Dispersion, evaporation and chemical kinetics of nanofuel sprays under external electrostatic fields

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Email: a.giusti@imperial.ac.uk (Presenter)

Context and Motivation

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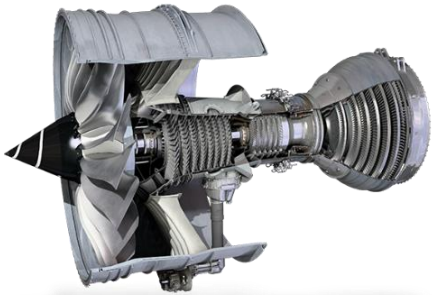

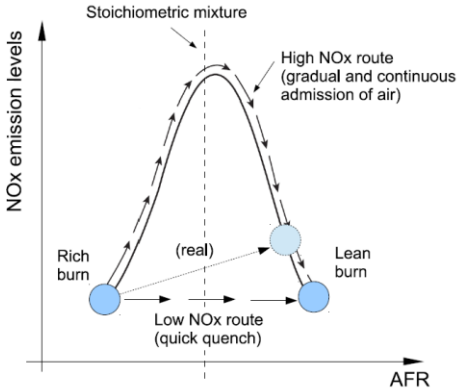

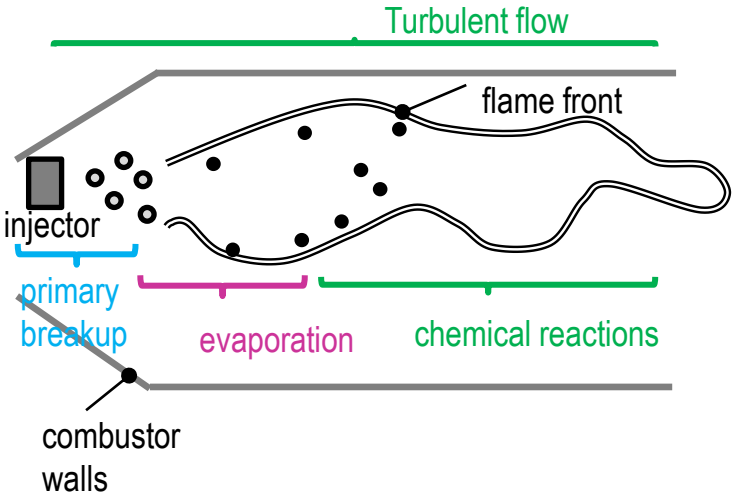

- Premixed/Non-premixed
- Azimuthal flames
- MILD combustion
- Fuel flexibility
- Dual fuel (hydrogen)

Mixing between air/fuel

- High-pressure ratio

Electrification of the aircraft

- Integration
- Distribution

➢ More electrical

➢ Hybrid thermal/electrical

➢ Fully electrical aircraft

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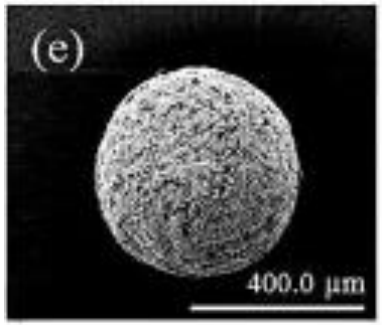
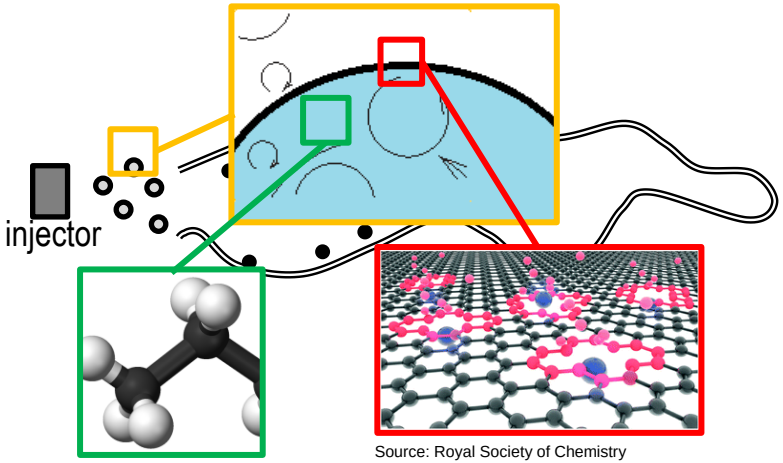


