



051176 - Computational Techniques for Thermochemical Propulsion
Master of Science in Aeronautical Engineering

Lagrangian Spray Modeling

Prof. **Federico Piscaglia**
Dept. of Aerospace Science and Technology (DAER)
POLITECNICO DI MILANO, Italy
federico.piscaglia@polimi.it

MULTIPHASE FLOWS *with DROPLETS and PARTICLES*

SECOND EDITION

Clayton T. Crowe
John D. Schwarzkopf
Martin Sommerfeld
Yutaka Tsuji



 CRC Press
Taylor & Francis Group

Clayton T. Crowe, John D. Schwarzkopf, Martin Sommerfeld, Yutaka Tsuji. "**Multiphase Flows with Droplets and Particles**", CRC Press, 2011.

SPECIAL TOPICS



- lagrangian sprays
- wall-film
- reacting flows
- combustion
- moving mesh
- multiphase flows (VOF, Euler-Euler)

Introduction



The atomization process is the mechanism that leads to increase the liquid-gas interfacial area in the combustion chamber. The different steps leading to combustion inside a combustion chamber can be summed up by:

- **primary atomization:** pulverization of the liquid jet into multiple droplets;
- **evaporation of the spray,** including the release of fuel vapors in the combustion chamber.
If fuel vapor is well mixed, it will be ignited and the combustion process will start;
- **evolution of the combustion process.**

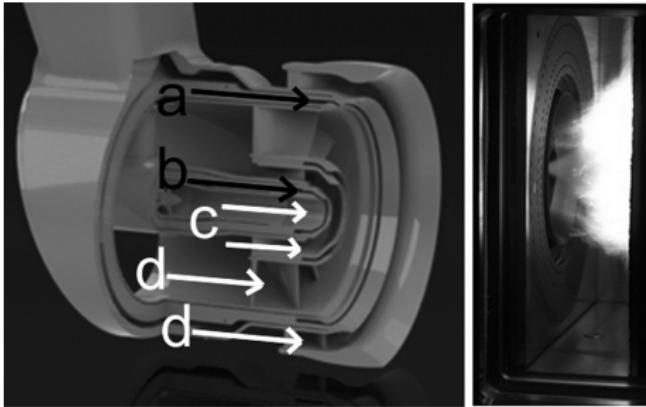
Atomization of a Liquid Jet

The purpose of an injector is to introduce the liquid fuel into a combustion chamber and, at the same time, to favor the mixing of the combustive agent and the combustible, in order to optimize the conditions of combustion. In industry, at least three main configurations of injector can be found:

1. in **pressure atomizers or single fluid atomizers**, high pressure forces the liquid to flow at high velocity through a small opening into a steady ambient atmosphere. Velocity difference between liquid and gas leads to the disintegration of liquid until obtaining a droplet clouds.
 - This type of injectors are widely used in industries, such as agriculture, cosmetics, automotive motors or aeronautic motors. They have the benefit to be simple and cheap to manufacture.
 - Droplet sizes can be controlled by adjusting the injection pressure: the higher the pressure, the smaller the droplets. On the other hand, the necessary energy to atomize the fluid increases very rapidly with the mass flow rate.



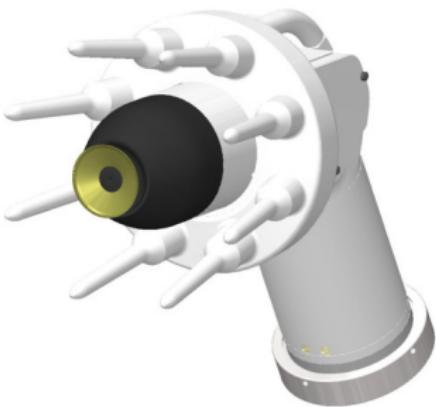
Atomization of a Liquid Jet



2. in **airblast atomizers (or twin fluid atomizers)**, the low speed fuel jet is usually first spread into a sheet and then exposed to a swirling gas flow, where the swirling motion enhances instabilities and increases the breakup.

- In principle, these mechanisms work at low relative speed and high air flow, as it happens for aircraft engines. Small part of high pressure air leaving out compressor stages is substituted and used in these injectors.
- Airblast atomizers have the benefit that, for a given mass flow rate, less energy is necessary to atomize the liquid, in comparison with a pressure atomizers. Higher fuel flow rate can thus be obtained.
- It is nevertheless necessary to have a high velocity gas flow to obtain a satisfying mixing.

