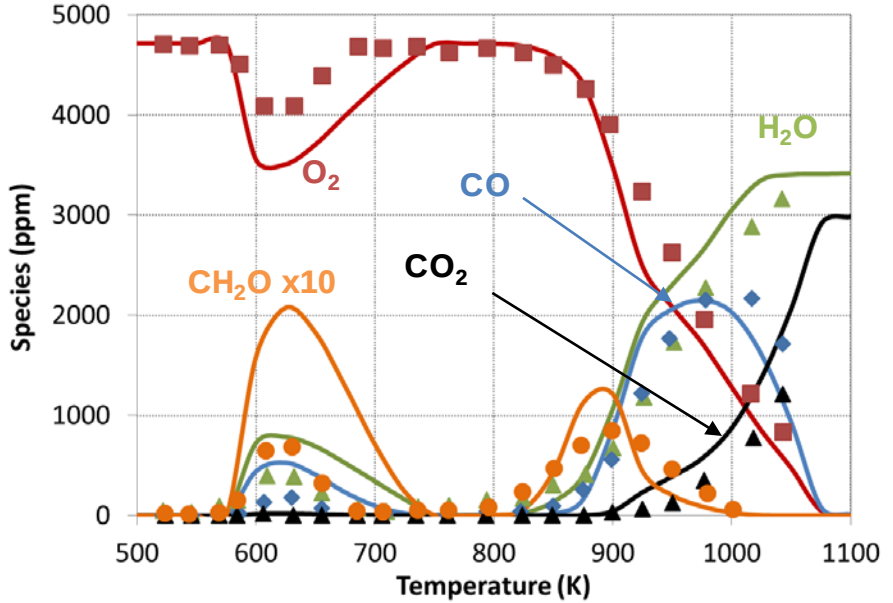

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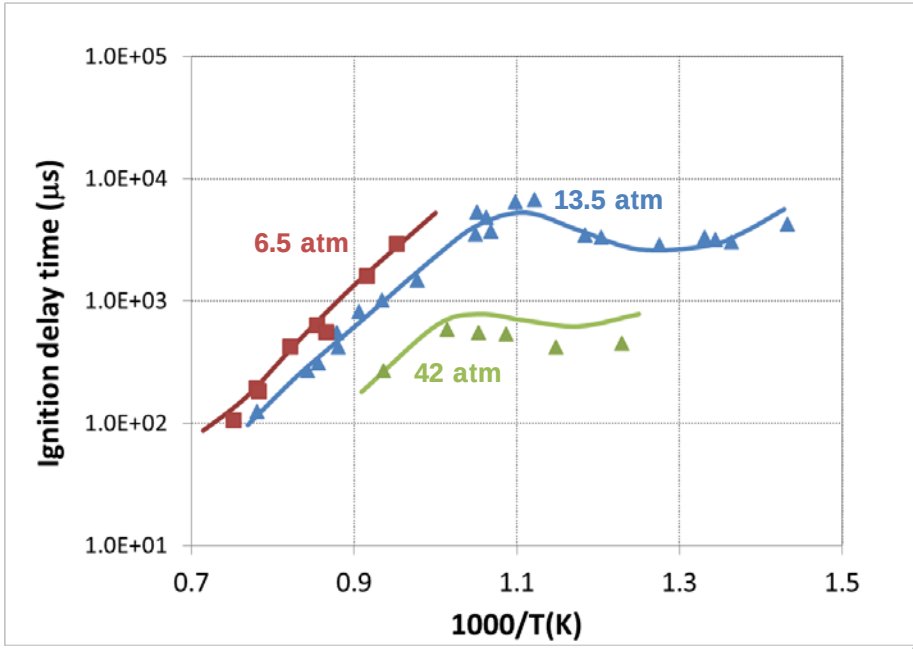
Validation of the kinetic mechanism: n-heptane

LLNL NC7 (658 species)

Shock-tube experiments



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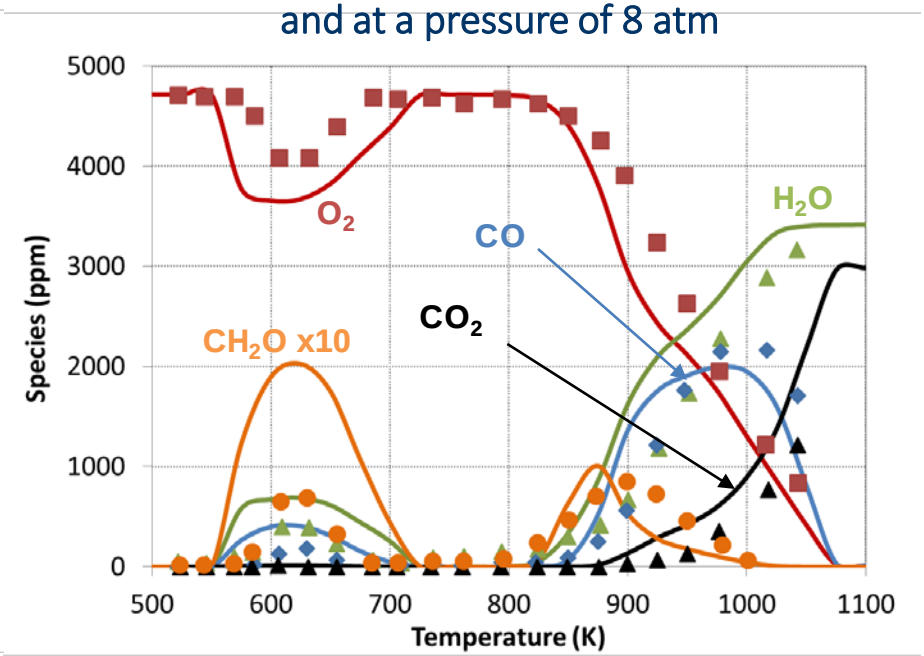

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n-heptane skeletal kinetic mechanisms

Skeletal mechanisms

Polimi-C1C16TOT (version 1212)

Species: 435
Reactions: 13,495

E. Ranzi, et al., Progress in Energy and Combustion Science, 38 (4), pp. 468-501 (2012)

Species: 100
Reactions: 1,567

Reduction factor: 4.35

Stagni A., *Lumping and reduction of detailed kinetic schemes: an effective coupling*, Submitted to Industrial & Engineering Chemistry Research

Lu-NC7

Species: 188
Reactions: 939

C.S. Yoo et al., Combustion and Flame, 158(9), p.1727–1741 (2011)

Reduction performed by the authors

Species: 88
Reactions: 387

Reduction factor: 2.13

C.S. Yoo et al., Combustion and Flame, 158(9), p.1727–1741 (2011)

LLNL-NC7

Species: 658
Reactions: 2,827

Mehl M. et al., Proceedings of the Combustion Institute33:193-200 (2011)

