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Droplet Breakup & Evaporation

AAE-E3030 Numerical Modeling of Multiphase Flows
4.3.2019

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Motivation

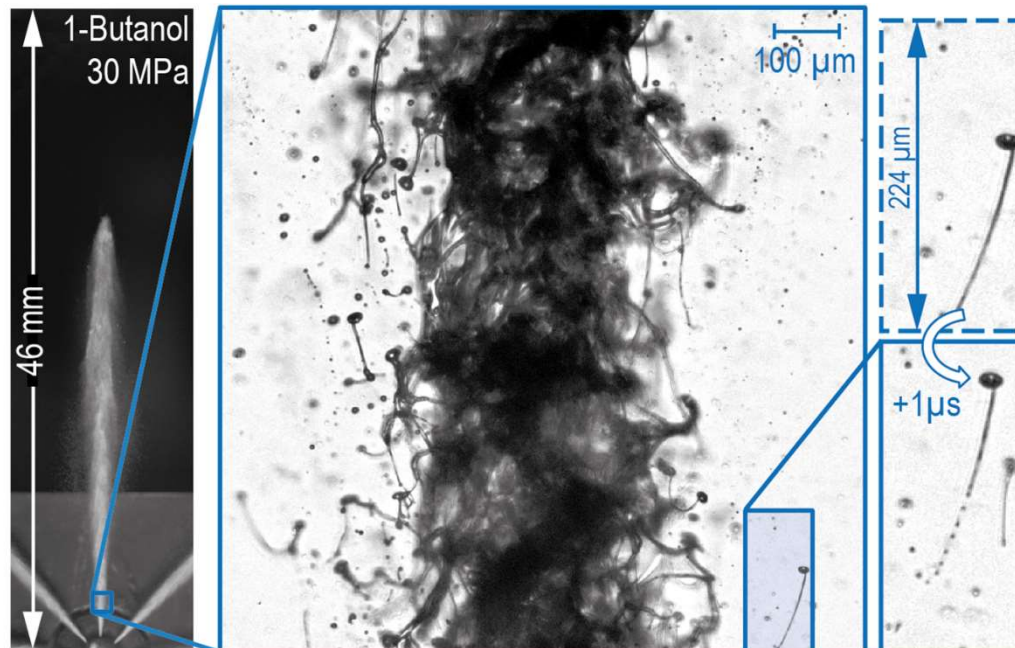
- **Why learn about the modeling of fuel sprays ?**
- **Modeling increases our understanding of sprays**
- **We can predict real life scenarios**
- **We can plan experiments**
- **We can improve the injection process**
- **We can reduce emissions**

Contents

- **Spray breakup phenomena**
- **Droplet evaporation**

Atomization and breakup

- **Basically two different phenomena**
- **Atomization: liquid column breaks up into various size ligaments, blobs, and droplets**
- **Secondary breakup: Already broken up droplets (or bigger structures) breakup again into smaller droplets**



Atomization

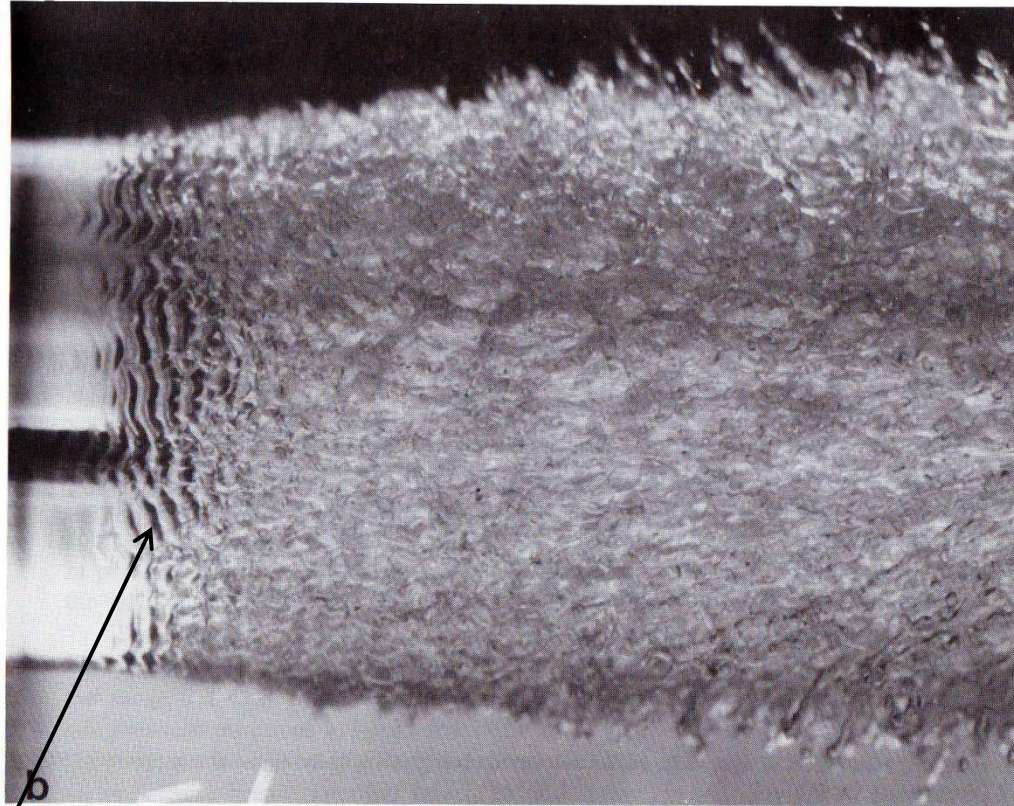


Figure by A.H. Lefebvre, Atomization and Sprays

K-H instability (discussed previously)



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Initial Drop Size Distributions

- **If only large (~ nozzle hole size) droplets are used for injection, this may not lead to totally realistic evaporation behavior.**

- **Power law**

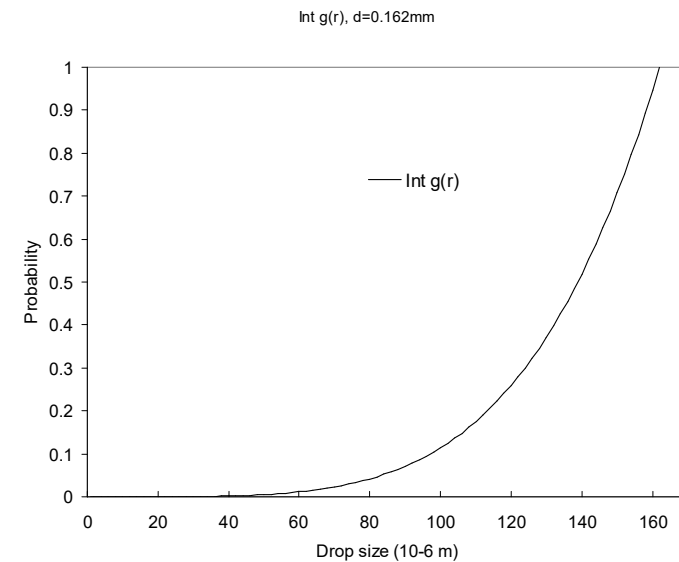
$$g(r) = \frac{n+4}{r_0} \left(\frac{r}{r_0} \right)^{n+3}$$

where r is drop radius and r_0 nozzle radius, and n is a coefficient, typically $n=0.5$.

- **Rosin-Rammler**

$$1 - Q = \exp\left(-\left(\frac{d}{X}\right)^q\right)$$

where d is drop diameter, Q is the fraction of the total volume contained in drops of diameter less than d , and X and q are constants. q is typically between 1.5...4. X is a drop diameter such that a certain fraction of the total volume is below the diameter.



