Evaporation, microexplosion and combustion of a nano-Al-particles-embedded single kerosene droplet under sub-atmospheric pressure

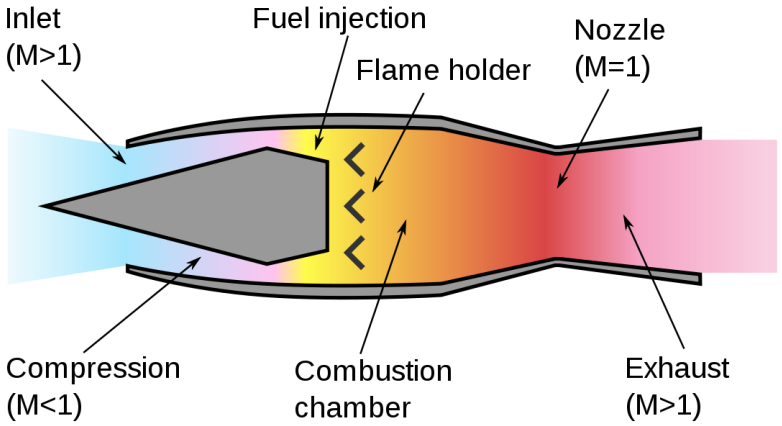
Hongtao Zhang, Jun Xia
Dept. of Mech. & Aero. Engineering
Brunel University

5th Combustion SIG workshop
University of Oxford, 23-24 September 2019

Introduction

- Background
- Kerosene droplet combustion
- Nano Al-particles embedded kerosene droplet combustion
- Vapor-Liquid Equilibrium Molecular Dynamics Simulation
- Conclusions

Background



Ramjet Engine

Flying in near space

↓

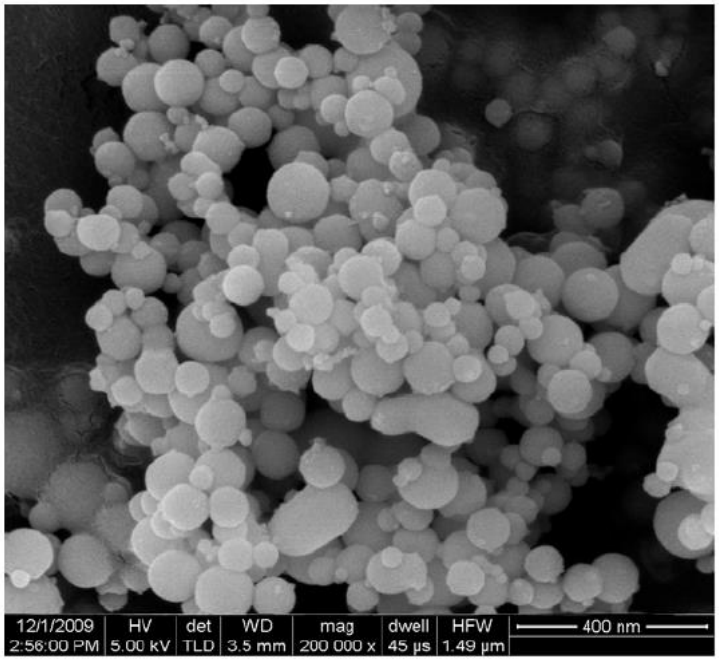
Inlet pressure: 0.1 ~ 0.3 bar

↓

Deterioration of fuel evaporation and combustion performance

Background

Additive to enhance energy density:
nano-Aluminum particles



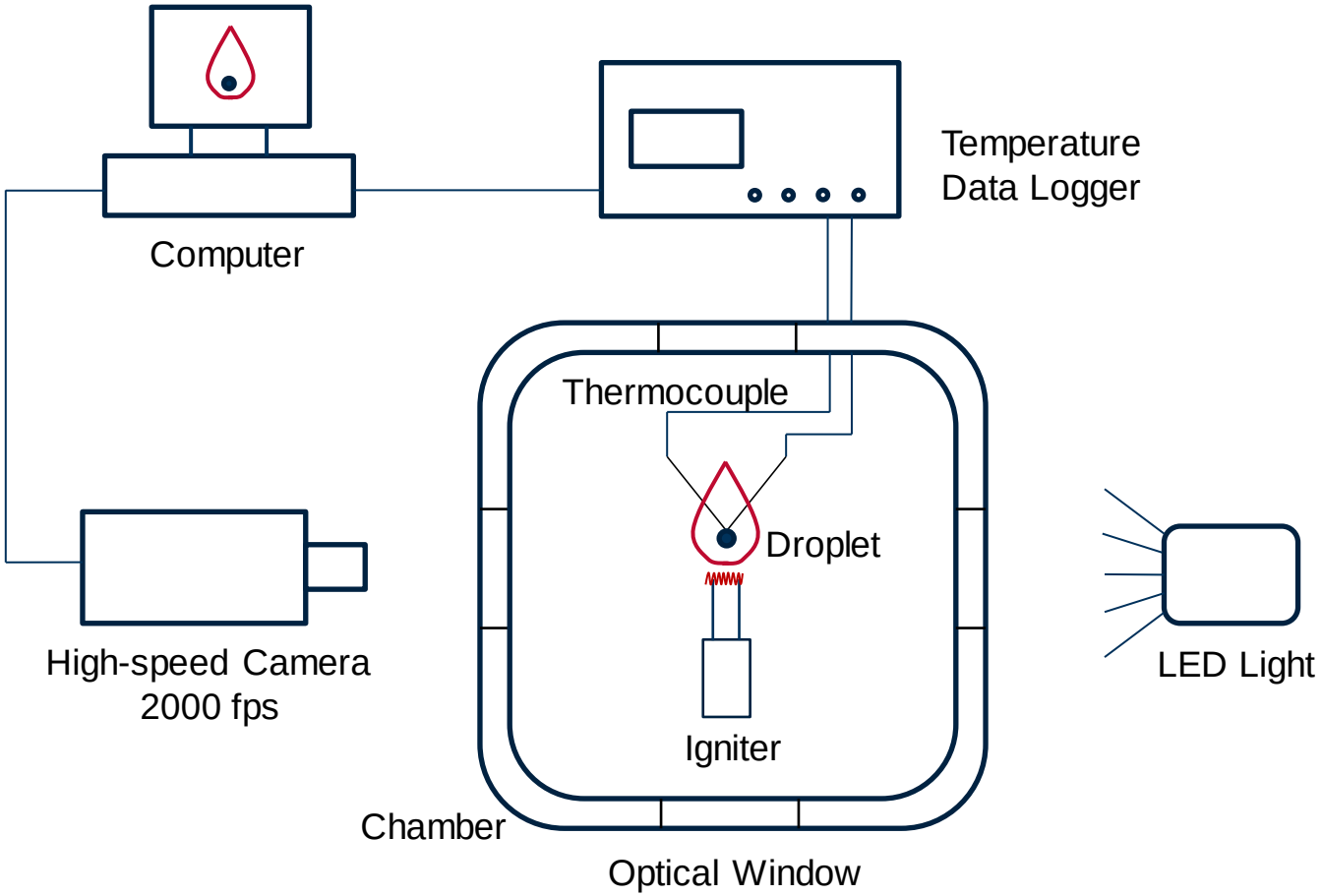
SEM photograph of 80nm nano-aluminium particles*