Reduction performed by the authors

Species: 160
Reactions: 1,540

Reduction factor: 4.11

Seiser H. et al., Proceedings of the Combustion Institute28:2029-2037 (2000)

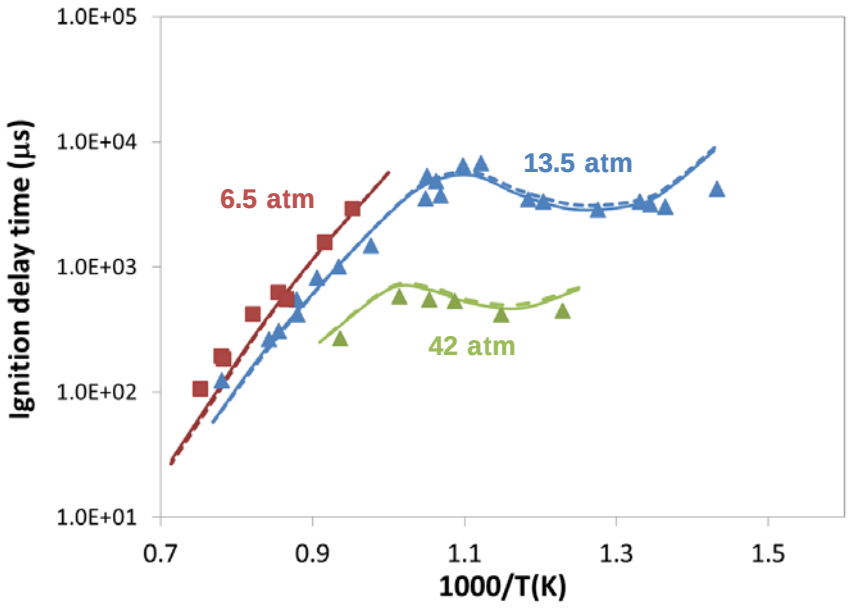
Validation of the kinetic mechanism: n-heptane

——— Original mechanism (435 species)

- - - - - Reduced mechanism (100 species)

Polimi C1C16TOT

Shock-tube experiments



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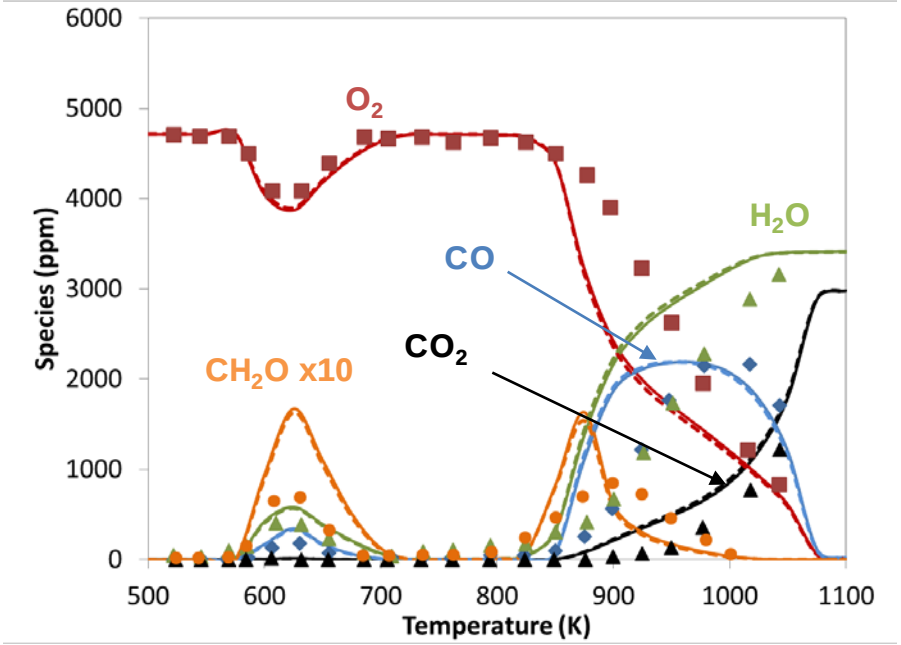

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Validation of the kinetic mechanism: n-heptane

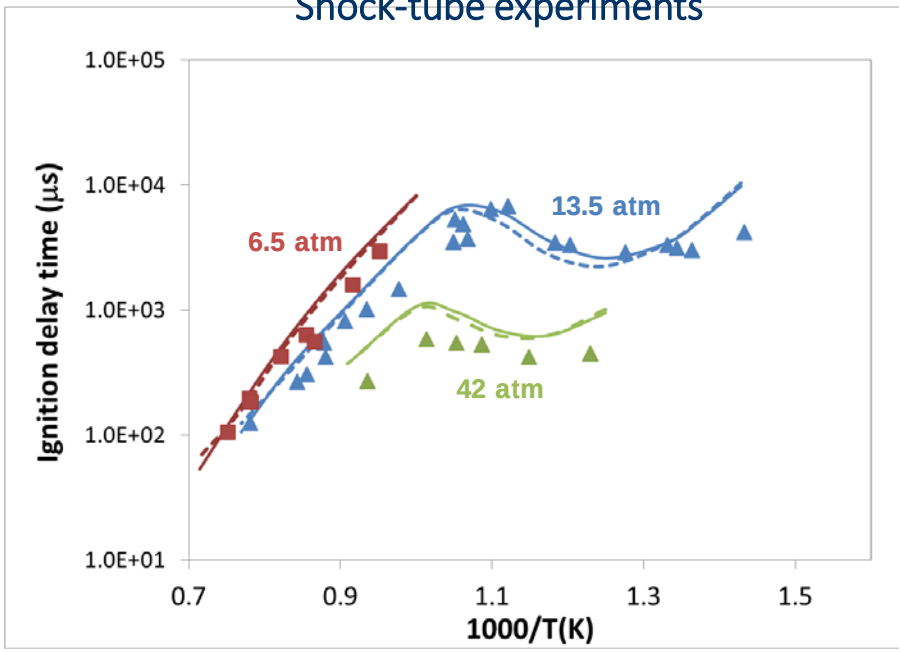
——— Original mechanism (188 species)