Spray Breakup Mechanisms

Current view of the most important mechanisms leading to spray/droplet atomization and breakup:

- **Aerodynamic breakup**
- **Cavitation**
- **Nozzle turbulence induced instabilities**

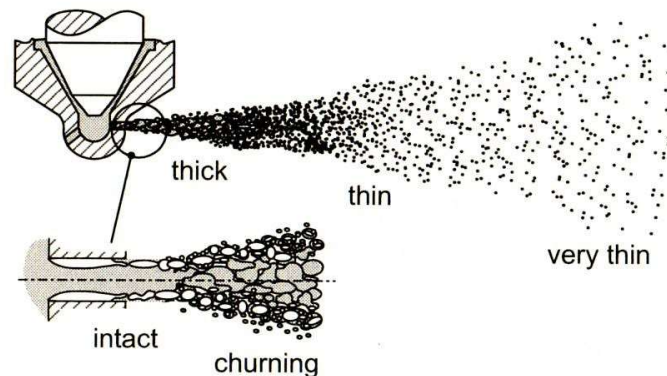




















Fig. 5.2. Schematic illustration of different flow regimes

Droplet Breakup

- Atomization → Secondary breakup

$$We = \frac{\rho_g d u_{rel}^2}{\sigma}$$

					Weber number			
We	↓	a) vibrational breakup	→ ○			~ 12		
		b) bag breakup	→ ○					< ~ 25
		c) bag / streamer breakup	→ ○					< ~ 50
		d) stripping breakup	→ ○					< ~ 100
		e) catastrophic breakup	→ ○					> ~ 100

Droplet Breakup

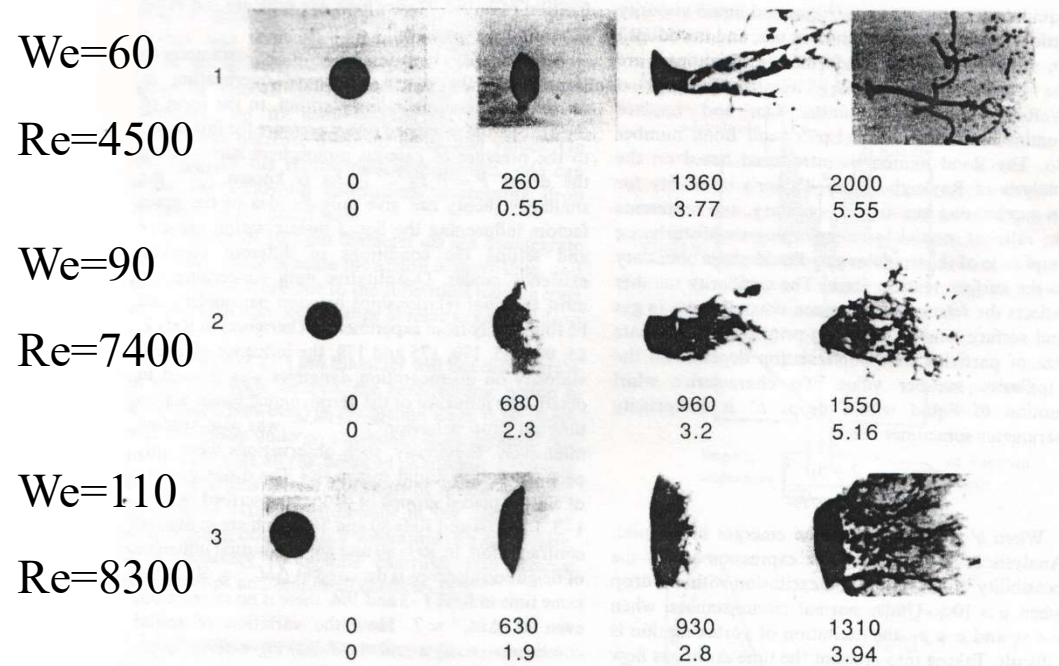
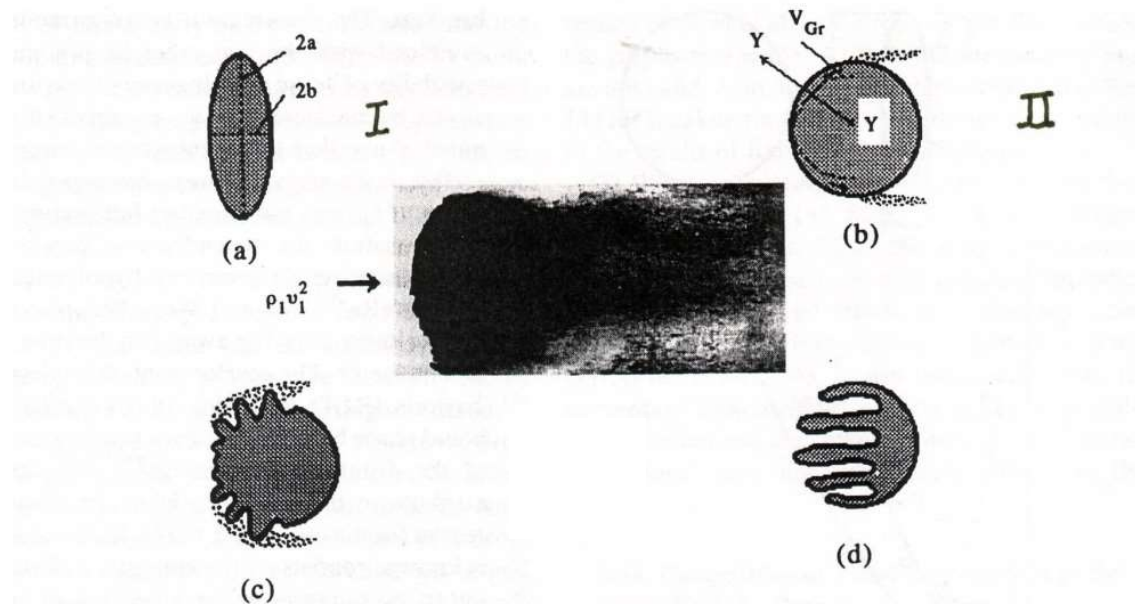


Fig. 12. Photographic sequence of viscous liquid (water + glycerine solution) droplet breakup by 'parachute + stamen' mode (photographs 1) and by the stripping of the thin liquid surface layer (photographs 2). Upper line of numbers—time in μsec , lower line of numbers—nondimensional time $\tau = t\tau_0^{-1}$.

Droplet Breakup



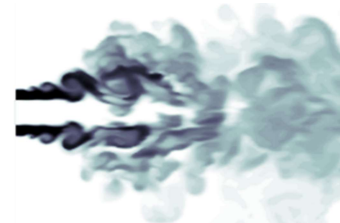
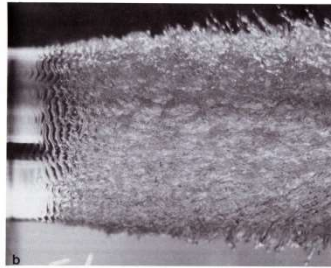
The main hydrodynamic phenomena accompanying droplet breakup: **(a)** deformation of droplet, **(b)** formation of boundary layer 'gas + liquid', **(c)** surface wave formation by Kelvin-Helmholtz (KH) instability, **(d)** surface wave formation by Rayleigh-Taylor (RT) instability



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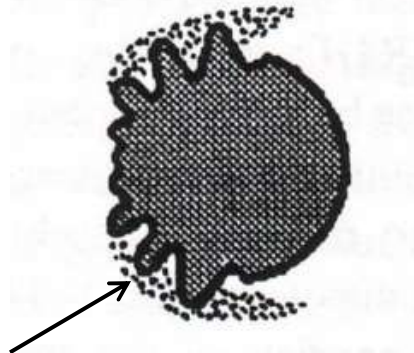
Kelvin-Helmholtz Instabilities

- **Already discussed with the context of jets and primary atomization**



Vuorinen, 2011

- **Can also be associated with droplet breakup**



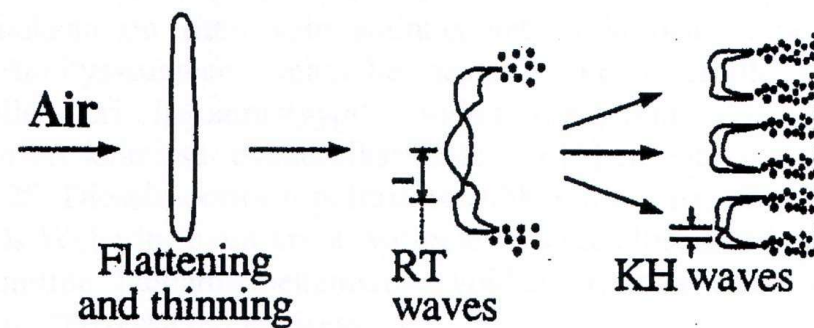
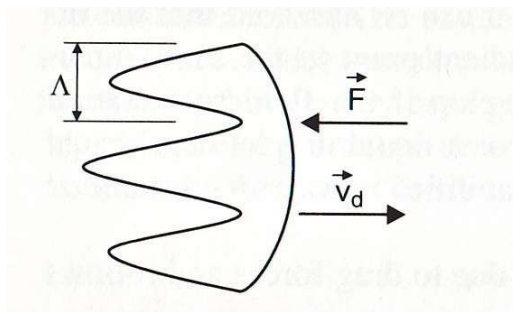
- **K-H wave formation leading to stripping breakup**



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Rayleigh-Taylor Instabilities

- **The Rayleigh-Taylor mechanism is incorporated into some breakup models.**
- **Typically R-T instabilities account for the large droplet formation near the nozzle.**
- **The K-H instabilities form the small droplets due to surface stripping.**