- Higher energy density
- Less CO_2 & NO_x
- Shortened ignition delay time
- Enhanced fuel oxidation by catalytic effect

*Y. Gan, L. Qiao / Combustion and Flame 158 (2011) 354–368

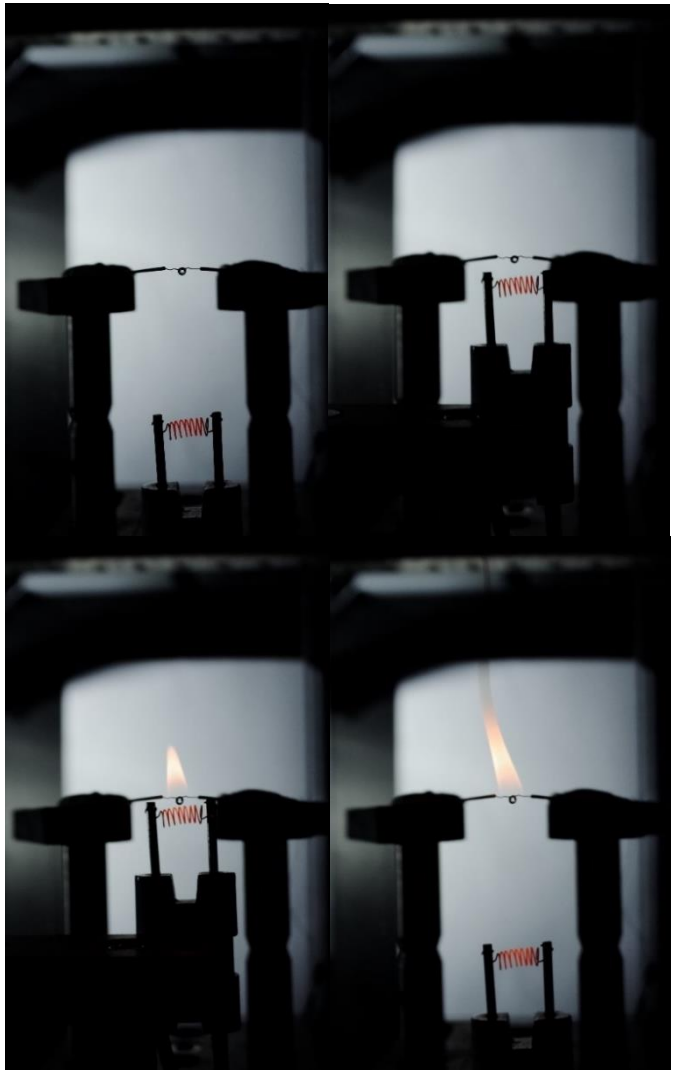
Kerosene droplet combustion

Experimental Setup @ Zhejiang University, China



Kerosene droplet combustion

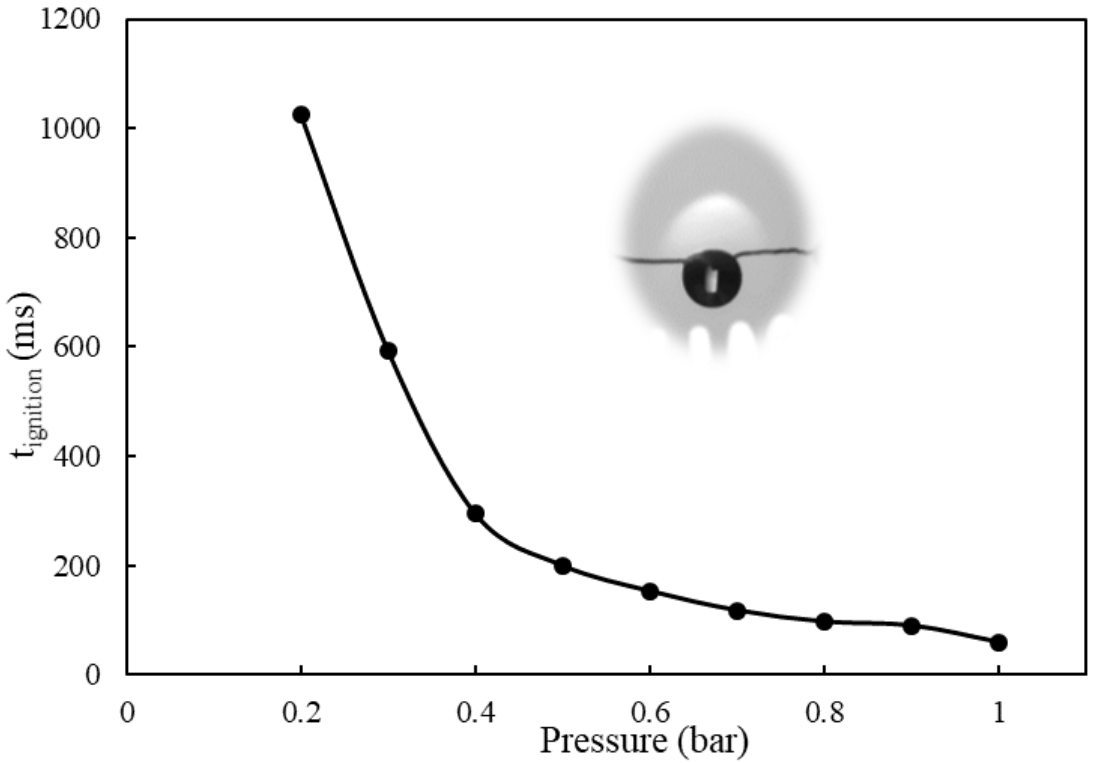
Experimental Setup



Kerosene droplet combustion

Major components of Chinese RP-3 kerosene (mass fraction)

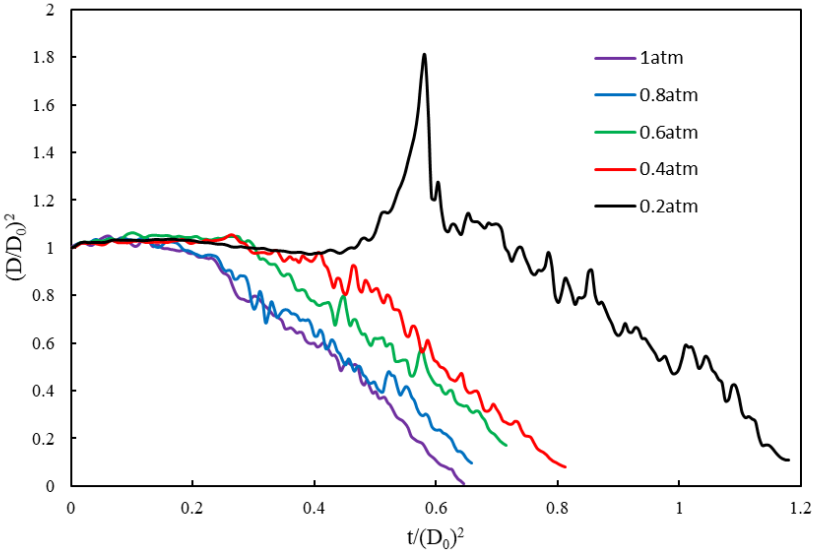
Saturated hydrocarbons				Aromatic hydrocarbons			
Alkanes	Naphthenes			Alkyl Benzenes	Indan & Tetralin	Naphthalene	Naphthalene derivatives
	Monocyclic	Bicyclic	Tricyclic				
52.2	33.8	6.0	0.1	5.1	1.3	0.6	0.9

