噴霧の微粒化・燃焼初期過程の詳細解析および実用シミュレーションへの展望

新城淳史

JAXA数値解析グループ

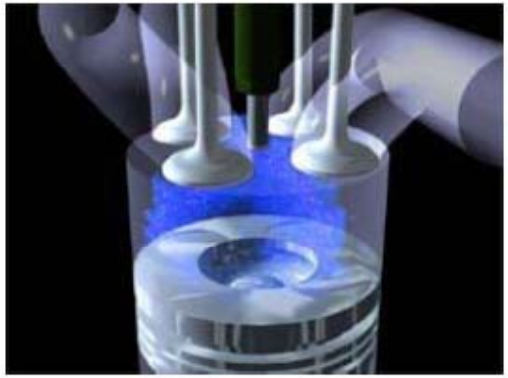
燃焼・乱流セクション

Jul 13, 2012

Background

- Liquid sprays for various engineering applications
  - Our main interest is in liquid-fuel engines

Rocket engine



Automotive engine

Jet engine

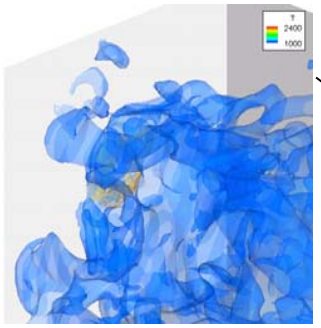
  - Others..

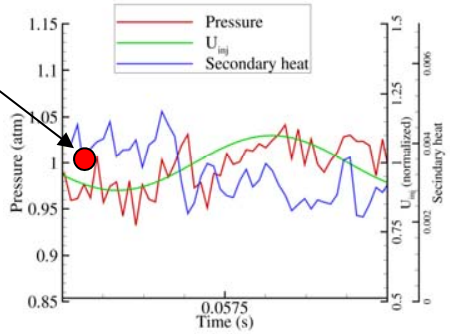
Spray

Agriculture

Recent research topics

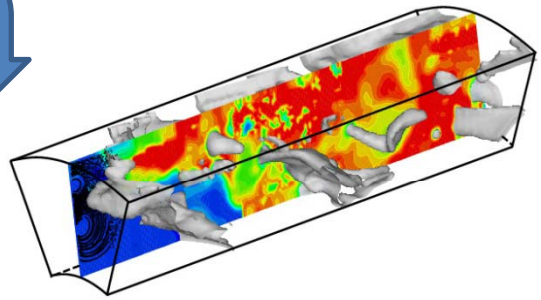
Combustion instability and control
(lean premixed CH_4 swirl combustor)





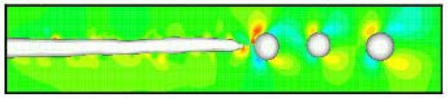
Tachibana et al., PCI 2007; Shinjo et al., CNF 2007

Shift from gas fuel to liquid fuel
for real engine applications

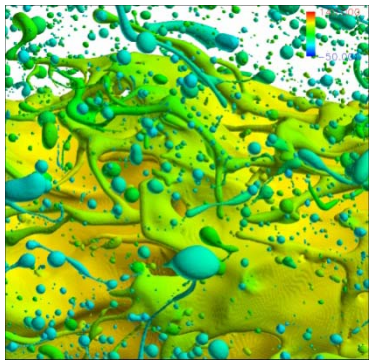


Spray combustion simulation
We still have many issues (physical mechanisms and modeling)!

Liquid atomization physics



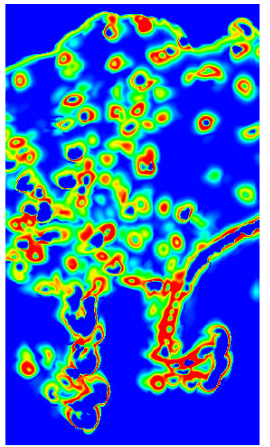
Rayleigh breakup



Turbulent atomization

Shinjo & Umemura, IJMF 2010, 2011, PCI 2011

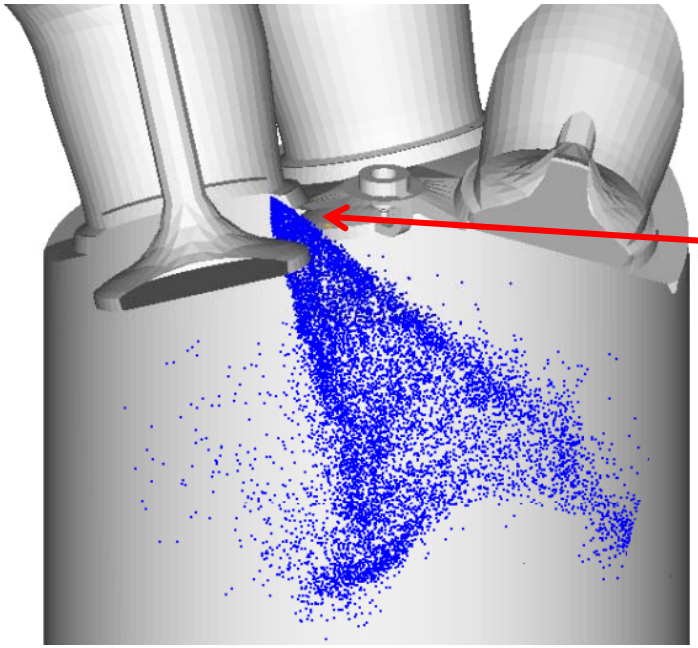
Spray combustion physics



Group combustion

Shinjo & Umemura, PCI (in press)

Spray simulation issues



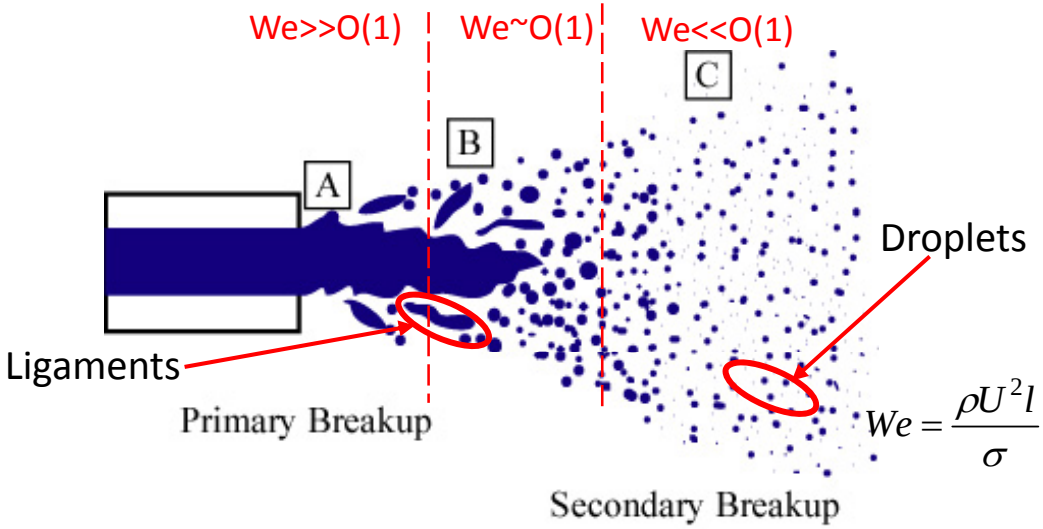
© Convergent Science

Primary atomization region

The incoming boundary of spray simulation
-cannot be resolved easily
-cannot be treated in the Lagrangian way

However, good models are not available now

Physical mechanisms should be understood for modeling



1. Liquid atomization study

- High-speed Diesel-like fuel injection -

Objectives and approach

- Investigate the primary breakup mechanisms
- Obtain modeling insight

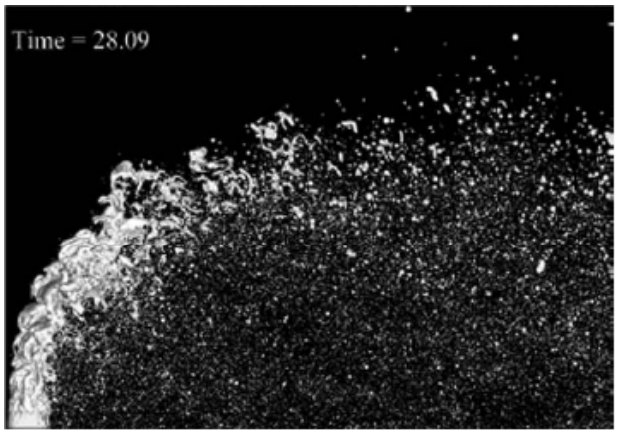
- Very detailed numerical simulation is used
  - No breakup model is employed
- Navier-Stokes eqs. + surface tension
  - Direct interface capturing by level-set/VOF method
  - Surface tension by CSF method

Recent primary atomization research

– High resolution data are becoming available to understand the underlying physics

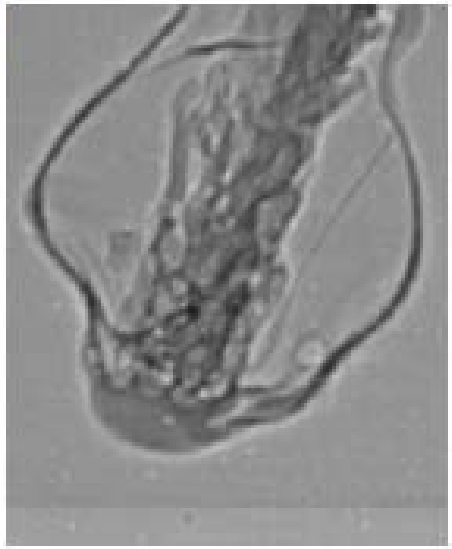
Simulation

(d) $q = 30, We_{cf} = 100, We_{liq} = 3000$



Liquid jet simulation in cross flow
(Left: Pai et al. 2008, right: Herrmann 2010)

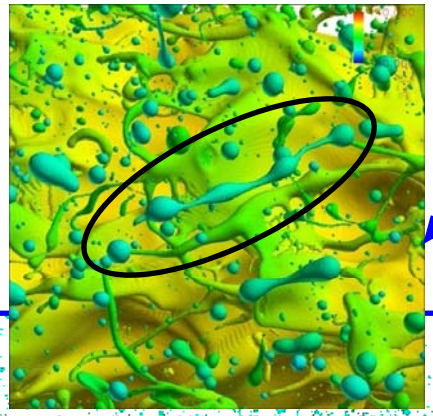
Experiment

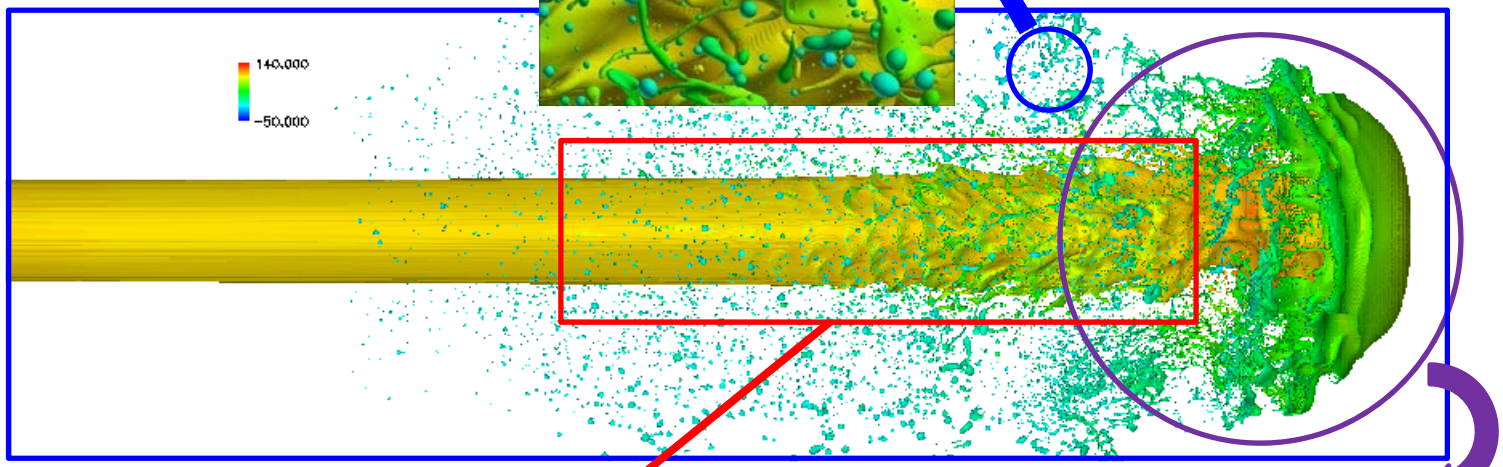


Exp photo of spray front
(Wang et al. 2008)

Our simulation of Diesel-like jet

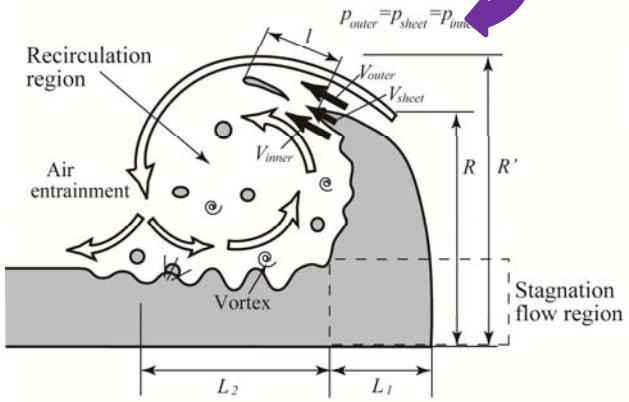
Overall characteristics and ligament/droplet dynamics (Shinjo & Umemura, IJMF 2010)





Surface instability development and atomization (Shinjo & Umemura, IJMF 2011)

Role of jet head (Shinjo & Umemura, PCI 2011)



Numerical methods

- Euler-Euler two-phase flow
  - 3D Navier-Stokes equations
    - Gas and liquid are Newtonian fluids
  - Pressure by Poisson equation
  - Advection by CIP method
  - Interface capturing by Level-Set method with MARS (VOF) method
  - Surface tension by CSF method

Flow conditions

- Liquid jet from a round nozzle
  - Three injection velocities
    - No excitation at the nozzle is given to exclude nozzle effects such as cavitation or liquid flow turbulence.