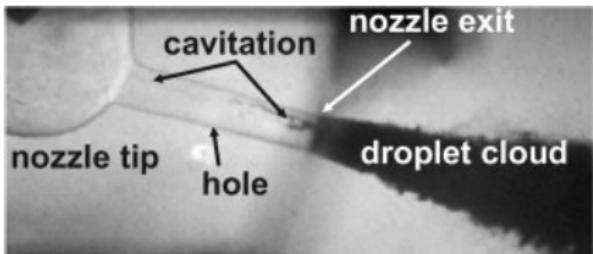
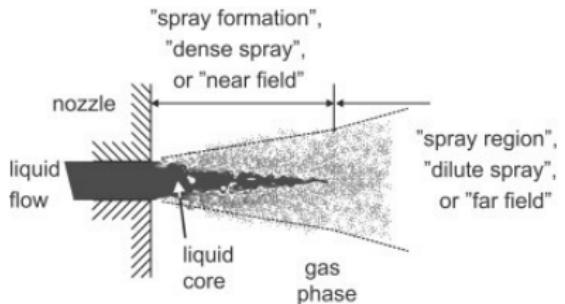
Atomization of a Liquid Jet



- **Rotary atomizers:** liquid is introduced at the center of a high-speed rotating disk. It is submitted to centrifugal forces and flows radially outward across the disk. At high flow rates, ligaments or sheets are generated at the edge of the disk and disintegrate into droplets. In contrast to pressure nozzles, rotary atomizers allows independent variation of flow rate and disk speed, thereby providing more flexibility in operation.

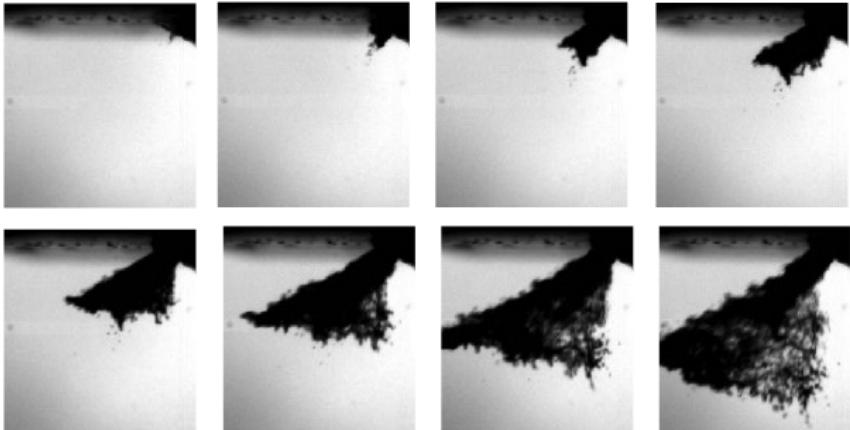
Spray regimes

A typical two-phase flow originated from a pressure atomizer can be divided into different regimes:



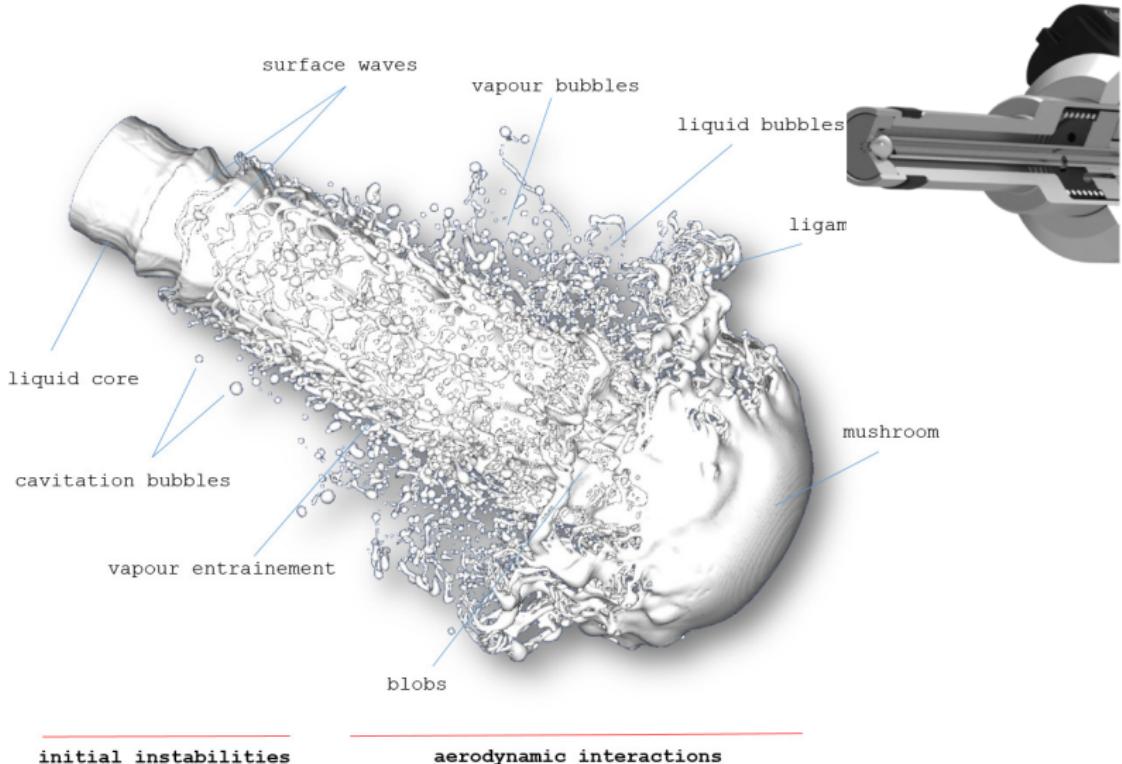
1. in the **primary atomization (or dense) zone**, an *intact core* of the liquid phase rapidly disintegrates into ligaments (churning flow) and further into droplets, but it still occupies a considerable fraction of the volume. In this region, the **high velocity gradients** between the liquid and the gas lead to shearing instabilities; these instabilities show sinusoidal waves of increasing amplitude at the liquid-gas interface in the direction of the liquid flow, provoking **detachments of liquid structures from the liquid core**. These structures remain relatively big compared to the liquid core size; on the other hand, the density of the liquid phase is significantly greater than the density of the gas phase, so its contribution to the total mass is still the most important.