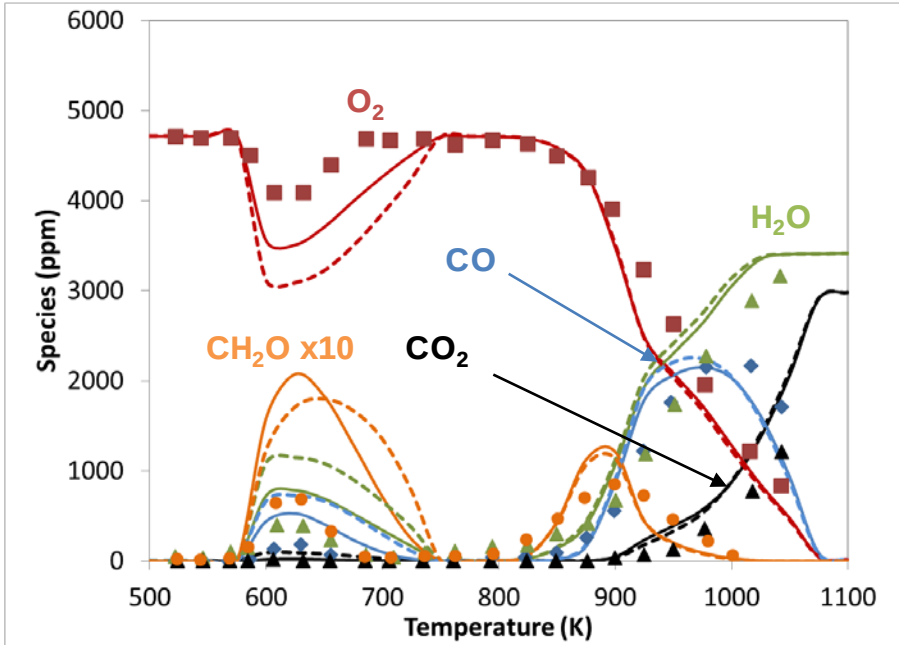
- - - - - Reduced mechanism (88 species)

Lu NC7

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

Shock-tube experiments





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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)

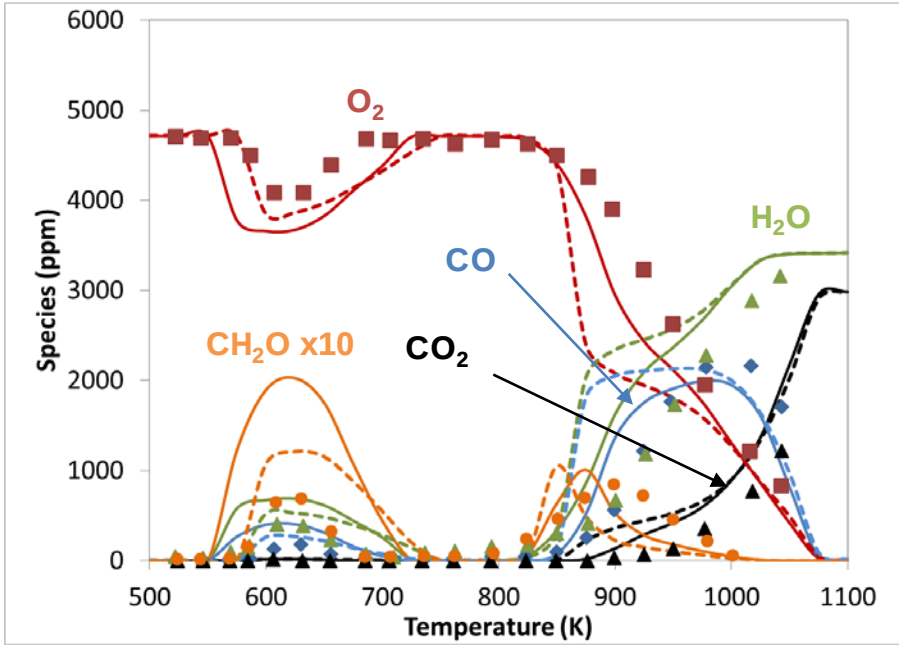
Validation of the kinetic mechanism: n-heptane

——— Original mechanism (658 species)

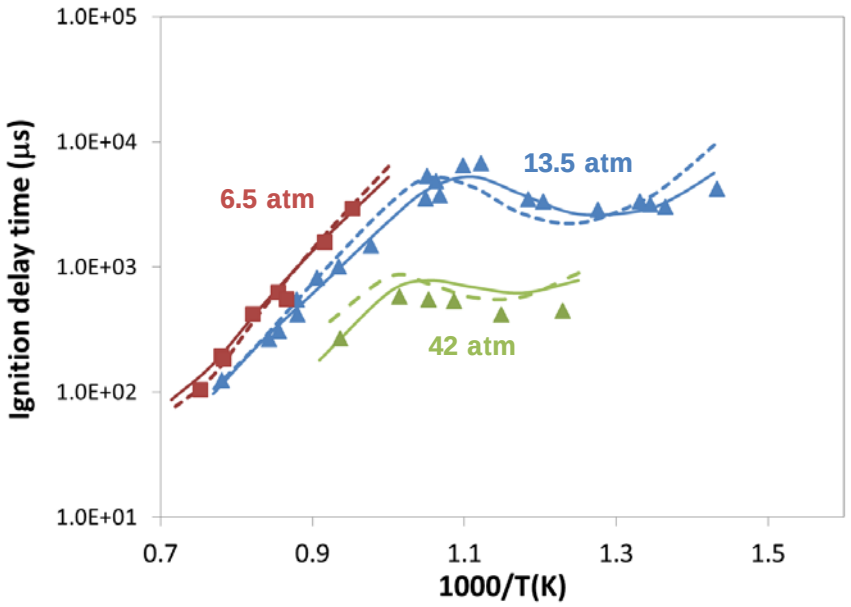
- - - - - Reduced mechanism (160 species)

LLNL NC7

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



Shock-tube experiments



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

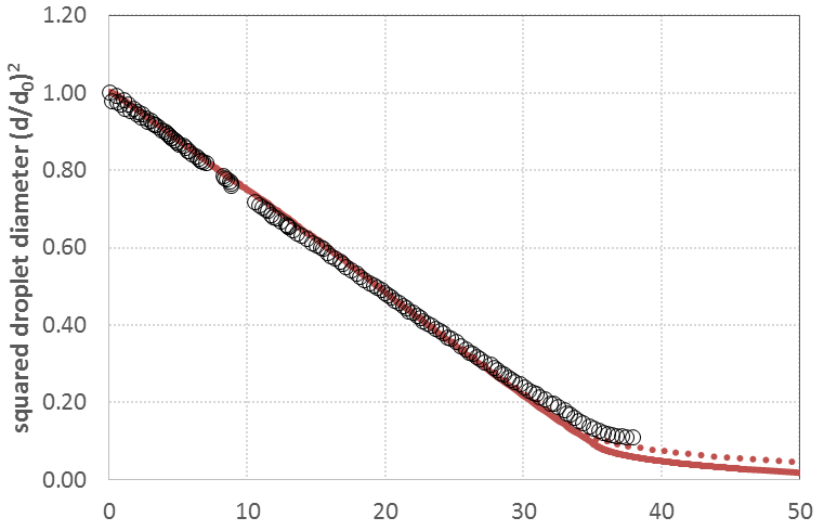
Experimental data from:
Veloo P.S., Jahangirian S., Dryer F.L., Spring Technical Meeting of the Central States Section of the Combustion Institute, Dayton, Ohio (2013)

