Australian Combustion Summer School
University of Sydney
December 2018

Sprays Session

Dr. Agisilaos Kourmatzis
A/Prof. Matthew Cleary

Topics:

1st hour-Dr. Agisilaos Kourmatzis

- **Two-Phase Flows Considerations and basic definitions**
- Unstable liquid-gas flows-atomization onset
- Atomization
- Turbulent sprays and spray combustion

2nd hour-A/Prof Matthew Cleary

- Two-phase flow modelling
- Combustion modelling
- Turbulence
- Droplet burning

General Considerations

Two-phase flows are a broad-reaching class of flows, in the general category of "multi-phase" flows.

Two-phase flows are generally characterized by the existence of one or several interfaces and discontinuities at the interface. We could have:

- Gas-solid mixture
- Gas-liquid mixture
- Liquid-solid mixture
- Immiscible-liquid mixture (e.g. oil and water, strictly not a two- "phase" flow…but we can treat it as such)

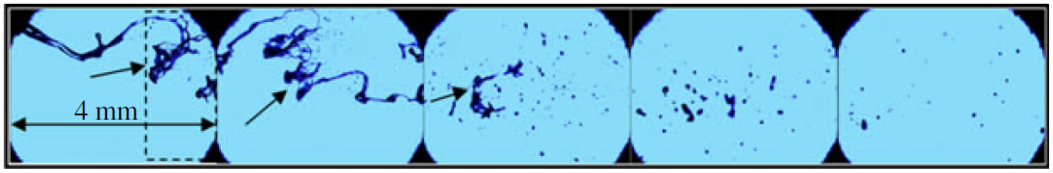
The typical spray in combustion: Separated->Transitional->Dispersed

Considering a fully turbulent liquid jet delivered into atmosphere is perhaps the best example where we can see all "categories" of two-phase flows in one single device.

Simulations are now getting pretty close to reality (see right) yet fully quantitative accuracy is still in progress. Experiments still critical.

Here we will focus on mixed/transitional flows (A) and dispersed flows (B)

M. Herrmann, J. Eng. Gas Turb. Power, 132(2), 2010.



Dimensionless groups

From our basic definitions we can already see one obvious non-dimensional number:
The Density Ratio: ρ_A/ρ_B.

A Buckingham-pi analysis of the physical variables (e.g. velocity, density, viscosity, surface tension, length-scale) will result in three more critical dimensionless groups

The Reynolds number (inertial : viscous)

- Note: We can now define either an "aerodynamic" Reynolds number using the gas phase density, or a liquid Reynolds number using liquid phase density
- Most widely used velocity scale is now U_{AB} (slip)
- Length-scale is the liquid jet diameter or droplet diameter.

The Weber Number (inertial : surface tension)

- $We=\rho U_{AB}^2 L/\sigma$ (again, can define "aerodynamic" Weber number or liquid Weber number)

The Ohnesorge Number (Viscous : inertial and surface tension)

- $Oh=\mu/(\rho\sigma L)^{1/2}$

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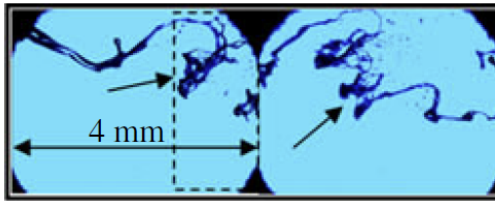
Unstable two-phase (liquid gas) flows

Instability is the norm in many practical applications (instabilities significant at high Weber number, more random at high Reynolds number)

Form on the interface between the liquid and gas shifting the two-phase flow from “separated” to “transitional”, if We very high (We>>15) can eventually turn to a dispersed flow.

This interfacial instability is ubiquitous in nature

Credit: Tim McKenna (theinertia.com)



Linear instability analysis

The general formal approach follows linear instability analysis, which would end up being a lecture on its own.

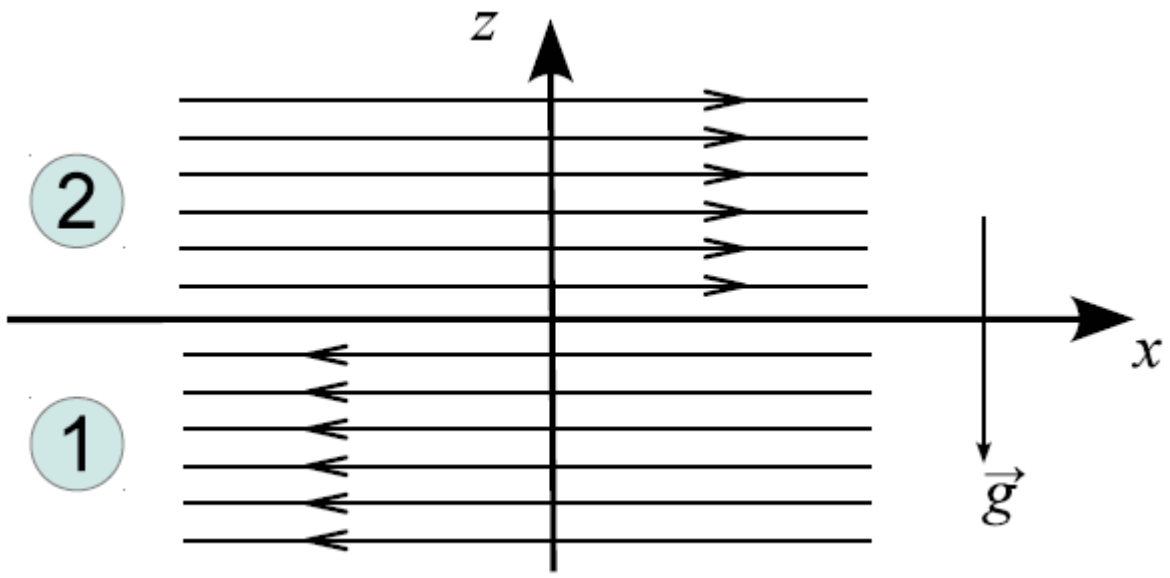
In general, we break instability analysis down into 5 key steps:

1. Add a perturbation to your equation and expand (e.g. f(y,t)=<f>+f')
2. Simplify the governing equation by removing all higher order terms (linearize it)
3. Consider a normal Fourier "mode" and assume that f'(y) will have a solution of that form
4. Substitute f'(y) into your linearized equation. After simplifying, this should be an eigen-relation (Df(y)=sf(y)) where D is a differential operator and s is an eigenvalue (which is also in the exponential term of the Fourier term). Now solve for f(y) for the general case.
5. Substitute f(y) back into your eigen-relation to determine the conditions where s>0 (unstable) and s<0 (stable).

Shear flow Instabilities

We do not have time to fully derive the instability conditions. But we can look at where they come from.

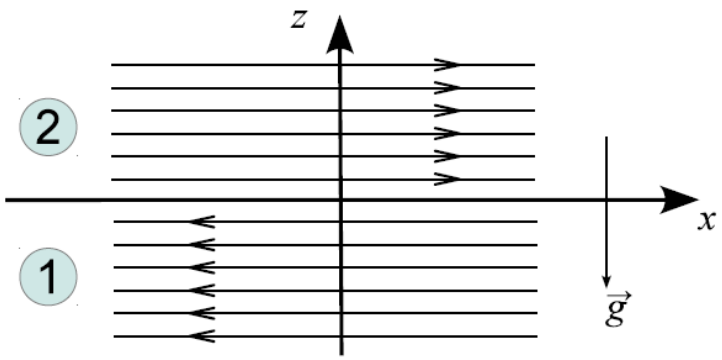
The General problem:



Shear flow Instabilities

We follow steps "1-5", but first formulating our governing equation

To make our lives easier, we are going to use potential flow theory (Laplace equation)



$$\nabla^2\phi_1 = 0$$

$$\nabla^2\phi_2 = 0$$

upper half: $\mathbf{v}_2 = \nabla\Phi_2$ for $z > 0$

lower half: $\mathbf{v}_1 = \nabla\Phi_1$ for $z < 0$

Linear momentum: $$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = \mathbf{g} - \nabla\left(\frac{P}{\rho}\right)$$

Shear flow Instabilities

Using potential function definition (and employing some simplifications…not too important) to re-write linear momentum (Navier-Stokes) as:

$$\frac{\partial \Phi}{\partial t} + \left(\frac{1}{2}\mathbf{v}^2\right) + gz + \frac{P}{\rho} = const$$

The above equation is just Bernoulli (with an unsteady term…).

So now (skipping lots of steps), we add a perturbation to the above and made use of the definition of a potential function: $\Phi_1=U_1x+\varphi_1$ and $\Phi_2=U_2x+\varphi_2$ (…$d\Phi/dx=u$).

I am also going to define a new governing equation to describe the position of my liquid air interface (not showing this but it is $\xi(x,t)=z$)

Shear flow Instabilities

$$\rho_1\left(\frac{\partial\phi_1}{\partial t}+U_1\frac{\partial\phi_1}{\partial x}+g\xi\right)=\rho_2\left(\frac{\partial\phi_2}{\partial t}+U_2\frac{\partial\phi_2}{\partial x}+g\xi\right)$$

OK, we have our perturbed, and linearized governing equation ("step 2"). The above is a governing equation in addition to our governing equations for ξ, these are as follows:

$$\begin{aligned}\frac{\partial\xi}{\partial t}+\frac{\partial\xi}{\partial x}U_1 &= \frac{\partial\phi_1}{\partial z}\\ \frac{\partial\xi}{\partial t}+\frac{\partial\xi}{\partial x}U_2 &= \frac{\partial\phi_2}{\partial z}\end{aligned}$$

The following must also be true (potential flow): $\nabla^2\phi_1=0$

$\nabla^2\phi_2=0$

Now time to look for Fourier mode solutions ("step 3"). We look for solutions for φ_1, φ_2 and ξ.

Plug in the Fourier Modes

Using normal Fourier modes (φ_1 is equivalent to φ_1'), e.g.

$$\phi_1' = \hat{\phi}_1(y)e^{ik(x-ct)} \qquad \phi_2' = \hat{\phi}_2(y)e^{ik(x-ct)}$$

And substituting these in the Laplace equation definition for potentials φ_1 and φ_2 will lead to the following simplified modes:

$$\begin{aligned} \phi_1 &= \hat{\phi}_1 \exp(kz)\exp[i(kx-\omega t)] \\ \phi_2 &= \hat{\phi}_2 \exp(-kz)\exp[i(kx-\omega t)] \\ \xi &= \hat{\xi}\exp[i(kx-\omega t)] \end{aligned}$$

Substituting the above Fourier modes in the governing perturbation equations from the previous slide, we can develop an algebraic instability equation for this flow, and for the case of no velocity (U=0),we can easily develop an instability criterion for ω ("step 5")

voila: the RT (Rayleigh-Taylor) and KH instability

If $U_1 = U_2 = 0$ then the relation is:

$$\omega^2 = \frac{(\rho_1 - \rho_2)kg}{\rho_1 + \rho_2}$$

So if the density of phase 2 is higher than phase 1 we will have unstable solutions with $\omega^2<0$. This would be a **Rayleigh-Taylor instability** (formulation for general flow-same instability in two-phase flows).

If the body force term is zero then solutions are given by (**Kelvin-Helmholtz instability**):

$$\omega_{1/2} = \frac{k(\rho_1 U_1 + \rho_2 U_2)}{\rho_1 + \rho_2} \pm i\frac{\sqrt{\rho_1 \rho_2}}{\rho_1 + \rho_2}|U_1 - U_2|$$

Any ABS(U_1-U_2)>0 can lead to instability, no matter how small.

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Atomization basics-plain orifice atomization

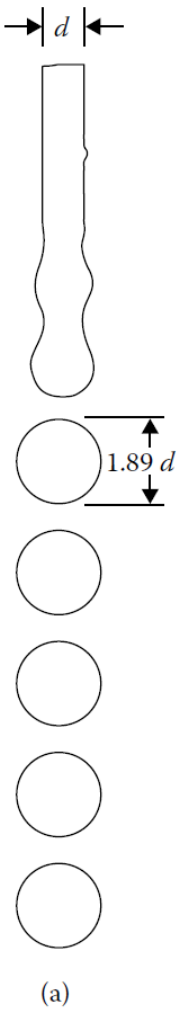
- Liquid jet ejected from an orifice. Atomization in this case can be dictated by a number of processes.
- One of the original analyses of these problems was by Rayleigh
- An instability analysis demonstrated that disturbances with a wavelength greater than the circumference of the liquid jet will grow with an optimum wavelength 4.51d.
- Assuming this cylindrical shape eventually turns into a sphere then:

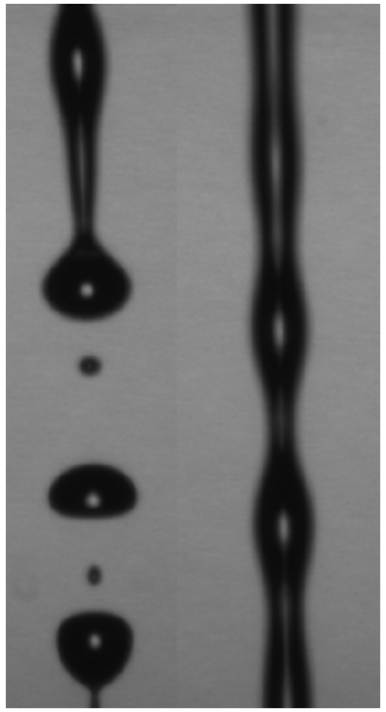
$$4.51d \times \frac{\pi}{4} d^2 = (\pi/6) D^3$$

$$D = 1.89d$$

Atomization basics-plain orifice atomization

- Experiments suggest this to be pretty close to the truth on average, another win for Rayleigh.
- Some revisions to the theory have followed but the overall story is the same, and we all generally agree that the most unstable Rayleigh wavelength is what leads to droplets forming.
- This all only valid at low Reynolds numbers.
- At higher Reynolds numbers…shear instabilities and turbulence start dominating.