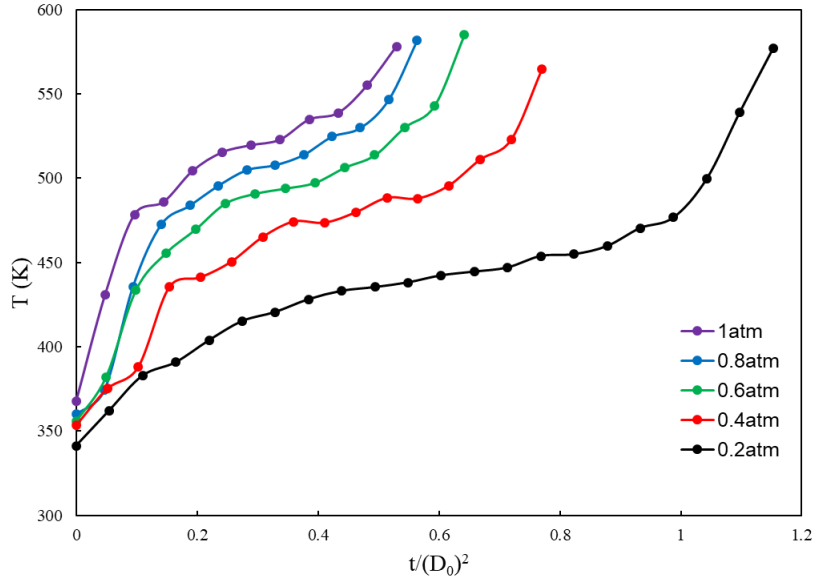


Ignition delay time at different pressures for RP-3 kerosene

Kerosene droplet combustion

P = 0.5bar

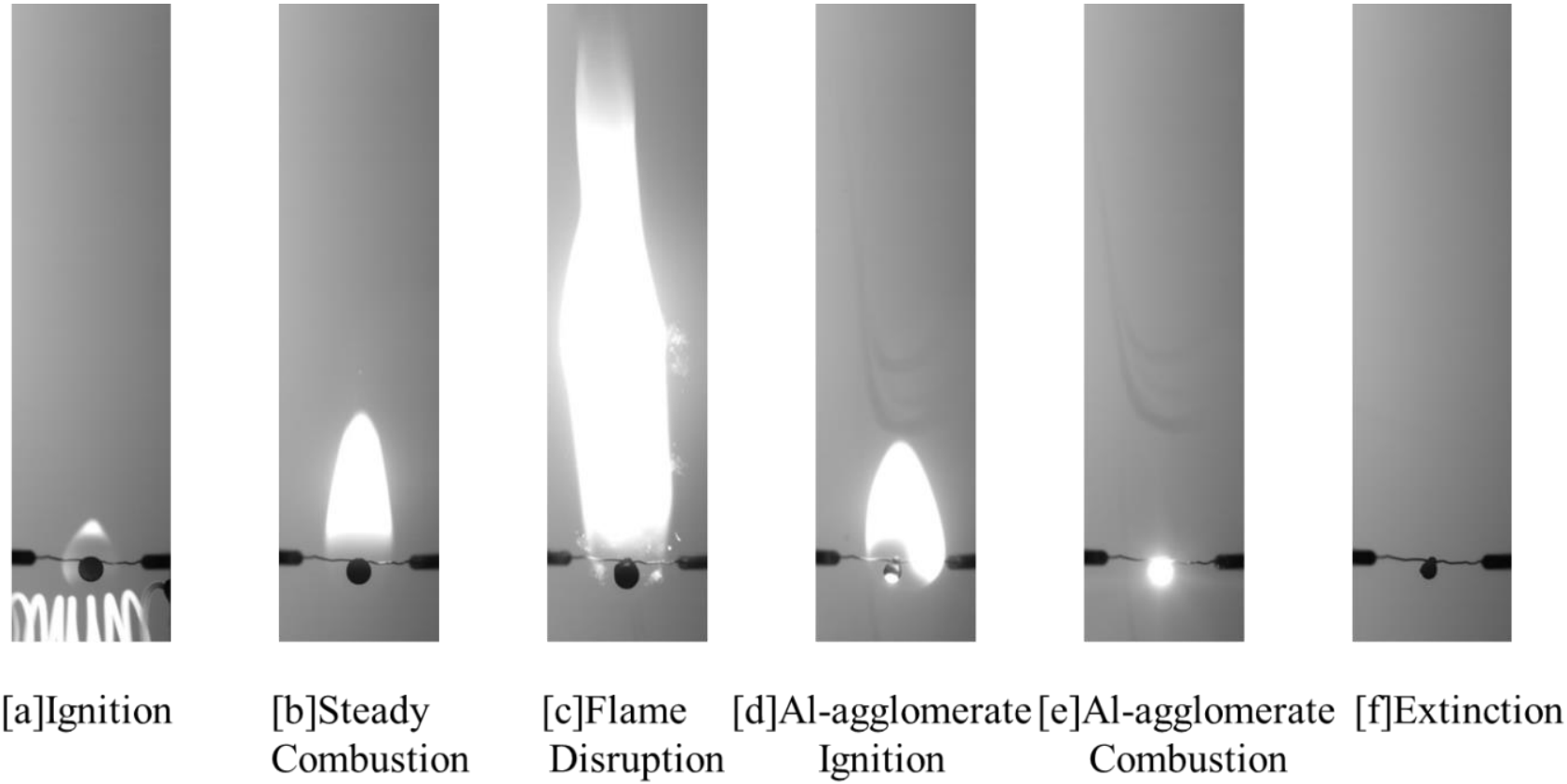