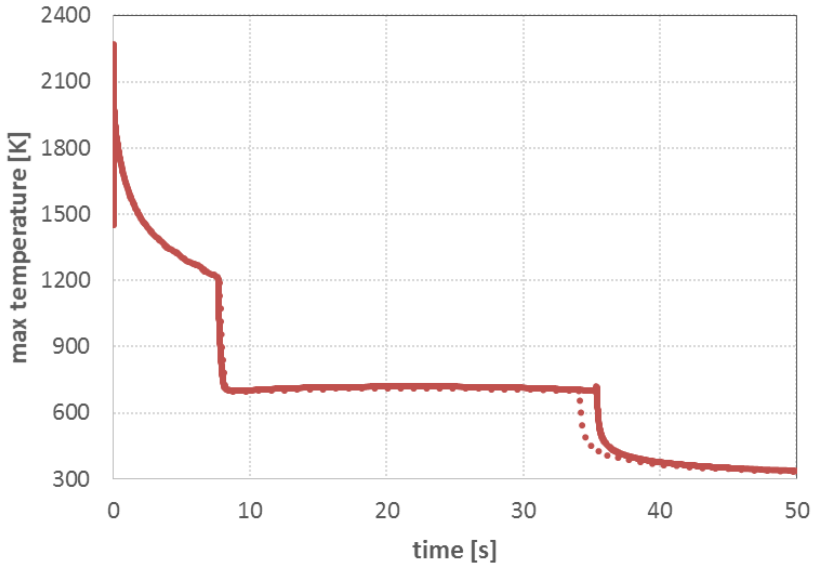
Detailed vs Reduced: Polimi-C1C16TOT

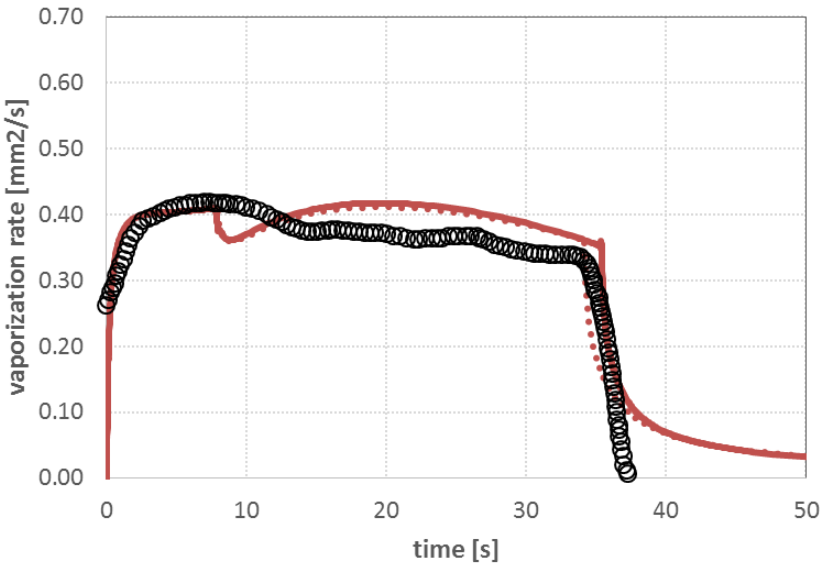
Polimi C1C16TOT

Original mechanism (435 species)

Reduced mechanism (100 species)