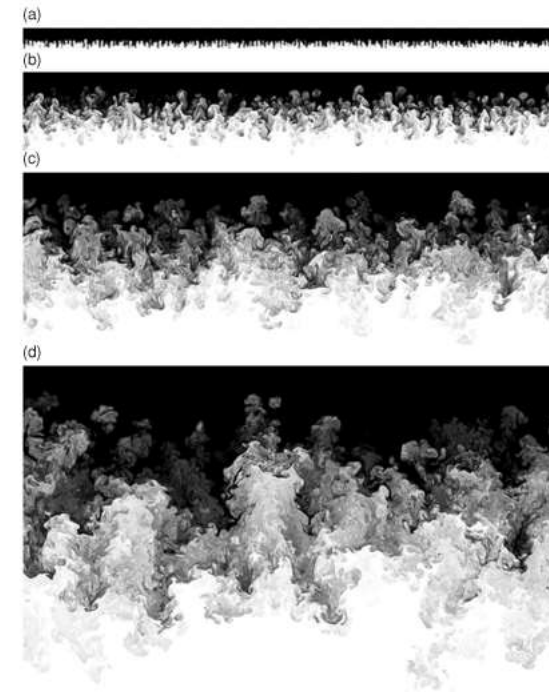
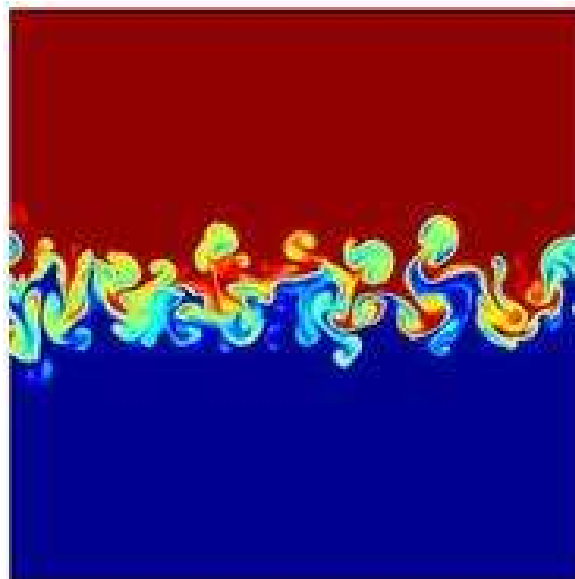




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Rayleigh-Taylor Instabilities

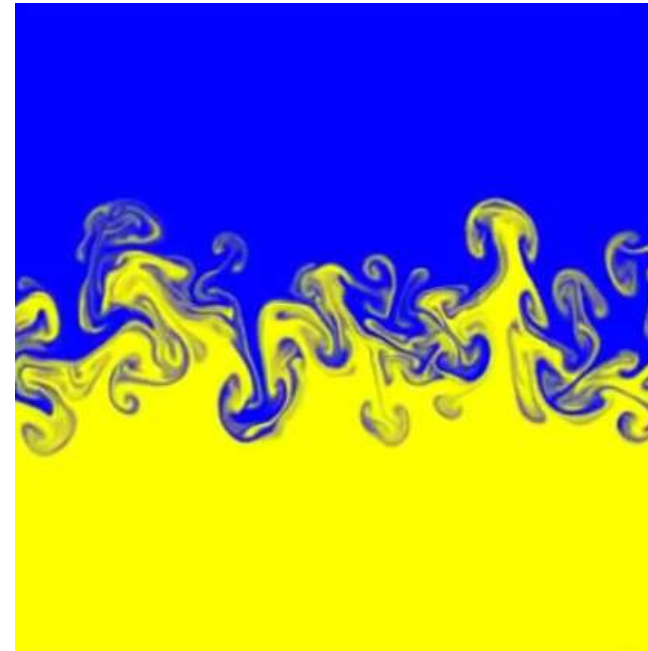
- **Occurs between fluids with different densities**
- **E.g. heavier fluid on top of lighter fluid. Gravity pulls the heavier fluid into the lighter one.**





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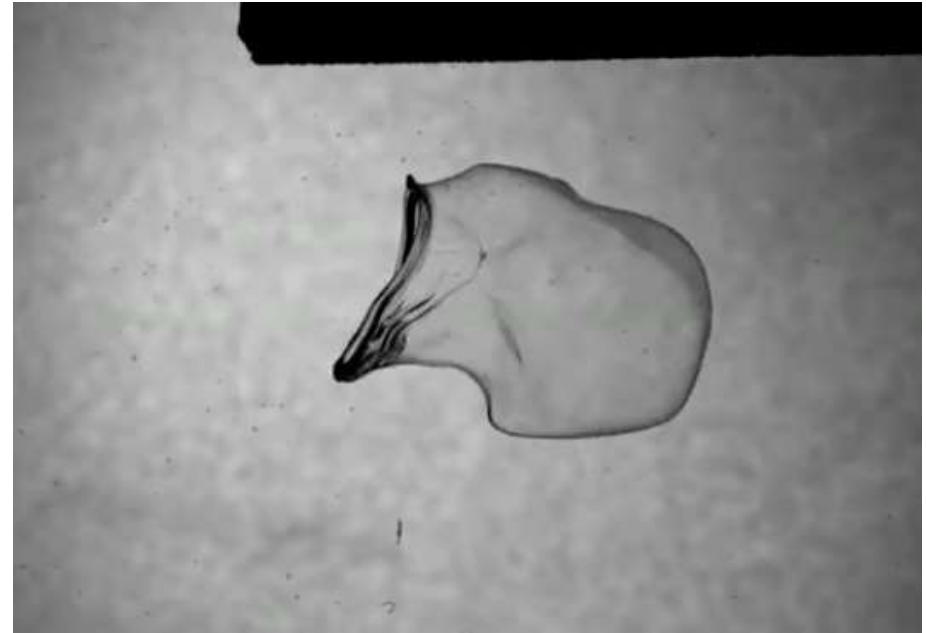
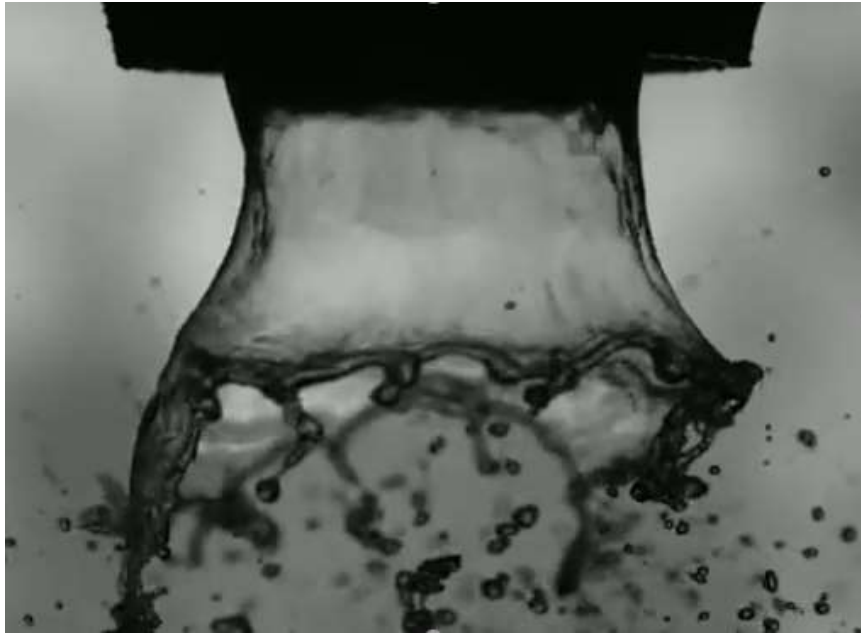
Rayleigh-Taylor Instabilities