From: Osman et al., J. Ind. and Chem. Eng., vol. 67, 2018



Source: Royal Society of Chemistry

- Design of fluid
- Nanomaterial able to self-organize
- Control of pore size through EM
- Tailored properties for evaporation and combustion

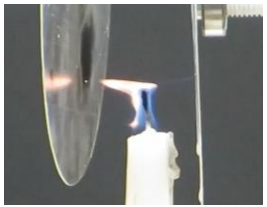
Nanofuels

- New material
- Nanoparticles in a liquid fuel
- Improve combustion characteristics

smart combustion

Electrification

EM effects



Shells of nanomaterials naturally forms during the drying process of a nanofluid

Objectives

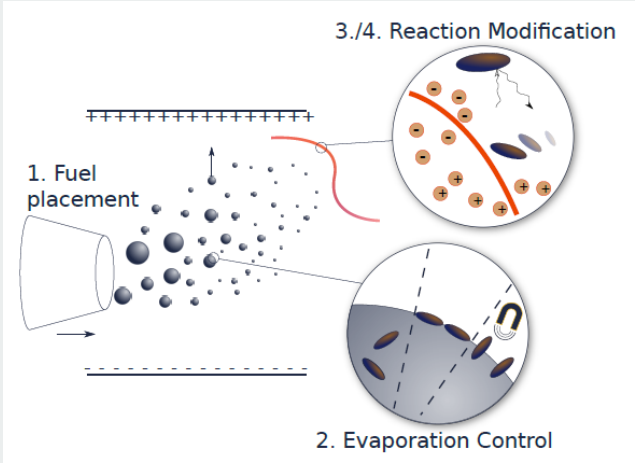
I. What is the effect of electrostatic fields on the dispersion of clouds of nanofuel droplets?
   - ➢ Direct Numerical Simulations in HIT of a spherical cloud

II. Can we control the location of the spray to change the mixing?
   - ➢ Large-Eddy Simulations of an electrospray in cross-flow

III. Does the electrostatic field affect the kinetics of nanofuel combustion?
   - ➢ Molecular Dynamics of n-dodecane oxidation with iron nanoparticles

Dispersion of a cloud of nanofuel droplets

- Investigate the competing effects of drag and electrostatic forces on the dispersion of a cloud of droplets
- Identify effects on the turbulence spectrum
- Develop regime maps



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Numerical approach

- Box of homogeneous and isotropic turbulence
- OpenFOAM, modified with electrostatic potential equation
- Two-way coupling, dilute spray

$$\frac{\mathrm{d}m_d}{\mathrm{d}t} = -\frac{\pi}{4}\rho_l d\, K \cdot \beta$$

Table 2. Overview of non-dimensional parameters in droplet cloud dispersion simulations.

Parameter	Symbol	Value
No. of trials per config.	N_t	6
Droplet cloud radius	$r_c/\mathcal{L}$	1/8
Init. droplet vol. frac.	$\overline{\phi}_0$	10^{-5}
Droplet diameter	$d_0/\mathcal{L}$	$4.143{\cdot}10^{-4}$
Density ratio	ρ_l/ρ_g	626.7
Droplet Stokes number	St	0.100
Nondim. charge group	Π_q	-11813
Nondim. potential group	$\Pi_{\Delta\Phi}$	4.123
External pot. difference	$\Delta\Phi/\Delta\Phi_0$	0, 0.5, 1, 2

Table 3. Droplet parameters for HIT simulations with evaporating nanofluid droplets.

Parameter	Symbol	Value
Initial diameter	$d_0/\mathcal{L}$	$4.143{\cdot}\ 10^{-4}$
Density ratio	ρ_l/ρ_g	626.7
Droplet lifetime	τ_v/τ	0.035, 0.07, 0.14
Nanop. Péclet number	Pe	50, 200
Init. droplet Stokes num.	St	0.1
Init. nanop. vol. frac.	$\varphi_{p,0}$	0.0016
Nanop. radius	$r_p/\mathcal{L}$	$3.694{\cdot}10^{-6}$
Nanop. contact angle	θ	40°
External pot. diff.	$\Delta\Phi/\Delta\Phi_0$	0, 1, 2