The droplet size and temperature histories at pressures 0.2-1.0 bar

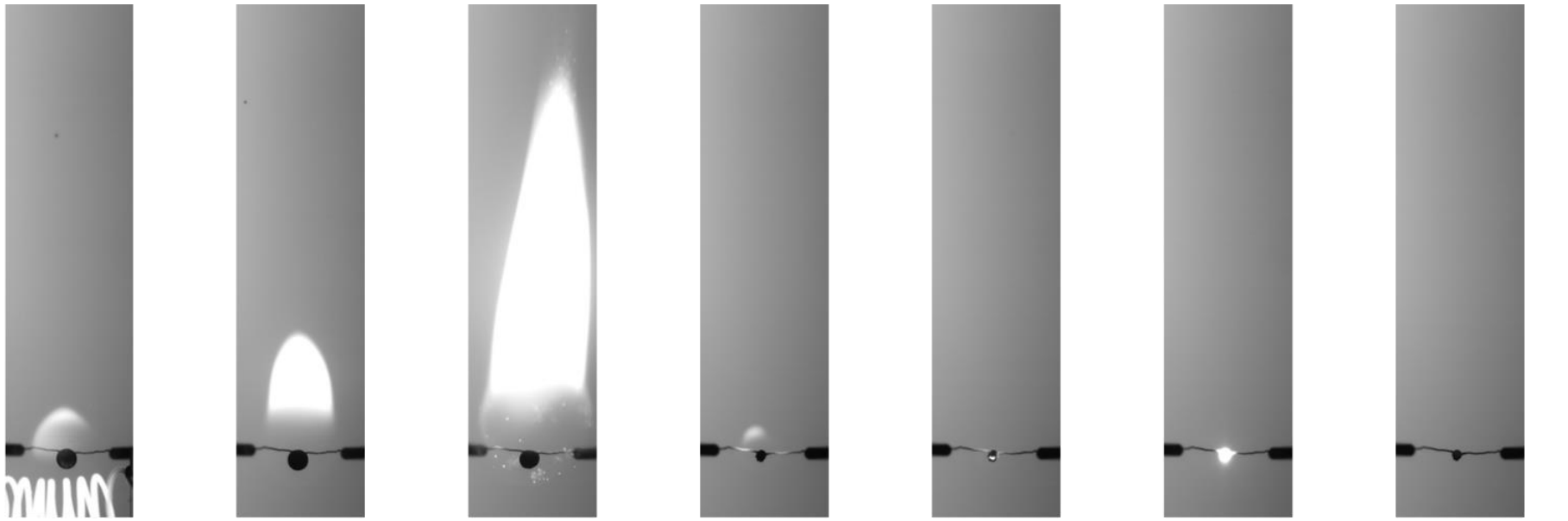
Nano Al-particles embedded kerosene droplet combustion