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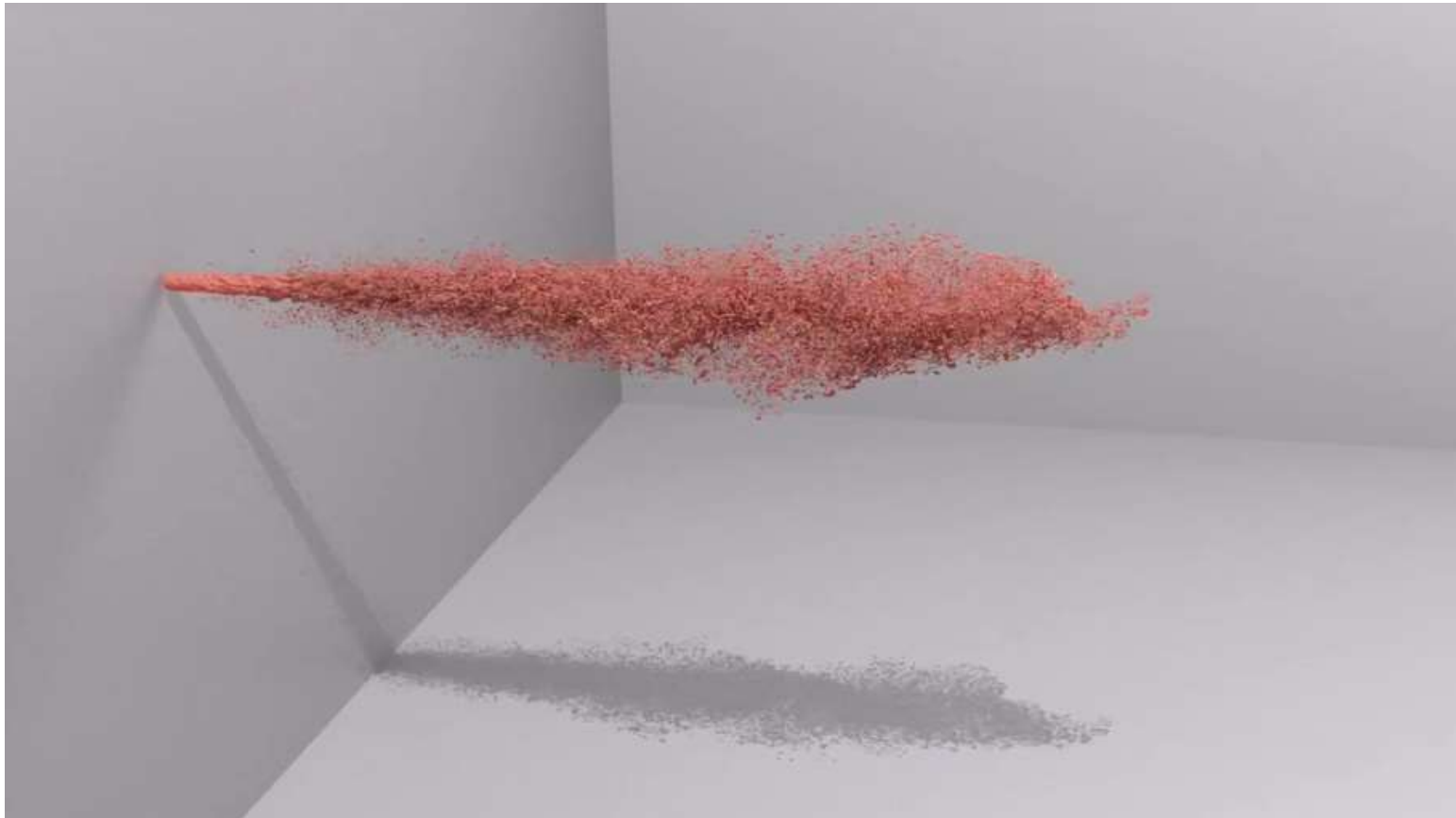
Atomization & Droplet Breakup





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Atomization & Droplet Breakup





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Droplet Breakup Modeling

- **Reitz-Diwakar model**

- **Breakup rate**
$$\frac{d(d)}{dt} = \frac{d - d_s}{\tau_b}$$

where τ_b is the breakup time scale and d_s is the stable droplet size .

- **For bag breakup, $We > 12$, the time scale is**
$$\tau_b = \frac{\pi \rho_l^{1/2} d^{3/2}}{4 \sigma^{1/2}}$$

- **For stripping breakup, $\frac{We}{\sqrt{Re}} > 0.5$, the time scale is**

- $$\tau_b = \frac{C_s}{2} \left(\frac{\rho_l}{\rho_g} \right)^{1/2} \frac{d}{|u - u_d|}$$
 , typically $C_s = 20$ (ranging between 2...30)



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Droplet Breakup Modeling

- From $\frac{d(d)}{dt} = \frac{d - d_s}{\tau_b}$ we get

$$d_2 = d_1 - \frac{d_1 - d_s}{\tau_b} dt \quad (3)$$

- **Eq. (3) can be used to assess the droplet breakup process.**
- **The stable Weber -number is obtained by assuming $We=12$ and calculating the equivalent droplet size.**



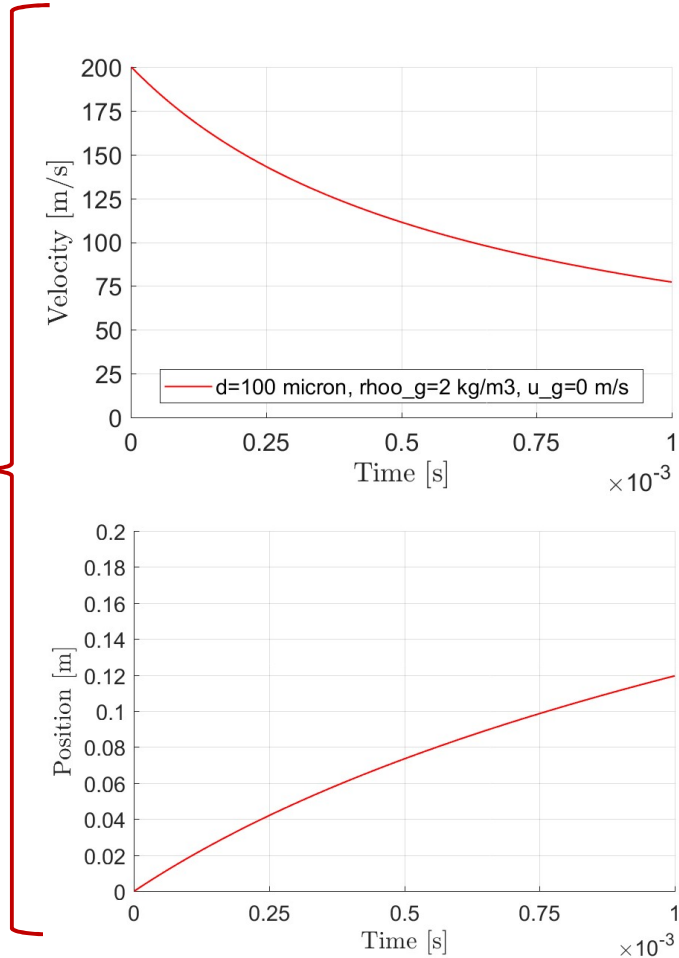
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Exercise

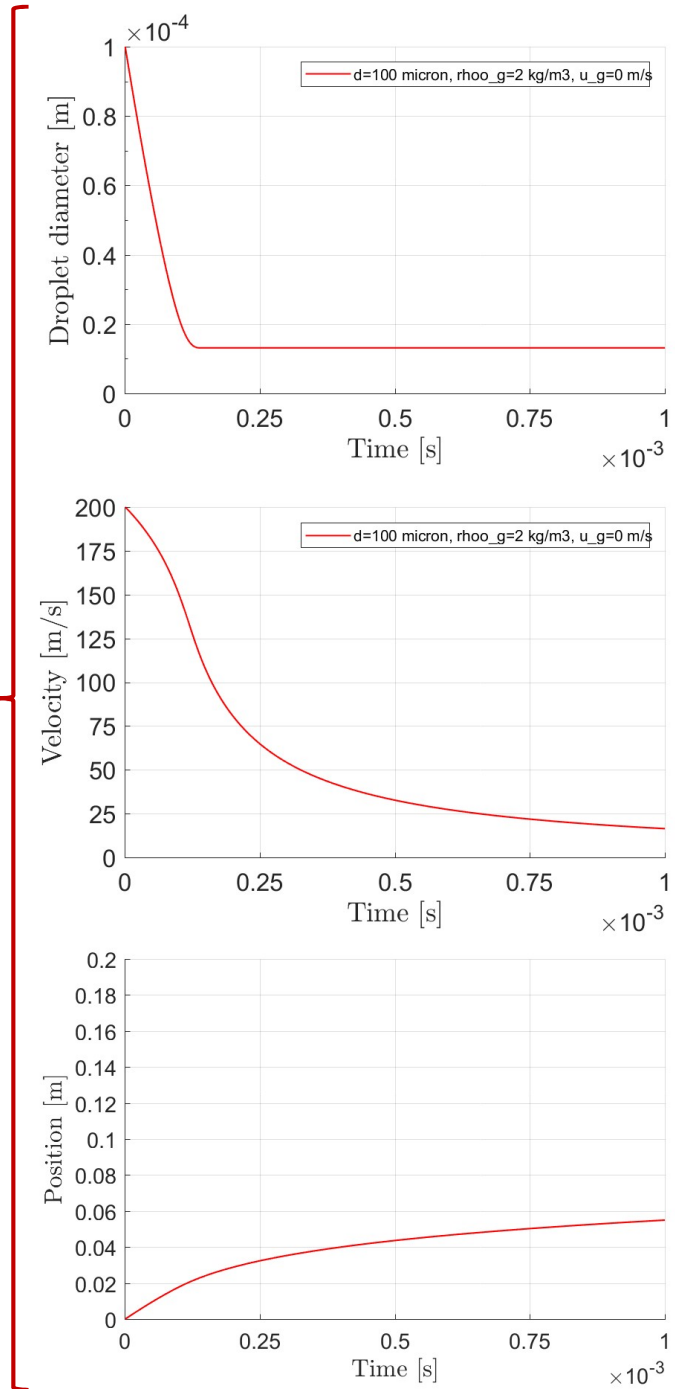
- **Droplet Weber number** $We = \frac{d \rho_g |u - u_p|^2}{\sigma}$ **is 20 and Reynolds number is 300. Fuel density is 800kg/m³, gas density is 1.2 kg/m³, surface tension is 0.03 N/m. The gas velocity is 100 m/s and the droplet velocity is 200 m/s. Droplet diameter is 50 μm**
- **Calculate**
 - 1. What is the stable droplet size (We=12) ?**
 - 2. Bag or stripping type of breakup mode ?**
 - 3. Calculate the new droplet diameter after one breakup. Dt=10 μs .**