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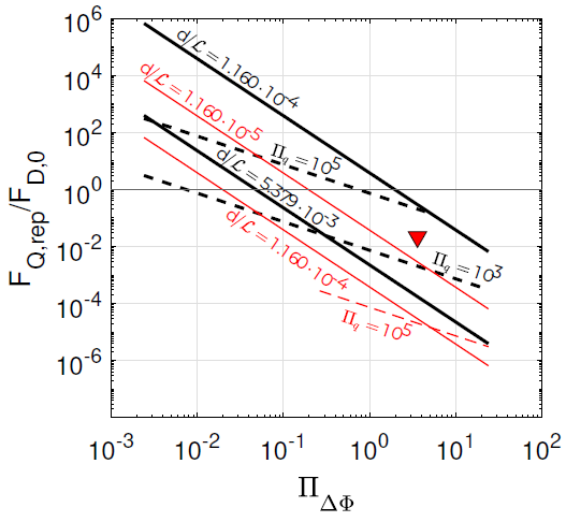
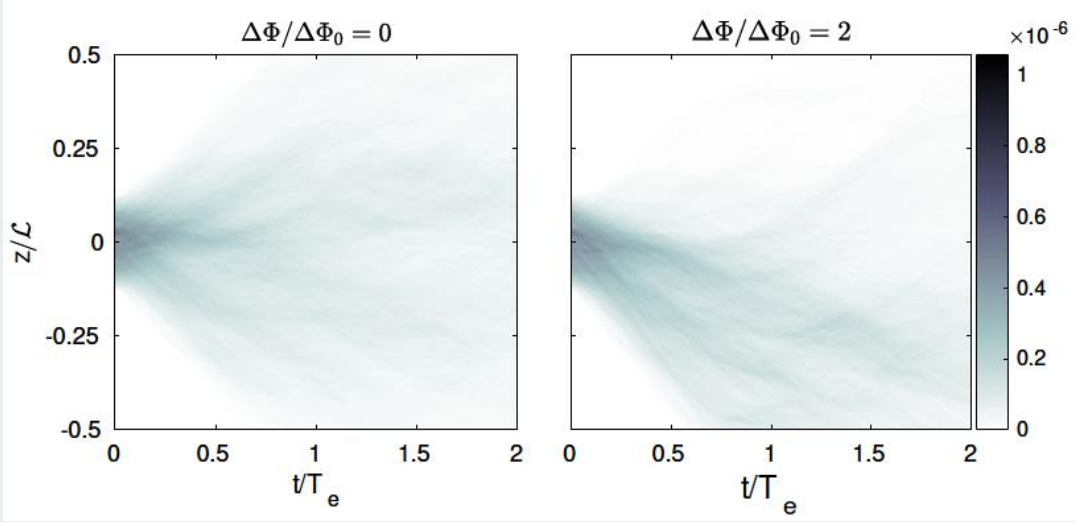
Some results