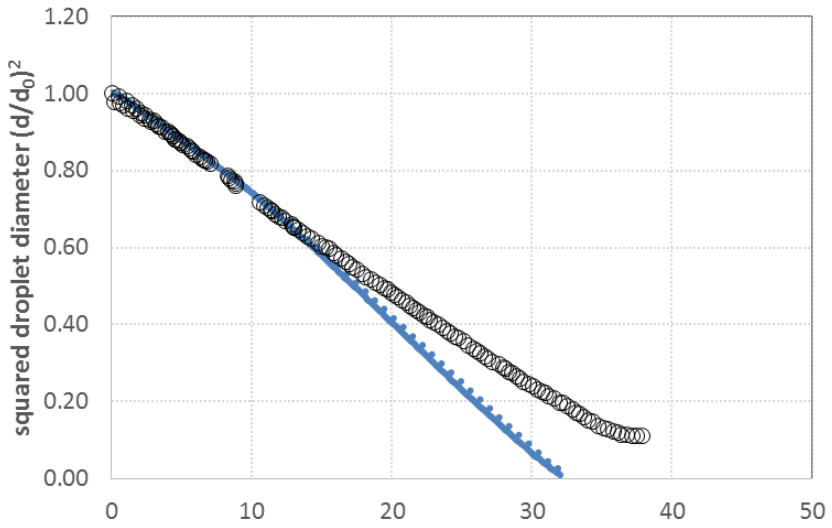


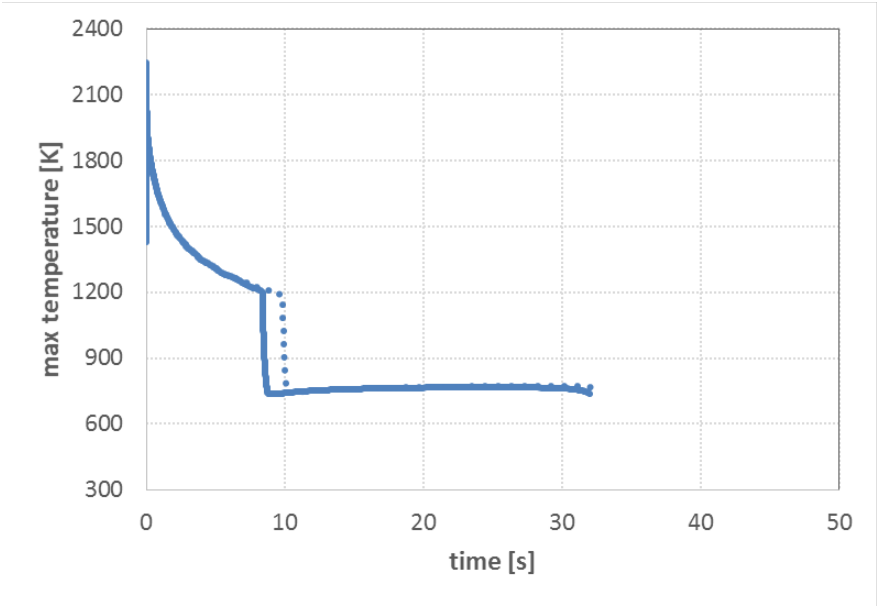
Detailed vs Reduced: Lu-NC7

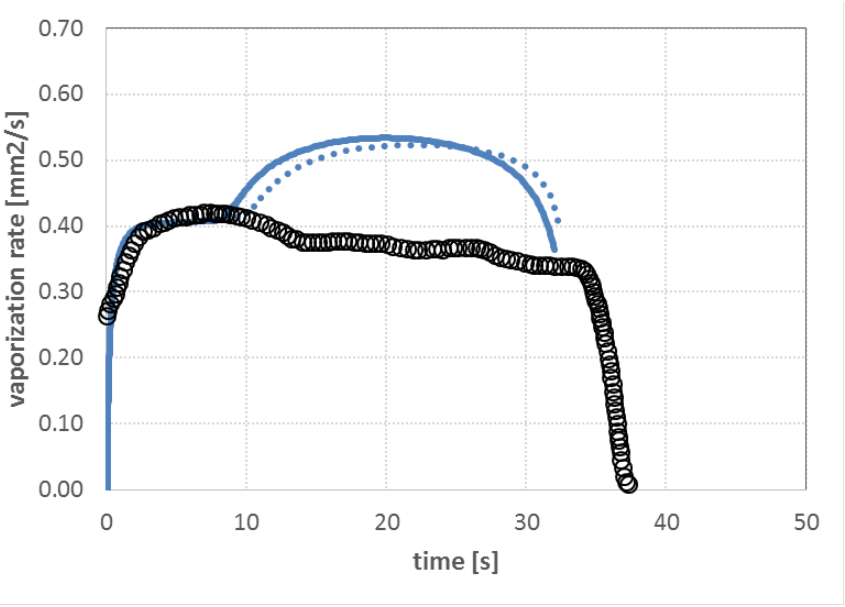
Lu-NC7

Original mechanism (188 species)

Reduced mechanism (88 species)





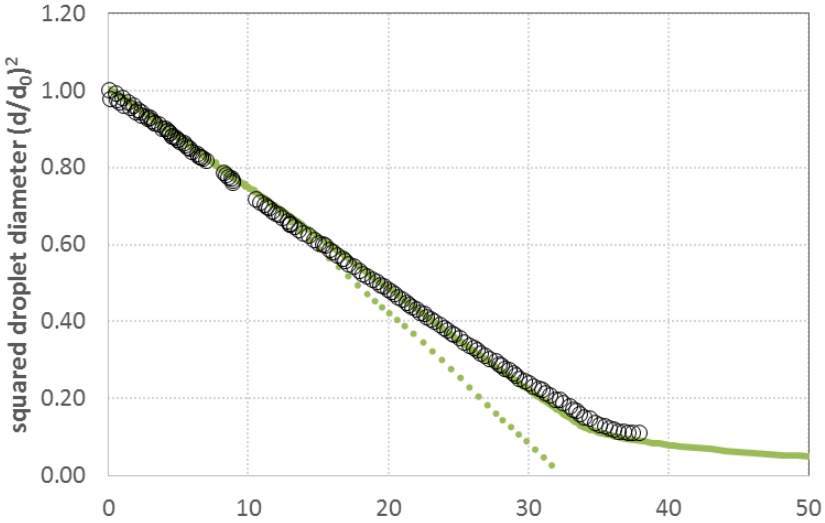


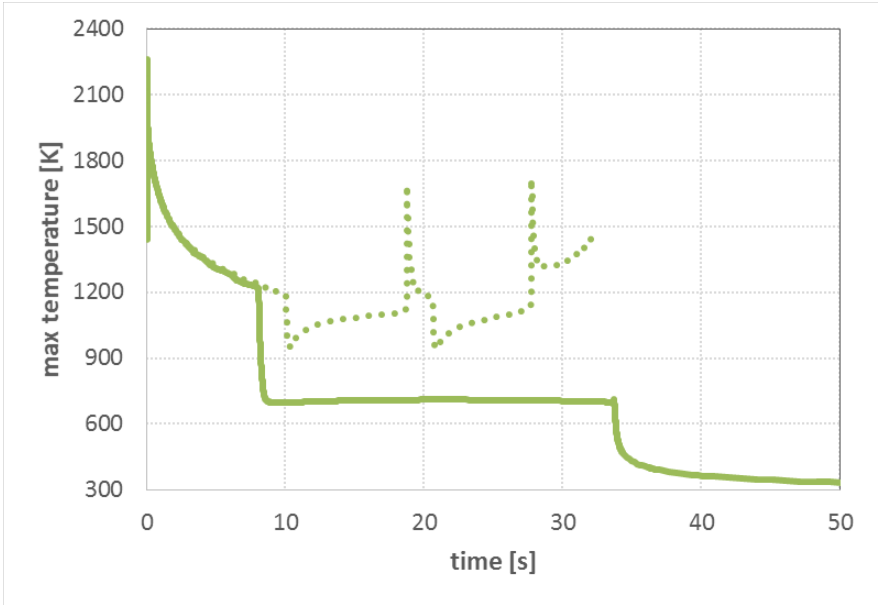
Detailed vs Reduced: LLNL-NC7

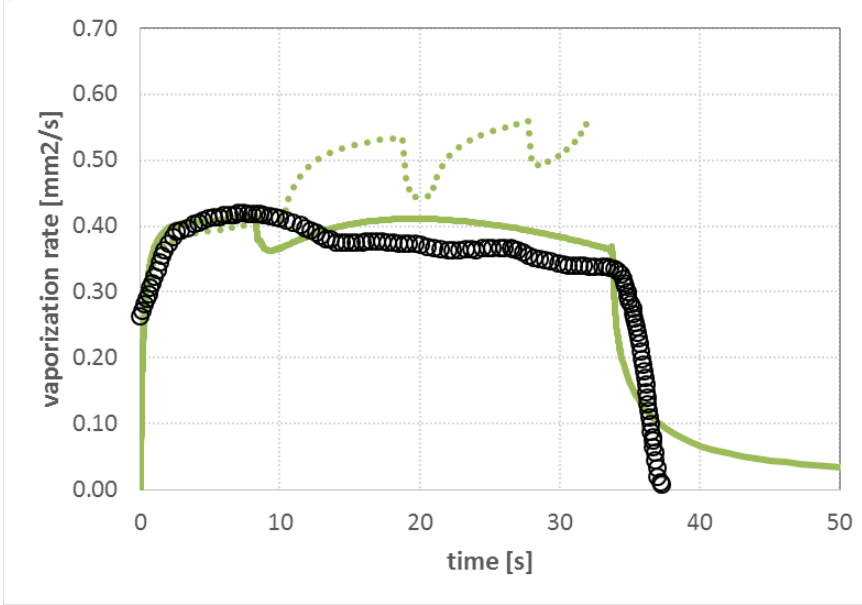
LLNL-NC7

Original mechanism (658 species)

Reduced mechanism (160 species)