0d Matlab results

No
breakup



Breaking
up drops





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Droplet breakup Modeling

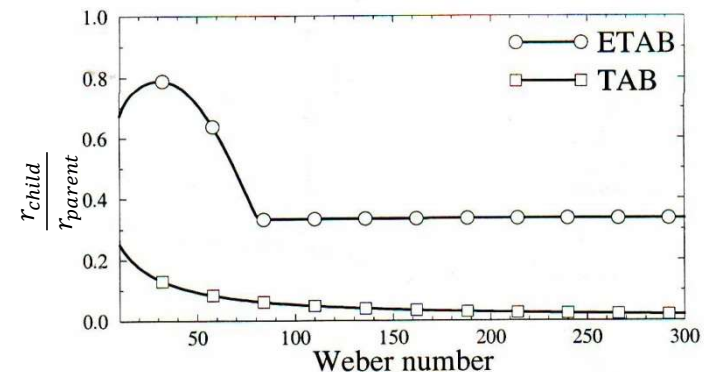
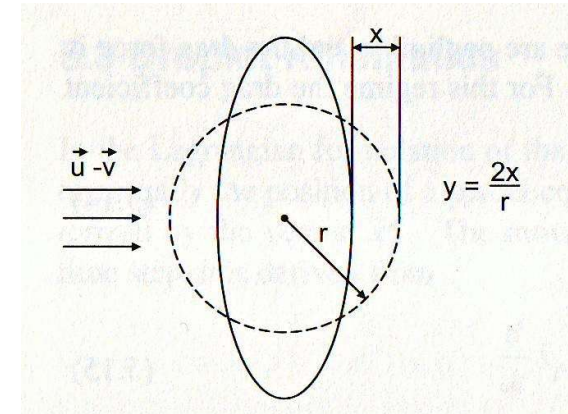
- **ETAB model**
- **Distortion of droplet by drop deformation parameter** $y = 2x/r$
- **Equation for y is given by the harmonic oscillator**

$$\ddot{y} + \frac{5\mu_l}{\rho_l r^2} \dot{y} + \frac{8\sigma}{\rho_l r^3} y = \frac{2\rho_g |U^2|}{3\rho_l r^2}$$

- **This can be solved for y**
- **The main idea of ETAB is to delay the first drop breakup in order to yield bigger droplets after breakup as the TAB model predicts generally too small droplets**
- **This is done by initializing drops with negative deformation velocity $\dot{y}(0) < 0$**
- **The breakup rate** $r_{child} = r_{parent} e^{-K_{br} t}$ **where**

$$K_{br} = \begin{cases} k_1 \omega & \text{if } We \leq We_t \\ k_2 \omega \sqrt{We} & \text{if } We > We_t \end{cases}$$

We_t is the transition We -number (typically assumed $We_t \sim 80$) between bag and stripping breakup, $k_1 = k_2 = 2/9$, $\omega = 8\sigma/\rho_l r^3 - 1/t_d^3$ and $t_d = 2\rho_l r^3/5\mu_l$

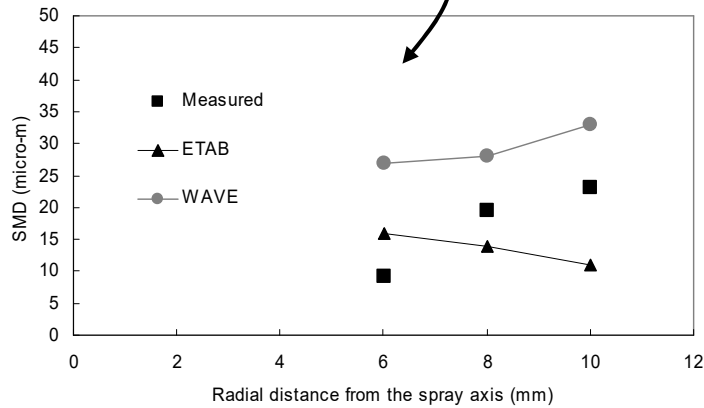
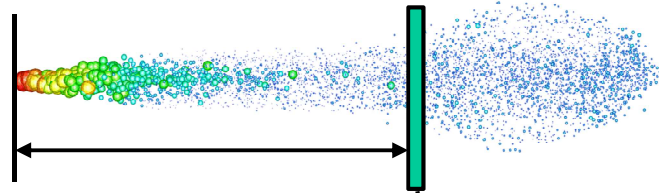




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Some Results

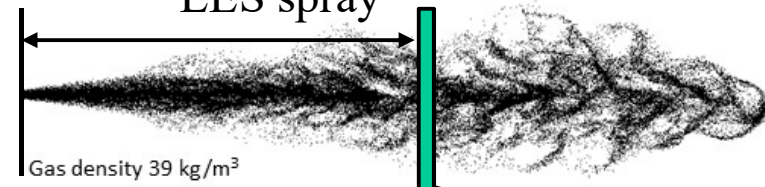
RANS spray



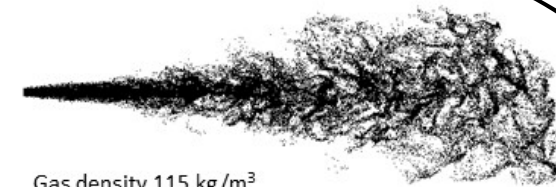
Kaario et al., Ilass 2002

- All SMD results are about 60mm from the nozzle
- At this distance, the correspondence between experiments and measurements is rather good
- However, little is known about the rate of breakup before the measurement point

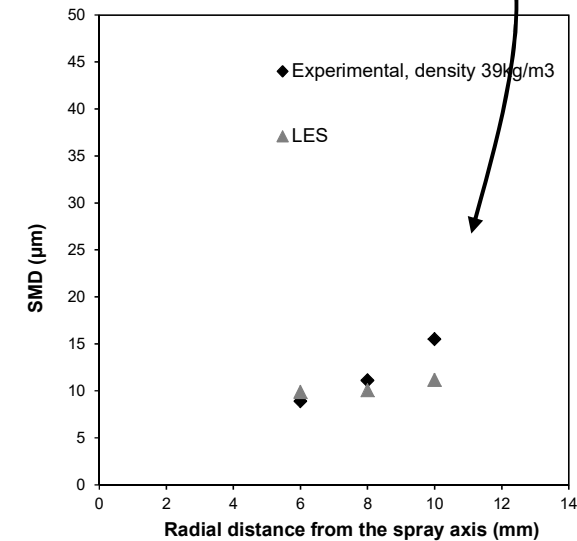
LES spray



Gas density 39 kg/m³



Gas density 115 kg/m³



Kaario et al., 2013



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Characteristic numbers

- **Sauter mean diameter (SMD)** $SMD = \frac{\sum_1^n d^3}{\sum_1^n d^2}$
- **Weber number** $We = \frac{d \rho_g |u - u_p|^2}{\sigma}$
- **Ohnesorg number** $Oh = \frac{\mu_l}{\sqrt{\rho_l \sigma d}} = \frac{\sqrt{We}}{Re} \sim \frac{\text{viscous forces}}{\sqrt{\text{inertia} \cdot \text{surface tension}}}$
- **Stokes number** $St = \frac{\tau_p}{\tau_f}$ $\tau_p = \frac{\rho_l d^2}{18 \mu_g}$ $\tau_f = \frac{D}{U_0}$

Group Work

Discuss in pairs (about 10 min):

- 1. What are the most important mechanisms leading to droplet breakup ?**
- 2. What two surface wave / instability types are responsible for final droplet breakup ?**
- 3. What dimensionless number governs the breakup phenomena ? What physical quantities in that number are most important ?**
- 4. How is the breakup phenomena described in the Reitz-Diwakar (Wave) breakup model ?**



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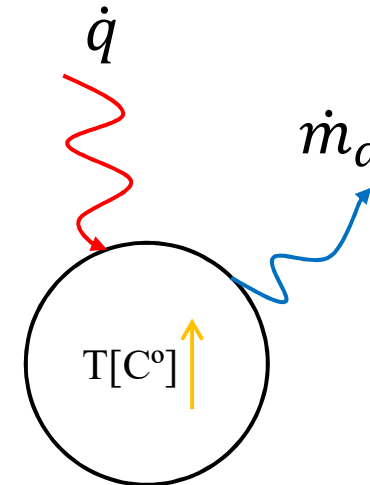
Evaporation



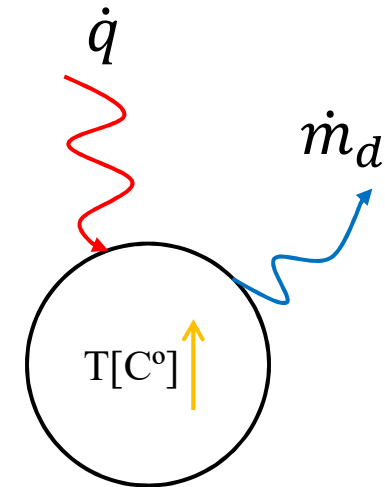
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Droplet Evaporation

- **Heat is transferred to the droplet (conduction, convection)**
- **Vapor is transferred from the droplet (conduction, convection)**
- **Possible temperature increase**
- **Overall rate depends:**
 - **Droplet properties:**
 - **Diameter**
 - **Temperature**
 - **Relative droplet-gas velocity**
 - **Surrounding gas properties:**
 - **Pressure**
 - **Temperature**
 - **Composition**



Droplet Evaporation



- **Droplet energy balance**

$$A_s \dot{q}_d = h_l \frac{dm_d}{dt} + m_d c_p \frac{dT_d}{dt}$$

where $\dot{q}_d = h(T_d - T)$ is surface heat flux, h is the heat transfer coefficient, and h_l is the latent heat of phase change.