    = Atomization is initiated from jet front only

Case	Nozzle diameter $D=2a$	Ambient pressure p	Gas density ρ_g	Liquid density ρ_l	Liquid viscosity μ_l	Surface tension coefficient σ	Liquid velocity $U_l=U$	Gas velocity U_g	Bulk liquid Reynolds number	Bulk liquid Weber number
1	0.1mm	3MPa	34.5kg/m^3	848kg/m^3	2870e-6 Pa·s	30.0e-3 N/m	30m/s	0m/s	440	1270
2							50m/s		740	3530
3							100m/s		1470	14100
4					957e-6 Pa·s				4410	

$$Re_{bulk} = \rho U a / \mu \qquad We_{bulk} = \rho U^2 a / \sigma$$

Computational resources

- Liquid jet from a round nozzle (D=0.1mm)
  - JAXA JSS system

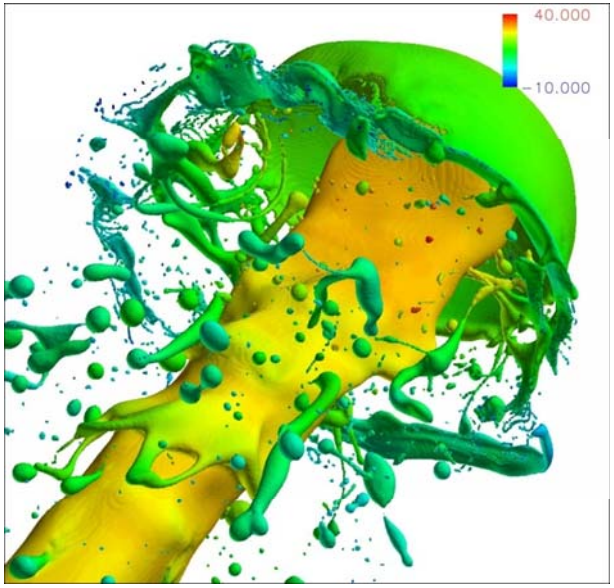
Case	# of grid points	Spatial resolution	# of CPUs (# of cores)	Computational time (Real clock time)
1	0.4 billion	1.5μm	320 (1280)	750hrs
2	1.2 billion	0.75μm	480 (1920)	700hrs
3	6 billion	0.35μm	1440 (5760)	400hrs
4	6 billion	0.35μm	640 (2560)	1100hrs

One of the world's largest computations at this time in this field.

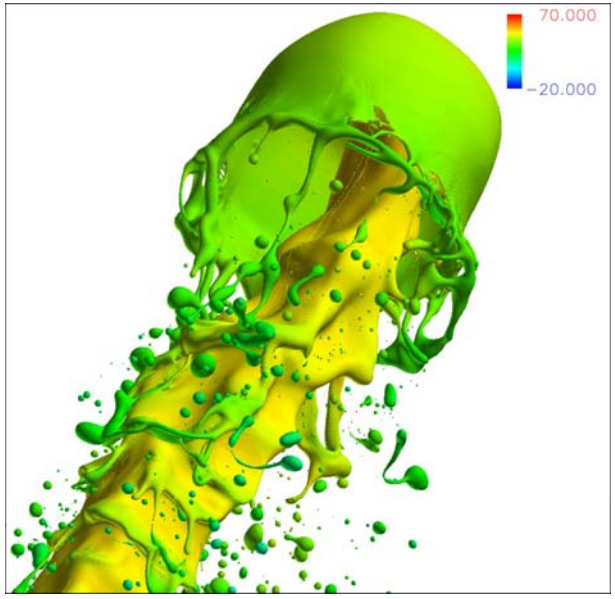
(1) Overview

– Ligament/droplet scale

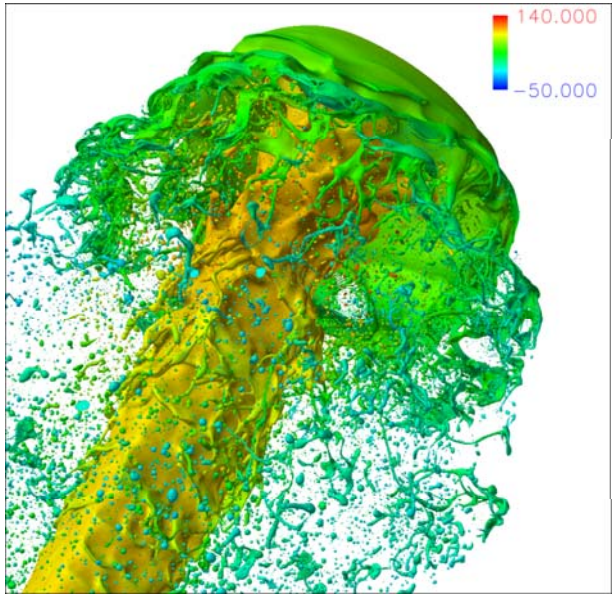
- As the liquid Weber number increases, generated structures get smaller



Case 1 (30m/s)



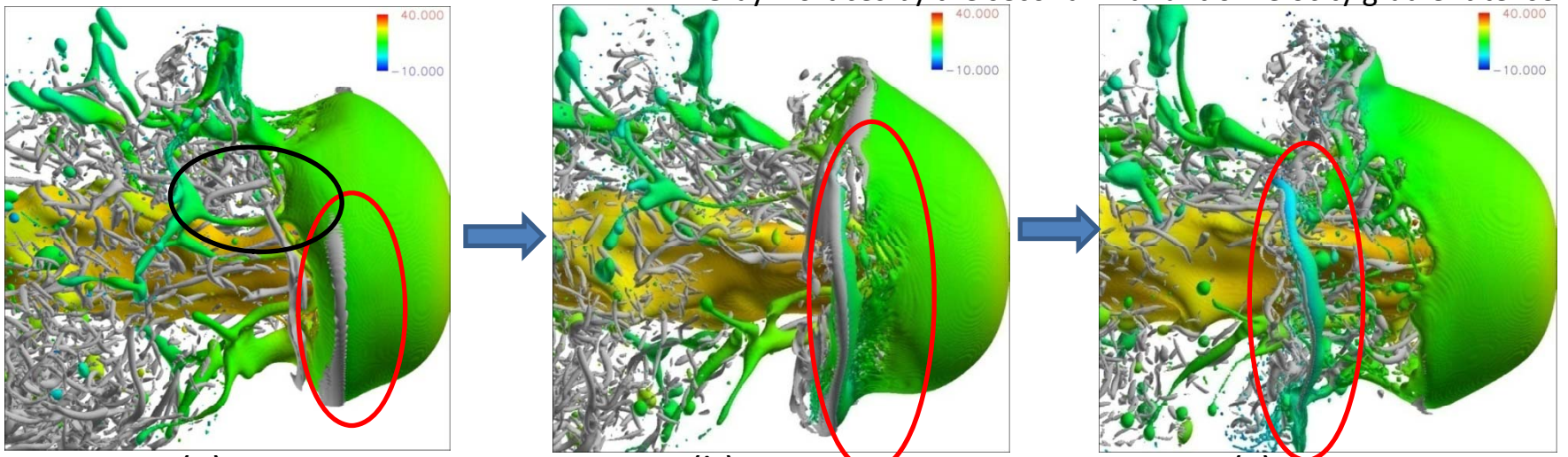
Case 2 (50m/s)



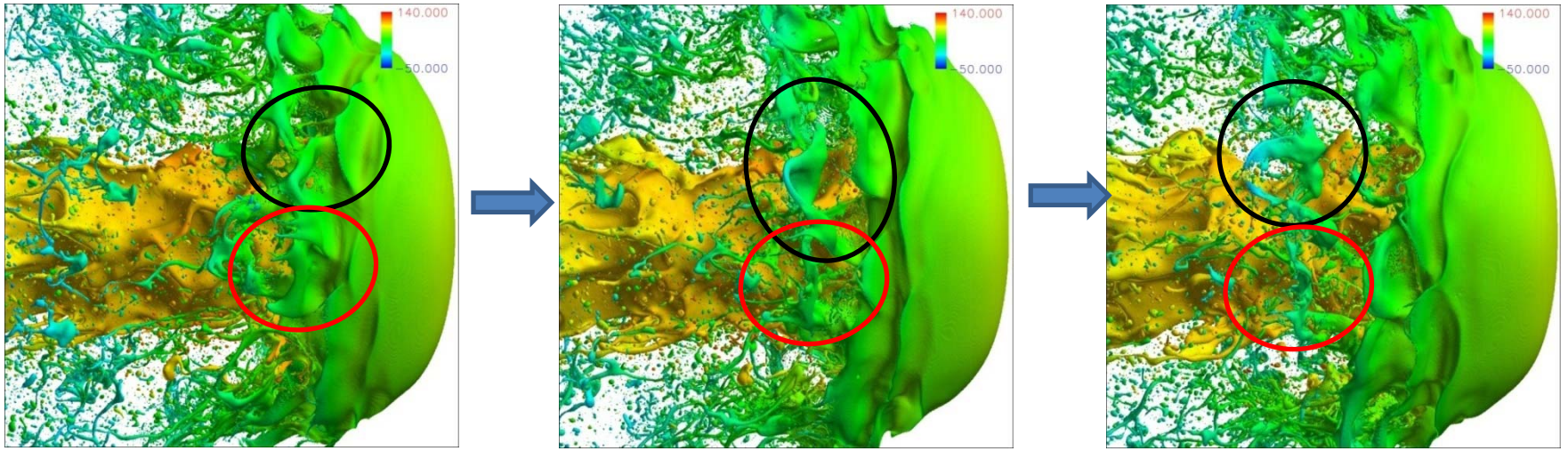
Case 3 (100m/s)

Ligament formation from front

Gray: vortices by the second invariant of velocity gradient tensor



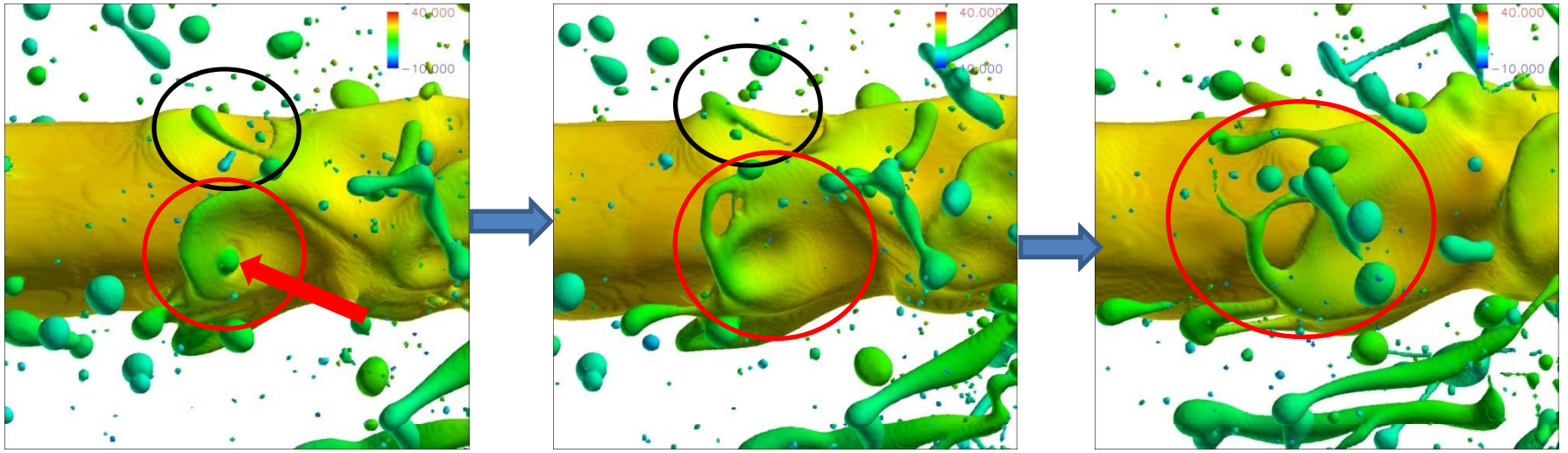
Case 1 (a) t=18.27 (b) t=19.67 (c) t=21.07



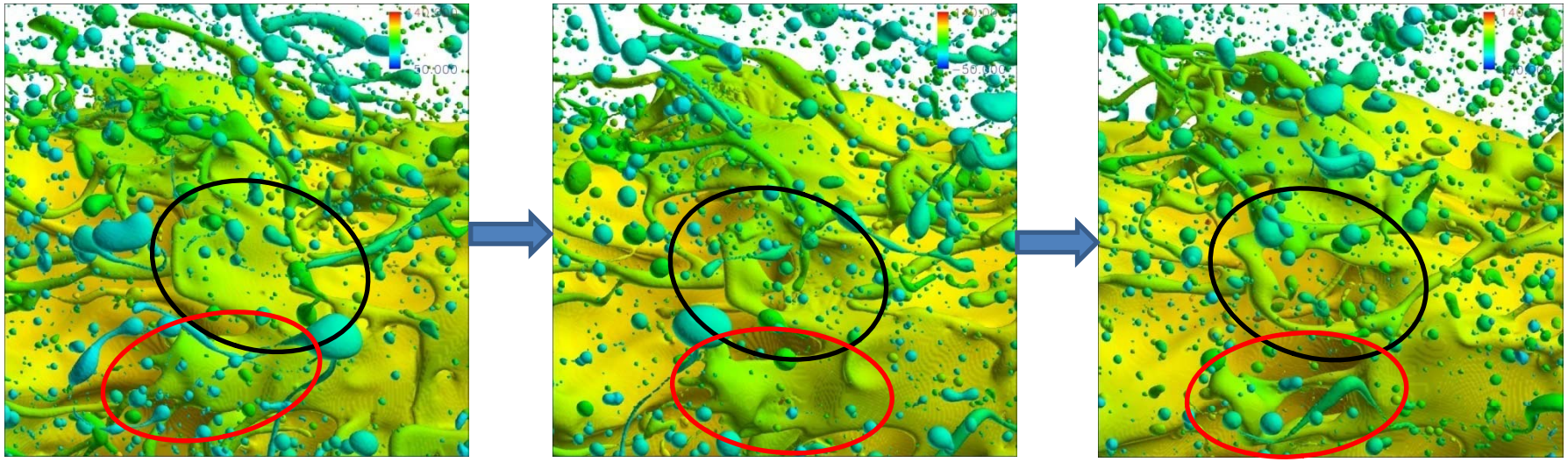
Case 3 (a) t=14.39 (b) t=15.11 (c) t=15.83

Roll-up vortices (circumferential and lateral) create ligaments.