Spray regimes

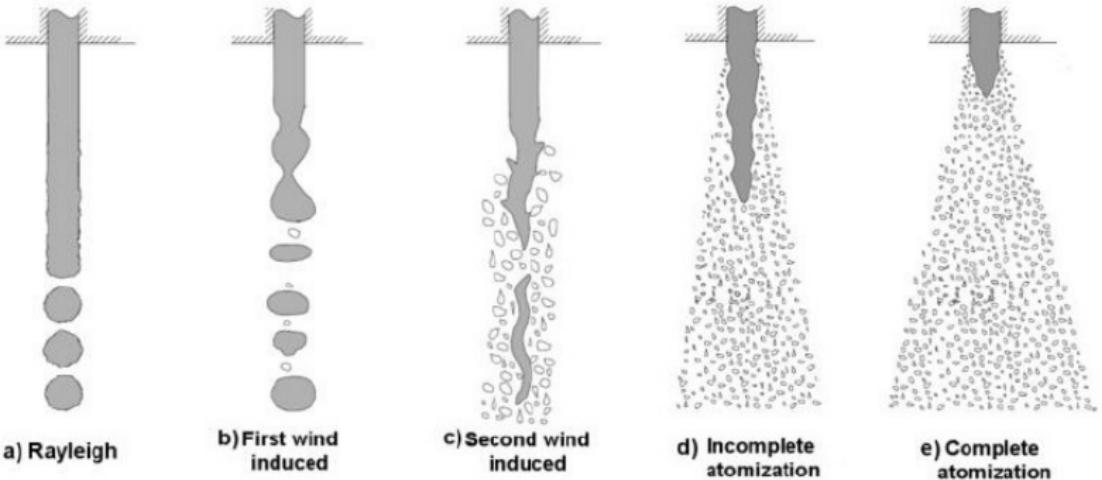


2. In a **secondary atomization (or diluted) zone**, the average spacing between droplets expands further downstream of the nozzle because of the conical spray shape and because of droplet evaporation; typical interactions between droplets are coalescence and collision (with breakup). The gas-phase fraction in this zone increases and approaches unity. However, due to the liquid to gas density ratio, the mass fraction of the liquid phase may still be noticeable.
3. A **diluted (or dispersed) spray region** is finally characterized by both volume and mass fractions of the liquid phase that are negligible compared to the ones of the gas phase.

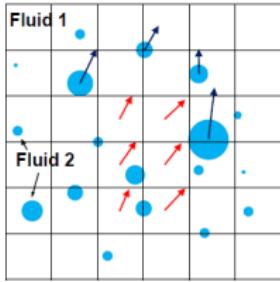
Primary atomization



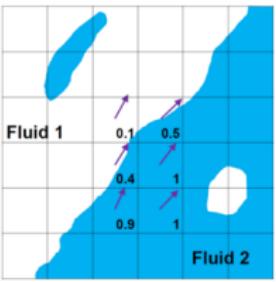
Spray regimes



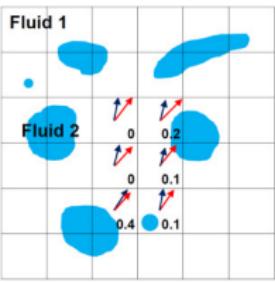
Spray modelling



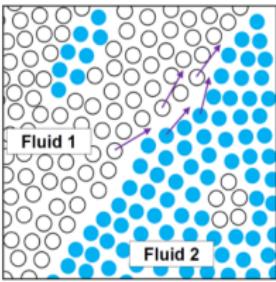
(a) Lagrangian Tracking



(b) VOF



(c) Eulerian two-fluid



(d) SPH

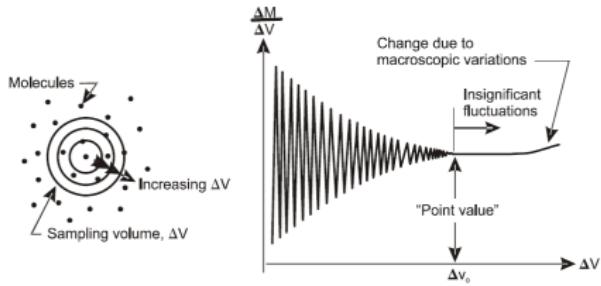
Three main methods exist to simulate the gas bubbles and to couple it with the liquid, namely:

1. Eulerian-Eulerian (EE), i.e. both the carrier phase and the gas phase are computed in an Eulerian framework;
2. Eulerian-Lagrangian (EL), i.e. the carried liquid is calculated as in (1) and the gas phase is treated as Lagrangian markers
3. Interface Tracking (IT), i.e. the carried liquid is calculated as in (1) and some features of the interface between liquid and gas phases are resolved by the numerical method.

Dispersed Phase Flows

Spray modelling

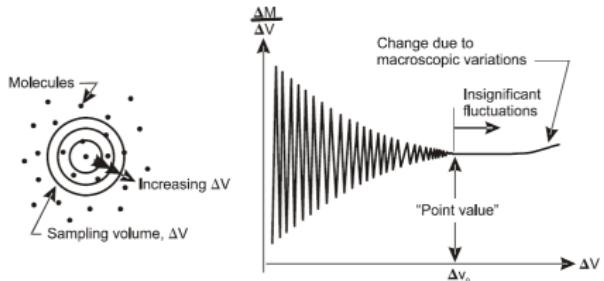
Dispersed phase flows are flows in which one phase, the dispersed phase, is not materially connected. These include gas-droplet, gas-particle and liquid-particle flows in which the particles and droplets constitute the dispersed phase. Bubbles in a bubbly flow also represent the dispersed phase.



Concept of a continuum

The concept of the continuum is important in the development of equations for multiphase flows. A fluid is regarded as consisting of continuous matter for which properties such as density and velocity vary continuously from point to point. As the volume is increased further the variations become progressively smaller. After the volume ΔV_0 (point volume) is reached, the variations become insignificant. As the volume is increased further, the density will change according to macroscopic variations such as shock waves, spatial density gradients or other macroscopic features.

Spray modelling



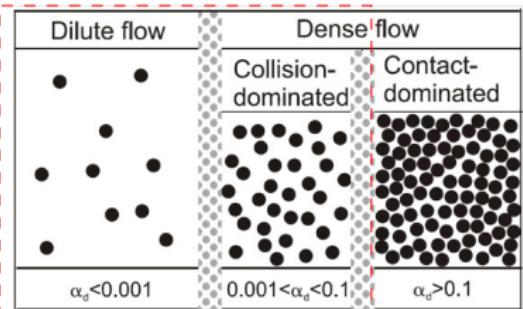
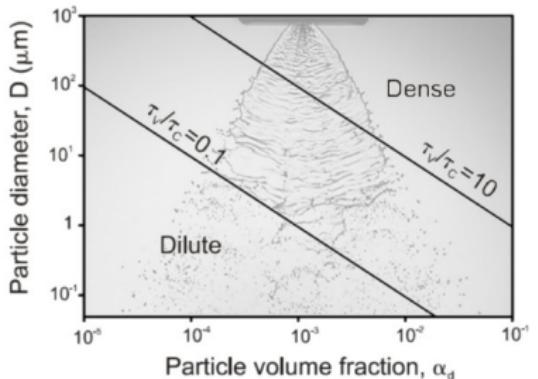
A small volume contains just few molecules, but by proceeding with the increment of its size, and therefore its volume, one obtains that new molecules get accounted within the latter. Due to this process, being the density

$$\rho \simeq \frac{\Delta m}{\Delta V}$$

ρ progressively varies until a specific volume Δv_0 is reached so that an insignificant variation of the density is perceived, even though the number of molecules and the dimensions are subjected to small variation. Thus, if $\Delta v > \Delta v_0$, it is expected to see a variation in density dependant on macroscopic events such as shock waves.

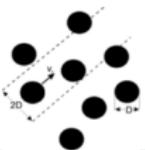
The size of sampling volume for a liquid to maintain insignificant variations is obviously less than the gas one

Classification of Multiphase Flows



Being τ_C the average time between particle-particle collisions, particle motion is controlled:

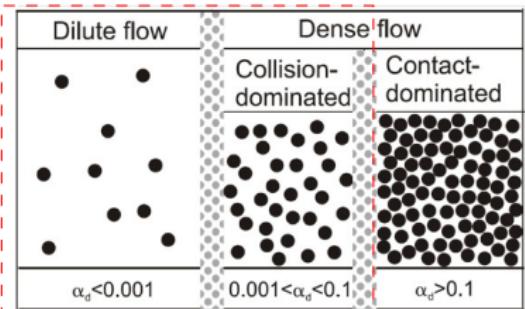
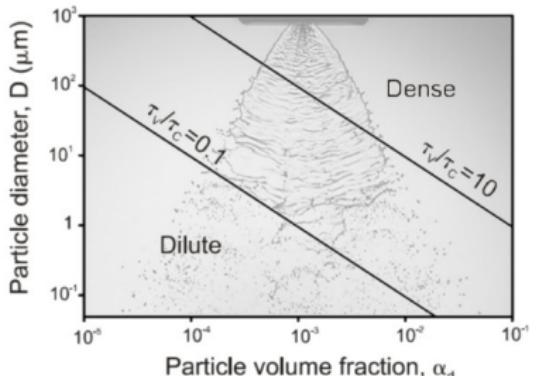
- by the fluid forces (drag and lift) in a **dilute/dispersed phase flow**: $\frac{\tau_v}{\tau_C} < 1$
- by collisions or continuous contact, in a **dense flow**: $\frac{\tau_v}{\tau_C} > 1$



The order of coupling between the dispersed and continuous phase is initially determined by the **volume (void) fraction** of the liquid:

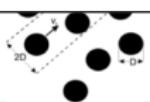
$$\alpha_p = V_{\text{liq}}/V$$

Classification of Multiphase Flows



Discrete-Particle (Lagrangian) Methods are used for dilute flows and dense (collision-dominated) flows!

- by collisions or continuous contact, in a **dense flow**: $\frac{\tau_v}{\tau_C} > 1$

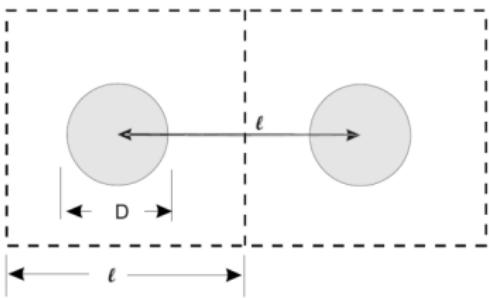


The order of coupling between the dispersed and continuous phase is initially determined by the **volume (void) fraction** of the liquid:

$$\alpha_p = V_{\text{liq}}/V$$

Particle or droplet spacing

The mechanics of a dispersed phase flow depends significantly on the **average distance between the dispersed phase elements**. This information is important to determine if a particle or droplet can be treated as an isolated element.

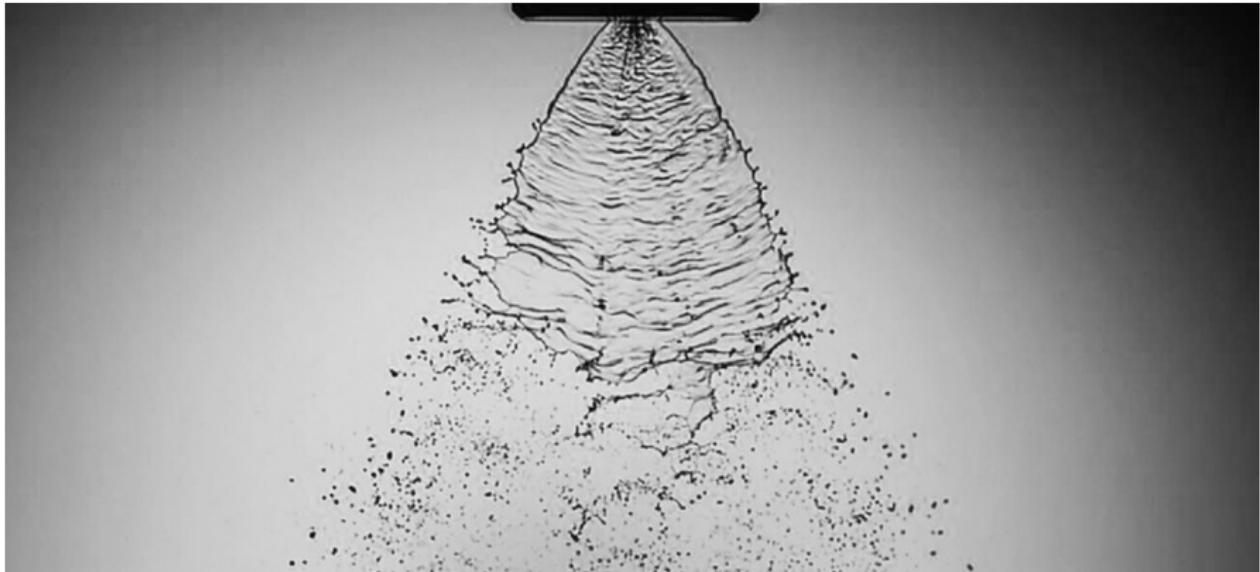


The particle or droplet spacing is related to the volume fraction by

$$\frac{l}{D} = \left(\frac{\pi}{6\alpha_d} \right)^{\frac{1}{3}}$$

- **If particles are dispersed**, individual particles or droplets could be treated as isolated droplets with little influence of the neighboring elements on the drag or heat transfer rate.
- **If particles are located less than 3 diameters apart**, the particle spacing is insufficient to treat the particles as isolated elements. Mass, momentum and heat transfer for each element are influenced by the neighboring elements.