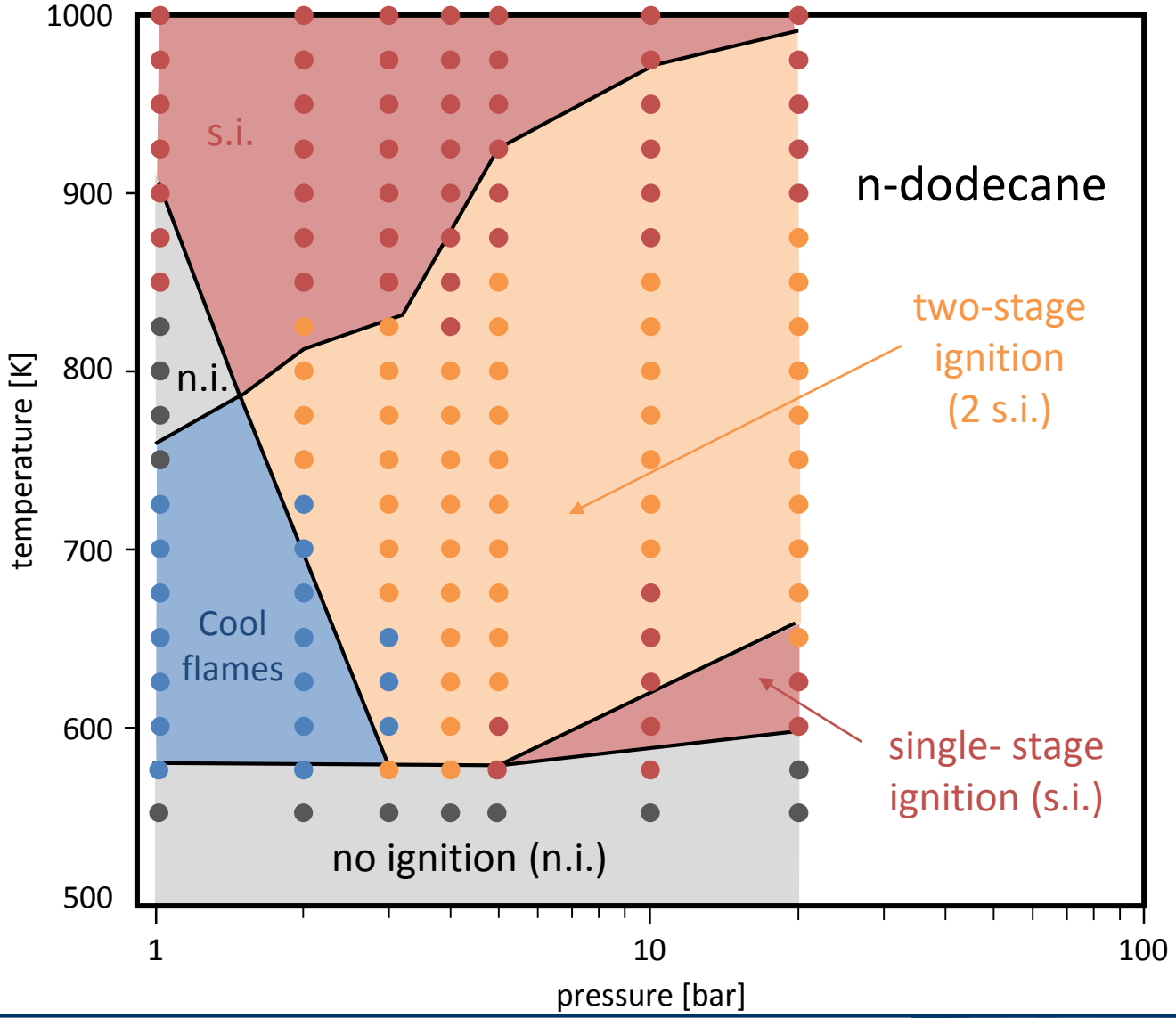






Autoignitions of nC12 droplets

Kinetic mechanism: POLIMI (Skeletal)



Ranzi E., Frassoldati A., Stagni A., Pelucchi M., Cuoci A., Faravelli T.

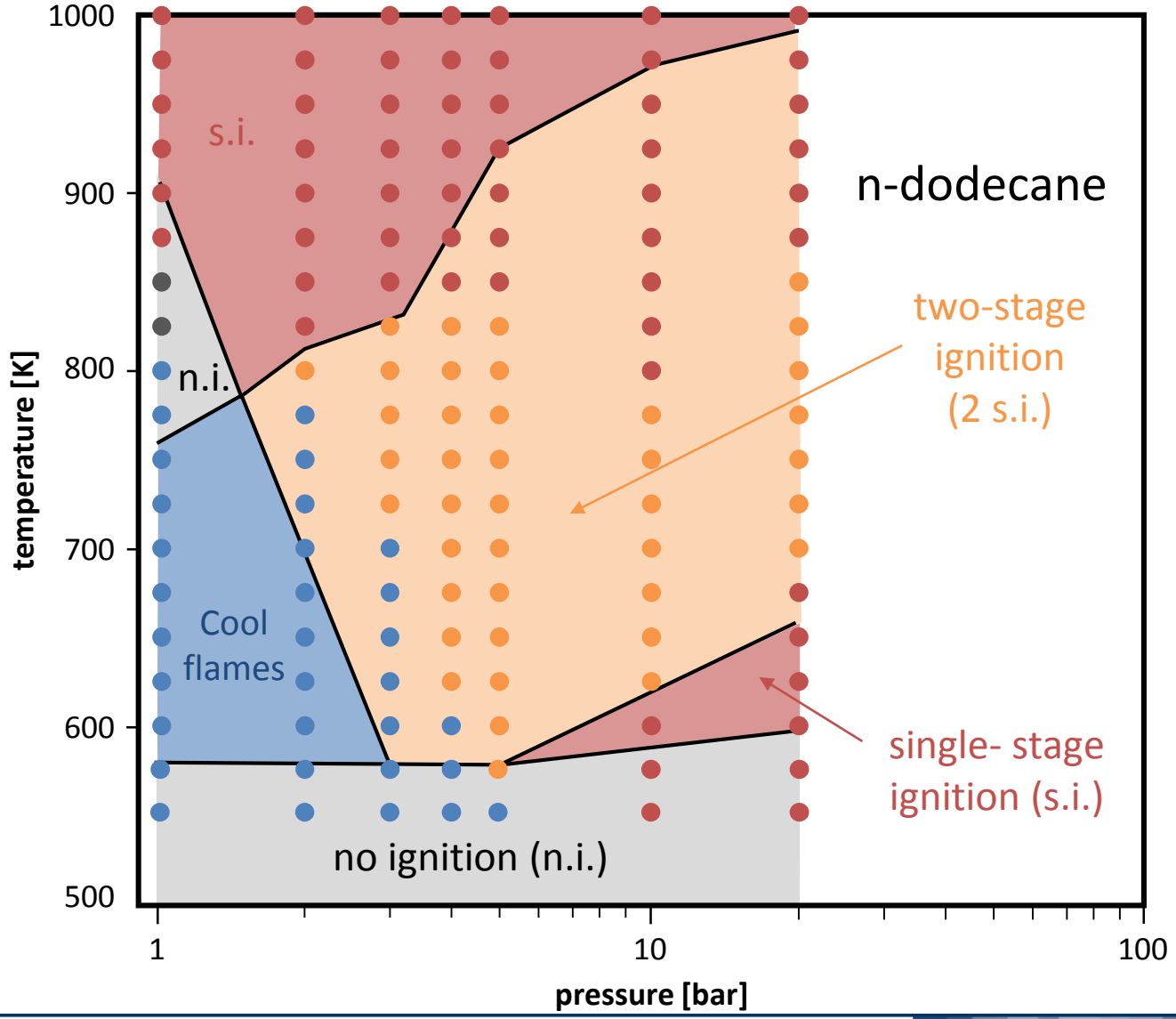
Reduced Kinetic Schemes of Complex Reaction Systems: Fossil and Biomass-Derived Transportation Fuels