- **Heat transfer coefficient has to be evaluated, typically correlations based on Nusselt number, conductivity and droplet size.**
- **Eventually wet-bulb temperature is reached (wet bulb temperature means droplet surface temperature during steady-state evaporation)**

Drop Evaporation

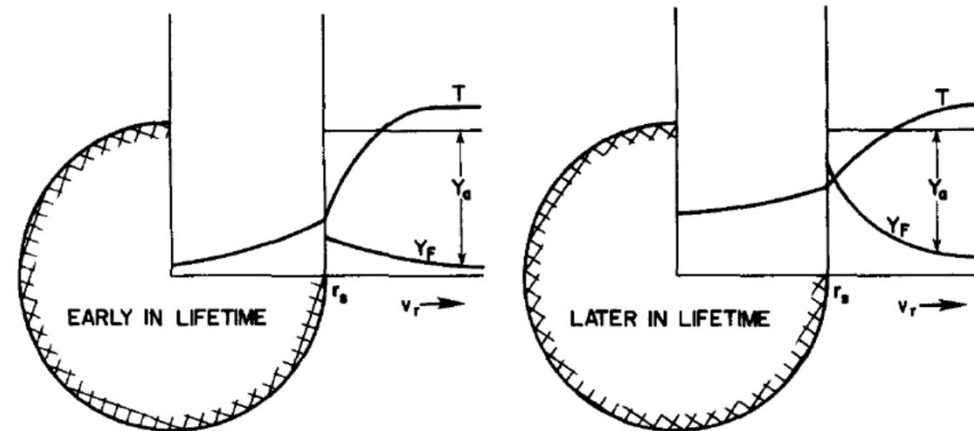


FIG. 10. Sketch of the drop vaporization process.

Figure G. M. Faeth

- **Heat up phase**
 - low fuel vapor concentration at the drop surface
 - strong temperature gradient
- **Later, increased fuel vapor concentration**
 - this reduces the heat transfer to the droplet
 - eventually the wet bulb temperature is reached where all the heat goes to the latent heat of evaporation



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Measurement of evaporation rate

- When droplet evaporation is measured, after an initial transitional period, drop diameter decreases according to

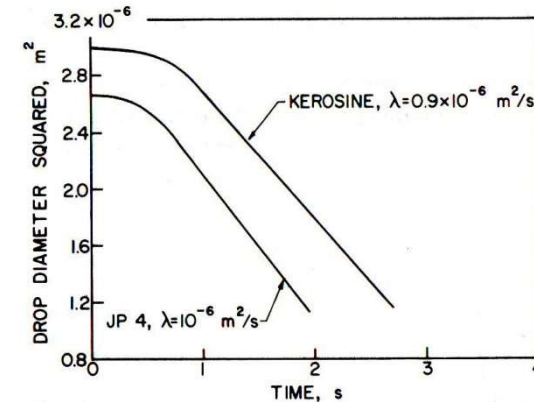
$$\lambda = -\frac{d(d^2)}{dt}$$

or

$$d_0^2 - d^2 = \lambda t$$

- This is called the “D² law” where λ is the *evaporation constant*
- Straight line indicates wet-bulb temperature
- Setting $d = 0$ gives us the evaporation time

$$t_e = \frac{d_0^2}{\lambda}$$



Figures A. Lefebvre, 1989

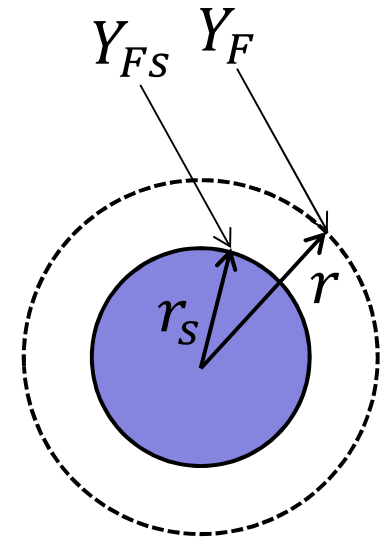
Table 8.1 Values of evaporation constant for various stagnant fuel-air mixtures

Fuel	λ (m ² /s)	λ (ft ² /s)
Gasoline	1.06×10^{-6}	11.4×10^{-6}
Gasoline	1.49×10^{-6}	16.0×10^{-6}
Kerosine	1.03×10^{-6}	11.1×10^{-6}
Kerosine	1.12×10^{-6}	12.1×10^{-6}
Kerosine	1.28×10^{-6}	13.8×10^{-6}
Kerosine	1.47×10^{-6}	15.8×10^{-6}
Diesel oil	0.79×10^{-6}	8.5×10^{-6}
Diesel oil	1.09×10^{-6}	11.7×10^{-6}



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Mass Transfer



- **Equation for the rate of evaporation of a fuel drop**
- **The derivation for the droplet evaporation equation is cumbersome and hence only main points are presented. Further reading in A. H. Lefebvre and G. M. Faeth (see end of presentation for more details).**
- **Assuming the driving force for species diffusion is the concentration gradient in the direction of the diffusion path, the following expression is obtained for an evaporating drop when starting from vapor phase *convection - diffusion equation*, and using the *ideal gas law*:**

$$\frac{\partial Y_F}{\partial r} = - \frac{RT}{DP} (\dot{m}_F Y_A)$$

- **From continuity of the mass rate of diffusion, we**

get from $\dot{m}_{FS} 4\pi r_s^2 = \dot{m}_F 4\pi r^2$

$$\frac{\partial Y_F}{\partial r} = - \frac{RT}{DP} (\dot{m}_{FS} Y_A) \left(\frac{r_s^2}{r^2} \right)$$

Y_F = fuel mass fraction
 Y_A = air mass fraction
 \dot{m}_F = mass rate of diffusion
(per unit area)
 D = diffusion coefficient
 P = pressure
 T = temperature



Mass Transfer

- **Rearranging gives** ($Y_A = 1 - Y_F$)

$$\frac{dY_F}{1 - Y_F} = - \frac{RT}{DP} \dot{m}_{FS} r_s^2 \frac{dr}{r^2}$$

- **Boundary conditions are**

$$r = r_s; \quad T = T_s; \quad Y_F = Y_{FS}$$

$$r = \infty; \quad T = T_\infty; \quad Y_F = Y_{FS} = 0$$

- **Integrating between $r=r_s \rightarrow r_\infty$**

$$[\ln(1 - Y_F)]_{Y_{FS}}^0 = \left[\frac{RT}{DP} \dot{m}_{FS} r_s^2 \left(-\frac{1}{r} \right) \right]_{r_s}^\infty$$

- **or**

$$0 - \ln(1 - Y_{FS}) = 0 - \frac{RT}{DP} \dot{m}_{FS} r_s^2 \left(-\frac{1}{r_s} \right)$$

- **We get**

$$\dot{m}_{FS} = - \frac{PD \ln(1 - Y_{FS})}{RT r_s}$$



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Mass Transfer

- **And the total mass flow rate**

$$\dot{m}_F = 4\pi r_s^2 \dot{m}_{FS} = 4\pi r_s \rho D \ln(1 - Y_{FS})$$

- **If we assume Lewis number of unity** $Le = \frac{k}{\rho D c_p} = 1$,
 ρD **can be replaced by** $\left(\frac{k}{c_p}\right)_g$ **and if we define**

$$B_M = \frac{Y_{FS}}{1 - Y_{FS}}$$

- **We obtain the droplet evaporation rate**

$$\dot{m}_F = 2\pi d \left(\frac{k}{c_p}\right) \ln(1 + B_M)_g \quad [\text{kg/s}]$$