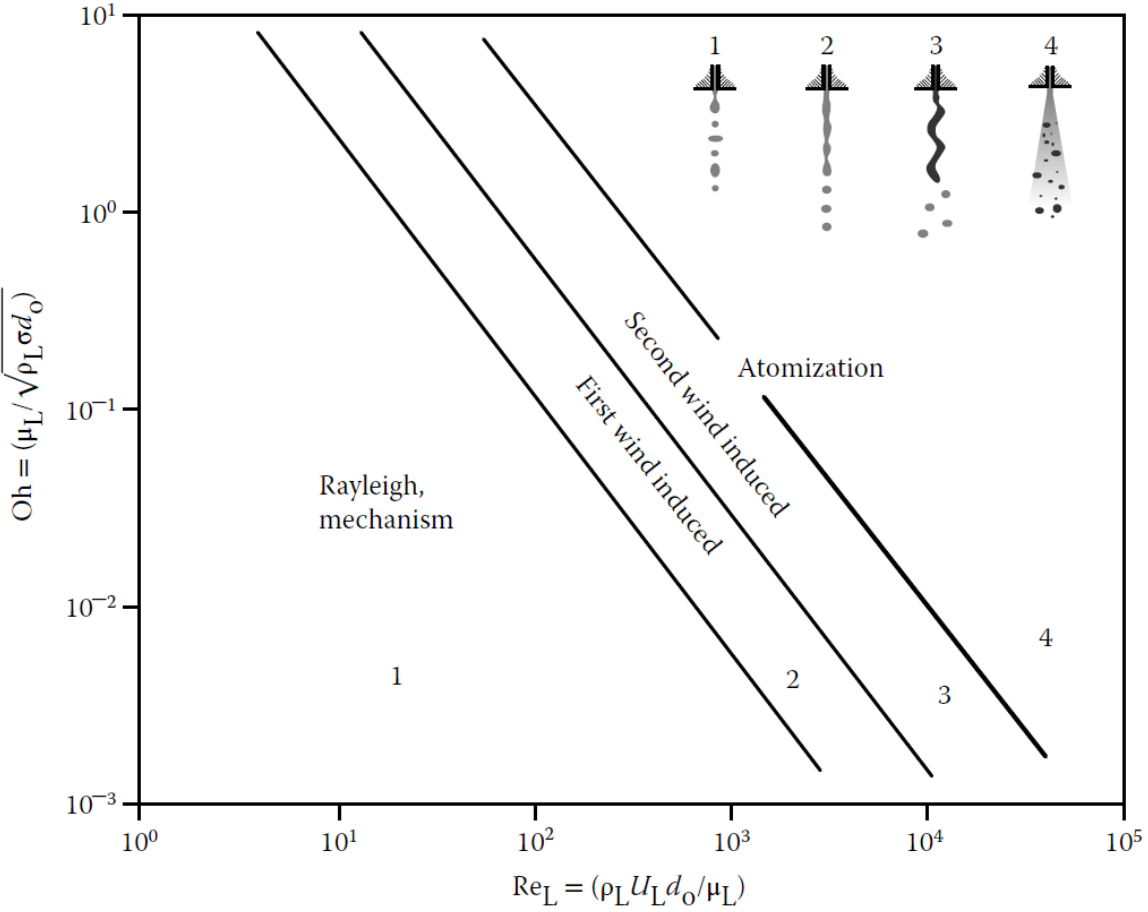




Left figure from Lefebvre
Right figure from Kourmatzis 2011

Primary break-up->core into ligaments/droplets

Atomization and Sprays A. Lefebvre



1	$We_A > 0.4$ $We_A > 1.2 + 3.4Oh^{0.9}$
2	–
3	$We_A > 40.3$ $We_A > 13,$
4	–

Reynolds number critical though also Ohnesorge number. Weber number can be used to describe aerodynamically assisted break-up, the above valid for liquid jet in stagnant air (plain-orifice)

Primary break-up->core into ligaments/droplets

Break-up length predictions:

Weber was the first to suggest that a small axisymmetric disturbance δ_0 will grow at some exponential rate qmax until δ_0=liquid jet radius. When that happens, we start seeing liquid distintegration.

According to Weber if t_b is the break-up time:

$$r_0 = \delta_0 \exp\left(q_{\max} t_b\right)$$

$$t_b = \frac{\ln\left(d/2\delta_0\right)}{q_{\max}} \qquad q_{\max} = 0.97\left(\frac{\sigma}{\rho_L d^3}\right)^{0.5}$$

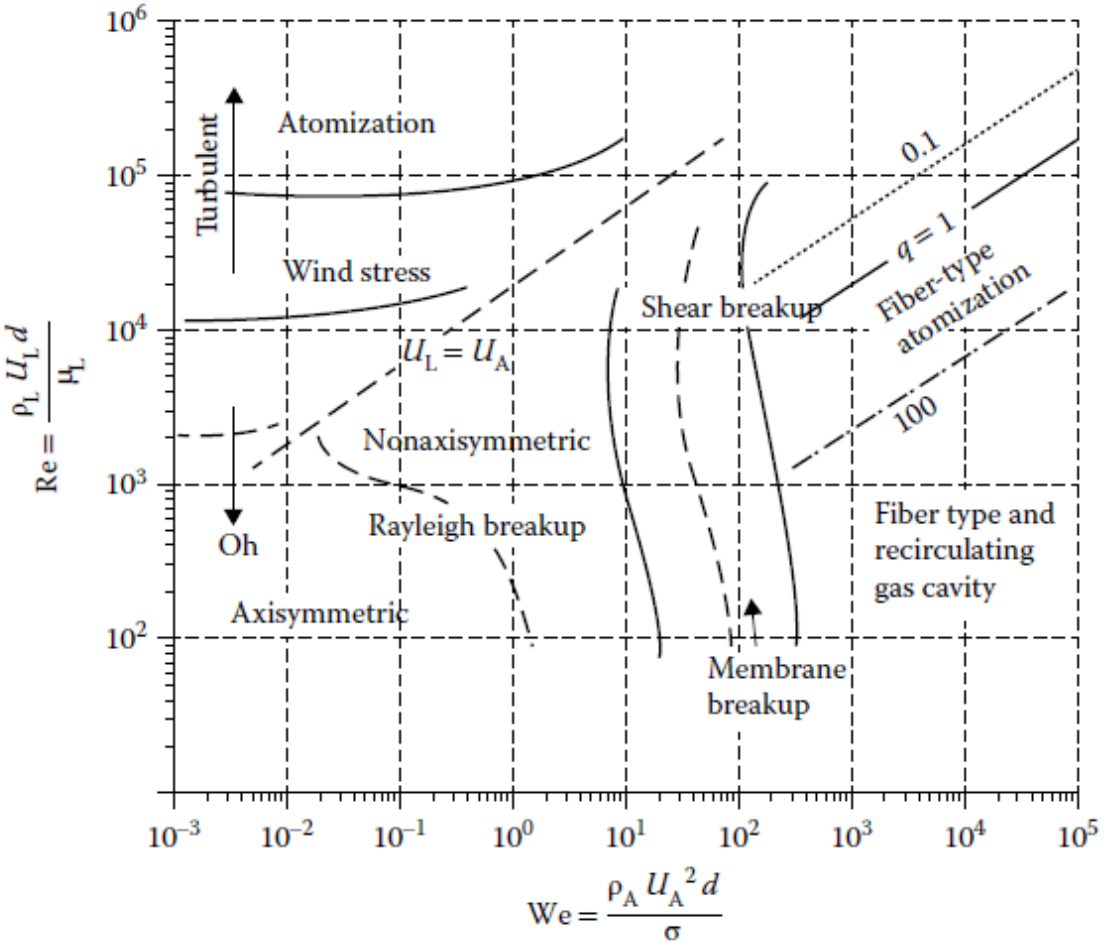
Leads to a break-up length: $L = 1.03\mathrm{d}\ \mathrm{We}^{0.5}\ln\left(d/2\delta_0\right)$ (from)

$$t_b = \frac{L}{U}$$

While the theory is sound…the correlation is a failure…

$$L = \frac{U}{q_{\max}}\ln\left(\frac{d}{2\delta_0}\right)$$

Primary break-up->core into ligaments/droplets



Lasheras et al., 2000 Ann. Rev. Fl. Mech

Where are we then?

What actually leads to atomization?

- **Instabilities on the surface** ultimately dictate the formation of droplets

$$\frac{\mathrm{SMD}}{\lambda_1} \approx \frac{0.68}{We_{\lambda_1}^{1/2}}$$

Varga et al. J. Fluid Mech. 2003

- **Boundary layer** at nozzle important (somewhat consistent between both pure pressure atomization and air assisted, see Varga et al J Fluid Mech, Raynal 1997 (PhD Thesis) and Kerstein et al. J Fluid Mech, 2017)

- **Turbulence inside the liquid jet** (at relevant Reynolds numbers) dictates the break-up of the jet.

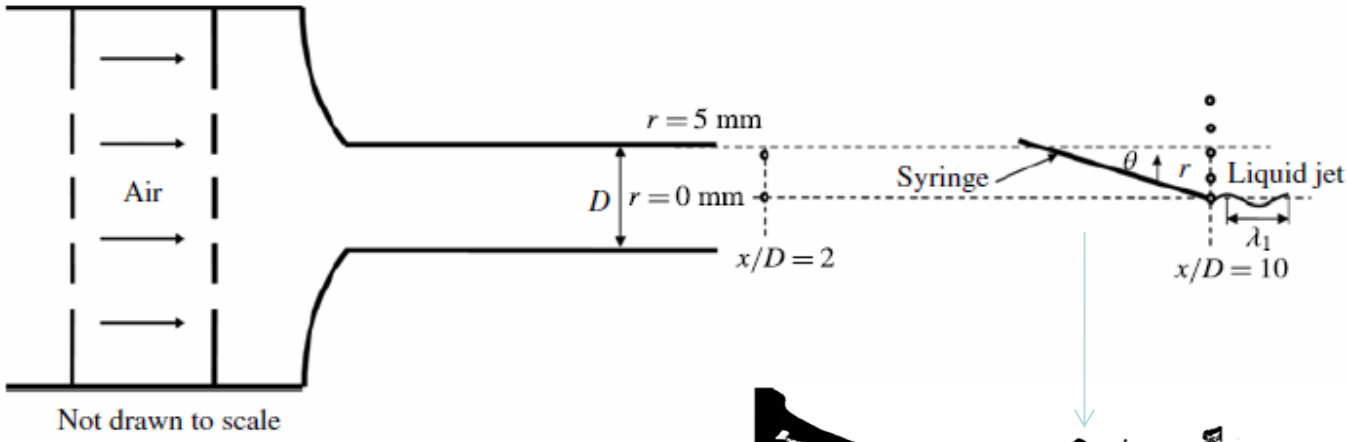
$$\rho_A \mathrm{SMD} u_o^2/\sigma = 12.9(x/\Lambda)^{1/3}(\rho_A/\rho_L)^{3/2}\mathrm{We}_{L\Lambda}^{5/6}/\mathrm{Re}_{L\Lambda}^{1/2}$$

Hsiang and Faeth, Int. J. Mult. Flow, 1995

How relevant are these mean dimensionless groups? Can we shift away from just morphologies?

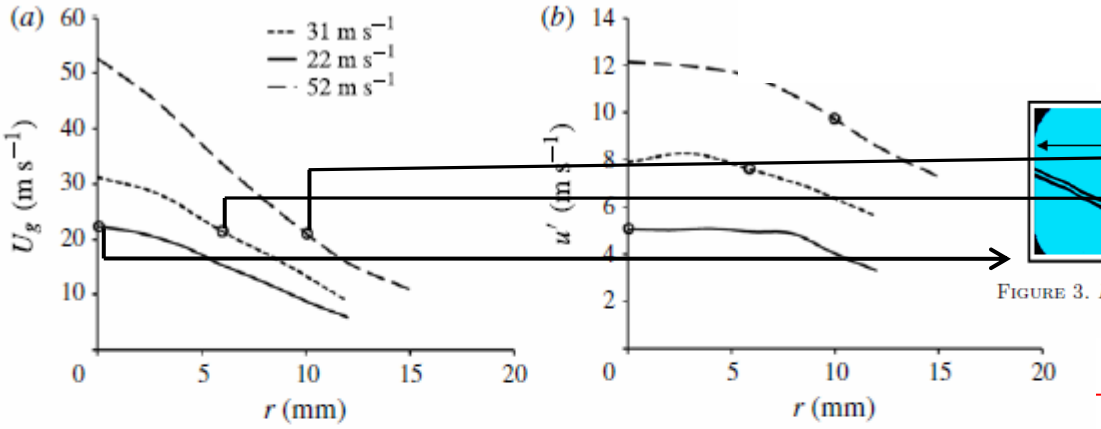
- Very little work on the influence of gas phase turbulence on sprays (believe it or not!)
  - Is the use of a single `mean' Weber number still useful/valid?
  - What is the influence of turbulence intensity on atomization?
  - Do existent models/schools of thinking apply when the velocity field is highly intermittent?
  - Are instabilities still key? Does turbulence change them?