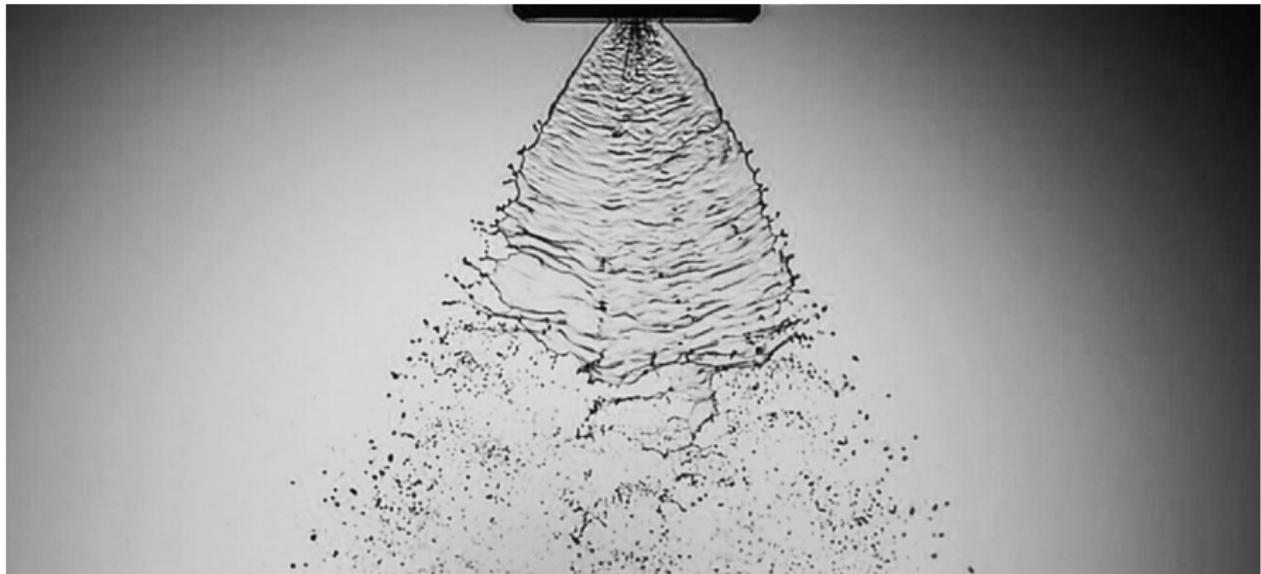
Spray regimes



The behavior of various droplets within different regimes of a spray is quite different:

- 1) **near the nozzle orifice**, droplet-droplet interactions such as collision and coalescence can be significant. Consequently, it can no longer be assumed that there is an undisturbed gas phase around the droplet in order to calculate the exchange processes between liquid and gas.

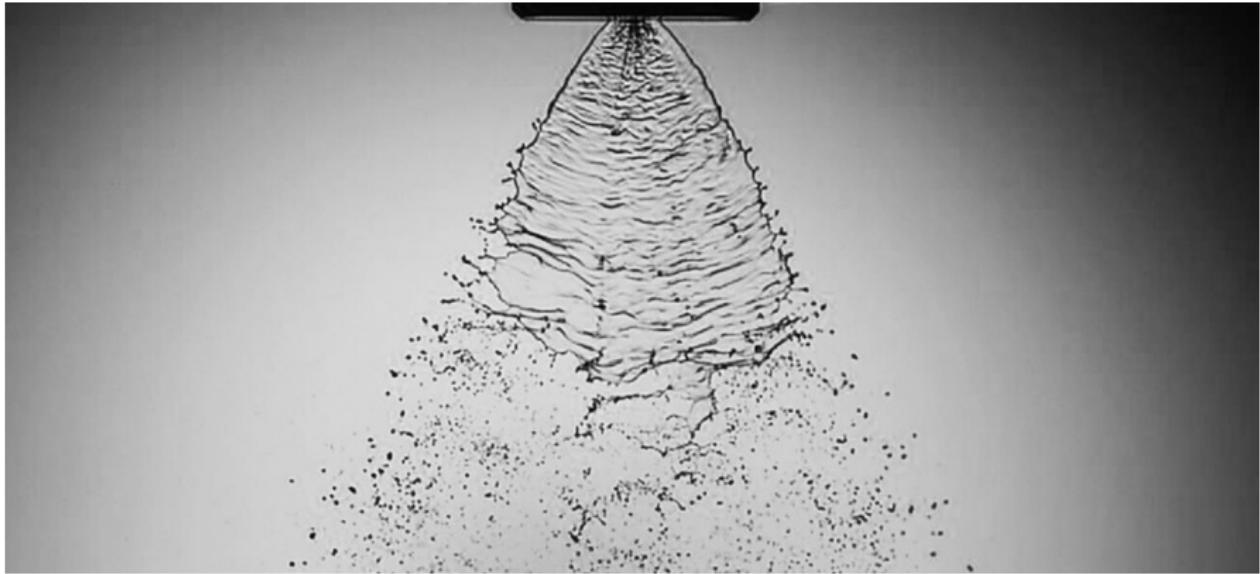
Spray regimes



The behavior of various droplets within different regimes of a spray is quite different:

- 2) **in the intermediate thin spray regime**, the liquid phase still accounts for a noticeable mass fraction. Thus, there is considerable momentum transfer from the droplets to the gas phase, which in turn affects other drop lets again. An example are the reduced drag forces on those droplets located in the wake of the spray tip that are decelerated by the gas less rapidly and may therefore overtake the droplets at the former spray tip that have been injected at an earlier.

Spray regimes



The behavior of various droplets within different regimes of a spray is quite different:

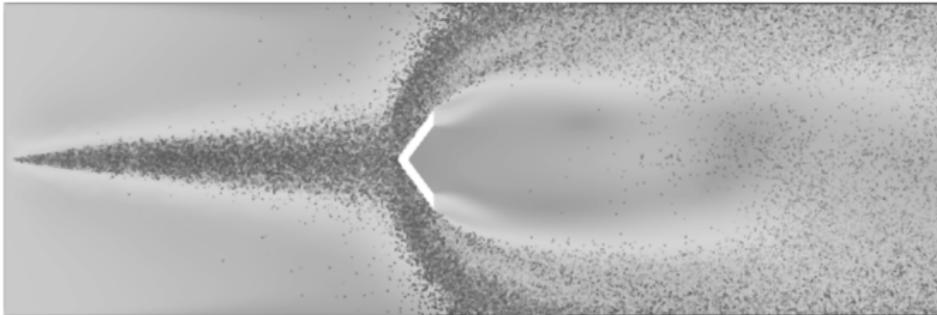
- 3) **in the dilute spray regime**, the droplet behavior can be calculated based on relations for an isolated droplet with good accuracy. There is still some mass, momentum and energy transfer between the droplets and the gas phase, but the influence that the droplets have on the gas phase is very small.

Most of the CFD-codes utilized in combustion simulations makes use of:

1. Eulerian multiphase flow simulation to simulate primary atomization of the thick spray, which is commonly valid for internal nozzle flows.
2. Simulation of (lagrangian) particle laden flows if the thin or dilute spray assumption is justified. This happens:
 - downstream of the injection nozzle where the spray has already been diluted by the gas phase;
 - for the very thin or dilute spray regime, which is characterized by both volume and mass fractions of the liquid phase that are negligible compared to the ones of the gas phase.

In this presentation, we will focus on the CFD modeling of particle laden flows in a Lagrangian-Eulerian framework.

Discrete Particle Method (DPM)



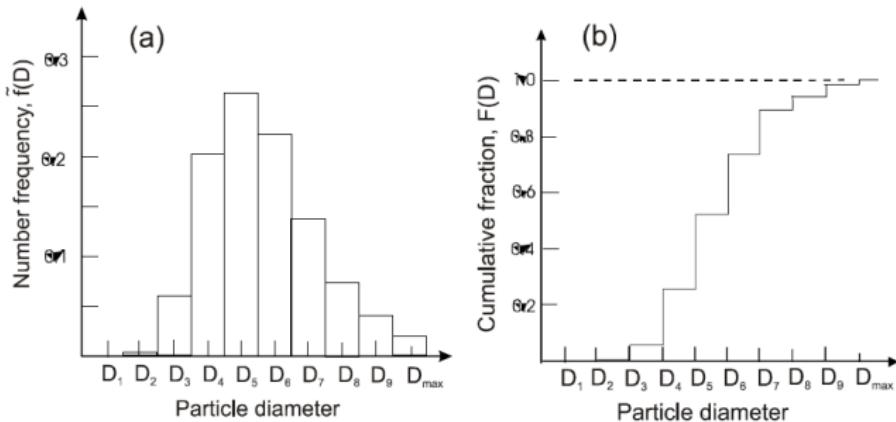
In CFD, the **Lagrangian particle tracking** (or in short **LPT method**) is a numerical technique for tracking Lagrangian particles within an Eulerian phase. It is also commonly referred to as **Discrete Particle Method (DPM)**.

Some simulation cases for which this method is applicable are:

- sprays
- small bubbles
- dust particles

The method is especially optimal for dilute multiphase flows with large Stokes number.