10%wt 80nm nano-Al, 2.5%wt surfactant



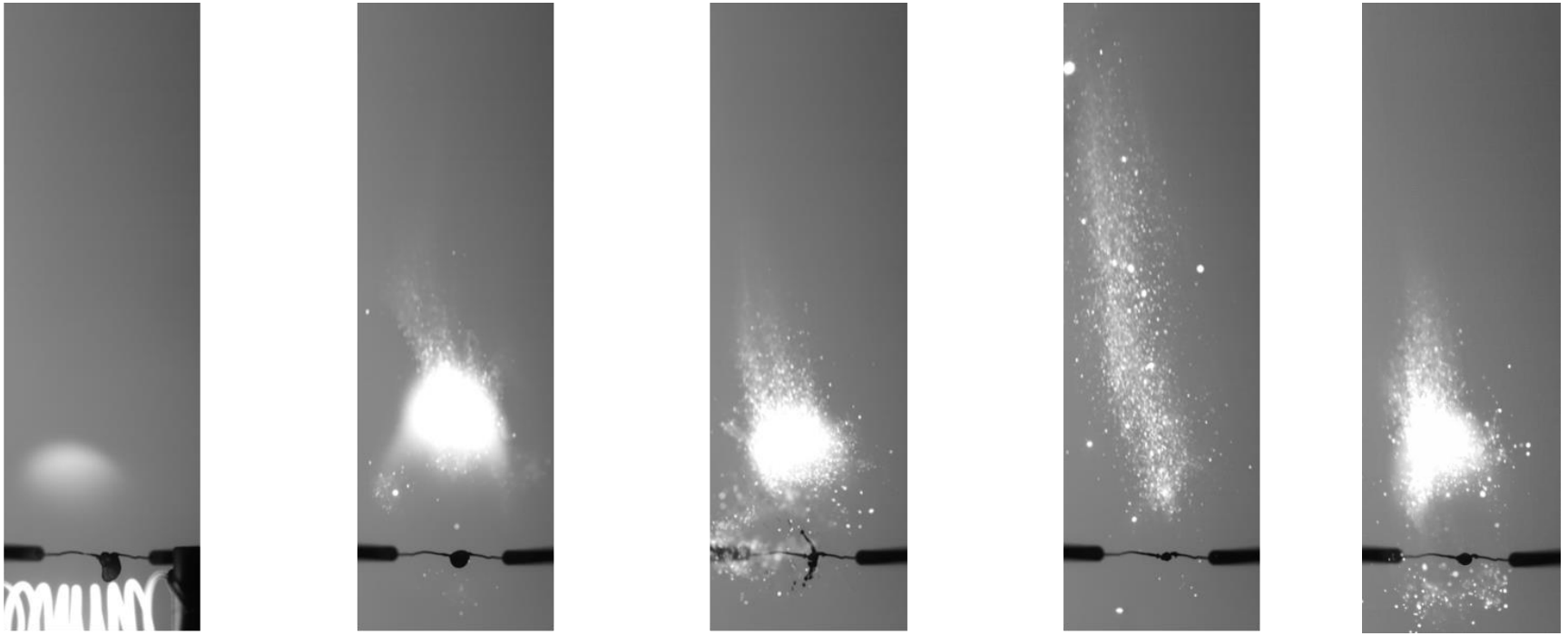
A burning sequence of RP-3/nano-Al droplet at 1bar

Nano Al-particles embedded kerosene droplet combustion



A burning sequence of RP-3/nano-Al droplet at 0.5bar

Nano Al-particles embedded kerosene droplet combustion

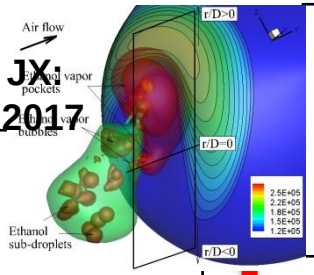


[a]Ignition [b]Flame Disruption [c]Micro explosion [d]Extinction

A burning sequence of RP-3/nano-Al droplet at 0.2bar

Multiscale framework

Navier-Stokes
Interface cap



JS, JX, PCI 2017

DNS
microexplosion

Immiscible
(emulsion)