Effects of turbulence-Controlling the turbulence intensity



λ_1 The primary instability wavelength

λ_{RT} The Rayleigh-Taylor wavelength



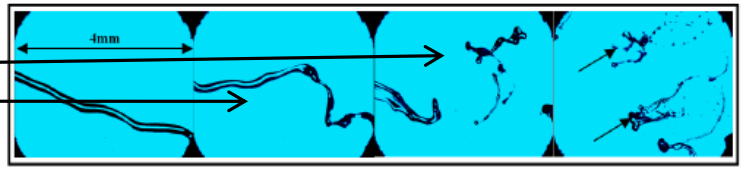
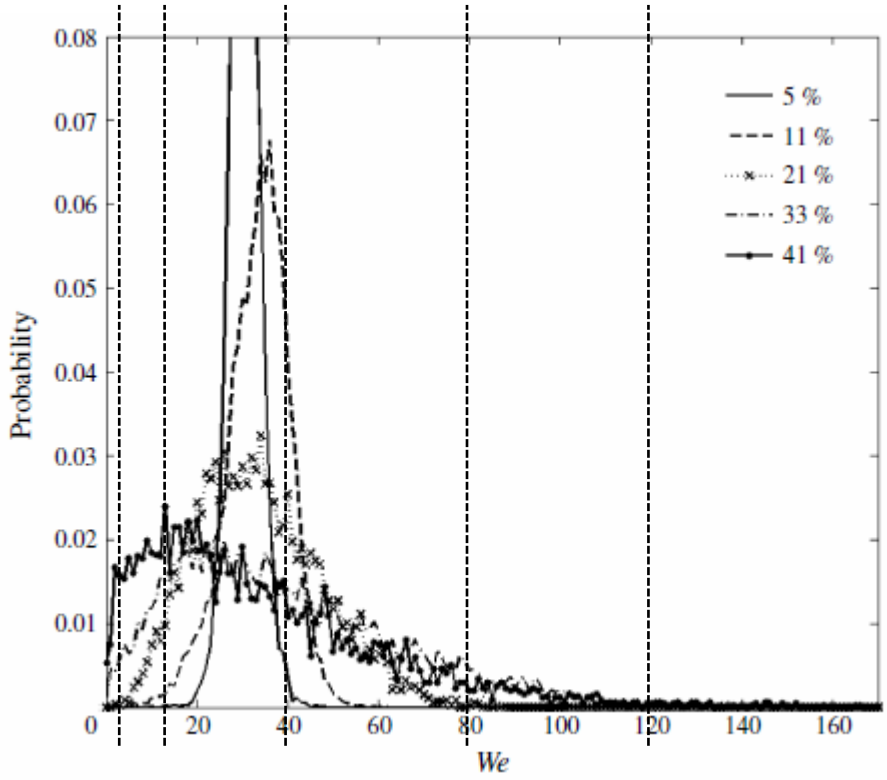
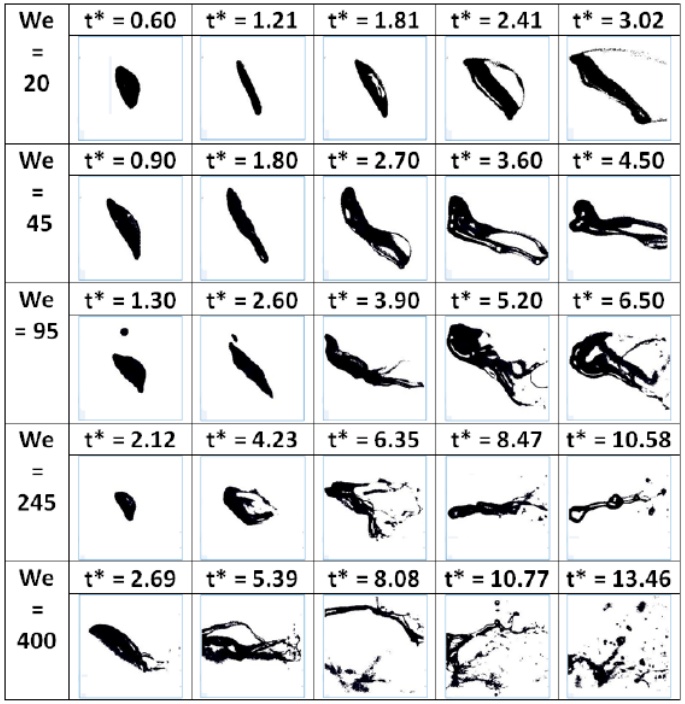


FIGURE 3. *Effect of turbulence intensity (3%, 25%, 35% and 41 % from left to right) on primary break-up morphology for case D2U2 at X/D1=14*

Distribution of Weber numbers

$$We_d = \frac{\rho_g (U - U_g)^2 D}{\sigma_l}$$



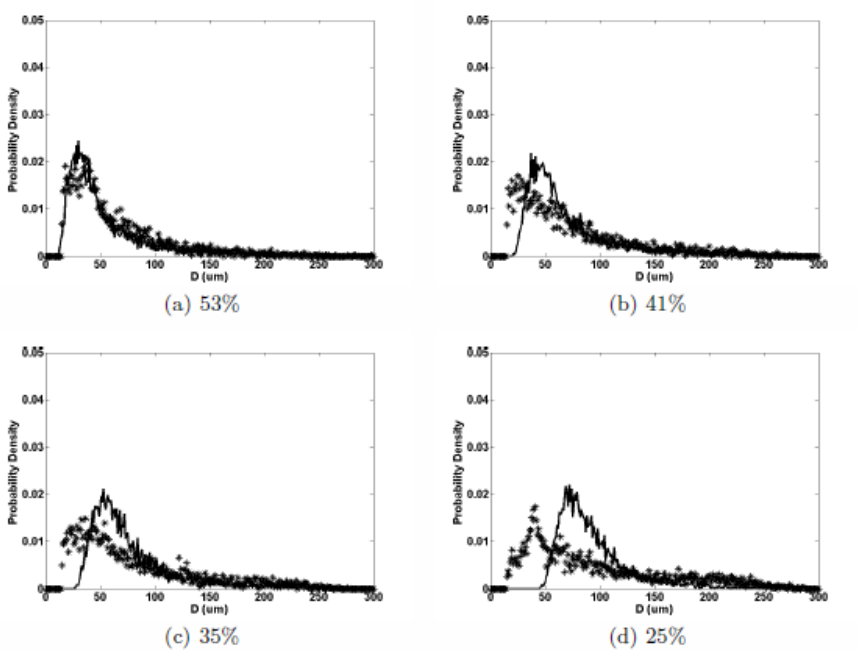


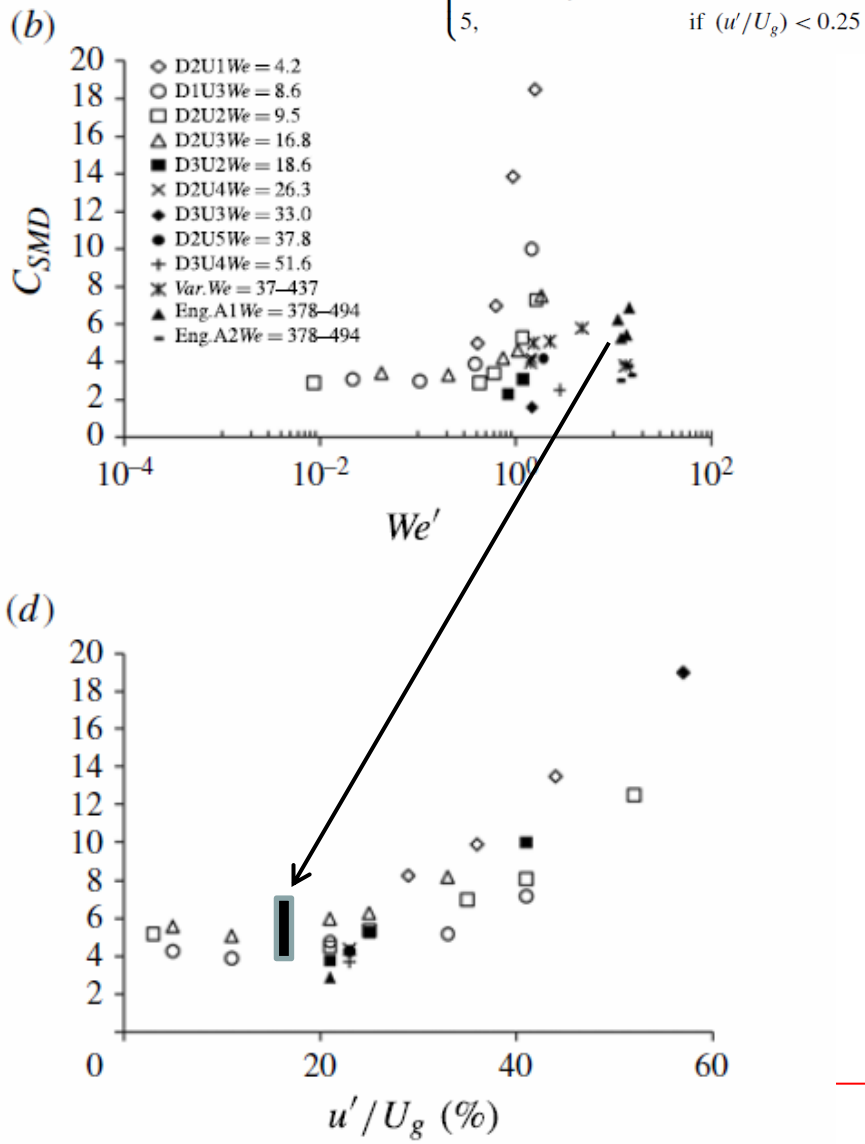
- Mean Weber number fixed whilst turbulence intensity increases.
- The turbulence level has never before been controlled in the gas phase in such atomization systems.
- This exposes the jet to a range of break-up regimes!

Instabilities and size distributions?

$$C_{SMD} = \begin{cases} 100m_1\left(\frac{u'}{U_g}\right) - 5, & \text{if } (u'/U_g) > 0.25 \\ 3.5, & \text{if } (u'/U_g) < 0.25 \end{cases}$$

$$C_{D10} = \begin{cases} 100m_2\left(\frac{u'}{U_g}\right) - 2.3, & \text{if } (u'/U_g) > 0.25 \\ 5, & \text{if } (u'/U_g) < 0.25 \end{cases}$$





- A full reconstruction of the measured droplet size histogram can be achieved by the model, however the wavelength must be normalized.

Kourmatzis and Masri, J. Fluid. Mech, 2015
Kourmatzis and Masri, Expts Fluids, 2015

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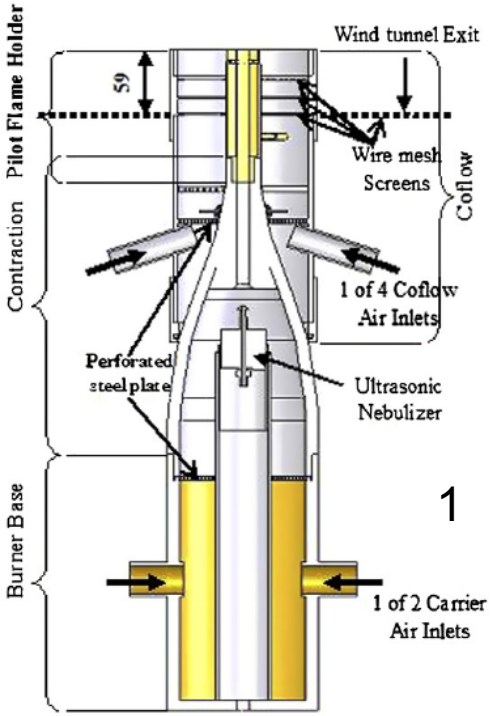
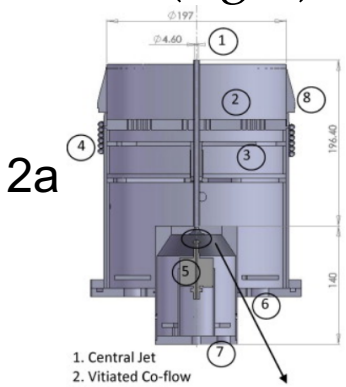
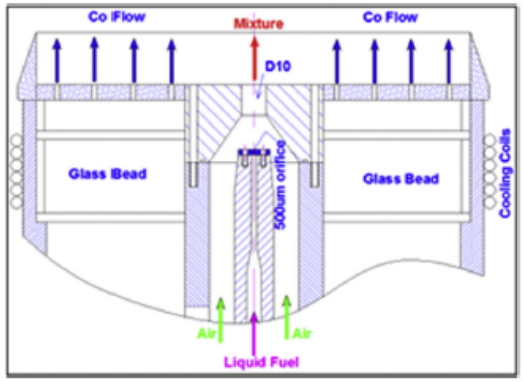
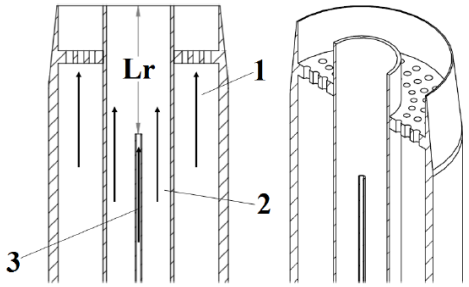
Spray burners