Ligament formation from jet core



Case 1 (a) t=18.97 (b) t=19.67 (c) t=21.07

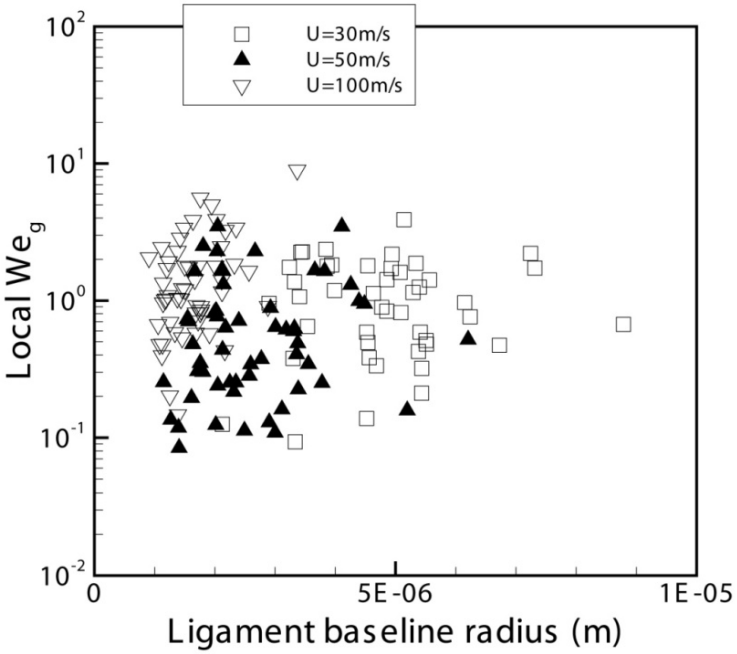


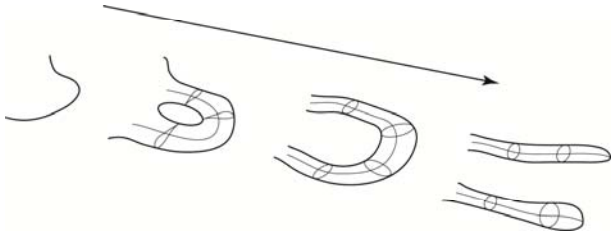
Case 3 (a) t=15.76 (b) t=16.33 (c) t=16.91

Flat crests break into multiple ligaments.

Ligament formation

- From spray front
  - Circumferential and lateral vortices create ligaments formation
- From jet core
  - A hole forms on crest structure and multiple ligaments develop.





Ligament condition: We_g~O(1)

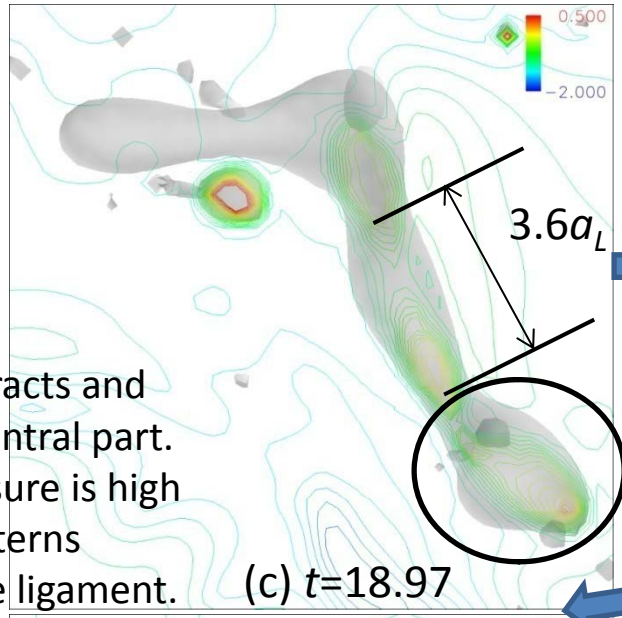
$$We_g = \rho_g \left|\mathbf{u}_l - \mathbf{u}_g\right|^2 a_L \Big/ \sigma$$

a_L: ligament radius

=(Aerodynamic force)/(surface tension)

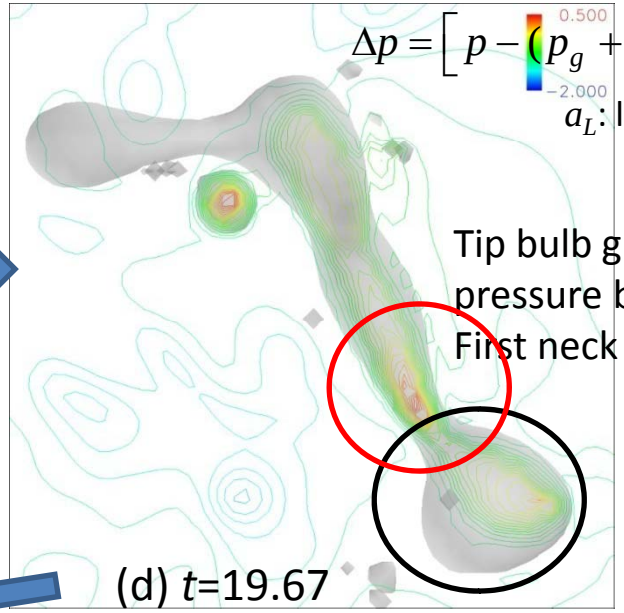
Droplet formation

Case 1



(c) t=18.97

Tip bulb contracts and pushes the central part. Tip bulb pressure is high and wavy patterns appear on the ligament.

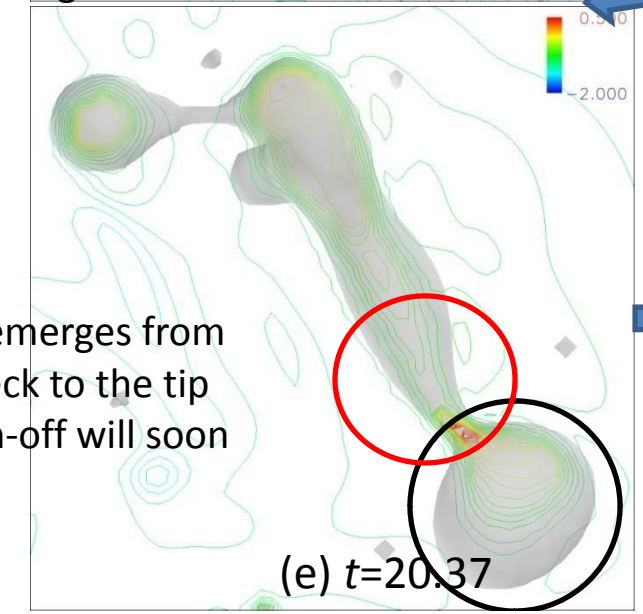


$$\Delta p = \left[p - (p_g + \sigma / a_L) \right] / (\sigma / a_L)$$

a_L: ligament radius

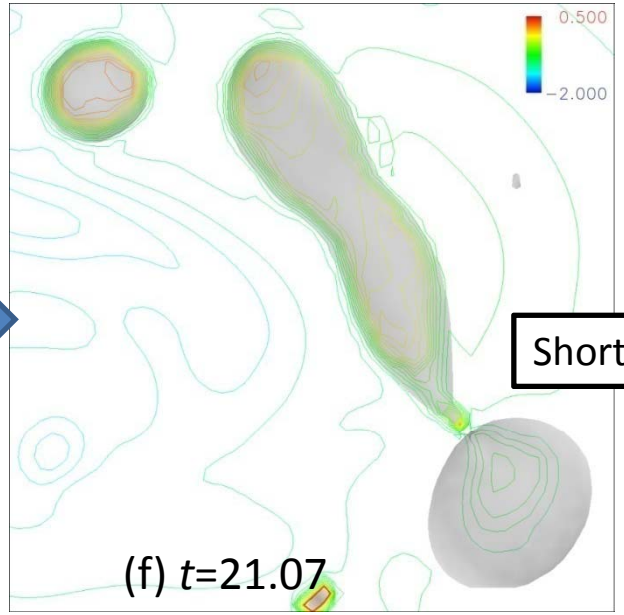
Tip bulb grows and the pressure becomes lower. First neck is destabilized.

(d) t=19.67



Liquid jet emerges from the first neck to the tip bulb. Pinch-off will soon follow.

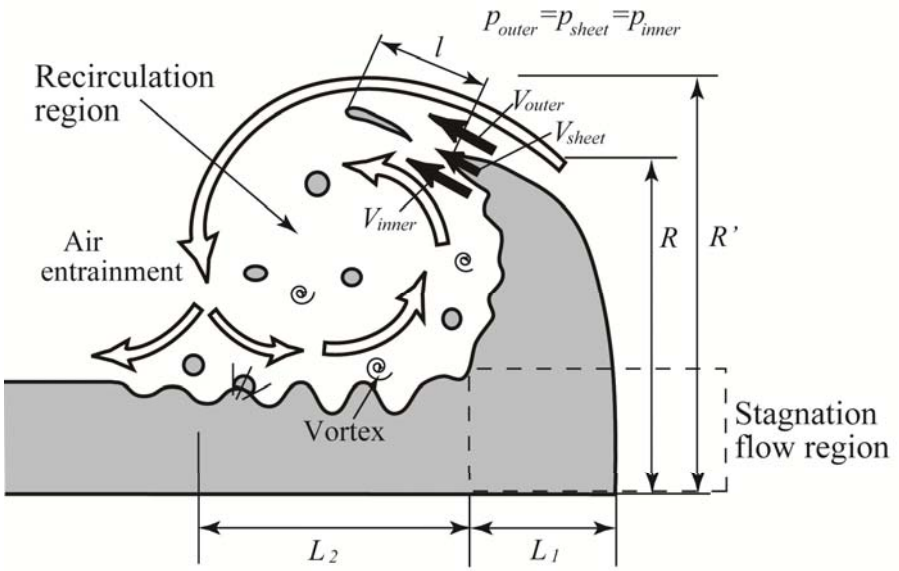
(e) t=20.37

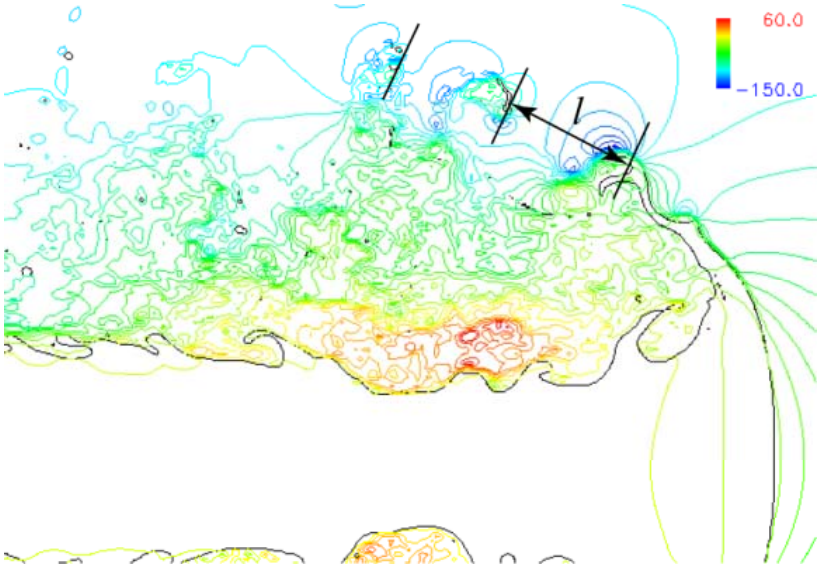


Short-wave mode

(f) t=21.07

(2) Head atomization loop





From theoretical consideration,

$$l = [(V_{outer(inner)} + V_{sheet})/2]\tau$$

$$(V_{sheet} - U_c)\tau = \left(V_{sheet} - \sqrt{\sigma/\rho_l a_{sheet}}\right)\tau = \lambda$$

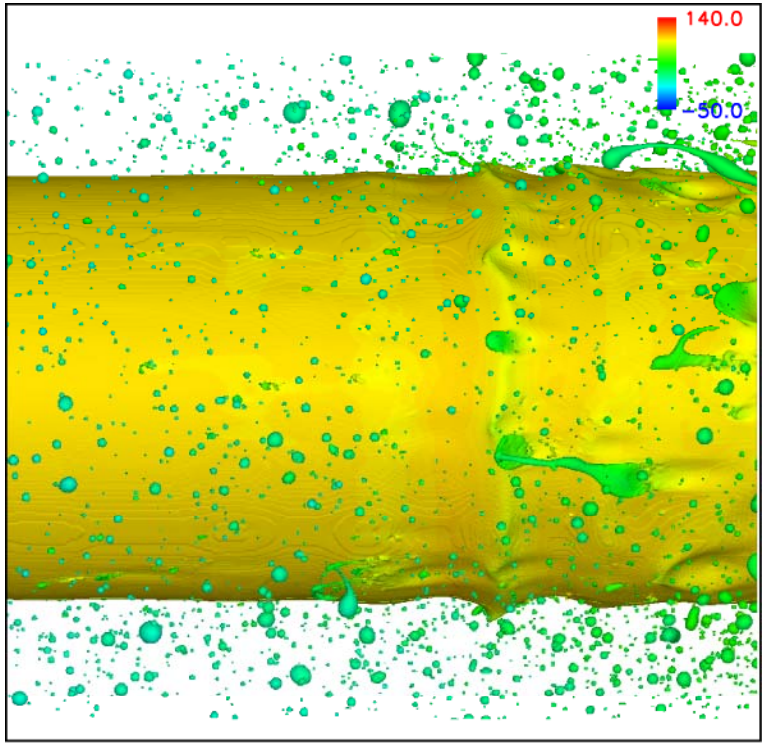
CFD result satisfies the above relations

$$\hat{V}_{outer(inner)} = 1.0, \quad \hat{V}_{sheet} = 0.5,$$
$$\hat{\lambda} = 0.37, \quad l = 0.6, \quad a_{sheet} = 0.04,$$
$$\hat{\tau} = 0.8$$

V_*: Edge velocity (fixed on spray front)
a_{sheet}: Thickness at edge
l: Spatial interval
σ: Surface tension
λ: Wavelength on edge
R: Edge radius
L_2: Recirculation zone length
τ: Time interval of atomization