Miscible

Initial
conditions

NanoP

Ambient P

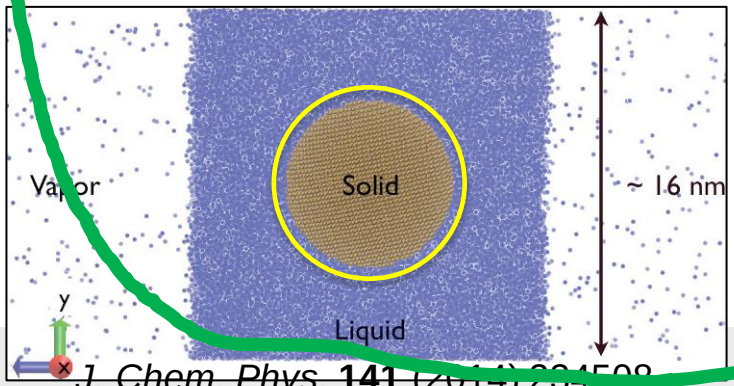
Nucleation

Nuclei size

Thermo
dynamic
state

Prediction
outcome

MD

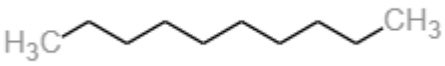


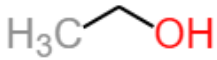
Objective of this Work

J. Chem. Phys. **141** (2014) 234508.

Vapor-Liquid Equilibrium Molecular Dynamics Simulation

Numerical setup

n-decane 

ethanol 

- Software: LAMMPS
- Force field: TraPPE-UA
  - Using single interaction sites to represent a carbon atom together with all of its bonded hydrogen atoms.
- Ensemble: NVT
  - Temperature was maintained by Nose-Hoover thermostat
- Molecule number: 1000
- T_{target}: 70, 75, 80, 85, 90% T_c

Vapor-Liquid Equilibrium Molecular Dynamics Simulation

Numerical setup

- pair style: lj/long/coul/long

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c \qquad E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

- bond style: harmonic

$$E = K(r - r_0)^2$$

- angle style: harmonic

$$E = K(\theta - \theta_0)^2$$

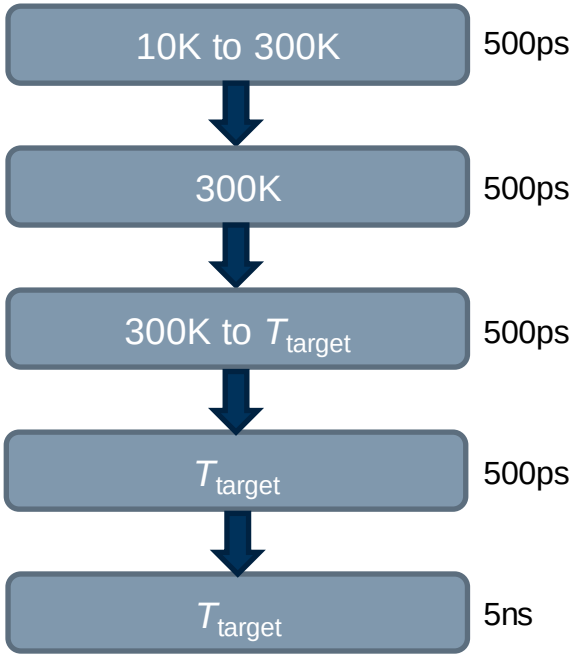
- dihedral style: opls

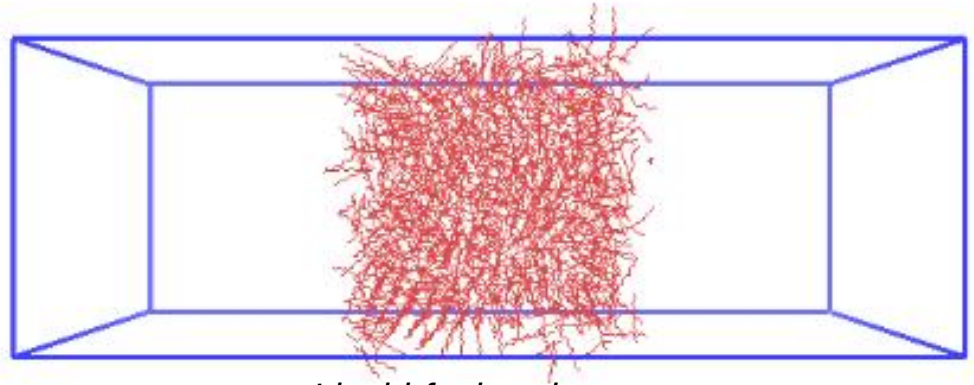
$$E = \frac{1}{2}K_1[1+\cos(\phi)] + \frac{1}{2}K_2[1-\cos(2\phi)] + \frac{1}{2}K_3[1+\cos(3\phi)] + \frac{1}{2}K_4[1-\cos(4\phi)]$$

- kspace style: pppm/disp
  - Add a long-range dispersion sum option for $1/r^6$ potentials and is useful for simulation of interfaces