From purely dilute sprays (left), to those enabling measurements of both atomization and combustion (right), autoignition (middle) and pilot stabilized (right)









Sydney Spray Burner
Gounder et al. 2012
Kourmatzis et al. 2013

Sydney Needle Burner
Lowe et al. (2015-2018)

Basic measurement considerations

- Microscopic (2.5-4mm FOV) backlit imaging of a particular spray, useful but has problems. **Main problems in imaging**: defocused objects, occlusion, droplet merging, asphericity
  - Series of Publications dealing with this issue:
    - Combustion and Flame 2015
    - Measurement Science and Technology 2016 & 2017
    - Experimental Thermal and Fluid Science 2017

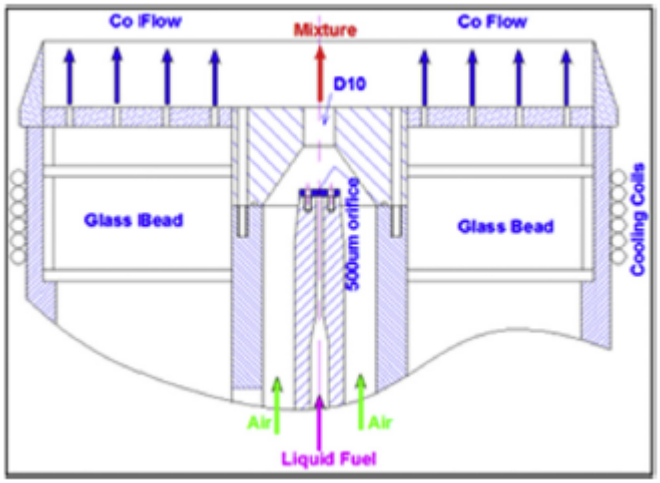
video

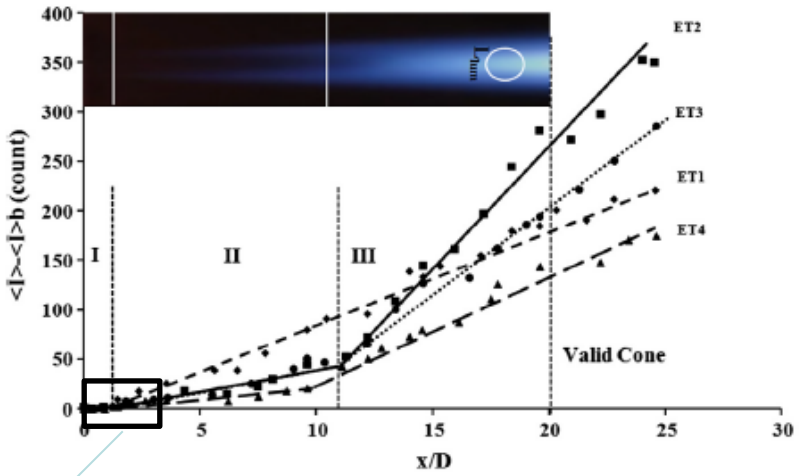
- Laser and phase Doppler anemometry for validation and comparison with image processing. **(spherical assumption only)**

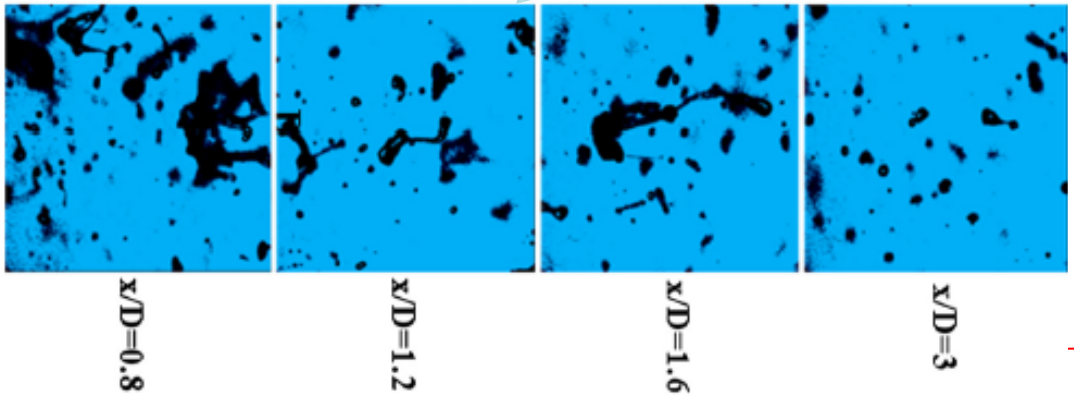
- Optical depth must be low enough for above to be used. These are not `dense' sprays, however they are atomizing sprays and have droplet-droplet interaction.
  - For spray diagnostics: *Spray measurement technology: a review (Fansler and Parrish, Meas. Sci. Tech., 2015)*
  - For dense sprays: *Imaging in the optically dense regions of a spray: A review of developing techniques (Linne, PECS, 2013)*

Measurement of Atomization and Combustion

- Most `fundamental' spray flames have all only provided quantities in the `dilute' region, where droplet-droplet interaction is absent, such as the`Sydney Spray burner'

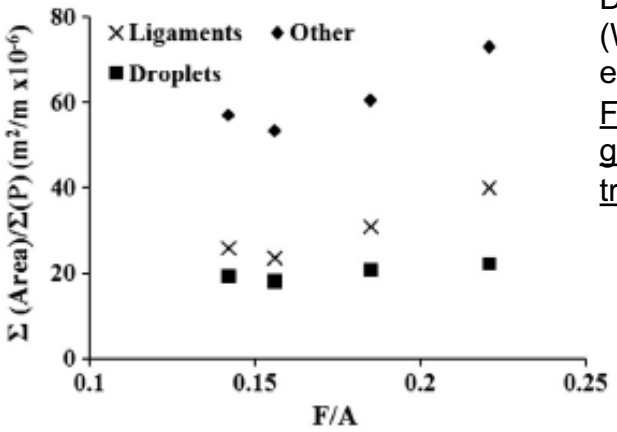


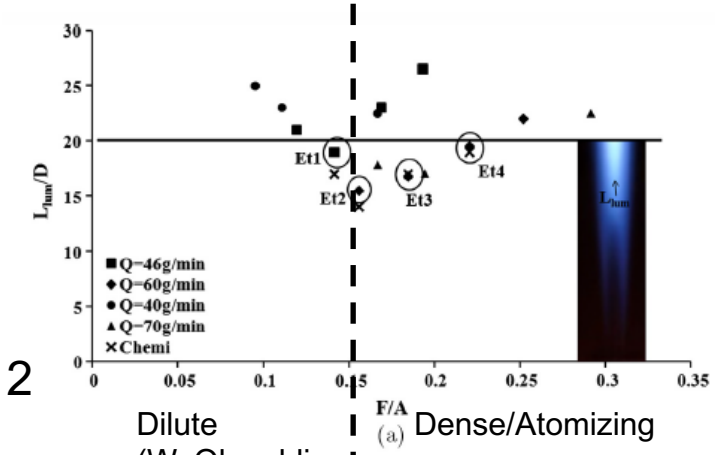




Relevance downstream?

- The lift-off of the flame is partly correlated to the size of the most non-spherical objects in the flow-field
- Pilot stabilized flame achievable with different atomization degrees at exit plane.





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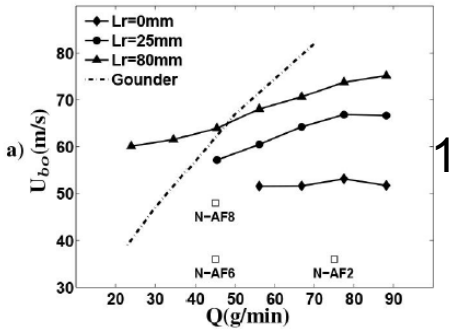
Dilute
(W. Oloughlin et al. 2015)
Follows pure gas phase trends

Dense/Atomizing

Atomization controlling



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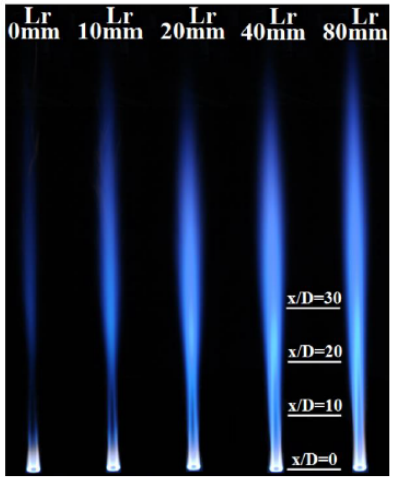
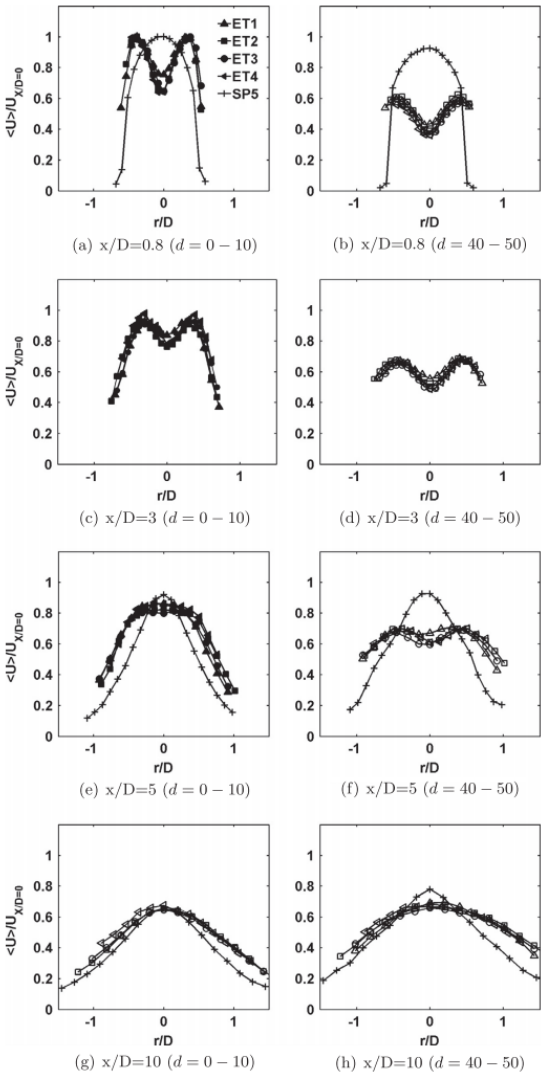
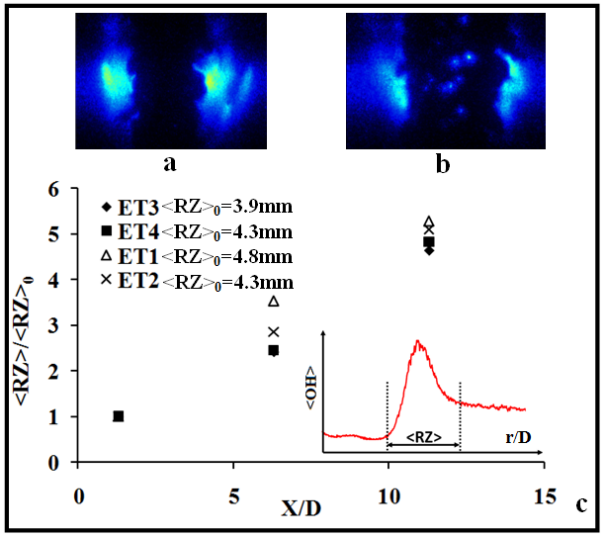