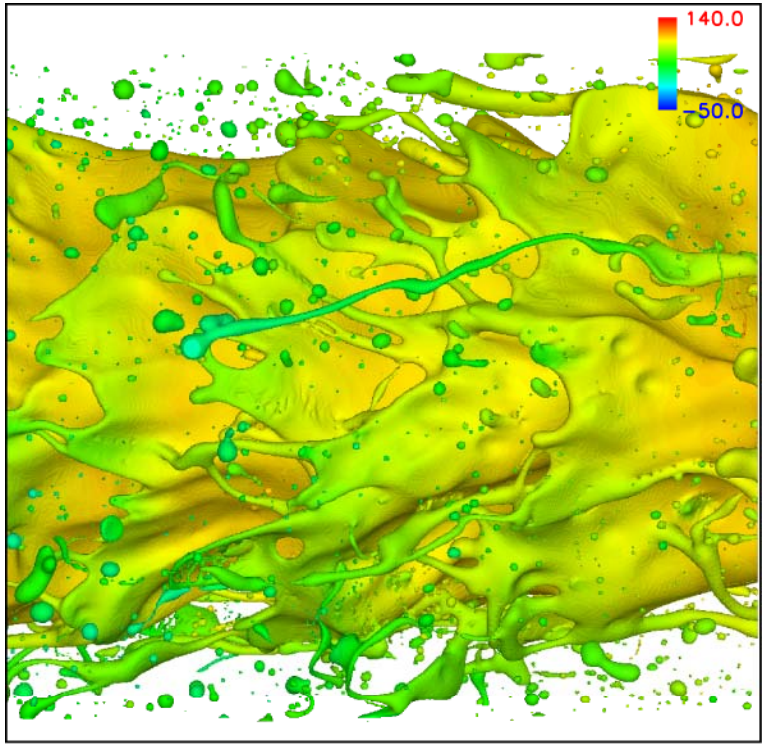
(3) Liquid core surface instability

- High-speed liquid jet



U=100m/s, t=8.27

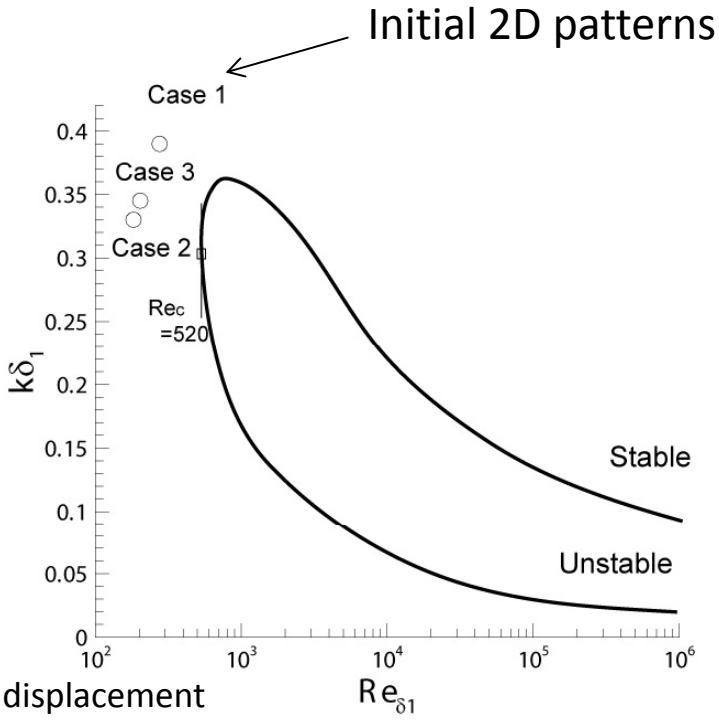
2D (axi-symmetric) patterns



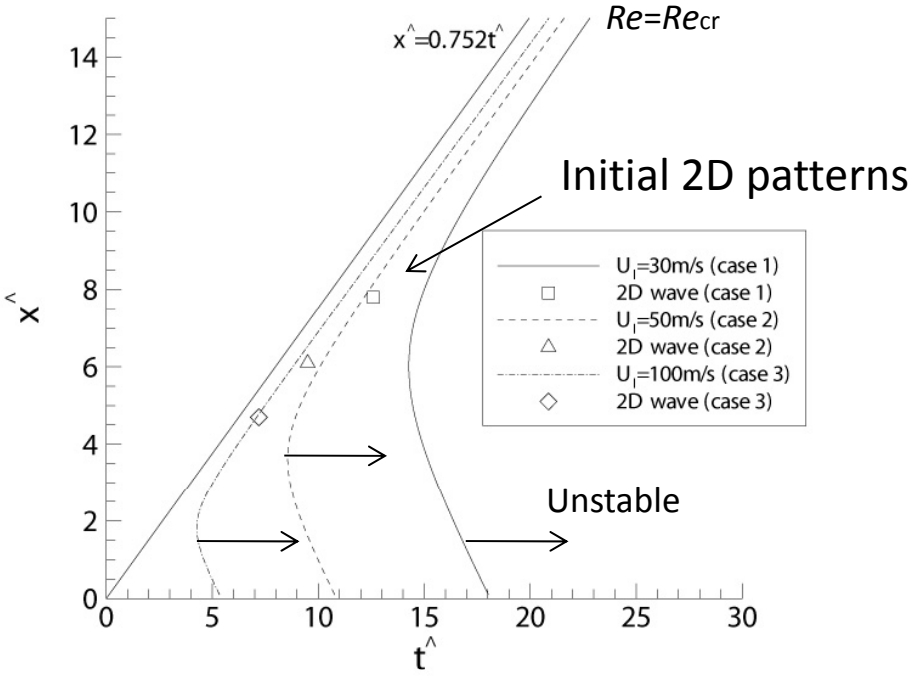
U=100m/s, t=15.47

3D patterns

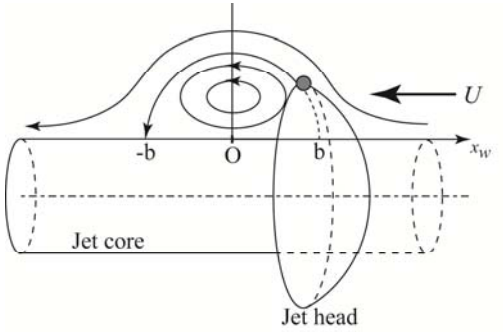
Initial 2D patterns and TS mode



δ_1: displacement thickness



<u>Without jet head wake effect</u>



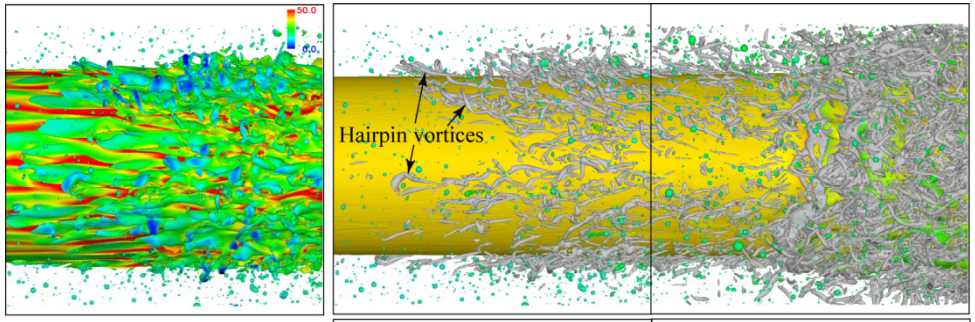
<u>With jet head wake effect modification</u>

$$\delta = K\sqrt{\nu\int_0^x \frac{dx}{U\left[1-\left(b/x'\right)^2\right]}}$$

$$Re_\delta = K\sqrt{\frac{U}{\nu}}\left[1-\left(\frac{b}{Ut-b-x}\right)^2\right]\sqrt{x-\frac{1}{2}b\ln\left(\frac{Ut-2b-x}{Ut-2b}\cdot\frac{Ut}{Ut-x}\right)+Ut}$$

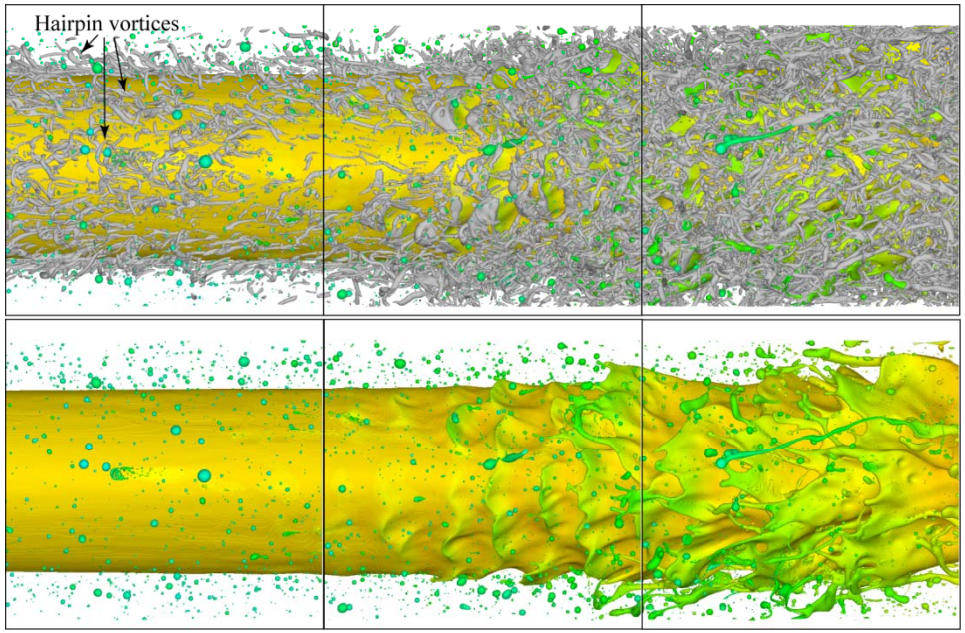
The results suggest that the <u>initial</u> 2D surface patterns are generated by TS waves.

Vortex structures



Streaks by velocity

t=11.33



t=15.47

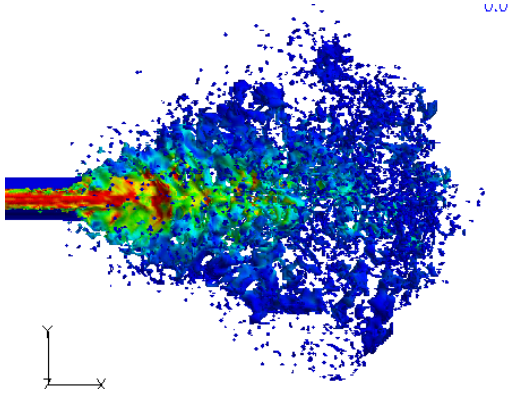
Similar to wall turbulence transition!

*True especially for high-speed liquid injection

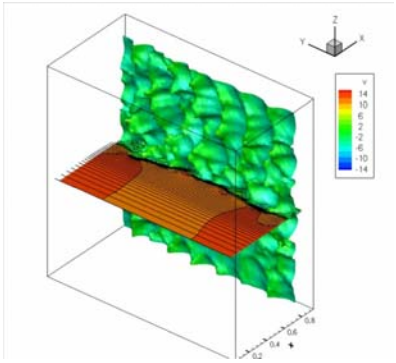
Summary of study 1

- High-speed liquid fuel injection
  - Atomization characteristics and mechanisms identified in this configuration
  - Modeling study underway

  - Investigation of sprays of other configurations
    - Impingement injector, wind wave, air-blast atomizer, etc.



Two-liquid mixing for a rocket-engine injection element



Wind wave simulation

2. Spray combustion study

- Vapor mixing and early flame kernel development -

Background

- Droplets and group combustion

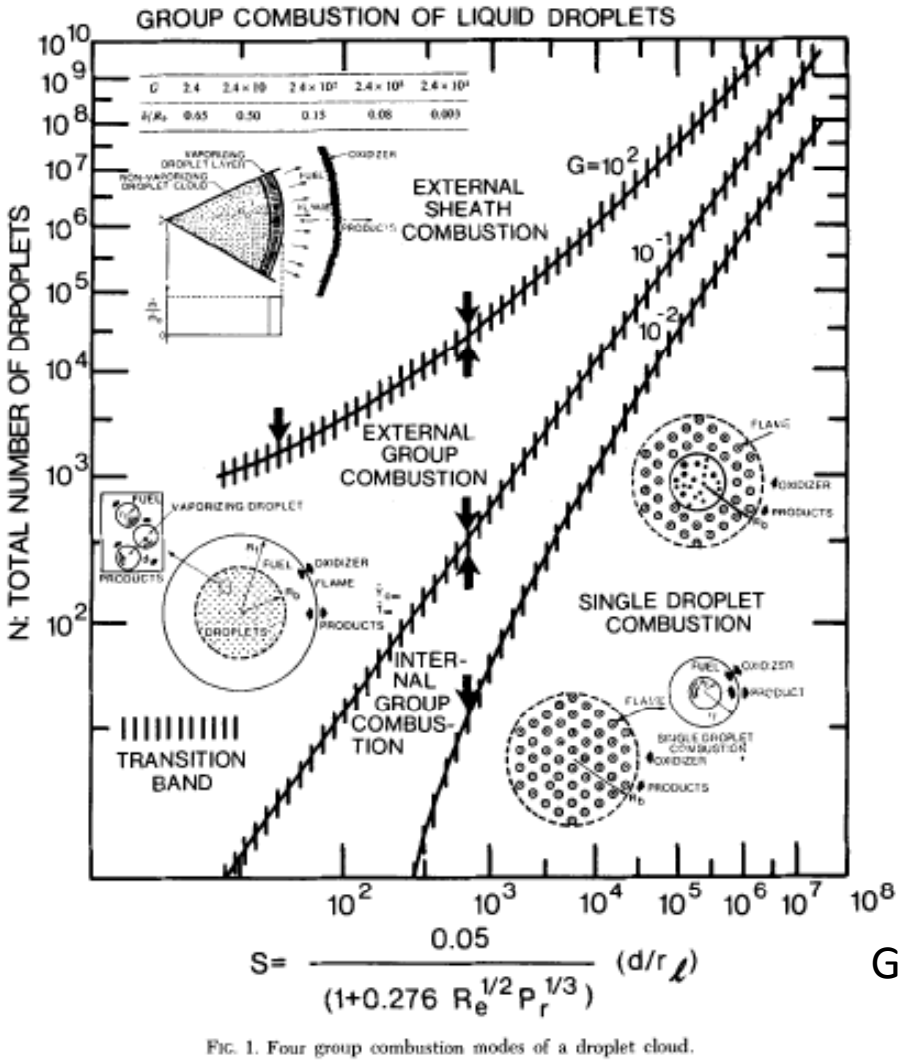


FIG. 1. Four group combustion modes of a droplet cloud.

- Single droplet combustion
- Internal group combustion
- External group combustion
- External sheath combustion

- In real sprays, however, the combustion mode is not well understood.

Group combustion diagram by Chiu (PCI 1982)

Previous work in the literature

- Eulerian-Lagrangian simulation
  - Turbulence scale >> droplet scale

Fig. 1. Initial gas velocity vectors and distribution of droplet locations (only 5% of the velocity vectors are shown for clarity).

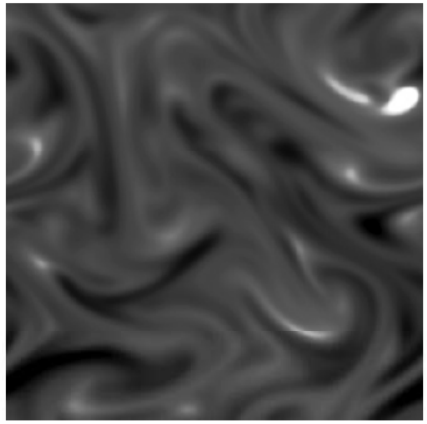


Fig. 2. Temperature contour at $t = 0.891$ ms for the $T = 1300$ K case (black = 1300 K; white = 2000 K).