- Operating point

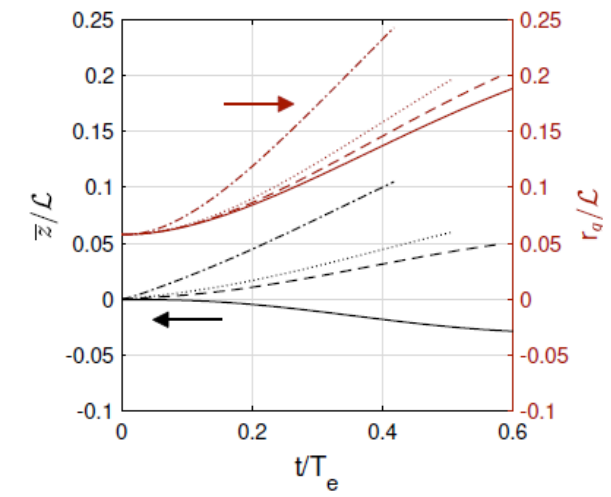


- Plane average droplet volume fraction

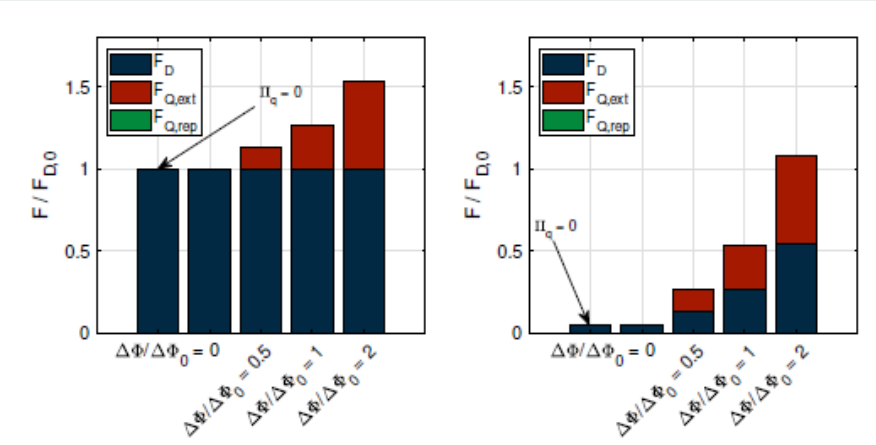


Some results

- Location of the centre of mass



- Force budget at t/Te = 0 and 0.35

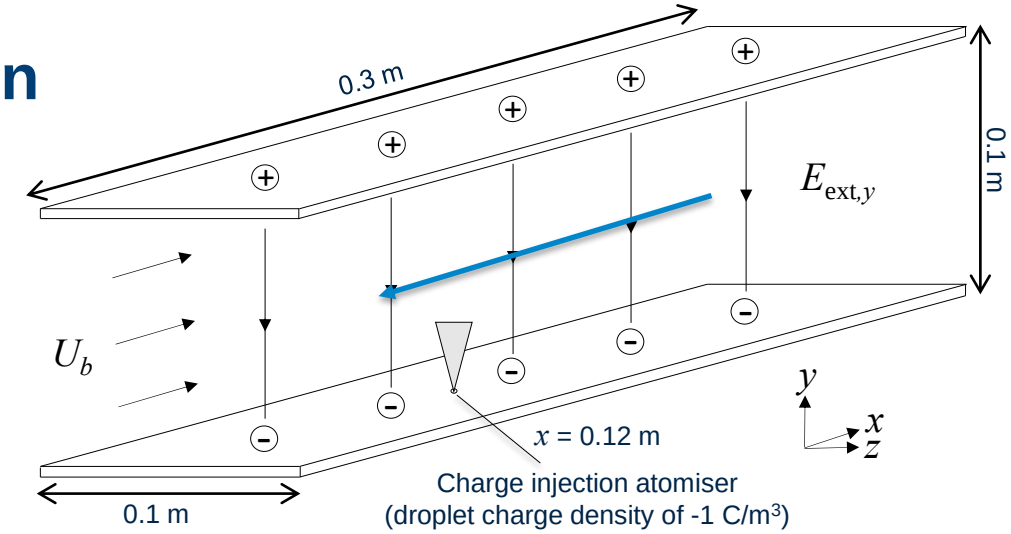


Electrospray in cross flow

- Modulate the trajectories of charged droplets in a bulk flow using external electrostatic fields.
- Increase the effective time available for droplet evaporation over a finite-length mixing region.
- Control the location of fuel vapour release – a concept introduced here as *‘targeted evaporation’.*

Hypothetical configuration

- ‘Electrospray in cross-flow’
- Air at atmospheric pressure
- Charged kerosene droplets w/ initial temperature of 300 K
- 3×10^6 mesh points



Case	$T_{g,0}$ [K]	U_b [m/s]	$d_{0,i}$ [μm]	$u_{d,y,0}$ [m/s]	θ_d [°]	$E_{\text{ext}}/E_{\text{ref}}$[1]	Orientation
A	300	2, 20, 80	{5:95}	30	±9	0, 0.1, 1	$\pm E_{\text{ext},y}$
B	700	10	50	10	0	0, 2	$E_{\text{ext},x}$

[1] E_{ref} = 1×10^6 V/m < Electrical breakdown of air (~ 3×10^6 V/m)

Numerical method

- Large eddy simulation (LES) with Eulerian-Lagrangian formulation
- Based on open-source CFD software package OpenFOAM
- Rapid mixing model[1] for droplet evaporation (secondary breakup neglected)
- Electrostatic forces computed in the Eulerian framework[2]
- Net charge of each droplet considered constant throughout lifetime[3]