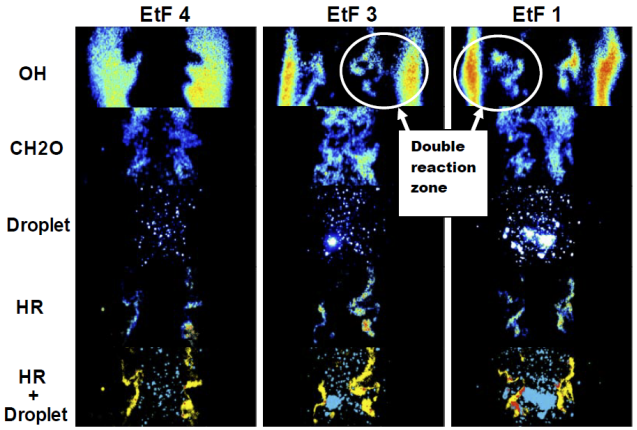
Development Downstream…





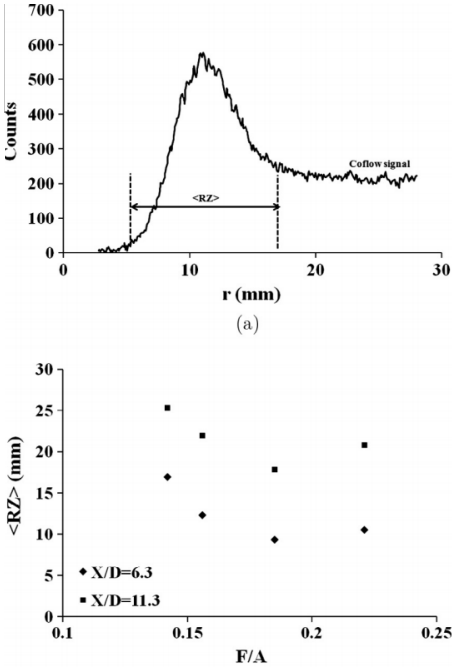
- **Mean reaction zone thickness grows at a faster rate for dilute spray (ET1)**
- **While non-spherical droplets do not survive downstream the initial spray conditions affect the onset location of auto-ignition and therefore the subsequent reaction zone structure.**
- **Mean flows start to look similar past the potential core (turbulent jets…)**

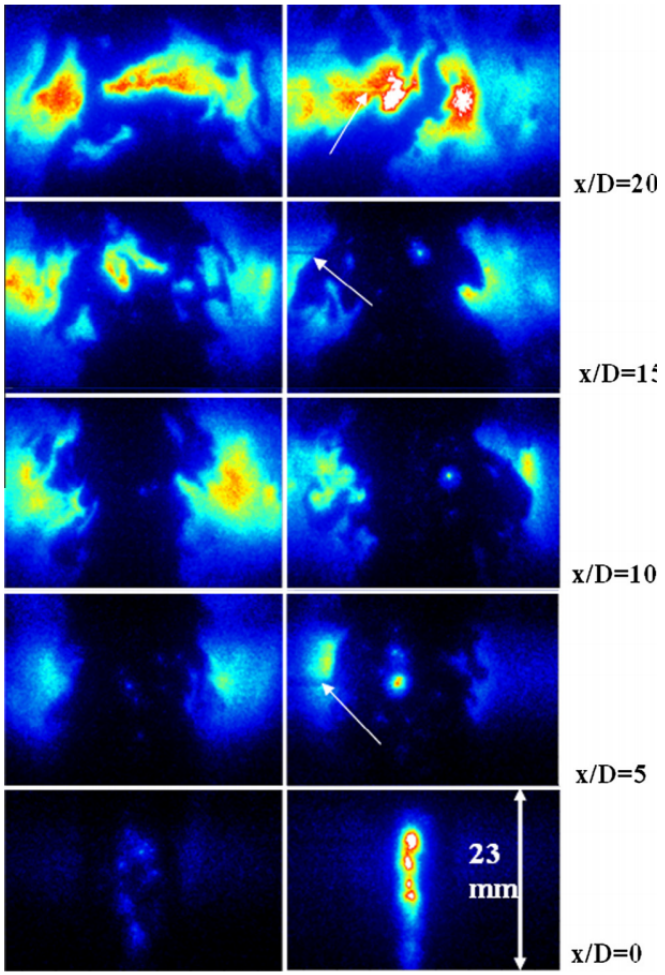
Reaction Zones Downstream



Gounder 2011

x/D = 5





Review papers you should read

- Drop and Spray Formation from a Liquid Jet (Lin and Reitz), *Annu. Rev Fluid Mech*. 1998
- Mixing, Transport and Combustion in Sprays (Faeth), *PECS*. 1987
- On the experimental investigation on primary atomization of liquid streams (Dumouchel), *Expts. Fluid*s. 2008
- Breakup phenomena in coaxial airblast atomizers (Engelbert et al.), 1995, *Proc. Roy. Soc*.
- Liquid jet instability and atomization in a coaxial gas stream (Lasheras and Hopfinger), 2000, *Annu Rev. Fluid Mech*.
- Advances and challenges in droplet and spray combustion. I. Toward a unified theory of droplet aerothermochemistry (Chiu), 2000, *PECS*
- Spray measurement technology: a review (Fansler and Parrish, *Meas. Sci. Tech.,* 2015)

Topics:

1st hour-Dr. Agisilaos Kourmatzis

- Two-Phase Flows Considerations and basic definitions
- Unstable liquid-gas flows
- Atomization
- Sprays and spray combustion

2nd hour-A/Prof Matthew Cleary

- **Two-phase flow modelling**
- Combustion modelling
- Turbulence
- Droplet burning

Separated and transitional flows

Most models in the near-nozzle and primary atomisation region are based on either the Volume of Fluid (VOF) or Level Set (LS) concepts.

Both are called o*ne-fluid models* because there is a single Navier-Stokes equation

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial P}{\partial x_i} - \rho g_i = \sigma \kappa n_i \delta_I$$

VOF:

Solve equation for liquid volume fraction (neglecting phase change):

$$\frac{\partial \alpha}{\partial t} + u_i \frac{\partial \alpha}{\partial x_i} = 0$$

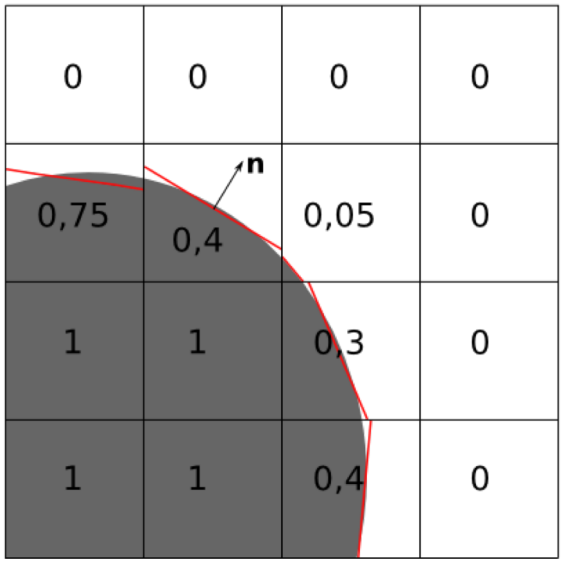
$\alpha(\boldsymbol{x}, t) = 0$ corresponds to pure gas

$\alpha(\boldsymbol{x}, t) = 1$ corresponds to pure liquid

$0 < \alpha(\boldsymbol{x}, t) < 1$ mixed cell, contains an interface

Density given by linear combination: $\rho = \alpha \rho_L + (1 - \alpha)\rho_G$

wikipedia



Smearing - special advection schemes for α.

Separated and transitional flows

LS:

The interface is defined implicitly as the iso-surface of a smooth function, ϕ, called the level set function.

Distance level set (traditional method):

$$|\phi(\boldsymbol{x}, t)| = |\boldsymbol{x} - \boldsymbol{x}_I|$$

$\phi(\boldsymbol{x}, t) < 0$ corresponds to one side of the interface

$\phi(\boldsymbol{x}, t) = 0$ corresponds to the interface

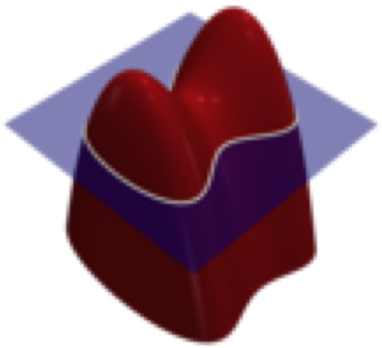
$\phi(\boldsymbol{x}, t) > 0$ corresponds to other side of the interface

Transport equation given by

$$\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = 0$$

Blending function used to smooth the density jump over a few cells around the interface.

wikipedia



Distortion, leading to non-smooth ϕ.

Special schemes to "re-initialise" ϕ.

Care needed, as the re-initialisation does not conserve mass.

Dispersed flows

Above methods do not account for interfacial shear at scales smaller than the numerical grid.

Problematic for dispersed sprays of small, heavy particles (large Stokes number).

Two-fluid models are cheaper and more accurate. Eulerian gas phase and Lagrangian point-particle dispersed phase.

For the liquid phase:

$$\frac{dx_{L,i}}{dt} = u_{L,i}$$

$$\frac{du_{L,i}}{dt} = \frac{u_{G,i} - u_{L,i}}{\tau} + g_i$$

$$\tau = \frac{1}{2} C_{drag} \frac{\rho_G}{\rho_L} \frac{A_L}{V_L} \left| u_{G,i} - u_{L,i} \right|$$

Additional terms if there is phase change.

For the gas phase:

$$\rho \frac{\partial u_{G,i}}{\partial t} + \rho u_{G,j} \frac{\partial u_{G,i}}{\partial x_j} - \frac{\partial \tau_{G,ij}}{\partial x_j} + \frac{\partial P}{\partial x_i} - \rho_G g_i = f_{drag}$$

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Scalar transport

Combustion modelling is conceptually very simple! We solve transport equations for reacting scalars.

Define a scalar field: $\phi = (\mathbf{Y}, \boldsymbol{N}, h) = (\text{mass fractions}, \text{number density}, \text{enthalpy})$.

Generic equation for scalar transport

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i \phi) - \frac{\partial}{\partial x_i}\left(\rho \mathcal{D} \frac{\partial}{\partial x_i}\phi\right) = \rho W_\phi$$

Assumes that particulate quantities move with the gas.

LHS is linear in ϕ.

Source terms are generally non-linear in ϕ:

- W_Y = chemical reaction rate, transfer rate from solid/liquid fuels;
- W_N = nucleation rate, breakage / agglomeration rate, … ;
- W_h = heat loss rate.

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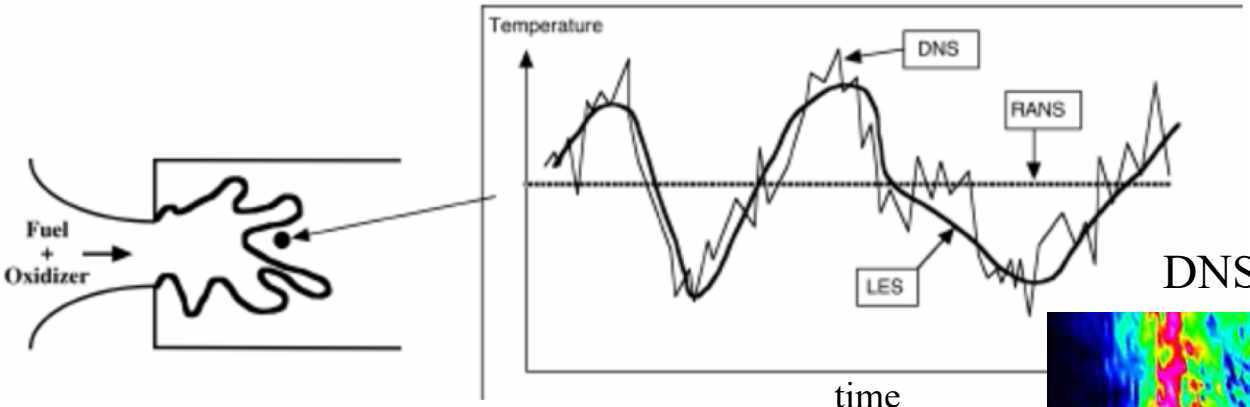
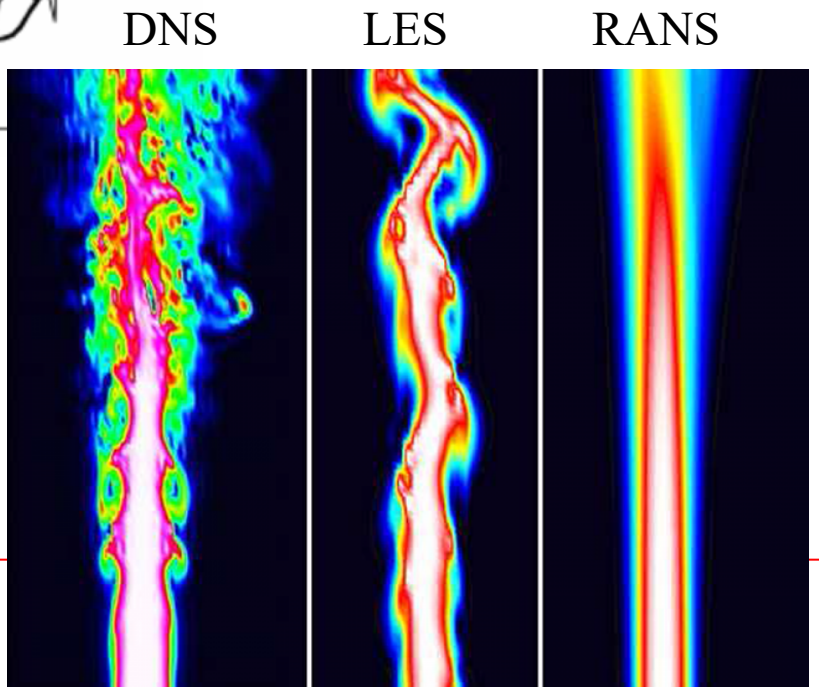
Turbulent flows and modelling strategies

Laminar flows can be viewed as having iso-layers with transport between the layers limited to molecular effects (i.e. viscous momentum exchange, and mass/heat diffusion).