Vapor-Liquid Equilibrium Molecular Dynamics Simulation

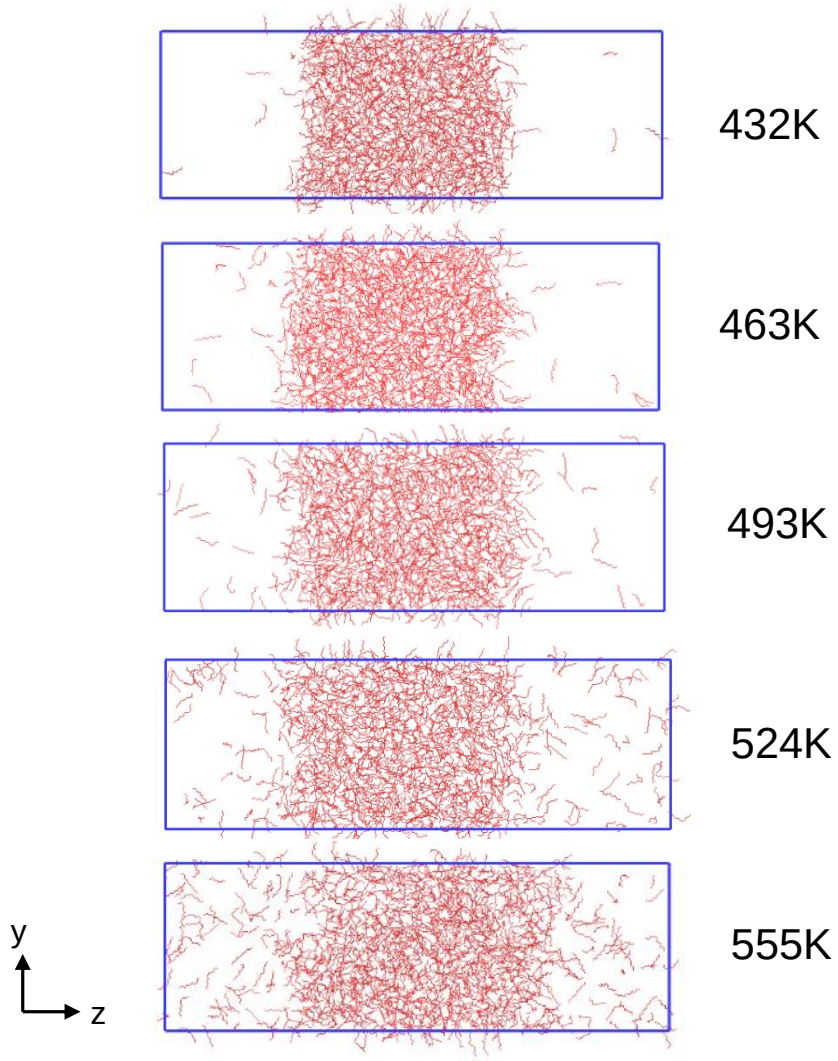
Numerical setup





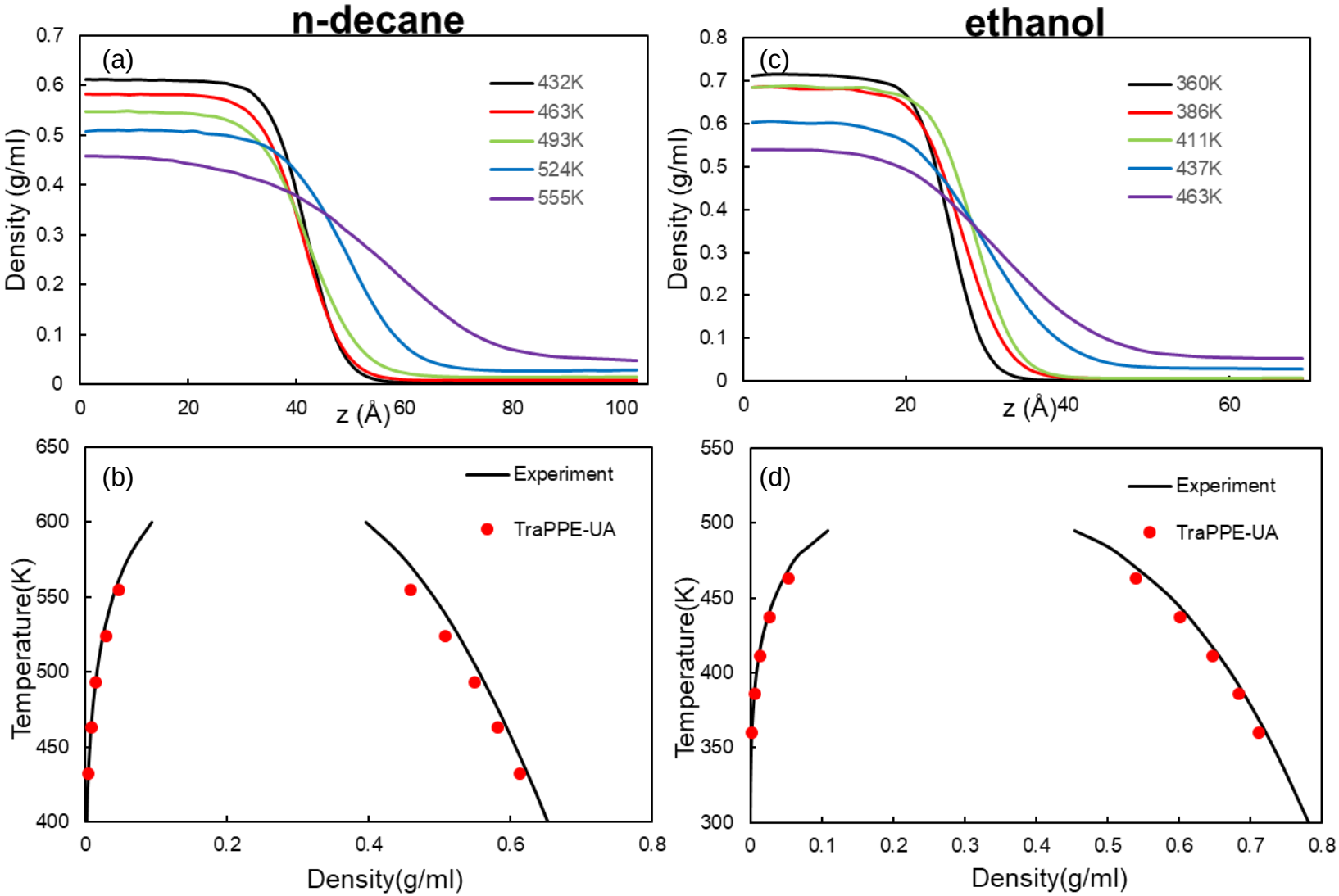
Liquid fuel: n-decane;
Domain size: 68.8, 68.8 and 206.4 Å in x, y and z directions