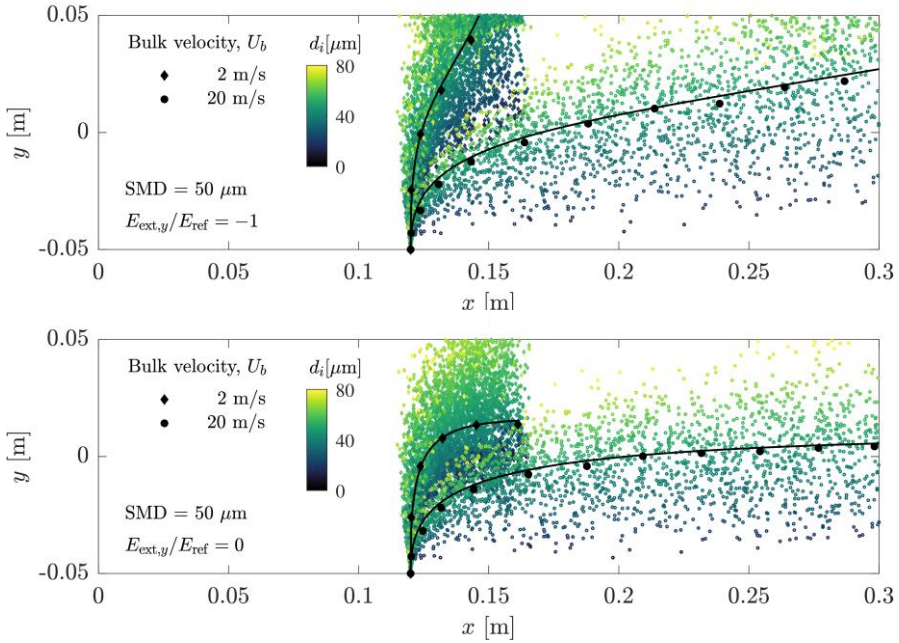
[1]Miller et al., International Journal of Multiphase Flow 24 (1998), 1025-1055.

[2]Weiand and Giusti, International Journal of Spray and Combustion Dynamics (2021), In review.

[3]Doyle et al., Journal of Colloid Science 19 (1964), 136-143.

Case A – Droplet trajectories

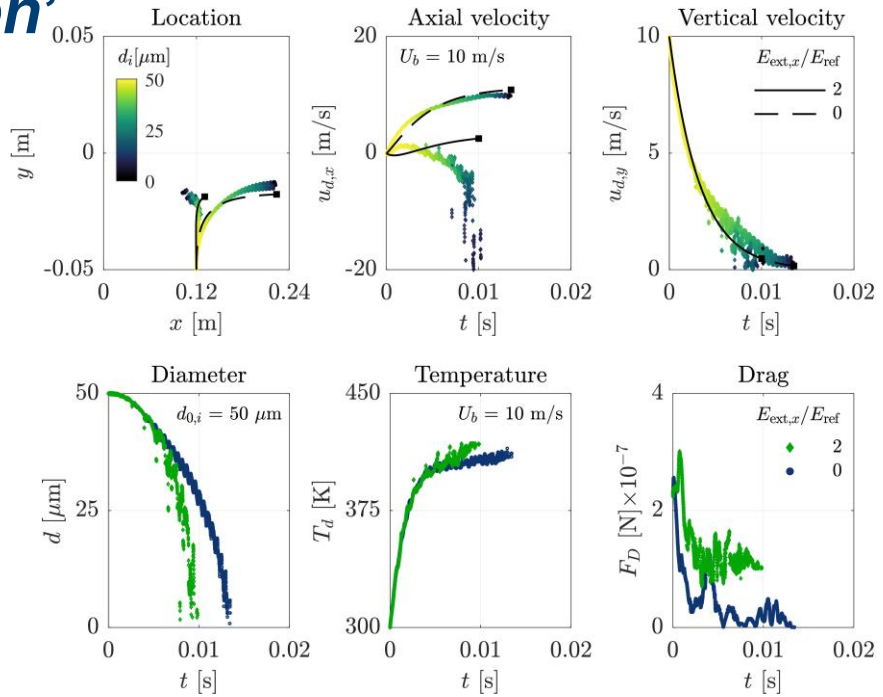
- *Symbols:* droplet bin-averages
- *Lines:* 2D analytical model based on drag and electrostatic forces
- *Setup:* el. field in the negative vertical direction (top figure only)
- *Conclusion:* mean droplet trajectories affected by el. forces



Fredrich, Weiand, and Giusti, J. Multiphase Flow, submitted

Case B -‘*Targeted evaporation*’