If the Reynolds number is high enough, the layers are disrupted and chaotic variations in fluid velocity and scalar properties occurs.



Staffelbach et al., International Conference on High Performance Computing for Computational Science. Springer, Berlin, Heidelberg, 2008.

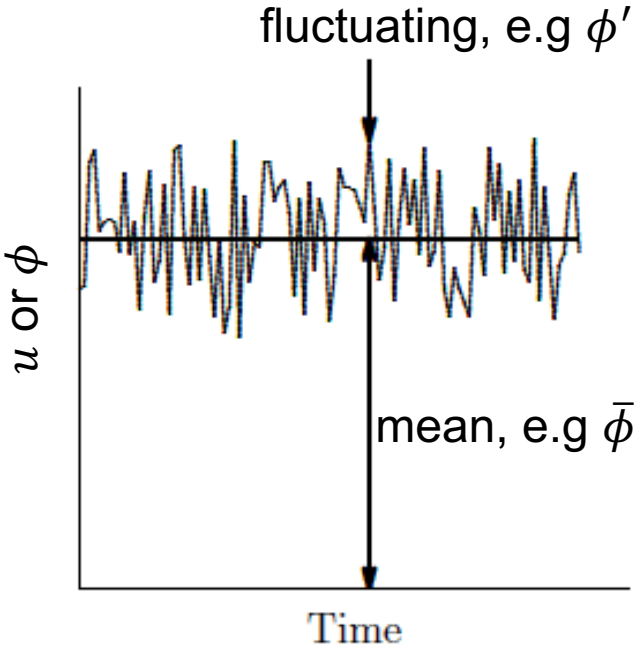


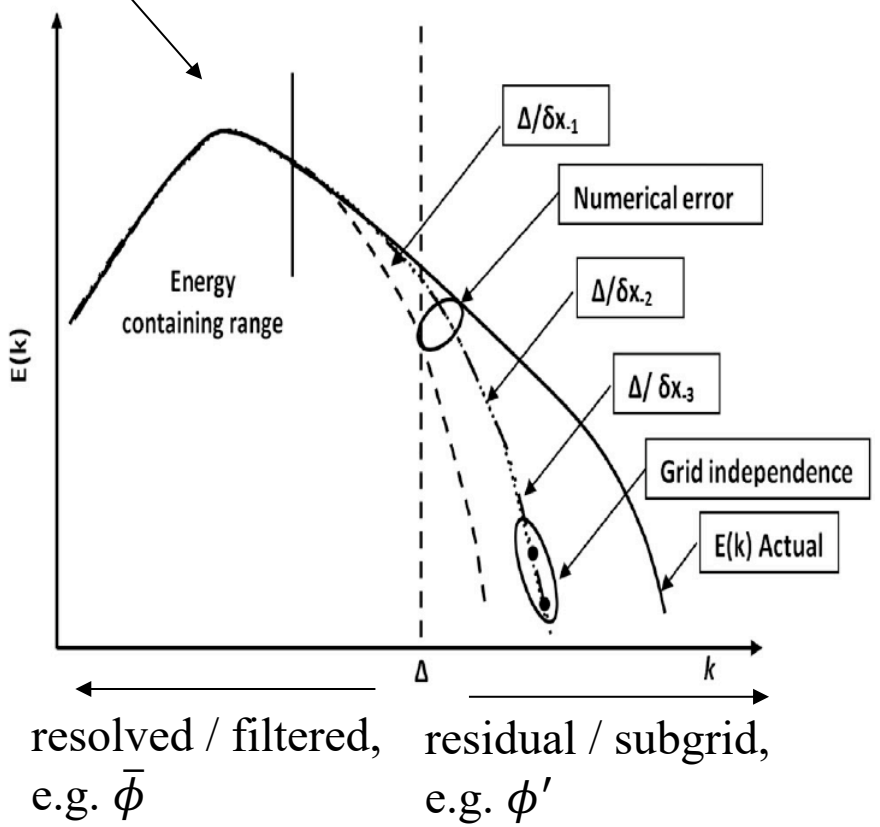
Maries, Adrian, et al., New Developments in the Visualization and Processing of Tensor Fields. Springer, Berlin, Heidelberg, 2012. 137-156.

Turbulent flows and modelling strategies

DNS is used for fundamental studies of canonical flows. (DNS of single-phase, laboratory jet flames is starting to emerge – see Evatt Hawkes et al. at UNSW)

Practical CFD relies on RANS (industry) and LES (research, some industry).





Sarwar, Mahfuz, et al., *International Journal of Heat and Fluid Flow* 65 (2017): 73-89.

Averaged / Filtered transport equations

RANS / LES deal with the moments of the statistical distribution.

Decompose ϕ and $\boldsymbol{u}$ into average/resolved and fluctuating/residual parts, e.g. $\phi = \bar{\phi} + \phi'$

Then spatially filter or average the transport equations:

$$\overline{\frac{\partial \rho\phi}{\partial t}} + \overline{\frac{\partial}{\partial x_i}(\rho u_i \phi)} - \overline{\frac{\partial}{\partial x_i}\left(\rho\mathcal{D}\frac{\partial}{\partial x_i}\phi\right)} = \overline{\rho W_\phi}$$

Favre average / filter introduced

$$\frac{\partial \bar{\rho}\tilde{\phi}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i}\tilde{\phi}\right) - \frac{\partial}{\partial x_i}\left(\bar{\rho}\mathcal{D}_e\frac{\partial}{\partial x_i}\tilde{\phi}\right) = \bar{\rho}\widetilde{W_\phi}$$

The source remains unclosed due to its non-linearity:

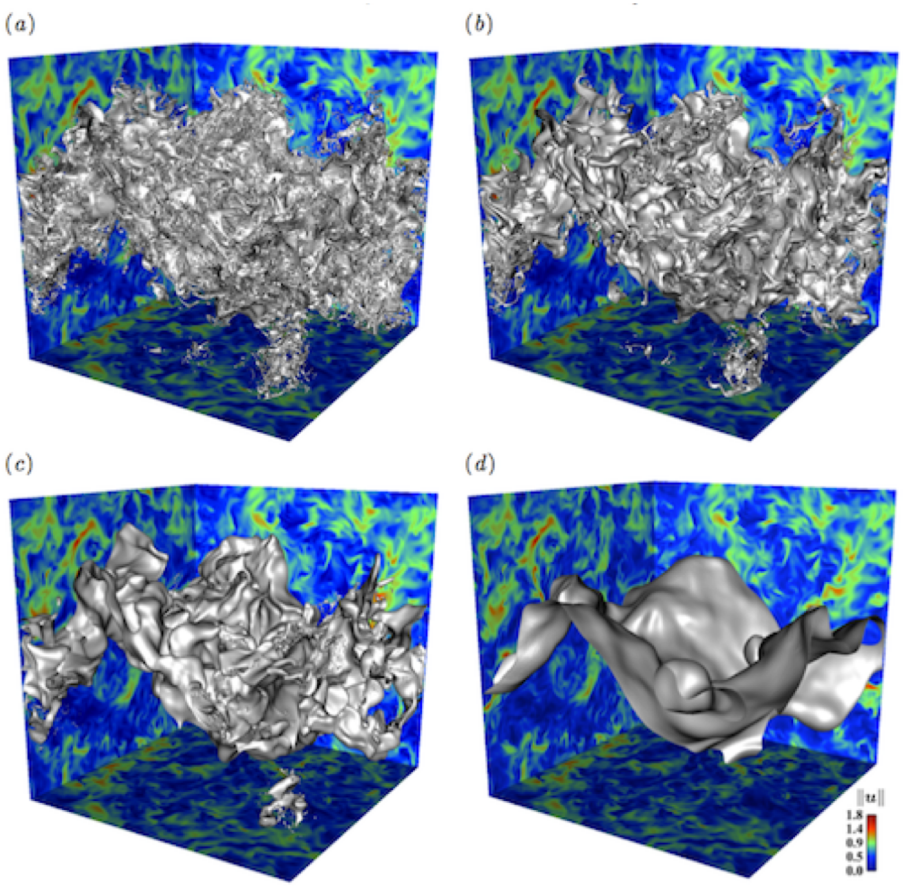
$$\widetilde{W_\phi(\phi)} \neq W_\phi(\tilde{\phi})$$

High order terms in Taylor series may be larger than leading order terms!

Averaged / Filtered transport equations

The same problem exists for two-phase flows. Interface between phases is not explicitly resolved, it fluctuates and the forces are multiscale and non-linear.

VOF and LS are grid sensitive. Some excellent work being done to improve numerical methods but quantitative DNS data is still elusive.



Direct numerical simulation of turbulence-interface interaction with different Weber numbers (surface tension force increases from (a) to (d)).

Olivier Desjardins, Cornell University
https://ctflab.mae.cornell.edu/atom4.html

Turbulent combustion models
1. Manifold methods – a) Flamesheets

Burke and Schumann developed the flamesheet concept in 1928.

Non-linearity is confined to an infinitely thin and fast reaction zone, by solving for a combined scalar

$$\beta = Y_F - \frac{1}{s}Y_O$$

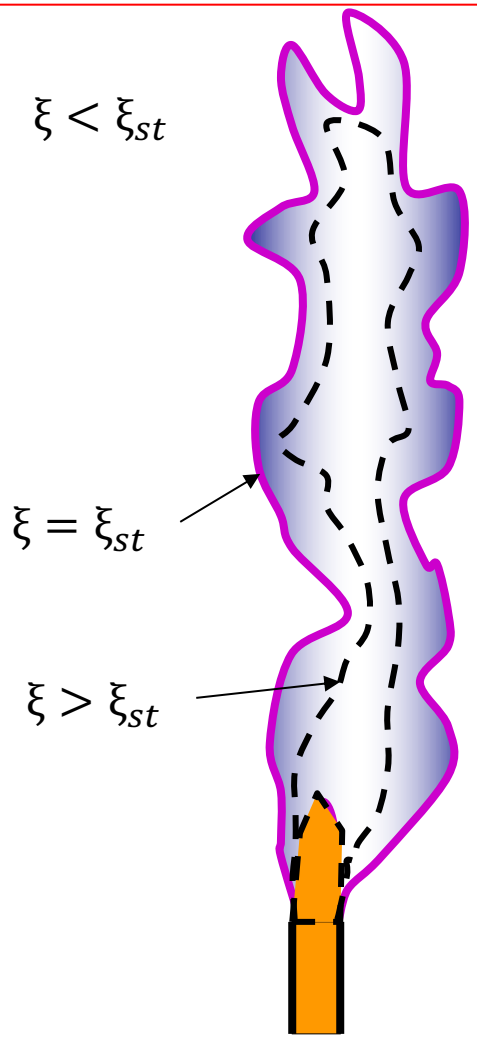
β is a conserved scalar. $W_\beta = 0$ everywhere and the equation for β is linear everywhere, even at the flamesheet.

Here , we define a normalised quantity (called the mixture fraction): $\xi = \frac{\beta - \beta_0}{\beta_1 - \beta_0}$

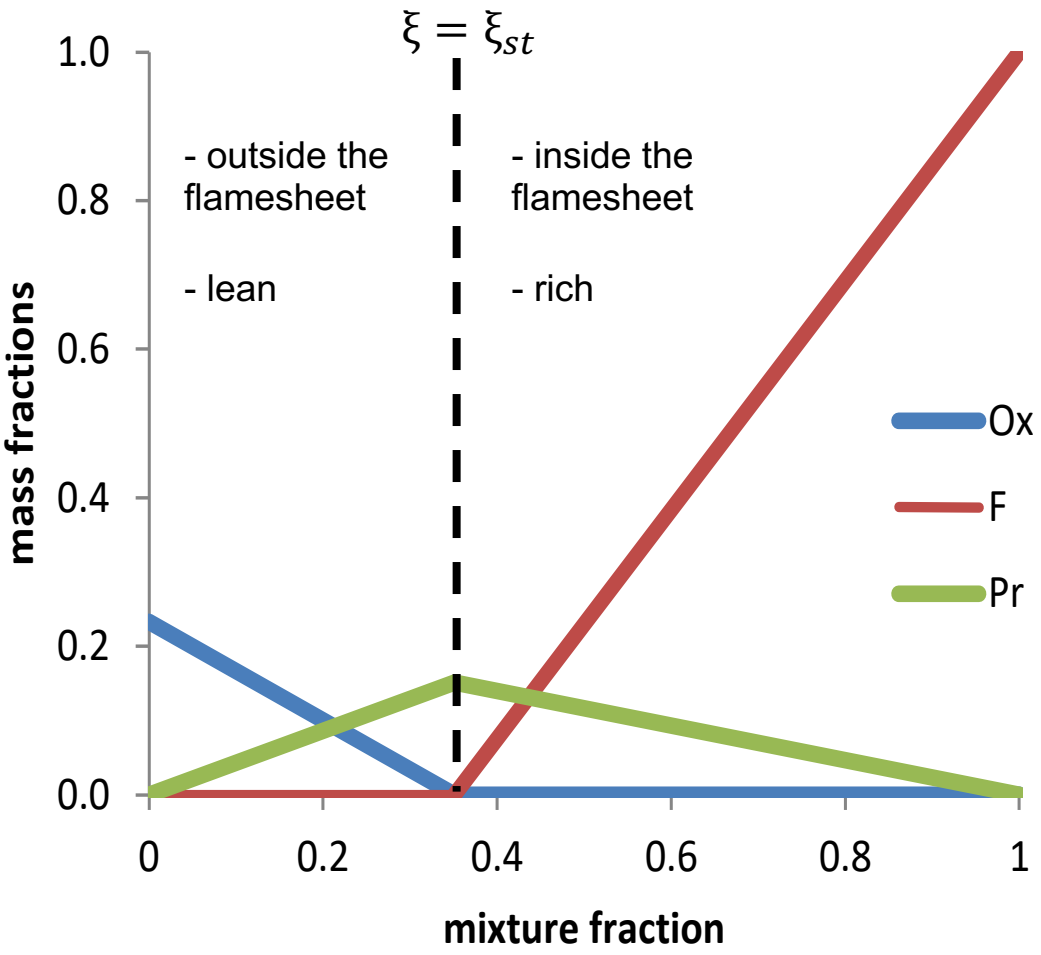
Averaged/filtered mixture fraction equation

$$\frac{\partial \bar{\rho}\tilde{\xi}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\tilde{\xi}\right) - \frac{\partial}{\partial x_i}\left(\bar{\rho}\mathcal{D}_e\frac{\partial}{\partial x_i}\tilde{\xi}\right) = 0$$