Wang & Rutland (PCI 2005)

- Gas-phase autoignition
  - Ignition occurs at small SDR

Viggiano (CNF 2010)

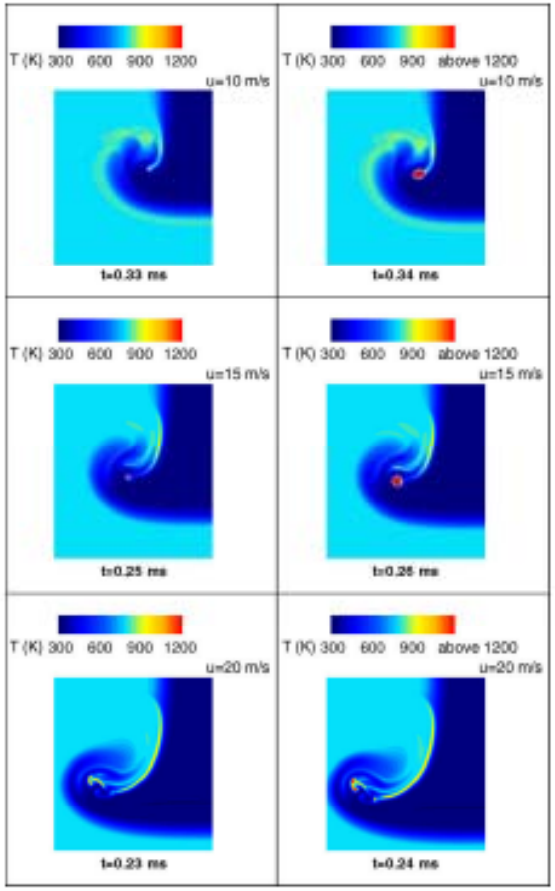
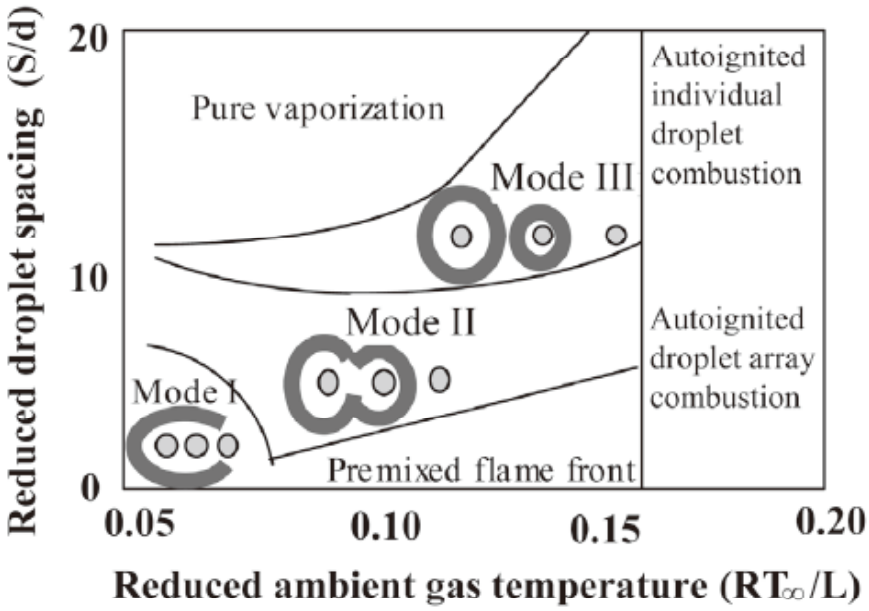


Fig. 12. Temperature fields by using the 30-step mechanism and different values of fuel stream velocity, in the case T_o = 800 K and T_f = 300 K, at the times when T_{max} is equal to 1200 K (on the left) and to 1700 K (on the right).

Previous work in the literature

- Simplified droplet array
  - Flame spreading mode analysis



Umemura (J. JSME 2002)

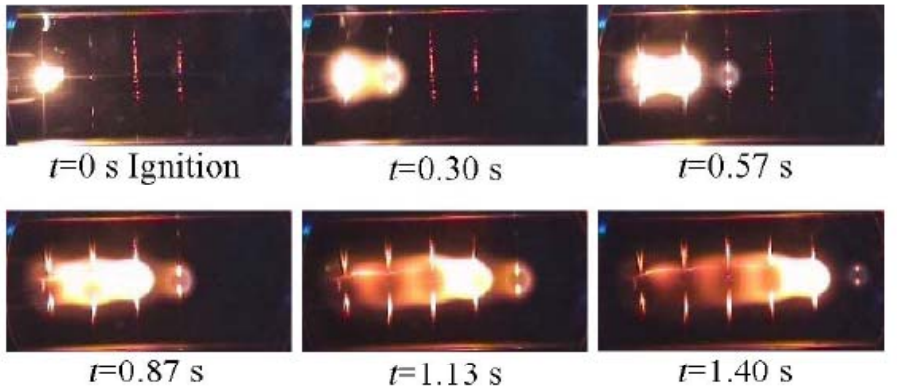


Fig. 8. Flame-spread behavior for $S = 8$ mm and $d_0 = 1.0$ mm at $T_a = 300$ K.

Mikami et al. (CNF 2005)

- Detailed measurement/computation possible
- Gap with the real sprays (scale, turbulence effect, etc.)

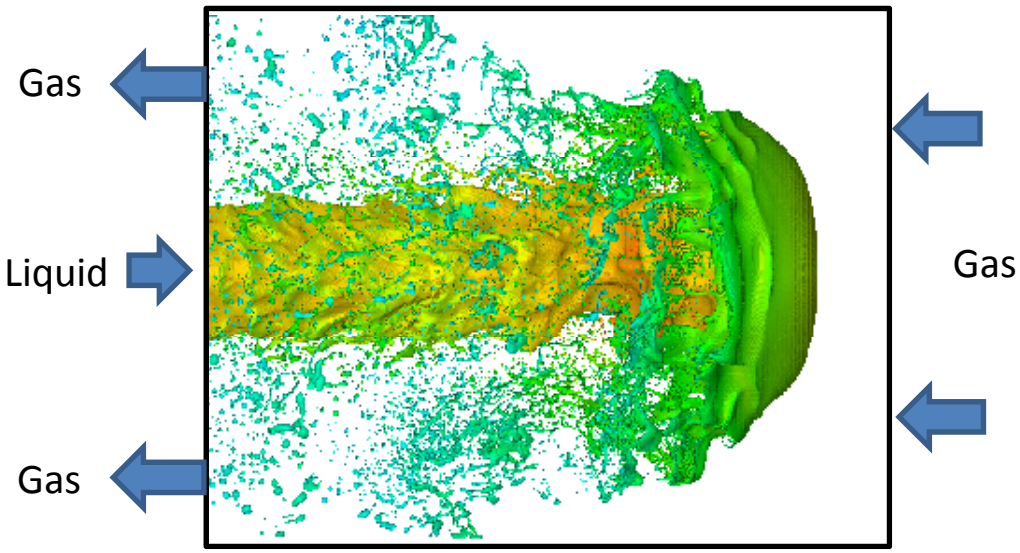
Objectives and approach

- Investigate autoignition of “dense” spray region using the previous droplet atomization data
  - Path leading to group combustion
    - Droplet distribution and number density
    - Gas-phase turbulence
    - Droplet shape effect
  - Find input to modify current models
  - Detailed simulation with evaporation, mixing and reaction
    - Flow field around each droplet is resolved
    - Computational domain is limited to small scale

*J. Shinjo, A. Umemura, *Proc. Combust. Inst.* (in press)

Computational setup

- Domain fixed on the head
  - Small spatial and temporal scales
  - "Flame" cannot be simulated, but early flame kernel development can be captured.



- 900K ambient air from $\hat{t} = 15.47$
- 30atm
- Equilibrium evaporation
- n-heptane (C_7H_{16}) global one-step reaction (Westbrook & Dryer, CST 1981)
- Physical properties from NIST data
- 2.2 billion grid points

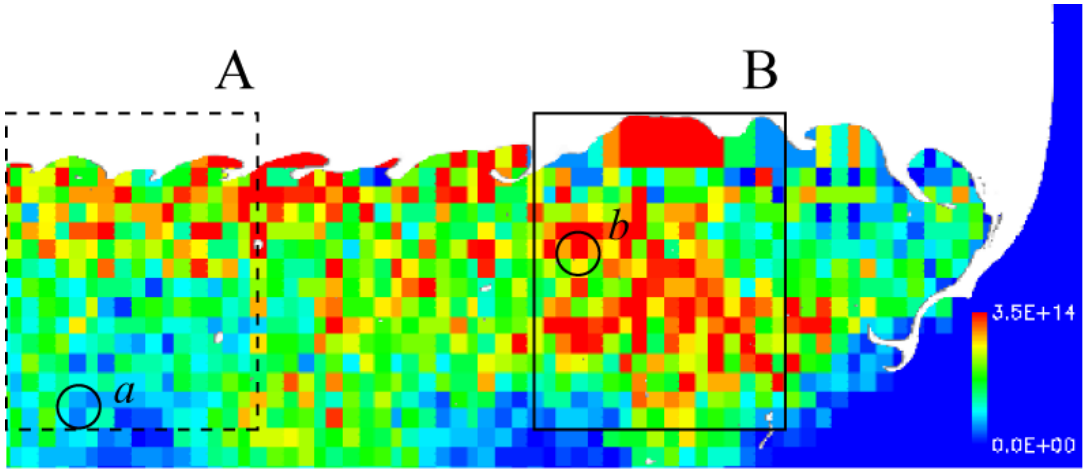
Nozzle diameter D_N	Ambient pressure p	Air density ρ_g	Liquid density ρ_l	Air temperature T_g	Liquid temperature T_l	Liquid injection velocity U_l=U	Air initial velocity U_g	Liquid viscosity μ_l	Air viscosity μ_g	Surface tension coefficient σ
0.1mm	3MPa	11.5kg/m^3	848kg/m^3	900K	300K	100m/s (Lab frame)	0m/s (Lab frame)	2.87e-3 Pa·s	3.90e-5 Pa·s	30.0e-3 N/m

Numerical methods

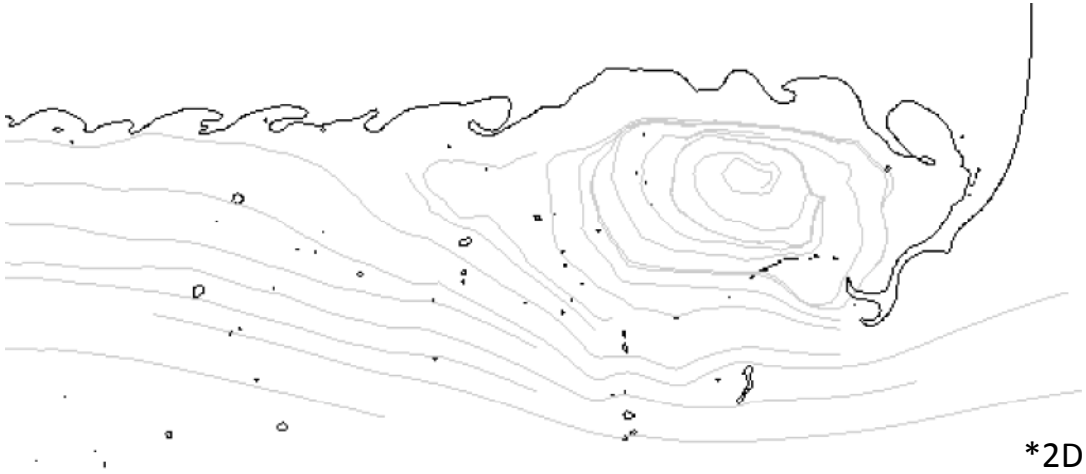
- Navier-Stokes equations
  - Density, velocities, temperature and chemical species
  - Compressibility included (perfect gas equation of state)
  - CIP for advection terms
- Level-set interface capturing
  - Combined with VOF-type method for volume conservation
- Evaporation
  - Equilibrium evaporation
  - Jump condition at interface
- Chemical reaction
  - One-step global reaction of n-heptane

Flow field

- Recirculation zone behind the head

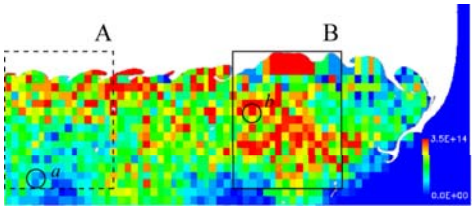


Color: droplet number density (1/m^3)

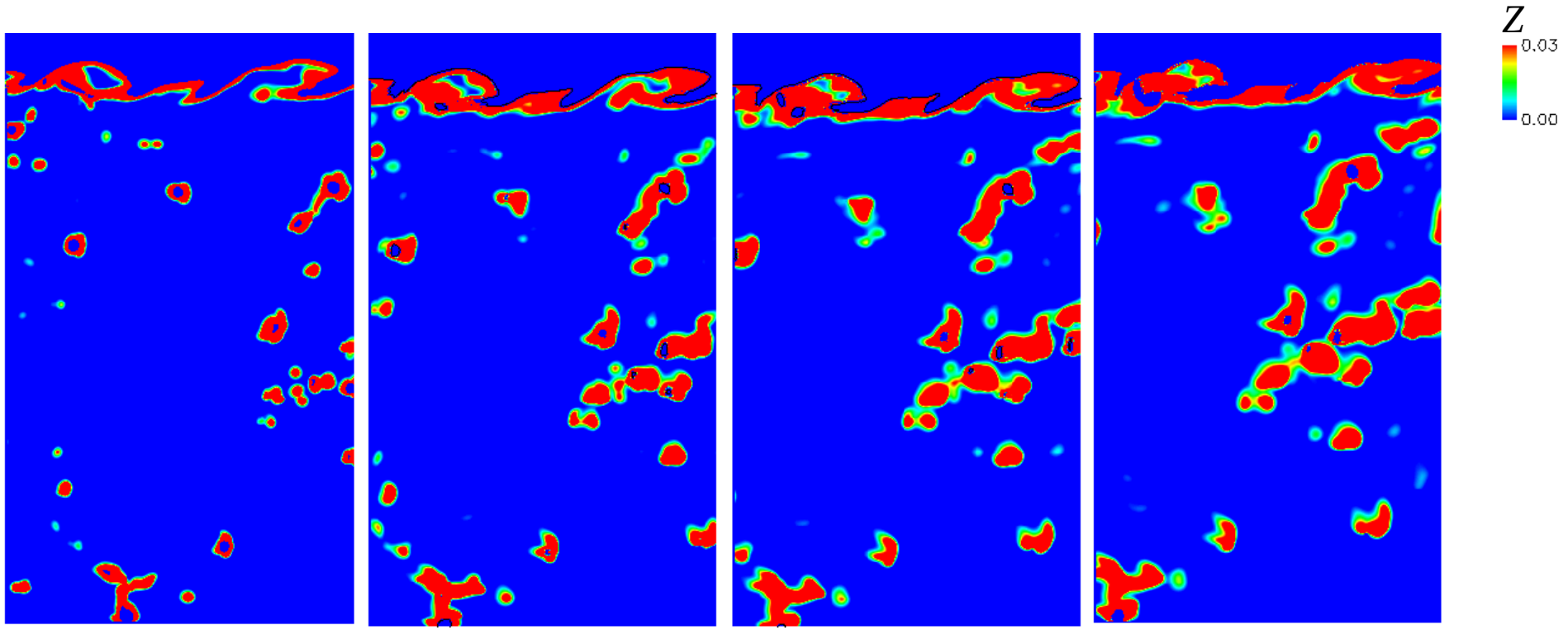


*2D slice image makes the impression that the number of droplets is small.