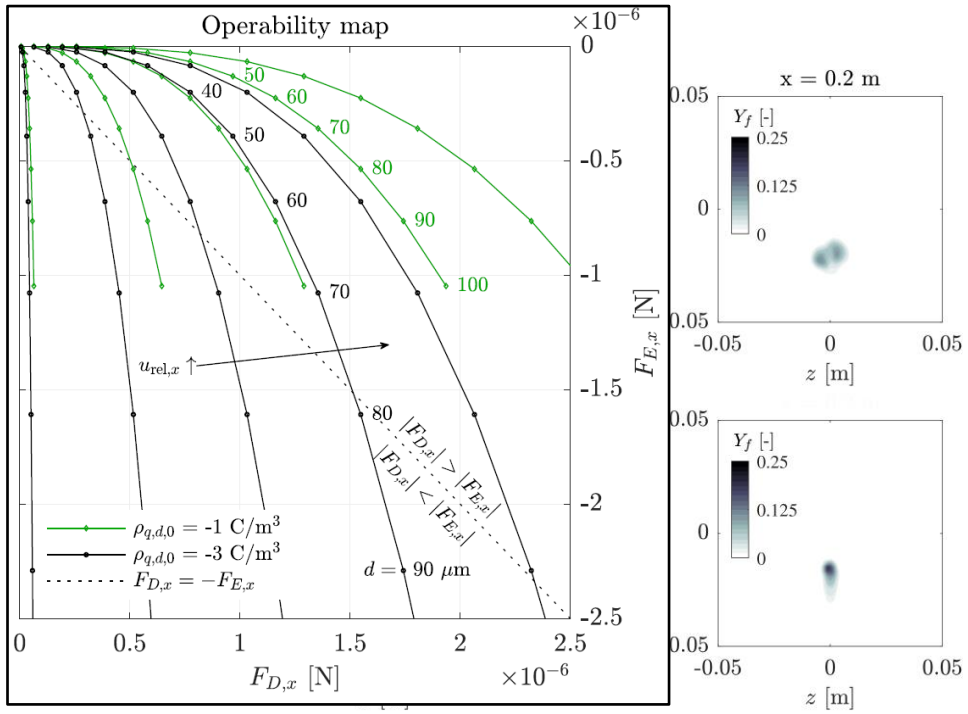
- Localised fuel vapour release
- Repulsion forces promote droplet separation and dispersion
- Quicker evaporation (-30%) due to higher droplet *Re* number (increased relative velocity)



Fredrich, Weiand, and Giusti, J. Multiphase Flow, submitted

‘*Targeted evaporation*’

- Enhanced mixing due to higher turbulence intensity in the continuous phase
- Smaller fuel vapour gradients downstream (more homogeneous mixture)



Fredrich, Weiand, and Giusti, J. Multiphase Flow, submitted

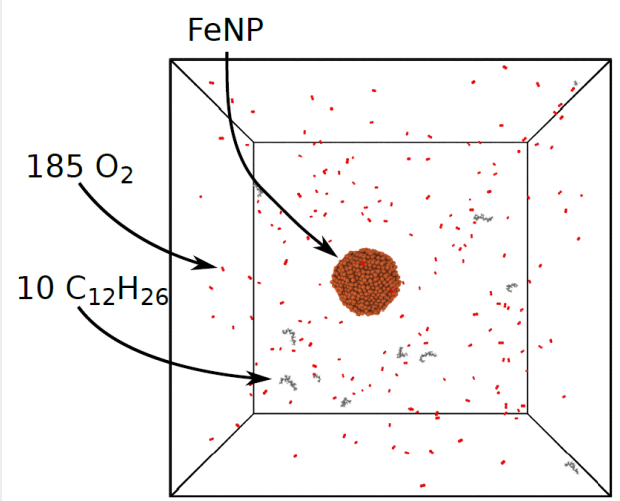
Chemical kinetics in nanofuel combustion

- The effect of electrostatic fields on combustion is mainly understood in terms of “ionic wind”
- Is there any direct effect on the chemistry?
  - Collision frequency: change of kinetic energy of ions and polarised molecules
  - Activation energy: change of the energy barriers

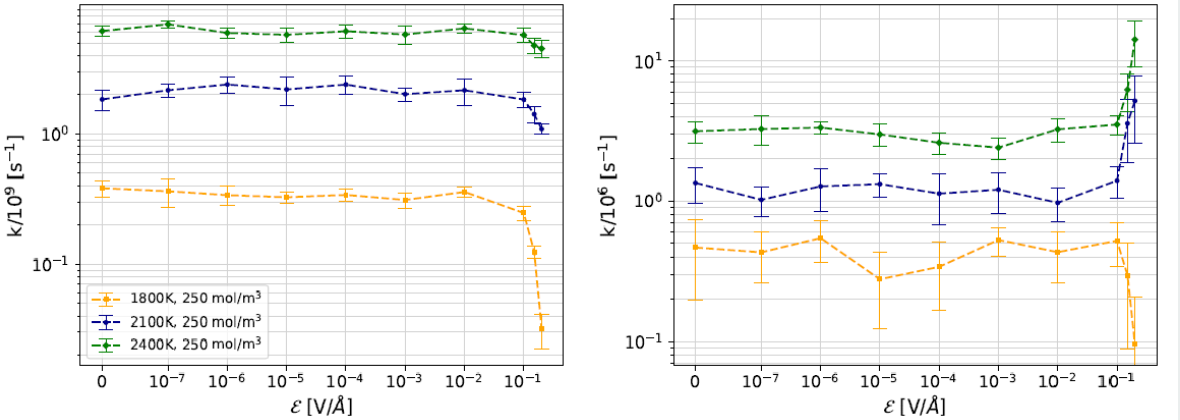
- Focus: local charge transfers due to close interactions