International Journal of Chemical Kinetics 46(9) (2014), pp. 512-542

~ 108 chemical species

~ 1,328 reactions

Kinetic mechanism: Luo

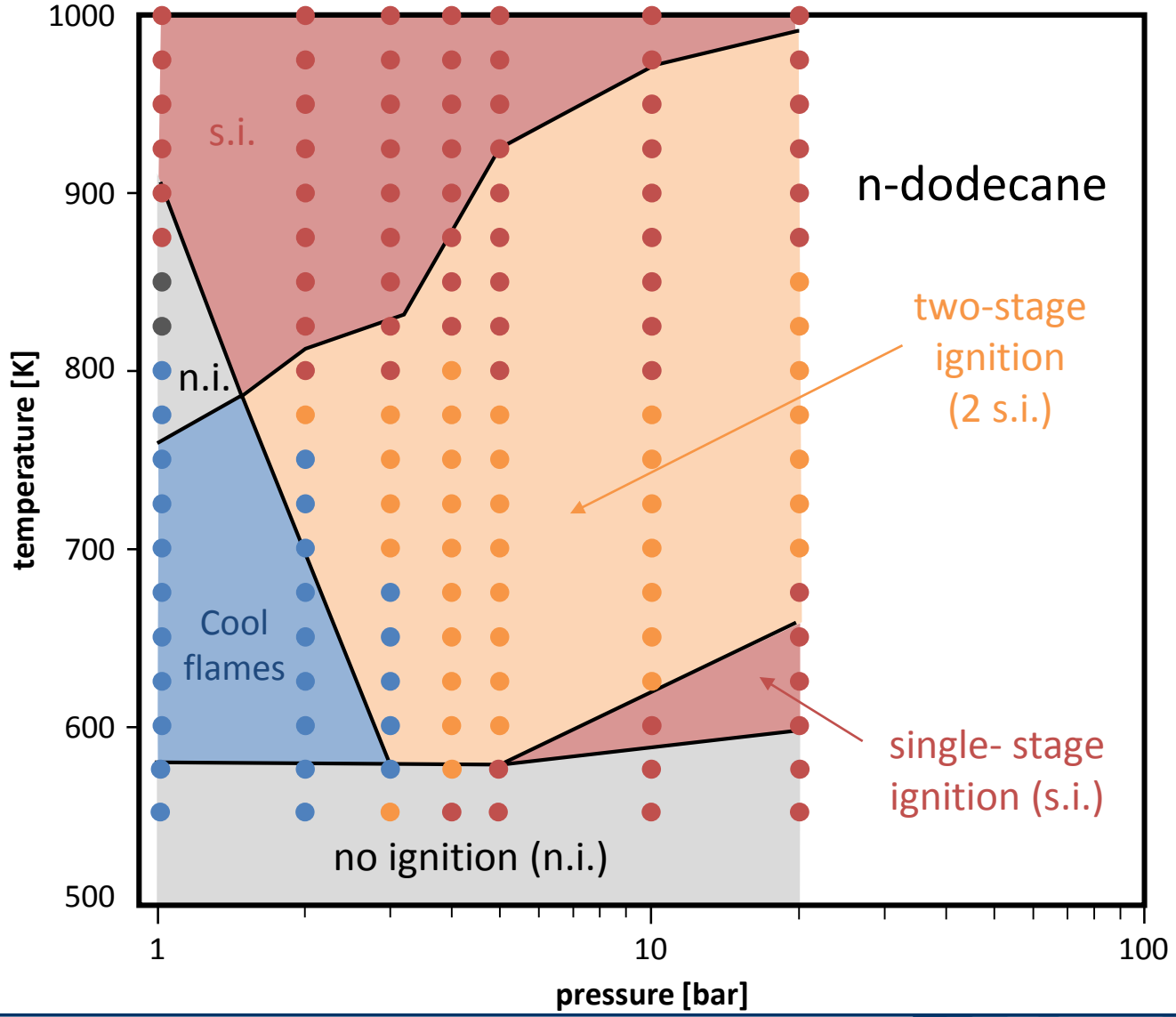


Luo, Z.,
Development of Reduced Chemical Kinetics for Combustion Simulations with Transportation Fuels
Doctoral Dissertations (2013)
Paper 232
University of Connecticut

~ 106 chemical species

~ 420 reactions

Kinetic mechanism: Narayanaswamy et al.



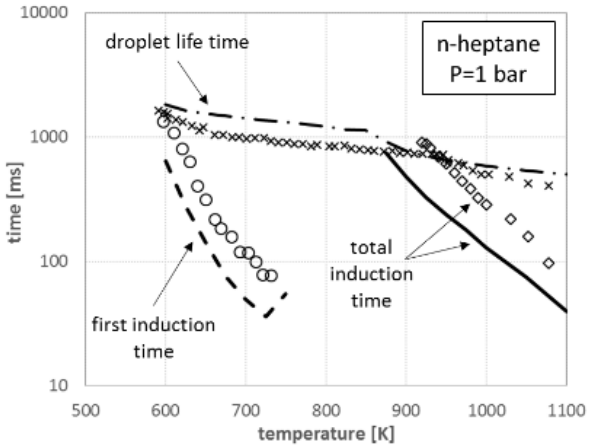
Narayanaswamy K., Pepiot P., Pitsch H.
A chemical mechanism for low to high temperature oxidation of n-dodecane as a component of transportation fuel surrogates
Combustion and Flame 161(4), p. 866-884 (2014)