Mixing of vapor/air



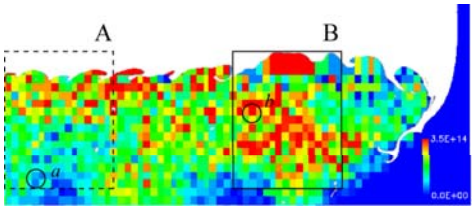
Region A



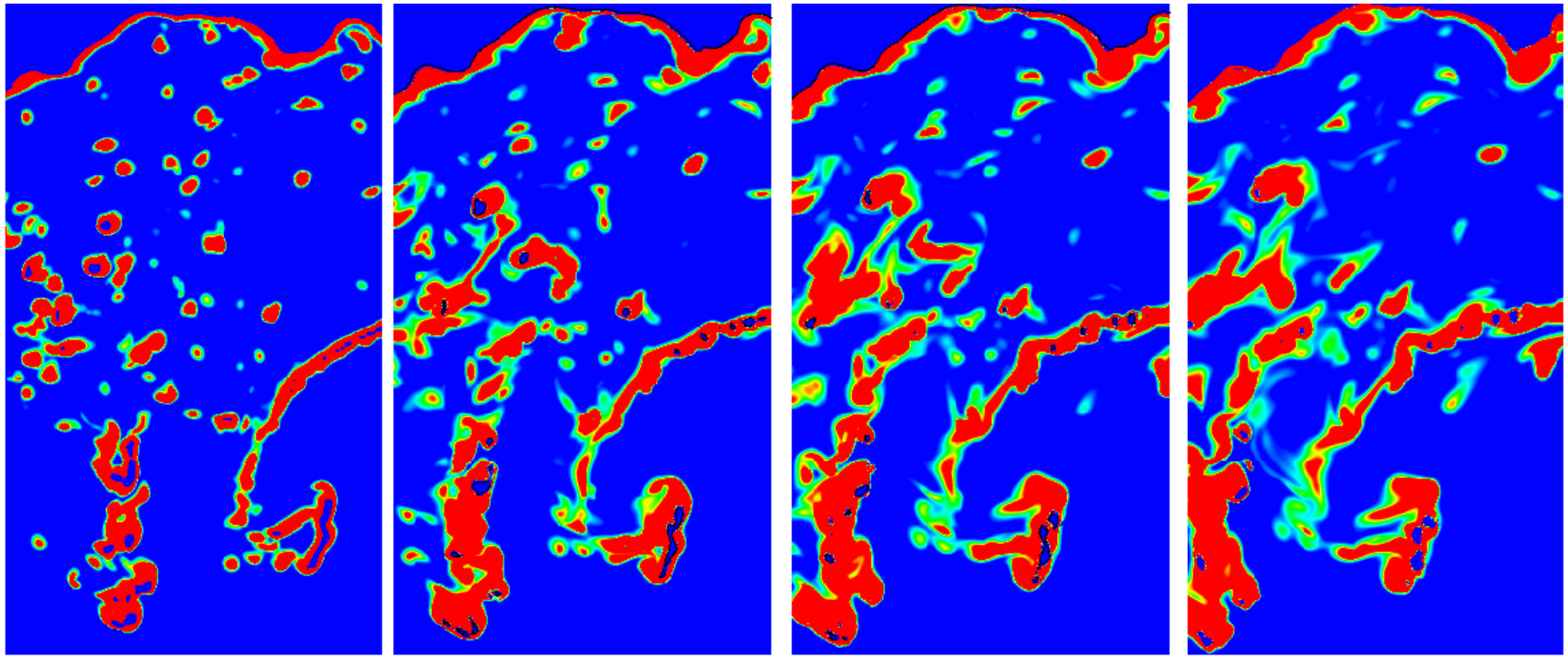
$\hat{t} = 15.62$ $\hat{t} = 15.81$ $\hat{t} = 15.93$ $\hat{t} = 16.03$

*Evaporation starts at $\hat{t} = 15.47$

Mixing of vapor/air



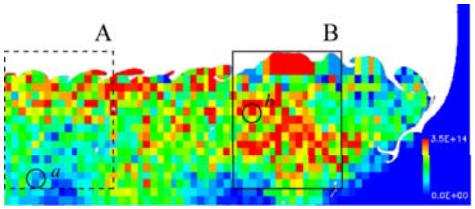
Region B

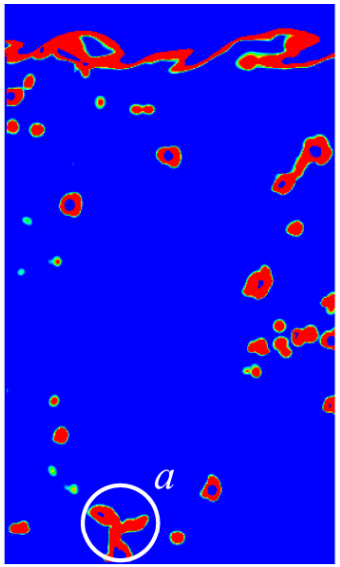


$\hat{t} = 15.62$ $\hat{t} = 15.81$ $\hat{t} = 15.93$ $\hat{t} = 16.03$

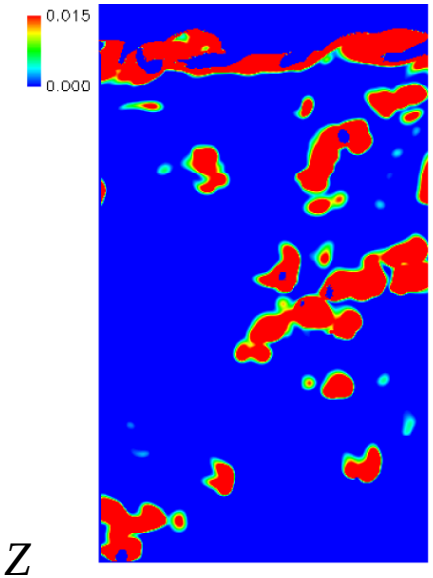
*Evaporation starts at $\hat{t} = 15.47$

Mixing of vapor/air

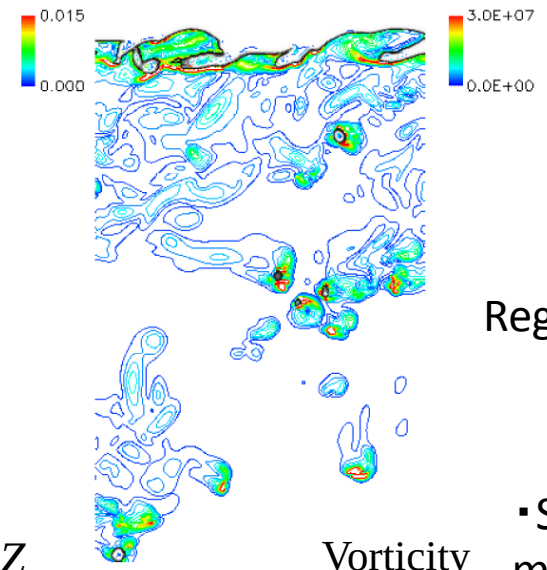




Z



Z



Vorticity

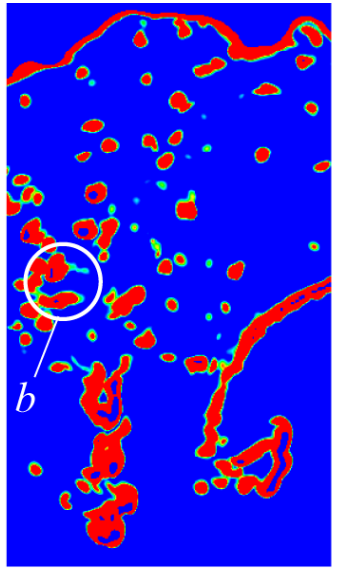
$\hat{t} = 15.62$

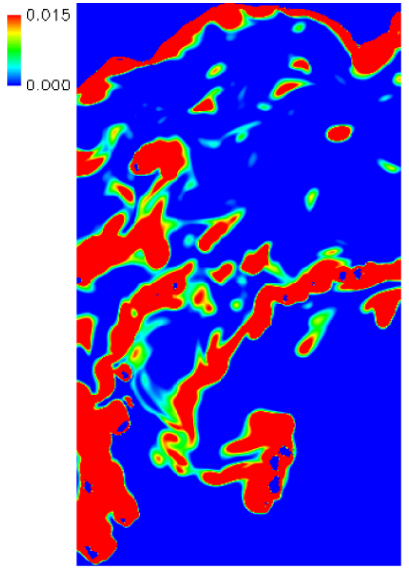
$\hat{t} = 16.03$

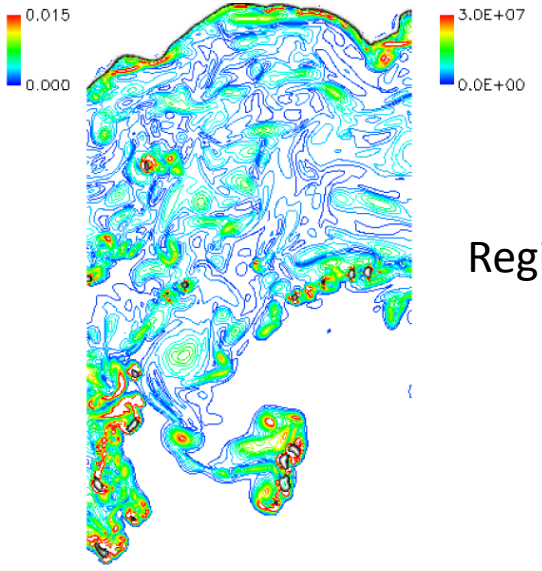
$\hat{t} = 16.03$

Region A

- Strong correlation between mixing and vorticity
- Faster mixing in region B





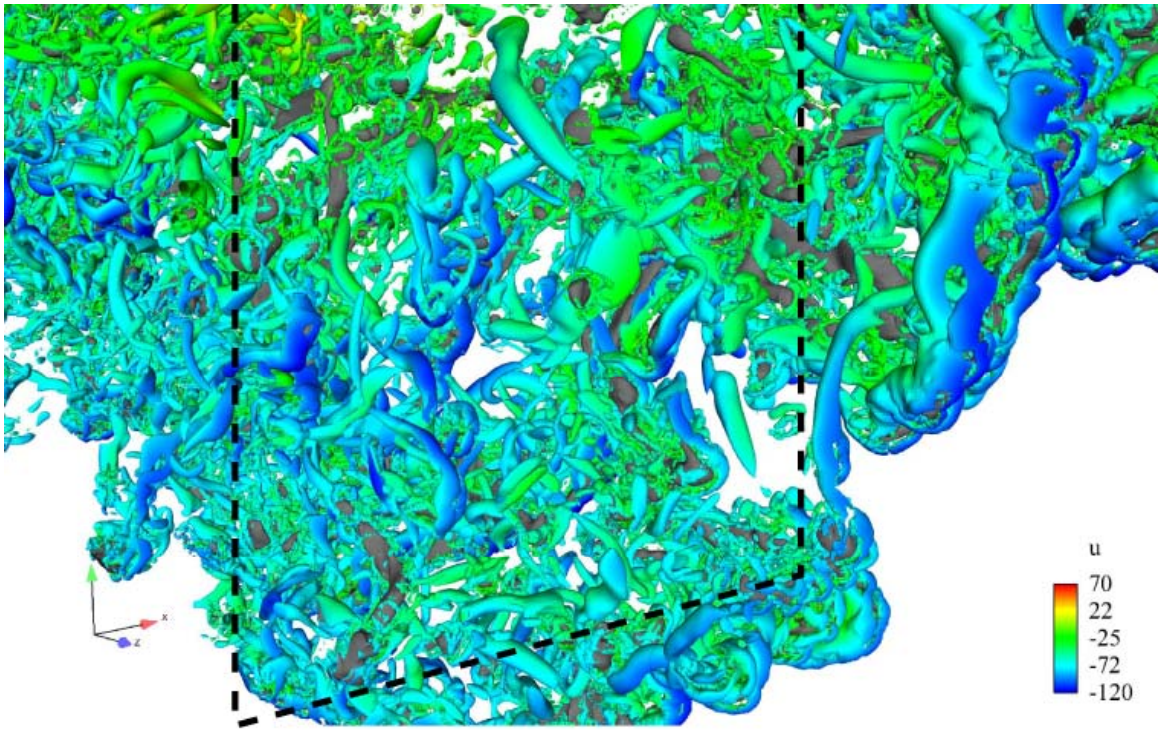


Region B

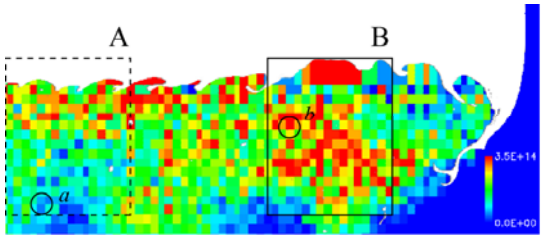
*Evaporation starts at $\hat{t} = 15.47$