Configuration and numerical methods

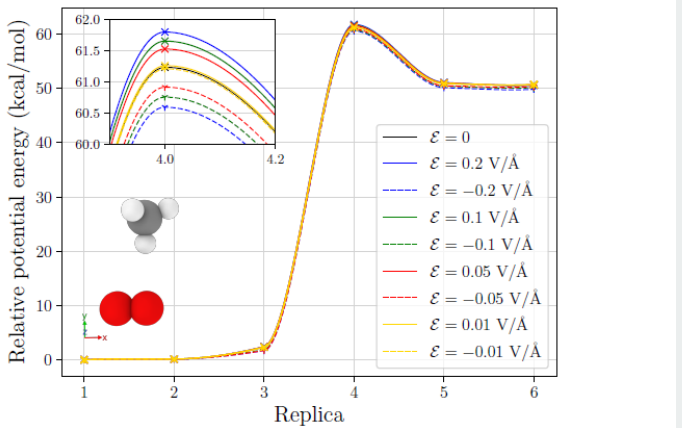
- Study of molecular interactions at nanoscale level
- ReaxFF force fields (tuned from QM computations)
- Qeq and QTPIE charge equilibration methods
- NVT and NVE ensemble simulations
- Amorphous FeNP, diameter 4 nm
- Ambient conditions:
  - Temperature: 1600 – 2400 K
  - Initial pressure: 5 – 40 atm



What is the effect of EF on n-dodecane combustion?



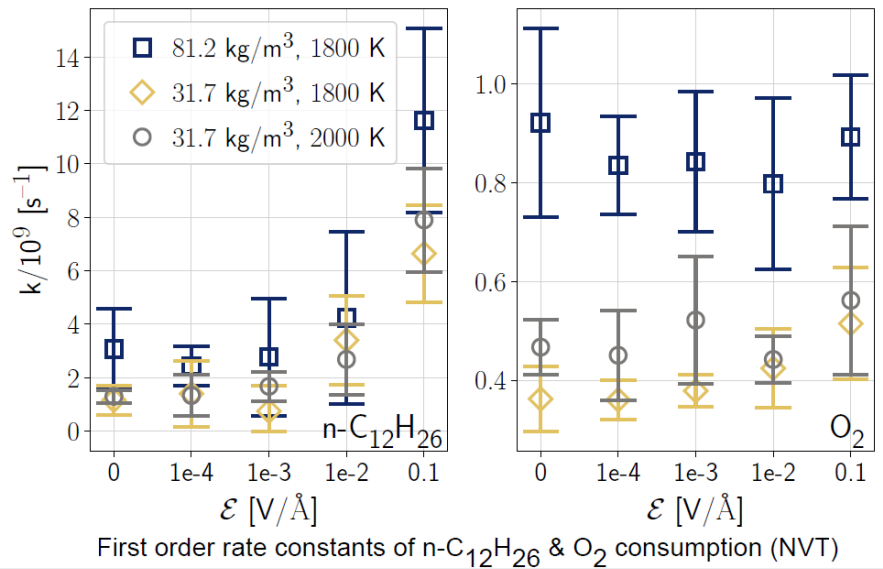
n-$C_{12}H_{26}$ (left) and O_2 (right) consumption rates