Turbulent combustion models
1. Manifold methods – a) Flamesheets



linear solution



Mean scalars: $\bar{\phi} = \int_a^b \phi(\xi) f(\xi)\, d\xi$

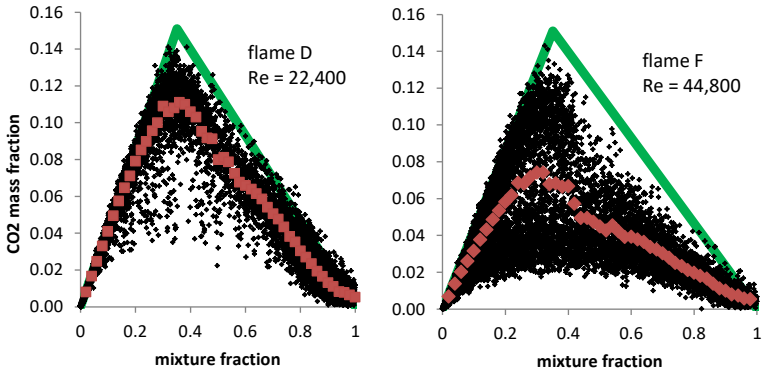
Turbulent combustion models
1. Manifold methods – b) CMC and flamelet

Conditional moment closure (CMC) and flamelet hypothesis:

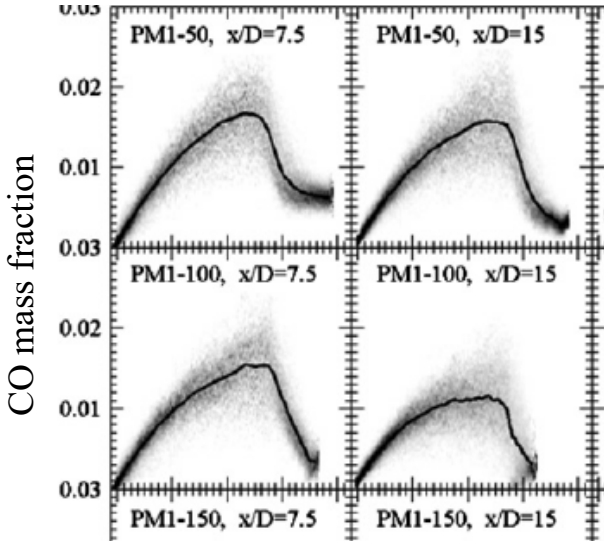
Although $\widetilde{W_\phi(\phi)} \neq W_\phi(\tilde{\phi})$, perhaps we can say that $\widetilde{W_\phi(\phi)}|\eta = W_\phi(\widetilde{\phi}|\eta)$

In non-premixed flames η is the mixture fraction and in premixed flames η is the temperature (or similar).

Generally, η is a low-dimensional manifold.



Barlow & Frank, Proc. Combust. Inst. 27 (1998)



Dunn, Masri, Bilger, Barlow, Wang, Proc. Combust. Inst. 32 (2009)

Turbulent combustion models
2. Probability density function (PDF) models

Probability density function (PDF) methods deal with the full statistical distributions.

Can model either

the joint PDF of both ϕ and $\boldsymbol{u}$

OR

the PDF of ϕ and use RANS / LES for the moments of $\boldsymbol{u}$.

Define the PDF as*

$$\int_a^b f_\phi(\psi; x, t)\, d\psi = Prob(a \le \phi < b)$$

Its transport equation is*:

closed form

unclosed, mixing models

$$\frac{\partial \bar{\rho} f_\phi}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i f_\phi - \bar{\rho}\mathcal{D}_e \frac{\partial f_\phi}{\partial x_i}\right) + \frac{\partial \bar{\rho} W_\alpha f_\phi}{\partial \psi_\alpha} = -\frac{\partial}{\partial \psi_\alpha \partial \psi_\beta}\left(\bar{\rho}\mathcal{D}\,\overline{\frac{\partial \phi_\alpha}{\partial x_i}\frac{\partial \phi_\beta}{\partial x_i}\,|\psi}\;\; f_\phi\right)$$

* Different interpretations for RANS and LES, but similar formulation

Turbulent combustion models
2. Probability density function (PDF) models

The PDF transport equation has as many dimensions as there are elements in ϕ.

Noting its similarity to the Fokker-Planck equation, it can be recast in stochastic form:

$$dx_i^{\ p} = \left[\tilde{u}_i + \frac{1}{\bar{\rho}}\frac{\partial}{\partial x_i}(\bar{\rho}\mathcal{D}_e)\right]^p dt + \left[\sqrt{2\mathcal{D}_e}\right]^p d\omega_i^{\ p} \quad (1)$$

$$d\phi^p = \left[W_\phi + S_\phi\right]^p dt \quad (2)$$

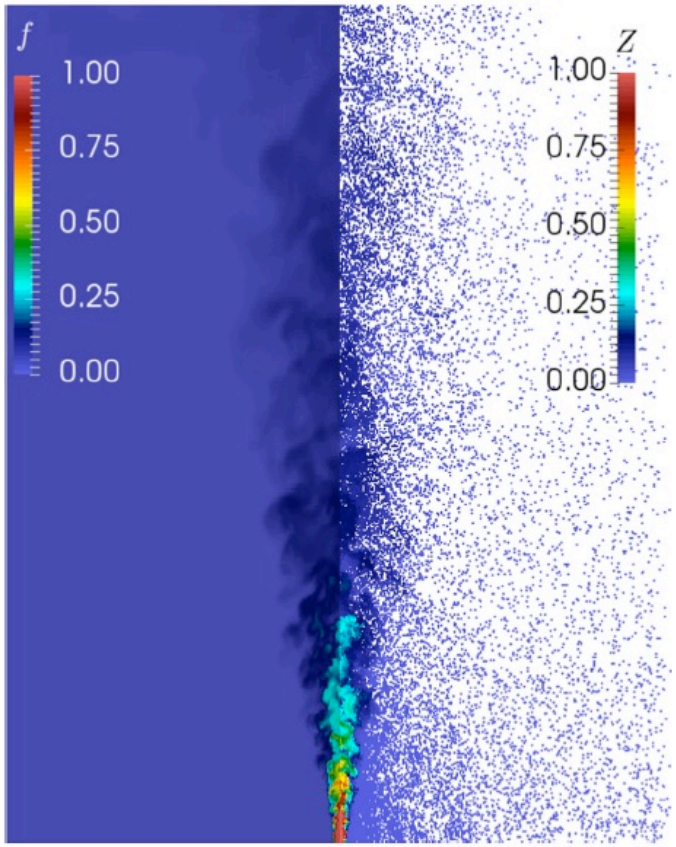
$$\overline{S_\phi|\boldsymbol{X}} = 0 \quad (3)$$

Solve Eq. (1) and (2) for an ensemble of notional particles. Constraint given by Eq. (3) is imposed by mixing between particles within a grid cell or that are local in composition space.

Usually interested in the moments of the distribution, e.g.

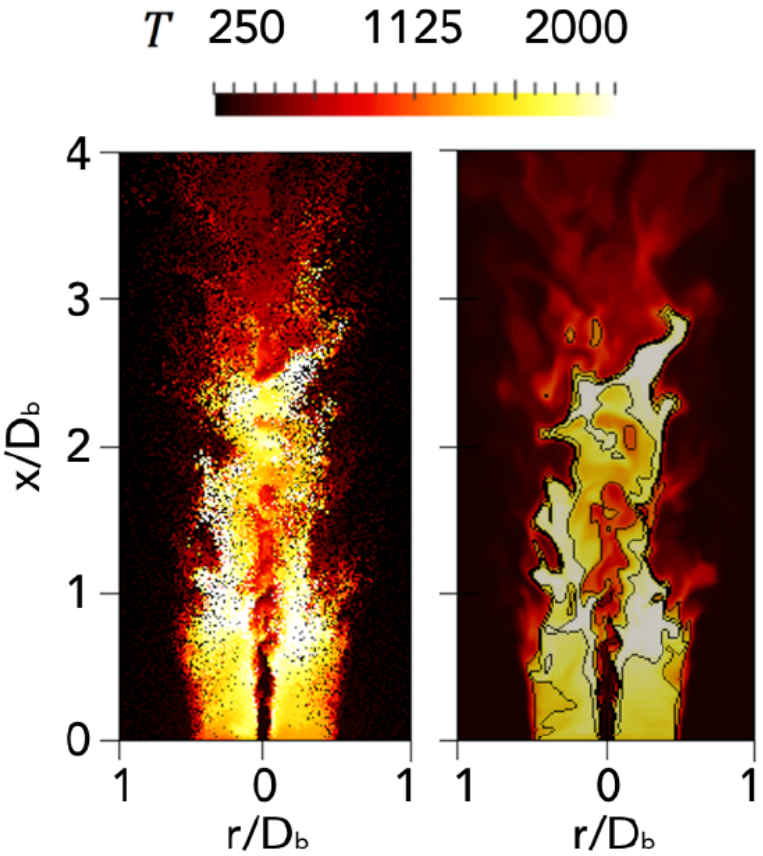
$$\bar{\phi} = \frac{1}{m_{tot}}\sum_{p=1}^{N} m^p \phi^p$$

Turbulent combustion models
2. Probability density function (PDF) models



Jet flame. Turbulent mixture fraction fields by a finite volume method (left) and a sparse stochastic method (right).

Neuber, Kronenburg, Stein, and Cleary, Chem. Eng. Sci., 2017.



Swirl flame. Instantaneous stochastic particle temperature field (left) and Eulerian equivalent temperature field (right).

Huo, Salehi, Galindo, Cleary, Masri, Proc. Combust. Inst, submitted 2017.

Turbulent atomisation models – separated and transitional regions

Let's look again at the VOF method.

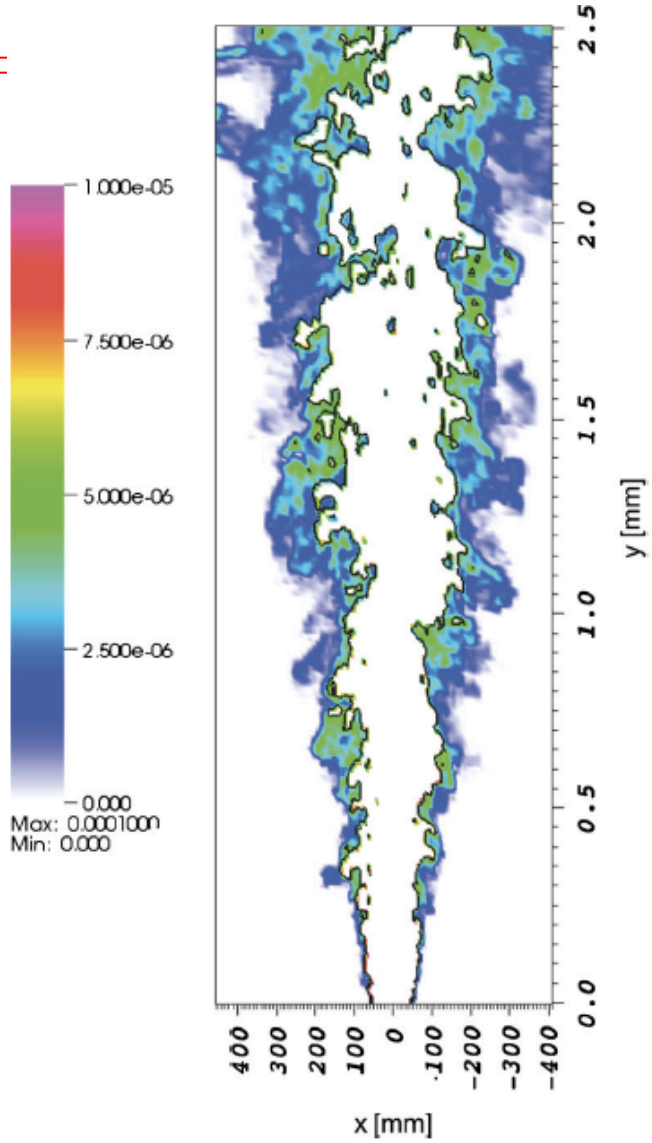
The Eulerian-Lagrangian Liquid Atomisation model (ELSA) models both α and surface density, Σ.