Droplet/turbulence interaction

- Droplet/turbulence scales



Droplets (gray) and eddies (Q-isosurface) near region B



Kolmogorov scale

$$\eta = \left(\nu^3/\varepsilon\right)^{1/4} \qquad \varepsilon = \nu\overline{u'_{i,j}u'_{i,j}}$$

$$\eta \sim 1\mu m = 0.23D_{32}$$

D_{32}: Sauter mean diameter

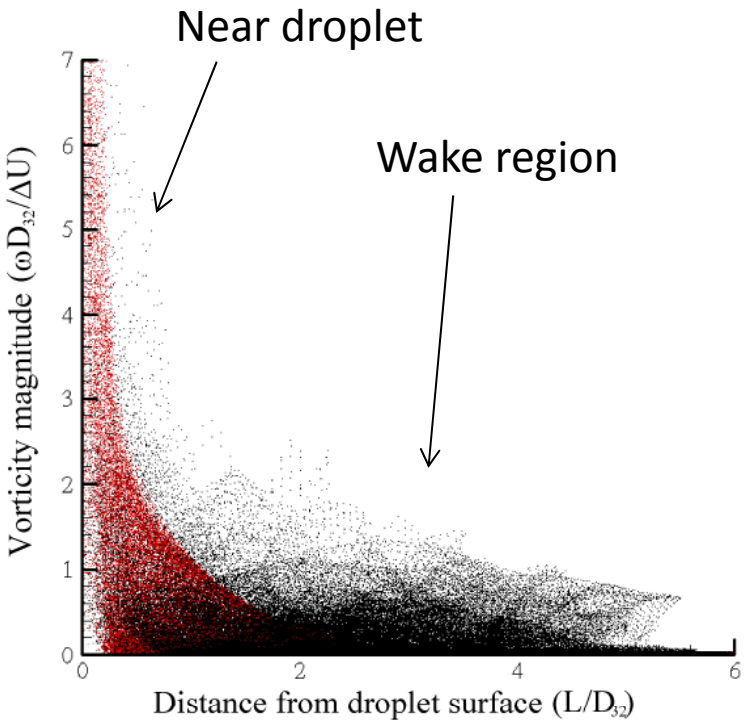
Droplet Stokes number

$$S_t = \rho_l {D_{32}}^2 U \big/ 18\mu_g L$$

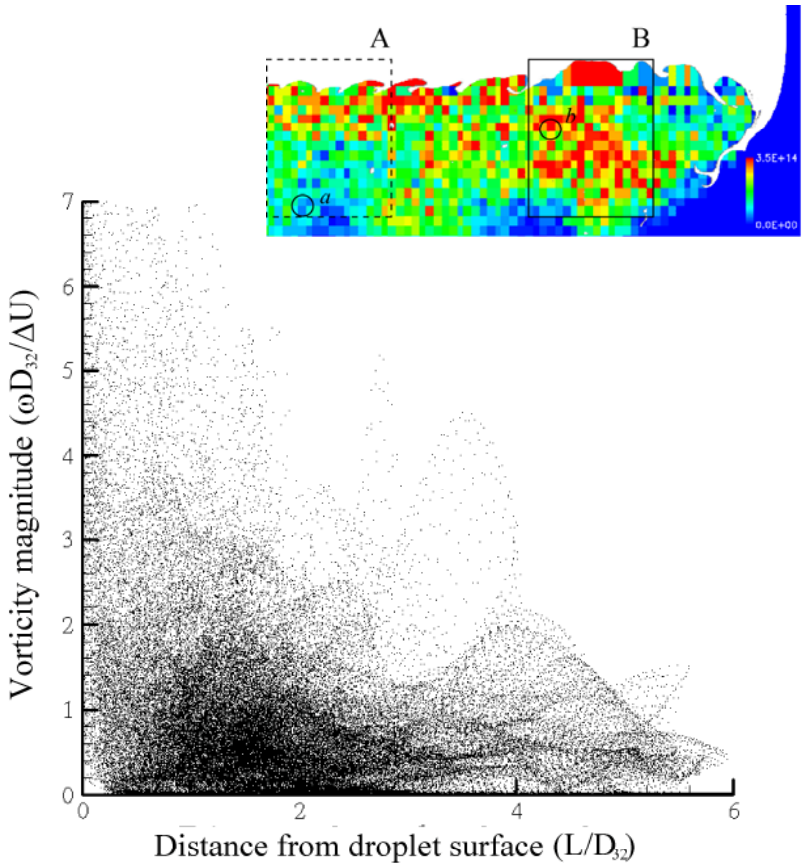
$$S_t \sim 22$$

- Slip velocity exists between droplet and gas
- Vorticity generation (eddy diameter~8-12η)
- Global energy feed from liquid to gas

Vorticity around droplet



Region A (low number density)

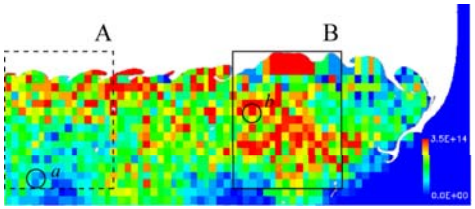


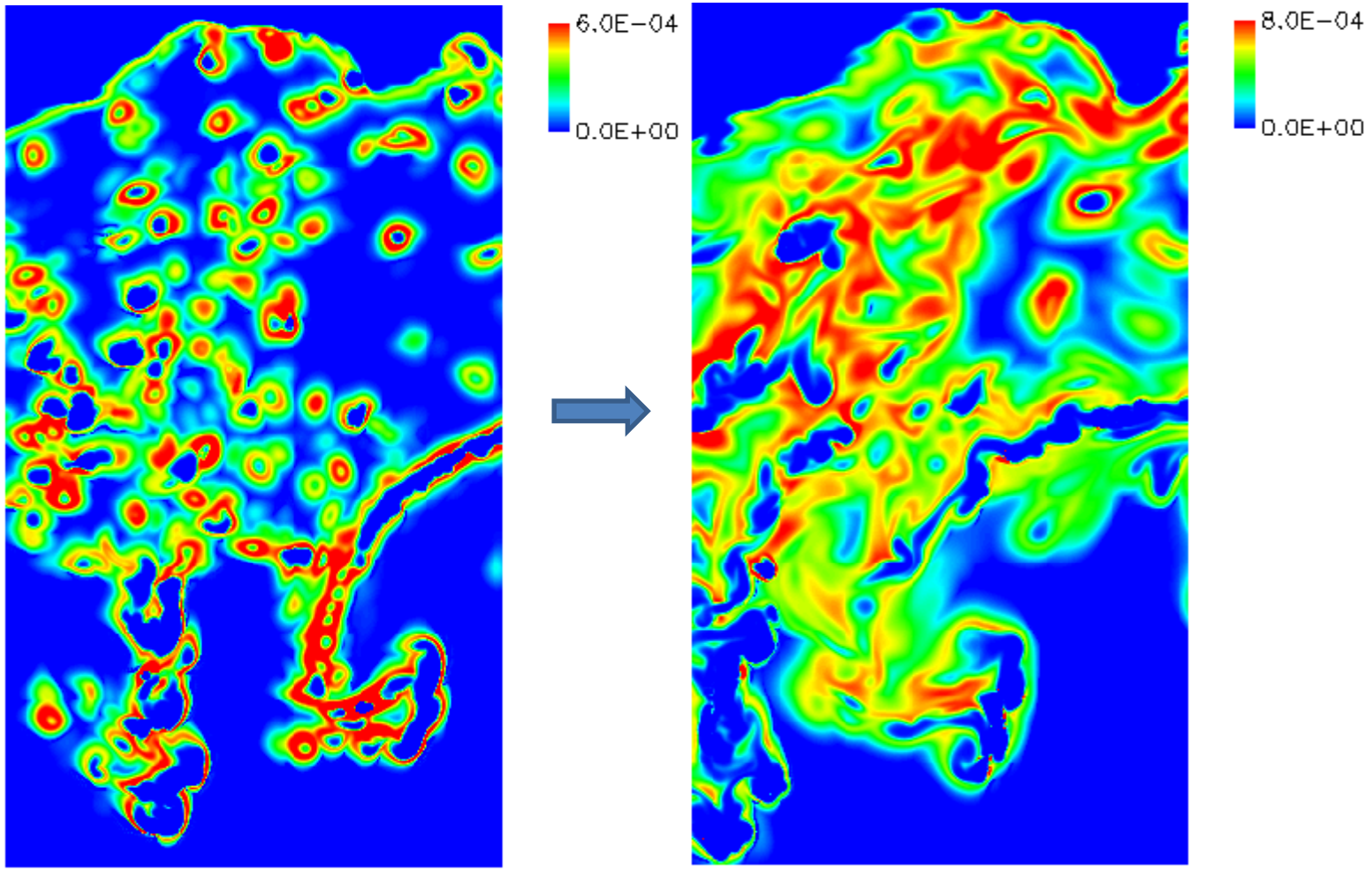
Region B (high number density)

*Red scatter points are from single droplet simulation of the similar Re (~40) with evaporation and reactions.

- Wake interaction is stronger in region B
- Mean inter-droplet distance: (A) $l=7.9D_{32}$ and (B) $l=3.3D_{32}$ $\quad l \sim n^{1/3}$

Formation of vapor clusters





Region B

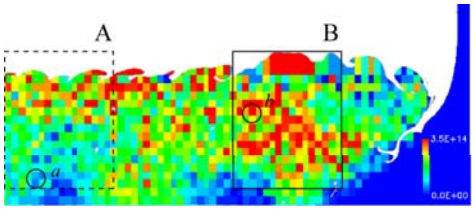
Fuel consumption rate (mol/cm^3/s)

Initially

Cluster formation

*Red shows the high reaction rate, but this is still not a “flame”

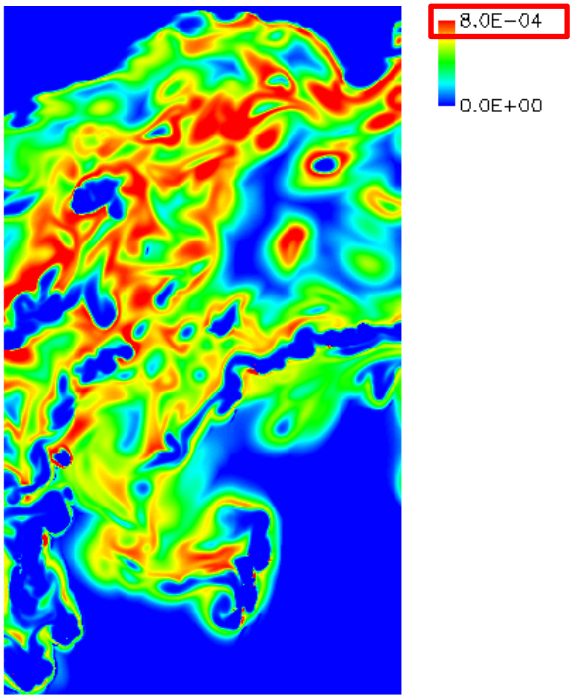
Formation of vapor clusters

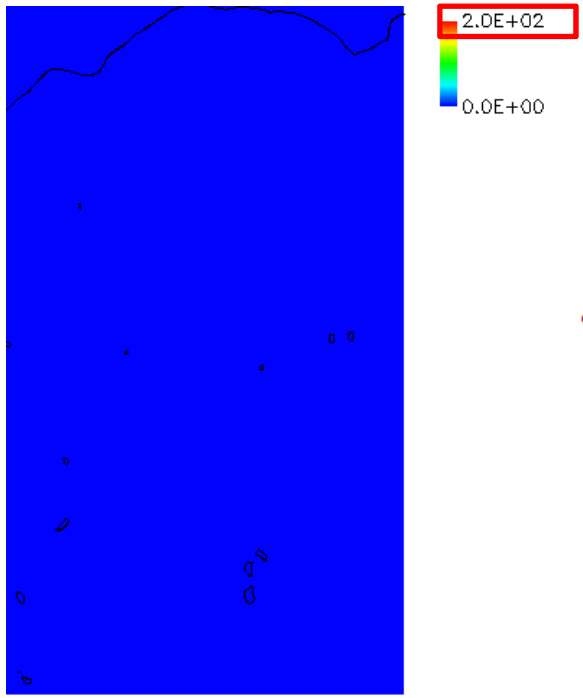


Note that the reaction rate magnitude is small at this early stage.

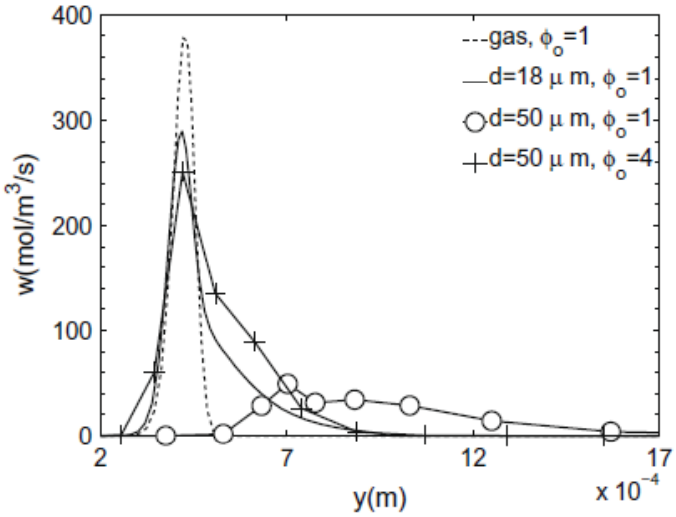
*Red shows the *relatively* high reaction rate, but this is still not a “flame”.

*Also note that the spatial scale is much smaller here.