Minimum energy path of $CH_4 + O_2 \rightarrow CH_3 + HO_2$

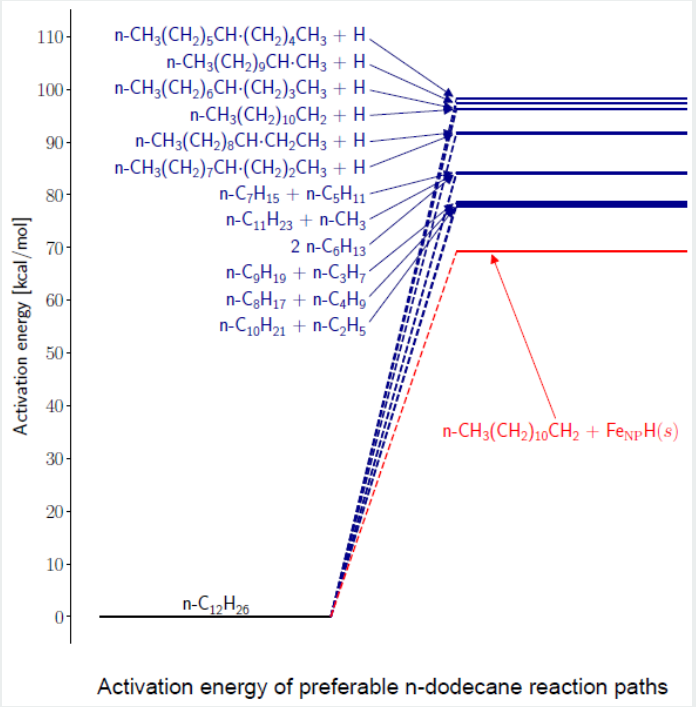
Kritikos and Giusti, Comb. Flame, 2022

What is the effect of NP addition?



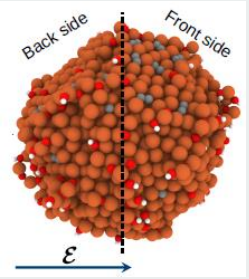
First order rate constants of n-$C_{12}H_{26}$ & O_2 consumption (NVT)

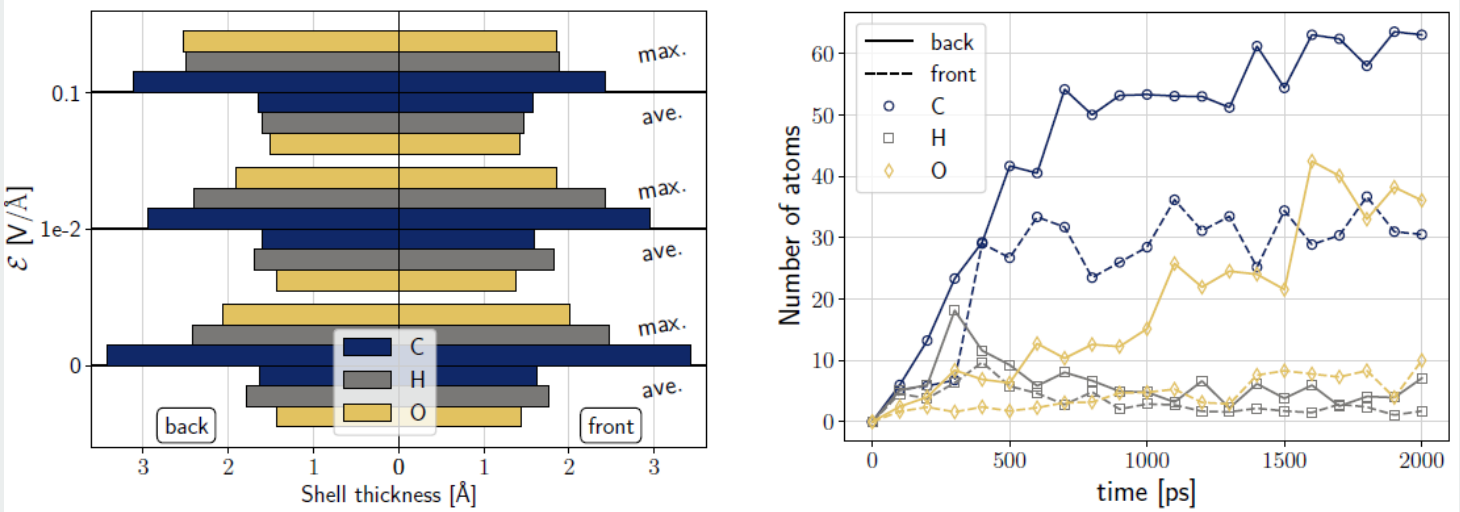
Kritikos and Giusti, Proc. Combust. Inst., 2023



Activation energy of preferable n-dodecane reaction paths

What is the effect of EF on NP combustion?





Shell thickness (top) and number of adsorbed atoms at 0.1 V/Å (bottom) at 31.7 kg/m^3 and 1800 K (NVT ensemble)

Kritikos and Giusti, Proc. Combust. Inst., 2023

Main takeaway

Interactions at the nanoscale level have the potential of opening up a wide range of new technologies to deliver tailored reacting flows

Acknowledgements

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Any questions?