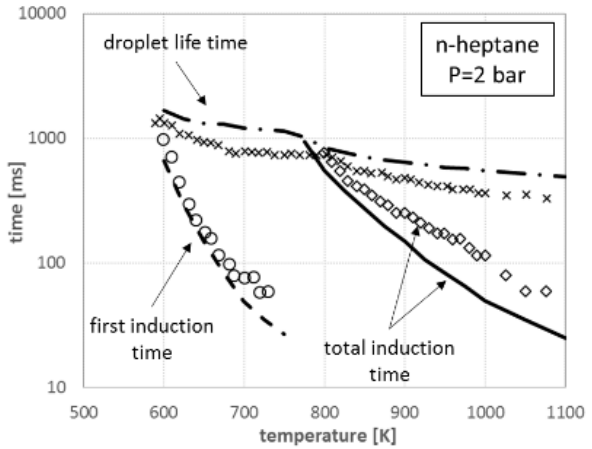
~ 255 chemical species

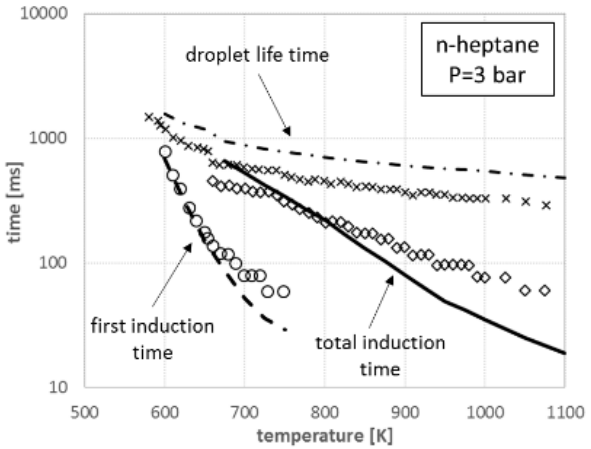
~ 1,509 reactions

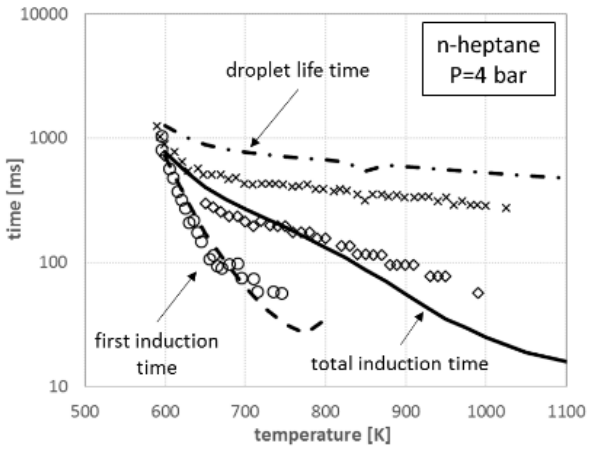
Autoignition times for n-heptane

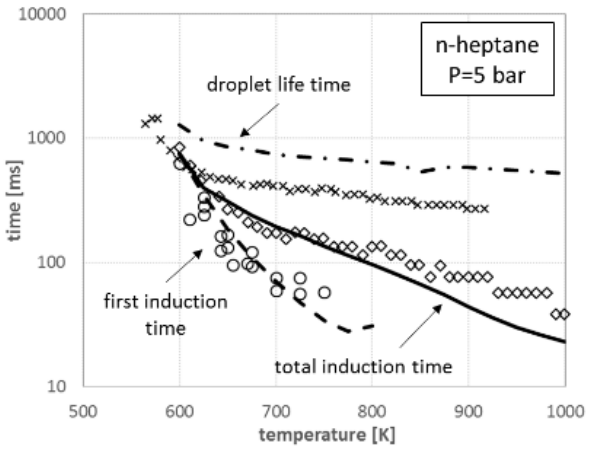
Autoignition times for n-heptane droplets

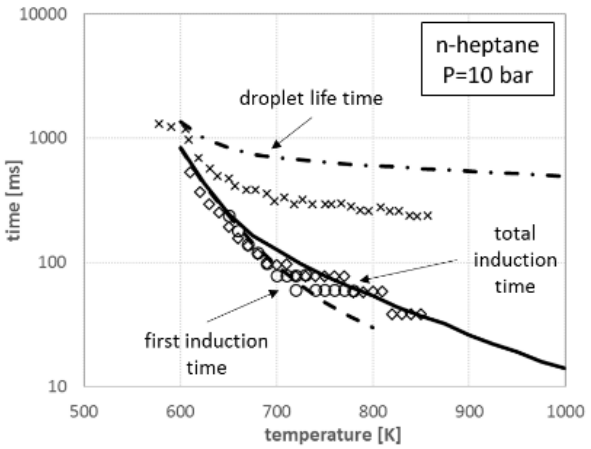




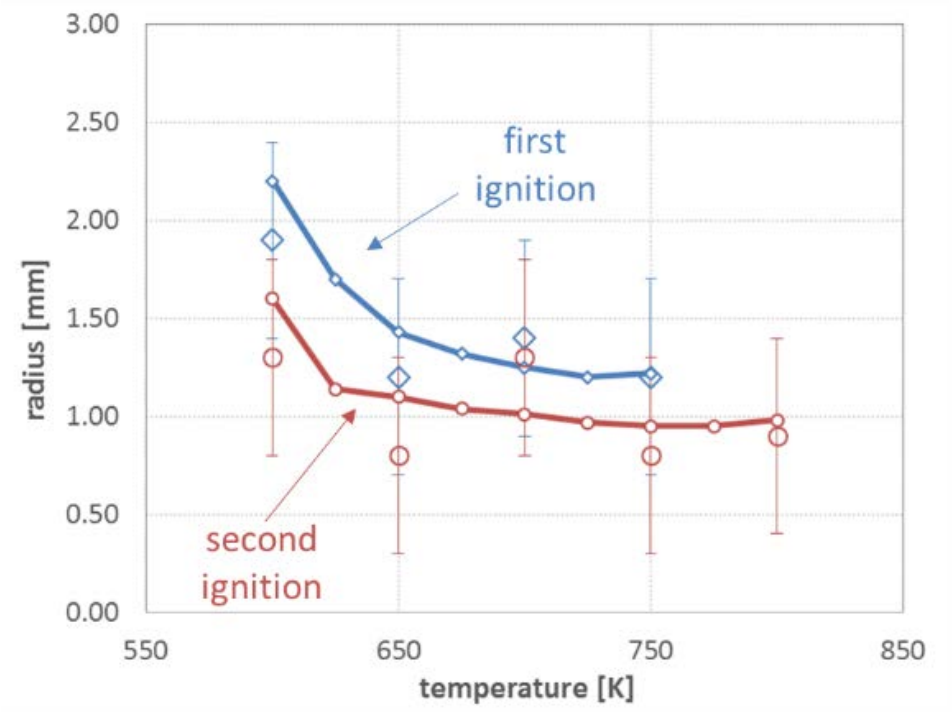








Ignition radius for n-heptane droplets



n-heptane
P=5bar
D0=0.70 mm

Exp. data: **S. Schnaubelt, M. Tanabe, C. Eigenbrod, H.J. Rath**, Proceedings of Drop Tower Days, (1998) 299-306