Fuel consumption rate (mol/cm^3/s)



(a) $C_7H_{16} + O \Leftrightarrow C_7H_{15} + OH$

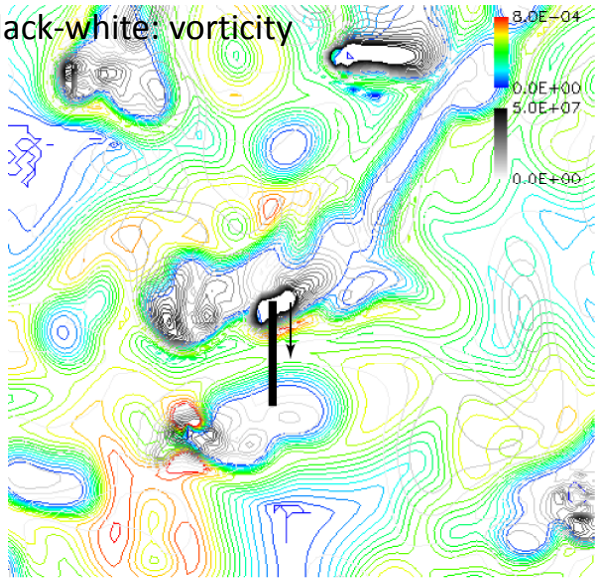
Neophytou & Mastorakos CNF 2009

Typical reaction rate magnitude

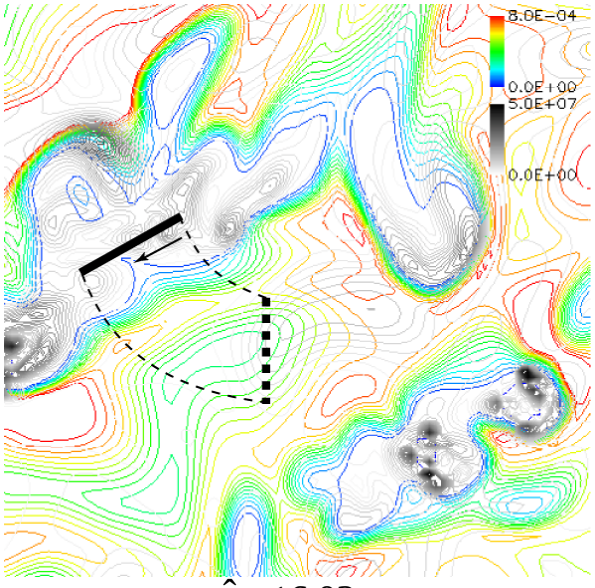
Formation of vapor clusters

Color: reaction rate

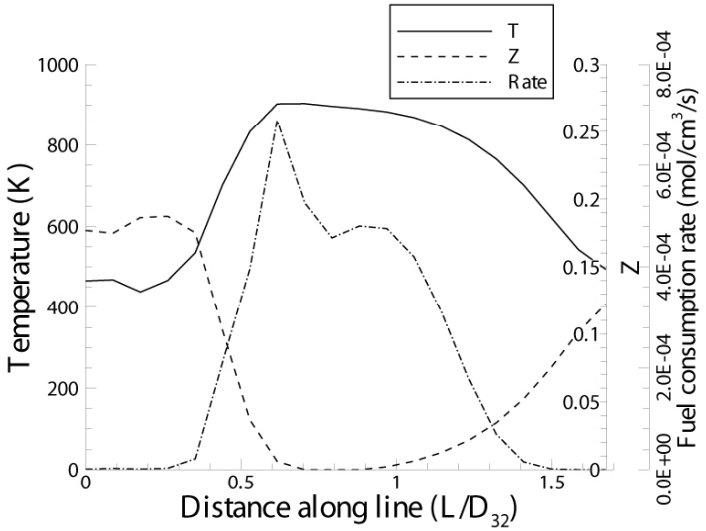
Black-white: vorticity

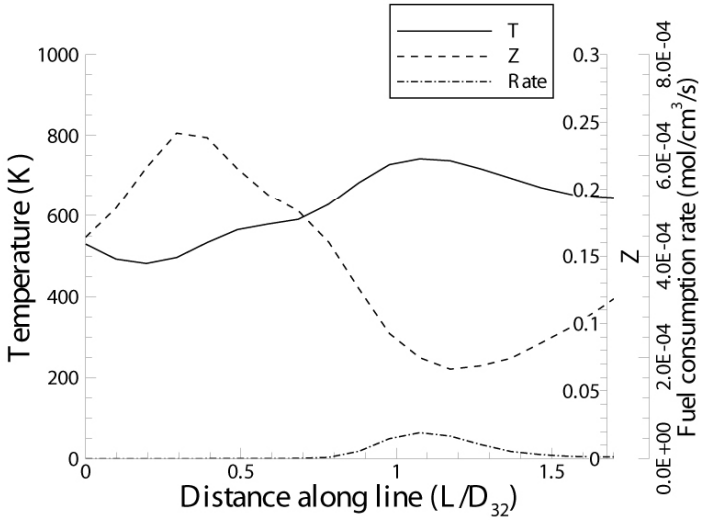


$\hat{t} = 15.71$



$\hat{t} = 16.03$





Molecular diffusion τ_d

$\tau_d = L^2 / D_{dif} = 5.4\text{e-}6\ \text{s}$

Or $\Delta\hat{t} = 5.4$

With

$D_{dif} = 3.4\text{e-}6\ \text{m}^2/\text{s}$

$L = D_{32} = 4.3\mu\text{m}$

Eddy turnover τ_e

$\tau_e = 4\pi / |\boldsymbol{\omega}| = 3.6\text{e-}7\ \text{s}$

Or $\Delta\hat{t} = 0.36$

With

$|\boldsymbol{\omega}| = 3.5\text{e}7\ \text{s}^{-1}$

Actual time difference

$\Delta\hat{t} = 0.32$

Already connected!

Eddy mixing is dominant.

Group combustion number

In region B,

$$G = 2\pi n D_{32} R_c^2 = 5.7$$

With

R_c=0.25D_N

n=3.4e14 m^{-3}

D_{32}=4.3μm

External Group Combustion

- Mixing by droplet-generated vorticity
  - Spherical and non-spherical droplets
- Inter-droplet interaction
  - Especially for high number density

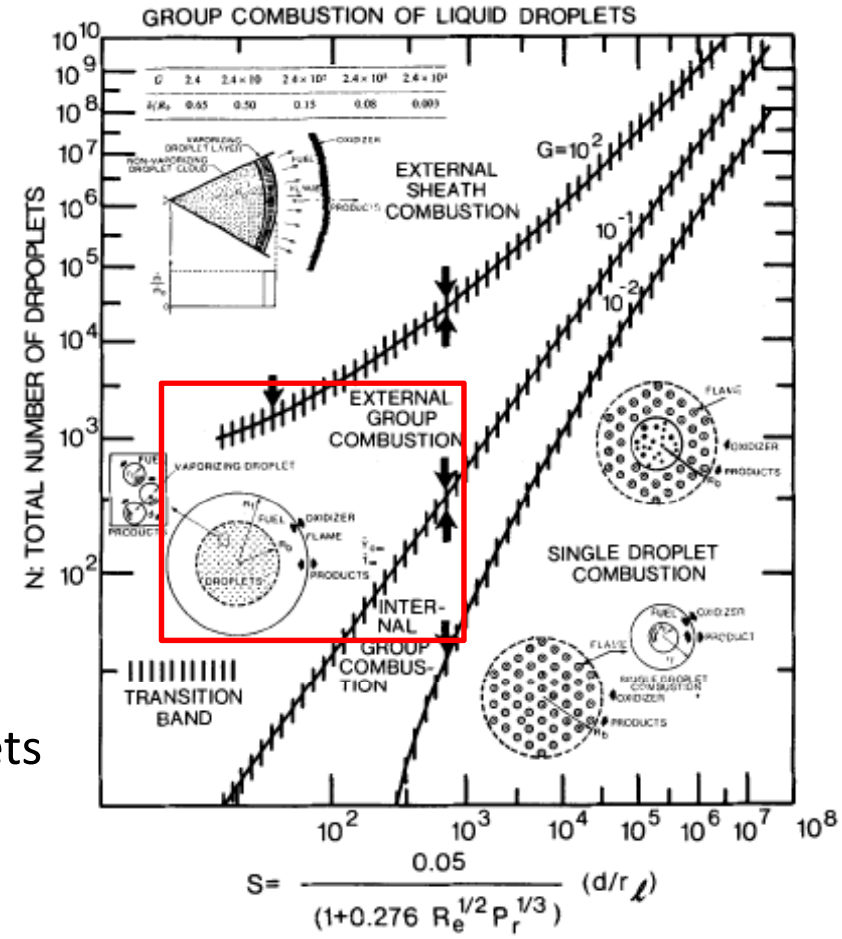


FIG. 1. Four group combustion modes of a droplet cloud.

Scale extension

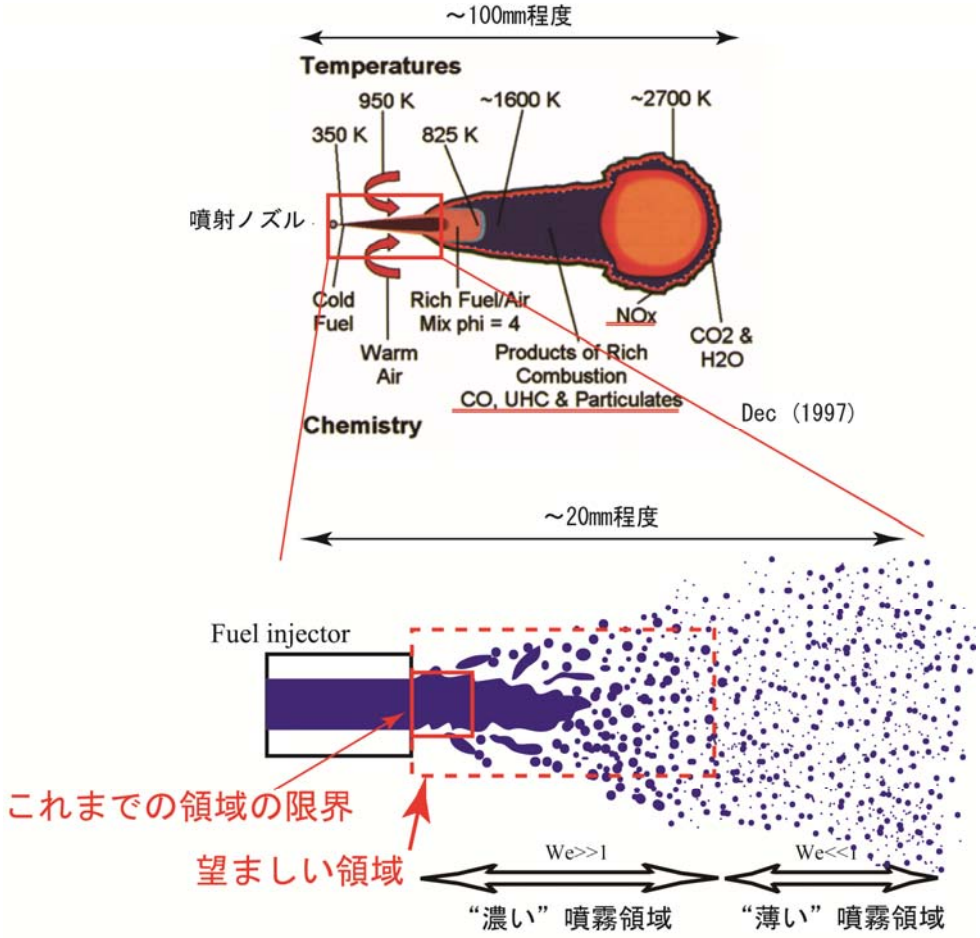
Based on DNS...possible by using a larger computer system such as “K”-class system)

•Spatial scale

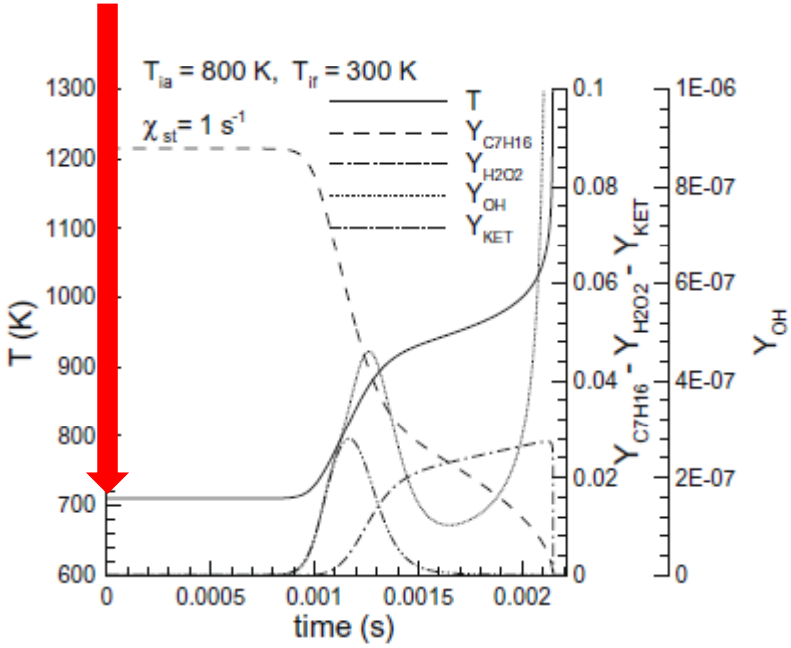
•At least, the primary atomization region should be covered.

•Temporal scale

•It is still far short compared to the ignition delay time.



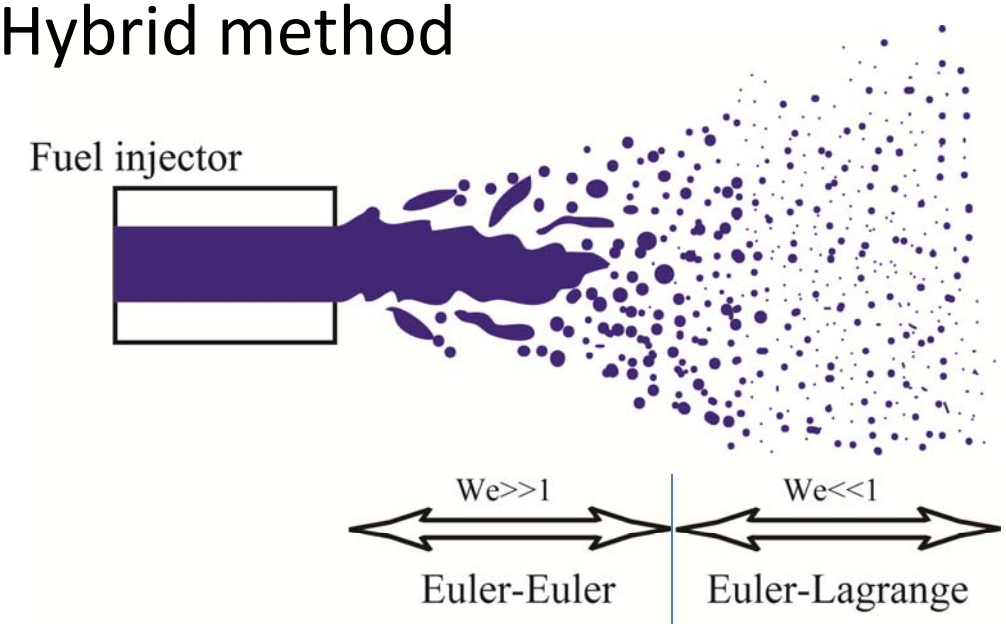
Current simulation time scale



Viggiano (CNF 2010)

Outlook

- Combustor scale simulation
  - Hybrid method



We will return to the initial starting point…
…but with more knowledge of physics and modeling of spray and flame

Summary of study 2

- Atomization data extended with evaporation, mixing and reactions
  - Droplet/turbulence interaction is very important in mixing
  - External group combustion expected in dense region
- Modeling
  - Must include the above effect
  - We are working on this now
- Others
  - Detailed reaction mechanisms
  - Spatial/temporal scale extension

Thank you!