Droplet lifetime

- **Now we have the Eq. for evaporation rate**

$$\dot{m}_F = 2\pi d \left(\frac{k}{c_p} \right) \ln(1 + B_M)$$

- **and the evaporation time**

$$t_e = \frac{d_0^2}{\lambda}$$

- **What would be the total evaporation time ?**
- **Droplet mass is**

$$m_d = \rho_d \left(\frac{\pi d^3}{6} \right)$$

- **And the rate of mass change is**

$$\frac{dm_d}{dt} = \rho_d \frac{d}{dt} \left(\frac{\pi d^3}{6} \right) \rightarrow \frac{\dot{m}_d}{\rho_d} = \frac{d}{dt} \left(\frac{\pi d^3}{6} \right) \stackrel{\text{derivate}}{=} \frac{\pi d^2}{2} \frac{d(d)}{dt}$$



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Droplet lifetime

- **Evaporation constant λ is**

$$\lambda = -\frac{d(d^2)}{dt} \xrightarrow{\text{derivate}} 2d \frac{d(d)}{dt} \rightarrow \frac{d(d)}{dt} = \frac{\lambda}{2d}$$

- **then**

$$\frac{\dot{m}_d}{\rho_d} = \frac{\pi d^2}{2} \frac{d(d)}{dt}$$

- **We have**

$$\frac{\dot{m}_d}{\rho_d} = -\left(\frac{\pi}{4}\right) \lambda d \quad \text{or} \quad \dot{m}_d = -\left(\frac{\pi}{4}\right) \rho_d \lambda d$$



Droplet Lifetime

- **Now the vapor mass rate must equal the droplet mass change**

$$\dot{m}_F = \dot{m}_d \rightarrow 2\pi d \left(\frac{k}{c_p} \right)_g \ln(1 + B_M) = - \left(\frac{\pi}{4} \right) \rho_d \lambda d$$

- **Solving for λ we get**

$$\lambda = \frac{8(k/c_p)_g \ln(1 + B_M)}{\rho_d}$$

- **Now we can use $t_e = \frac{d^2}{\lambda}$ to obtain the equation for the droplet lifetime without convection**

$$t_e = \frac{\rho_F d^2}{8(k/c_p)_g \ln(1 + B_M)} \quad [\text{s}]$$

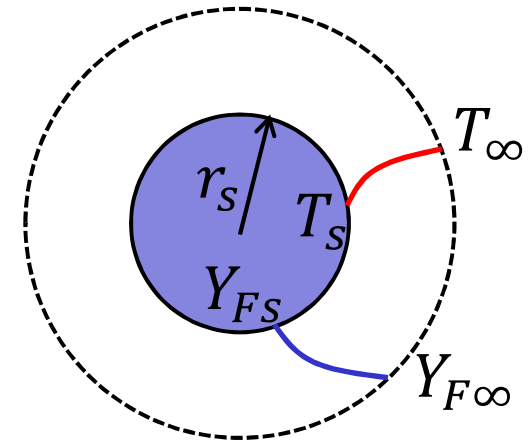


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Calculation of Mean Properties

- **The accuracy of the below equation is dependent on the choice of the values for k and c_p .**

$$\dot{m}_F = 2\pi d \left(\frac{k}{c_p} \right)_g \ln(1 + B_M)$$



- **Average mixture or film properties can be estimated e.g.**
 - **One-third or two-thirds rule**

$$T_m = \frac{(2T_s + T_\infty)}{3}$$

$$Y_{Fm} = \frac{(2Y_{Fs} + Y_{F\infty})}{3}$$

In OpenFOAM

- **50-50 rule**

$$T_m = \frac{(T_s + T_\infty)}{2}$$

$$Y_{Fm} = \frac{(Y_{Fs} + Y_{F\infty})}{2}$$

In Star-CD



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Calculation of Mean Properties

- **Mixture (film) specific heat and thermal conductivity**

when $Y_{Fm} = 1 - Y_{Am} \Rightarrow Y_{Am} = 1 - Y_{Fm}$

$$c_{pg} = Y_{Am} c_{pA}(\text{at } T_m) + Y_{Fm} c_{pv}(\text{at } T_m)$$

$$k_g = Y_{Am} k_A(\text{at } T_m) + Y_{Fm} k_v(\text{at } T_m)$$

- **Assuming fuel concentration is zero in the far field** $Y_{F\infty} = 0$

and $Y_{Fs} = 0.68$

- **Two-thirds rule gives**

$$Y_{Fm} = \frac{2}{3} Y_{Fs} = 0.4533$$

- **50-50 gives**

$$Y_{Fm} = \frac{1}{2} Y_{Fs} = 0.34$$



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Effect of Convection

- **When there is relative velocity between surrounding gas and droplets, the rate of evaporation can be greatly enhanced.**
- **A 100 times increase is possible.**
- **It has been shown that the effects of convection can be taken into account by a correction factor.**
- **Correlations by N. Frössling, and Ranz & Marshall**

$$Sh = \frac{\text{convective mass transfer}}{\text{mass diffusion}} = 2 + 0.6 Re^{0.5} Sc^{0.33}$$

$$Nu = \frac{\text{convective heat transfer}}{\text{heat conduction}} = 2 + 0.6 Re^{0.5} Pr^{0.33}$$

- **First one is used when diffusion effects are controlling and the lower one when heat transfer rates are controlling.**

$$Sc = \frac{\nu}{D} \quad Pr = \frac{c_p \mu}{k} = \frac{\nu}{\alpha} \quad Re = \frac{\rho_g |U - U_p| d}{\mu_g}$$



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Effect of Convection

- **Rate of fuel evaporation with convection is**

$$\dot{m}_F = 2\pi d \left(\frac{k}{c_p} \right)_g \ln(1 + B_M) (1 + 0.30 Re^{0.5} Pr^{0.33})$$

- **Droplet lifetime can be now calculated from**

$$t_e = \frac{\rho_F d^2}{8 \left(\frac{k}{c_p} \right) \ln(1 + B_M) (1 + 0.3 Re^{0.5} Pr^{0.33})} \quad [s]$$



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Alternative formulation of droplet mass transfer

- **Droplet evaporation rate can also be formulated as (Bird et al.)**

$$\frac{dm_d}{dt} = -A_d K_g p_g \ln \frac{(p_g - p_{v,\infty})}{(p_g - p_{v,s})}$$

where p_g is the ambient pressure, $p_{v,s}$ is the vapor pressure in the droplet surroundings, and $p_{v,\infty}$ is the vapor pressure at the droplet surface.

- **The mass transfer coefficient is given by**

$$K_g = \frac{Sh D_m}{R_m T_m d}$$

- **D_m is the mixture (film) vapor diffusivity, R_m is the mixture gas constant, and T_m is the mean temperature.**
- **This droplet evaporation model is used e.g. in Star-CD**

Model by Bird et al.

- **From the rate of mass change**

$$\frac{dm_d}{dt} = -A_d K_g p_g \ln \frac{(p_g - p_{v,\infty})}{(p_g - p_{v,s})}$$

- **We get to the new droplet mass by**

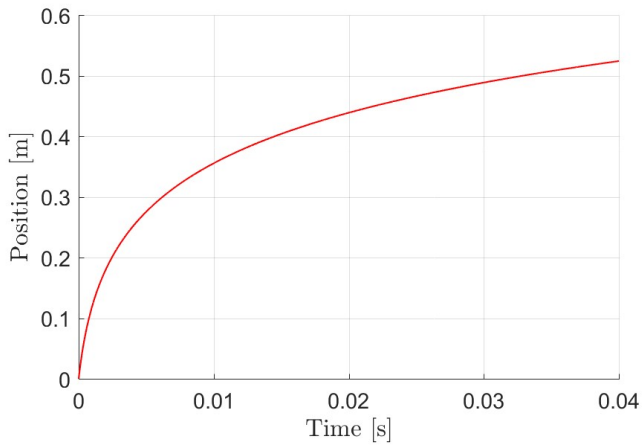
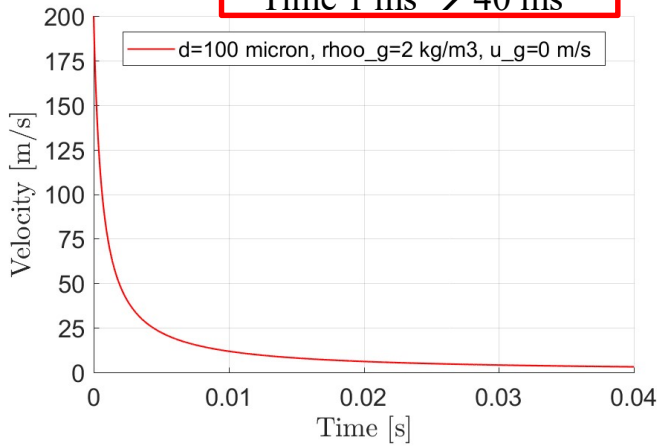
$$m_{d,new} = m_{d,old} - A_d K_g p_g \ln \left(\frac{p_g - p_{v,\infty}}{p_g - p_{v,s}} \right) dt \quad (4)$$