Vapor-Liquid Equilibrium Molecular Dynamics Simulation



Evaporation of n-decane at different temperatures

Vapor-Liquid Equilibrium Molecular Dynamics Simulation



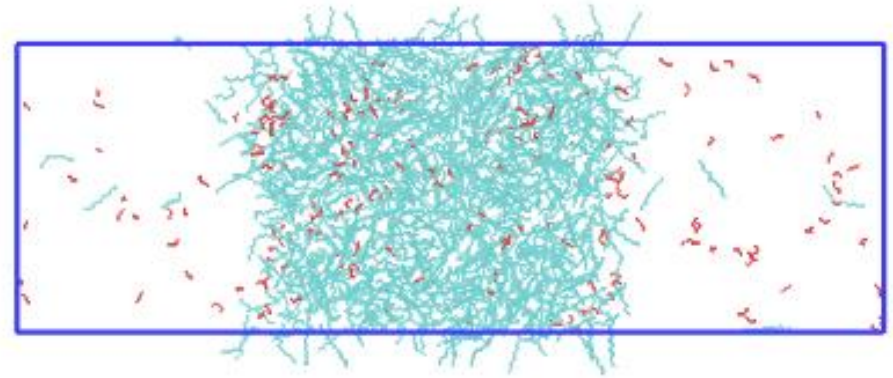
(a) (c) Density as a function of distance from the liquid-slab center of mass

(b) (d) Vapor-lquid coexistence curve

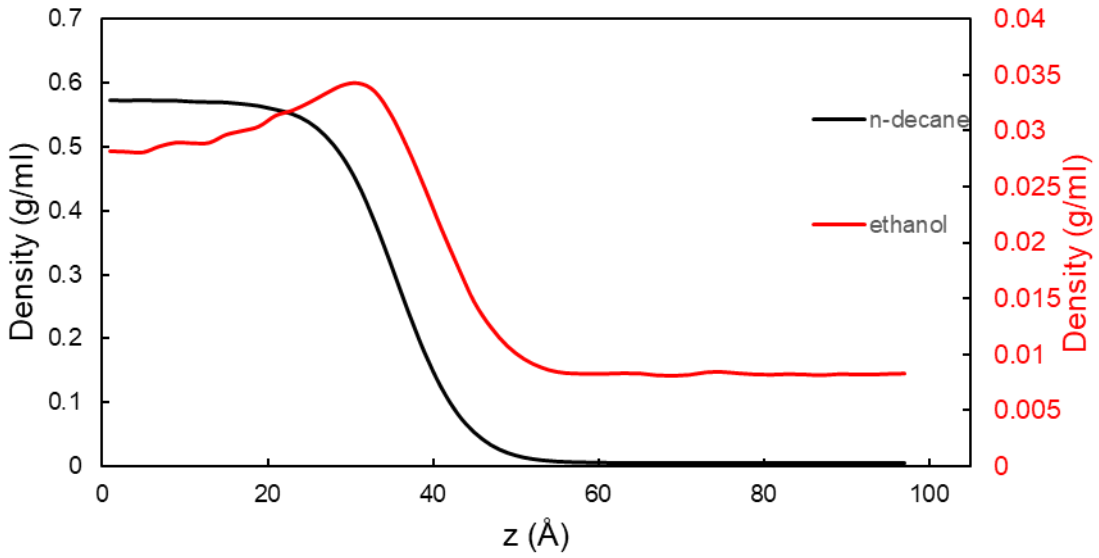
Vapor-Liquid Equilibrium Molecular Dynamics Simulation

80% n-decane + 20% ethanol

T = 437K (85% $T_{c\text{-ethanol}}$)



No experimental data; DSMC benchmarking?



Density as a function of distance of z for n-decane/ethanol mixture

Conclusions

- Decrease of ambient pressure increases the ignition delay time of kerosene droplet burning and enhances the probability of inner boiling, leading to puffing.
- Six distinctive stages (ignition, droplet combustion, flame disruption, surfactant flame, Al-agglomerate ignition, Al-agglomerate combustion) were identified for nano-Al particles embedded kerosene droplet combustion.
- Much more intense puffing was observed for nano-Al particles embedded kerosene droplet combustion, with micro-explosion occurring at 0.2 bar.
- Molecular dynamics simulation with TraPPE-UA force field and long-range LJ interaction properly predicts vapor-liquid equilibrium.
- Future work: MD simulation of evaporation and nucleation of multicomponent liquid mixture embedding nano particles.

Acknowledgements

- Financial support by the China Scholarship Council (CSC) for a research visit of Hongtao Zhang to Brunel University London is gratefully acknowledged.

Brunel University London

Thank you for listening!

Any questions?