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial u_i \Sigma}{\partial x_i} = \sum n_j n_i \frac{\partial u_j}{\partial x_i} = W_\Sigma$$

SMD: $d_{32} = \frac{6\alpha}{\Sigma}$; Curvature: $\kappa = -\nabla \cdot \boldsymbol{n} \approx \frac{\boldsymbol{\Sigma}}{\boldsymbol{\alpha}}$

In a turbulent flow, α and Σ are going to fluctuate at scales smaller than the grid (unless DNS is used). Navarro-Martinez (2014) introduced an Eulerian PDF form of ELSA.

Solve joint PDF, f_ϕ, where $\phi = (\alpha, \Sigma)$. PDF of SMD and curvature easily obtained.



Mean d_{32} in an atomising jet. Navarro-Martinez, Int. J. Mult. Flow (2014).

Turbulent atomisation models – dispersed regions

Modelling of turbulent dispersed sprays is much better understood. Again, the PDF concept is very powerful - see the excellent review by Minier and Peirano (2001).

A related concept, which combines population balance equation modelling and the PDF method, was recently developed by Salehi, Cleary and Masri (2017).

Need a turbulent dispersion and break-up model that provides statistical distributions of droplet size and shape; $N(v, s)$.

$$\frac{\partial N}{\partial t} + \frac{\partial}{\partial x_i}(u_i N) + \frac{\partial}{\partial v}(\dot{v} N) + \frac{\partial}{\partial s}(\dot{s} N) = W_N$$

Following normal procedure, derive an equation for the PDF of number density, f_N, and recast it in stochastic form and solve on ensemble of stochastic particles.

$$dx_i^p = u_i^p \; dt$$

$$du_i^p = a_i^p \; dt$$

$$dN^p = {W_N}^p dt$$

Turbulent atomisation models – dispersed regions

Acceleration given by particle timescale:

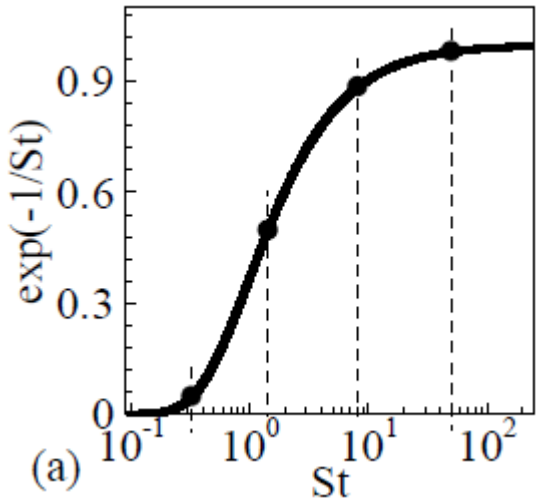
$$du_i^p = a_i^p \, dt$$

$$a_i^p = \frac{1}{\langle \tau \rangle}\left(u_{f,i}^p - u_i^p\right)$$

In general, the ensemble of stochastic particles needs to be partitioned.

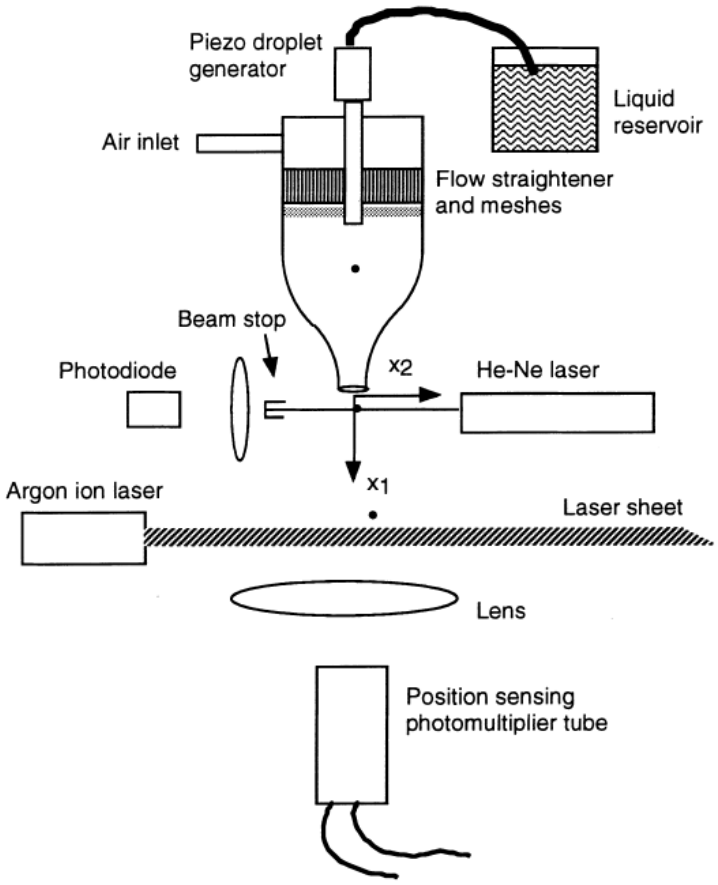
Integrate velocity, taking into account the model for acceleration leads to

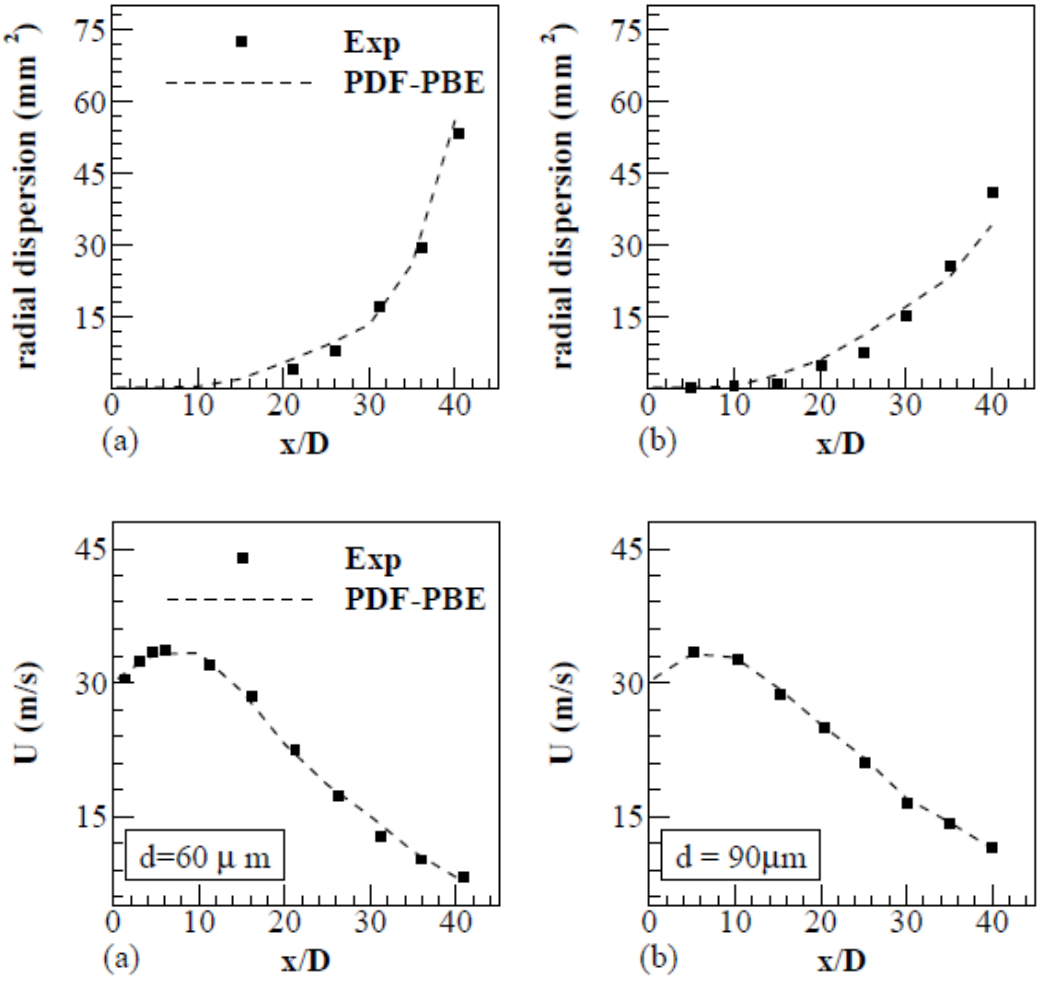
$$u_i{}^p(t_0 + \tau_f) = u_i{}^p(t_0) + \left(u_i{}^p(t_0) - u_{f,i}{}^p\right)\left(\exp\left(-\frac{1}{\langle St \rangle}\right) - 1\right)$$



Dynamically partition the ensemble into Stokes bins.

Turbulent atomisation models – dispersed regions





Salehi, Cleary, Masri, J. Fluid Mech. (2017).

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- **Droplet burning**

Single droplet combustion

Droplet heat and mass transfer rates are determined by composition and enthalpy gradients at the droplet surface.

These gradients are never known explicitly*.

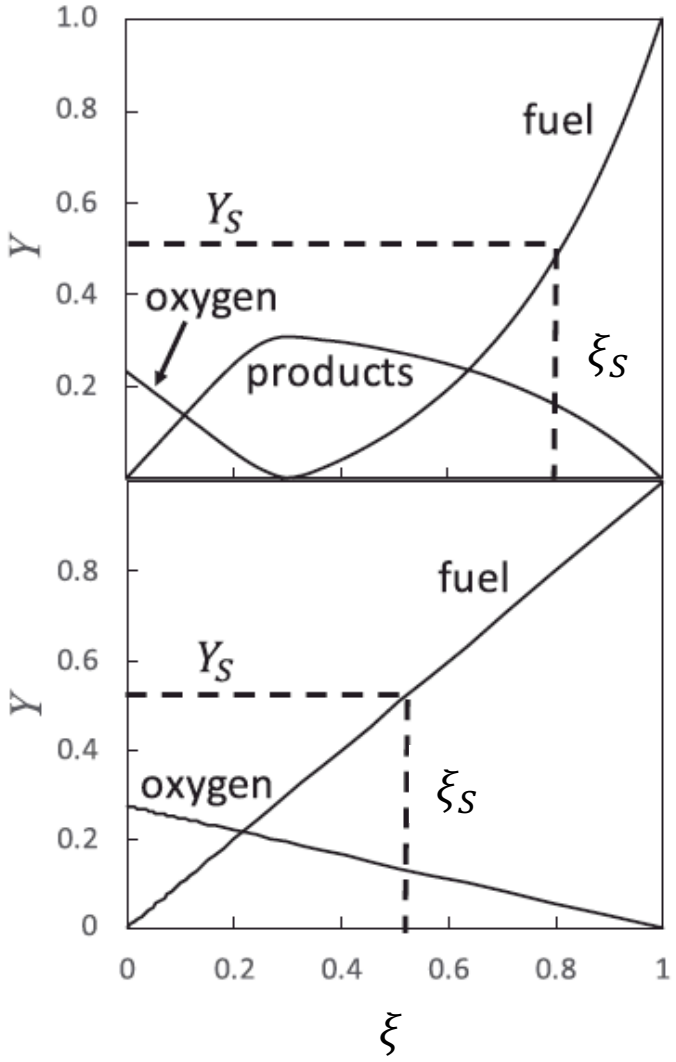
Conserved scalars and the flamesheet concept (Burke and Schumann, 1928) provides an elegant solution.

$$\dot{m}_L = \frac{\rho \mathcal{D}}{\delta} ln(1 + B_M)$$

$$B_M = \frac{\xi_G - \xi_S}{\xi_S - 1} \quad \text{if burning in air} \left(B_M = \frac{\xi_S}{1 - \xi_S} \right)$$

Spalding derived this in 1953, but almost all modern publications use non-conserved scalar relations.

Khan et al. demonstrate this simple model in the context of PDF modelling of a turbulent spray flame.



* Carrier-phase DNS does not resolve the boundary layer. Fully resolved DNS is very rare.

Modelling summary

- Two-phase flow models divided into those used in the separated and transition regions (Volume of Fluid and Level Set methods) and those used in the dispersed region (Lagrangian point-particle method).
- Combustion modelling is conceptually simple; solving the scalar transport equation is much easier than solving the Navier-Stokes equation.
- Both two-phase and combustion modelling become challenging when turbulence is added. The problem is the closure of averaged / filtered forms of the non-linear source terms.
- Turbulent combustion modelling has two broad approaches – manifold methods and PDF methods.
- Manifolds are simple and remain useful as submodels in sprays with isolated burning droplets (as long as researchers don't forget the past!).
- PDF methods are more complex but are superior to other methods as they eradicate the primary closure problem.
- PDF methods are relatively new for separated and transitional regions of two-phase flows. Cost and grid sensitivity of VOF and LS methods should drive further PDF development.
- PDF methods for dispersed two-phase flows are mature but new, computational efficient methods are still being developed.

Modelling papers you should read

- Hirt CW, Nichols BD. Volume of fluid (VOF) method for the dynamics of free boundaries. Journal of computational physics. 1981;39:201-25.
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