0d Matlab results

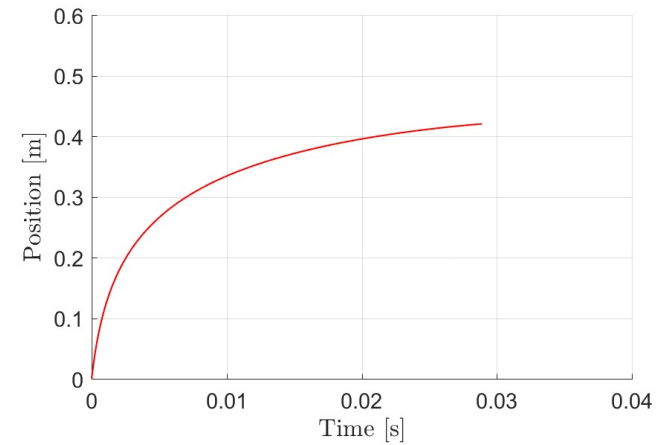
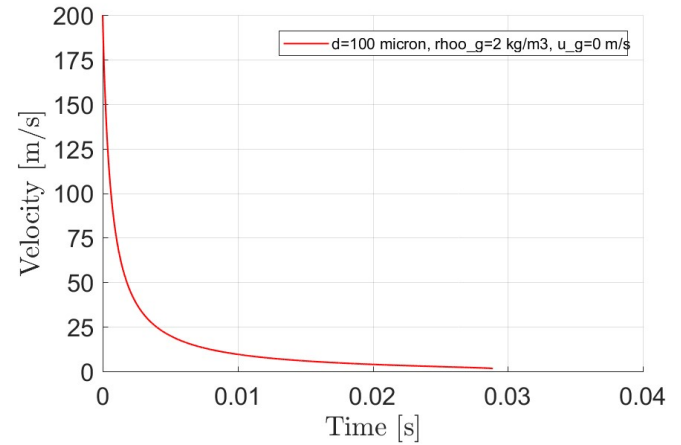
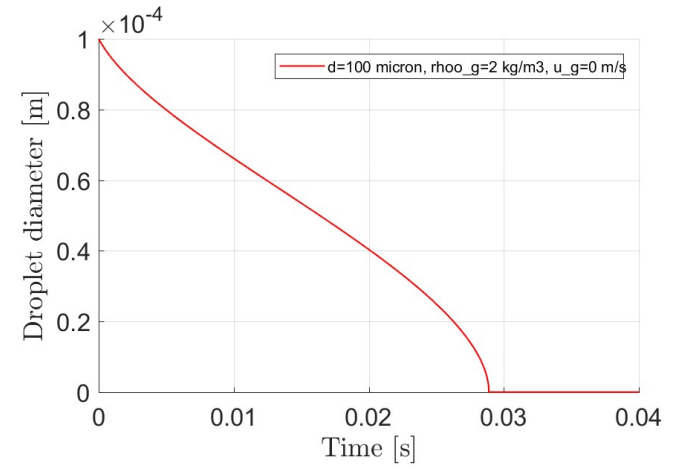
Conditions

$p_{v,\infty} = 0 \text{ Pa}$
 $p_{v,d} = 1.3e + 5 \text{ Pa}$
 Time 1 ms \rightarrow 40 ms

No evaporation, no breakup



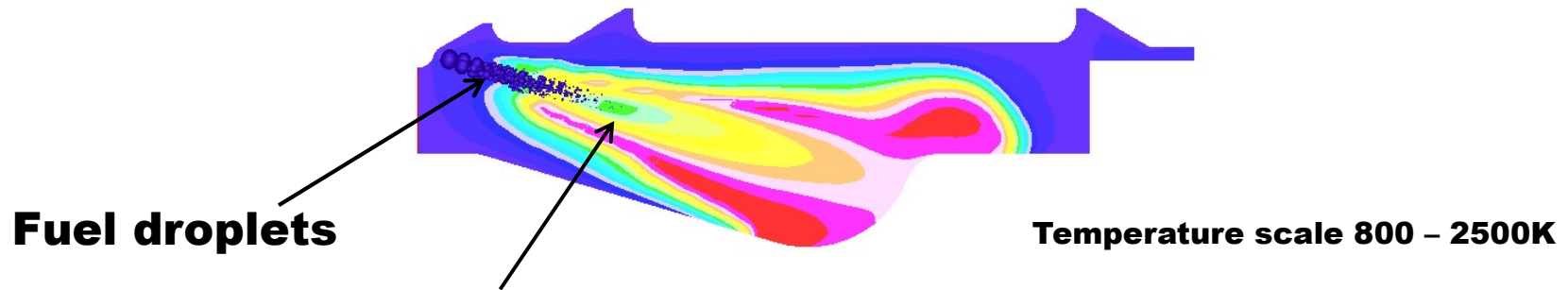
Evaporating drops, no breakup





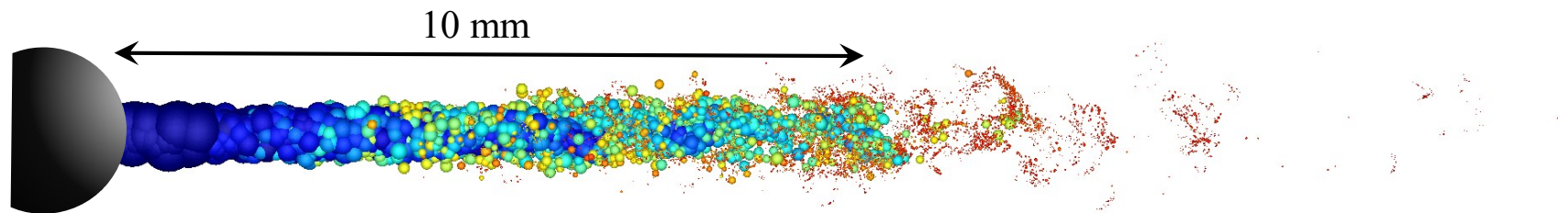
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Some Results



- Moderate temperatures within the fuel spray $\sim 1000\text{K}$
- High fuel concentration $\sim 30\%$
- High gas pressure $\sim 100\text{bar}$

LES: Evaporation and breakup of a spray



- Drop sizes between $10 - 0.01 \mu\text{m}$
- Drop temperatures between $363 - 580 \text{ K}$



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Dimensionless numbers

- **Lewis number is the ration of thermal and mass diffusivities**

$$Le = \frac{\alpha}{D} \quad \text{where} \quad \alpha = \frac{k}{\rho c_p} \quad \text{and } \mathbf{D} \text{ is mass diffusivity}$$

– It can also be expressed as $Le = \frac{Sc}{Pr}$

- **Prandtl number is the ration of momentum and thermal diffusivities**

$$Pr = \frac{c_p \mu}{k} = \frac{\nu}{\alpha}$$

- **Schmidt number is the ration of momentum and mass diffusivities**

$$Sc = \frac{\nu}{D}$$



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Dimensionless numbers

- **Sherwood number is dimensionless concentration gradient at the surface**

$$Sh = \frac{hL}{D}$$

- **Nusselt number is dimensionless temperature gradient at the surface**

$$Nu = \frac{hL}{k}$$

Primary Factors Influencing Drop Lifetime

- 1. The physical properties of the ambient gas (T, P, C_p ..)**
- 2. The relative velocity between the drop and the surroundings**
- 3. The properties of the liquid and its vapor (P_v, k_v, C_{pv} ..)**
- 4. The initial condition of the drop, especially size**



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Exercise

- 1. A $200\mu\text{m}$ n-heptane fuel droplet is evaporating in 900K environment without convection. Density of the fuel is 700kg/m^3 , the mean k and c_p can be assumed to be 0.04W/mK and 1000J/kgK respectively. The fuel vapor mass fraction at the droplet surface is assumed to be $Y_{Fs} = 0.68$. Calculate the time needed to evaporate the droplet.**
- 2. The same situation as in 1) but now the relative velocity between the droplet and the surrounding gas is 10 m/s which yields a Reynolds number of 200 . Calculate the time needed to evaporate the droplet.**

Additional Reading

- **B.E. Gelfand, Droplet breakup phenomena in flows with velocity lag, Prog. Energy Combust. Sci., Vol. 22, pp. 201-265, 1996.**
- **Reitz, RD, Modeling atomization processes in high-pressure vaporizing sprays, Atomization and spray technology, vol. 3, pp. 309-337, 1987.**
- **F.X. Tanner, Liquid jet atomization and droplet breakup modeling of non-evaporating diesel fuel sprays, SAE paper 970050, 1997.**
- **A., H., Lefebvre, Atomization and Sprays, ISBN 0-89116-603-3, 1989.**
- **Crowe, C.T., Schwarzkof, J.D., Sommerfeld, M., and Tsuji, Y., Multiphase Flows with Droplets and Particles, 2nd edition, CRC Press, ISBN 978-1-4398-4050-4, 2012.**