Size distribution

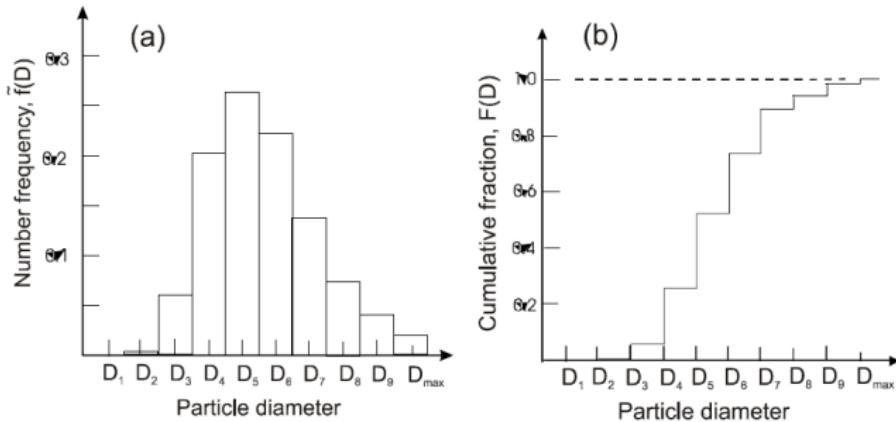


The most general definition of the spread of the particle size distribution is **monodisperse** or **polydisperse**.

- A **monodisperse distribution** is one in which the particles are close to a single size;
- **polydisperse** suggests a wide range of particle sizes. An approximate definition of a monodisperse distribution is one for which the standard deviation is less than 10% of the mean particle diameter.

Assume that the sizes of many particles in the sample have been measured: the results would be plotted in the form of a histogram (bar chart).

Discrete size distribution - number freq.



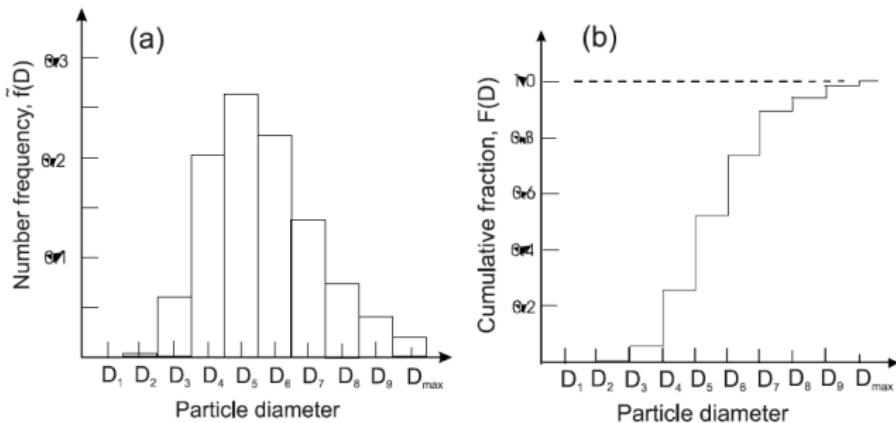
a) This is identified as the discrete number frequency distribution for the particle size 1 . The ordinate corresponding to each size interval is known as the **number frequency**, $f_n(D_i)$.

- The sum of each bar is unity since the number since the number in each size category has been divided by the total number in the sample. The distribution has been normalized:

$$\sum_{i=1}^N f_n(D_i) = 1$$

where N is the total number of intervals.

Discrete size distribution - mass based



b) Another approach to describe size distribution is to use the **particle or droplet mass (or volume)** instead of the number as the dependent variable.

- Thus the mass of each particle would be obtained, or inferred, from measurement and the fraction of mass associated with each size interval would be used to construct the distribution.
- This is known as the **discrete mass frequency distribution** and identified as $f_m(D_i)$. With this distribution, one can calculate the mass-average particle diameter and mass variance.

Discrete size distributions



For each distribution, one can calculate the (mass- or number-) average particle diameter:

$$\bar{D}_m = \sum_{i=1}^N D_i \tilde{f}(D_i)$$

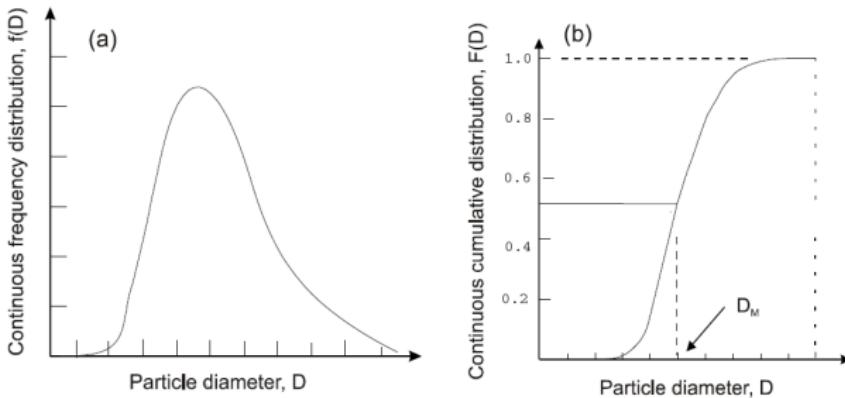
and mass (or number-) variance,

$$\sigma_m^2 = \sum_{i=1}^N (D_i - \bar{D})^2 \tilde{f}(D_i) = \sum_{i=1}^N D_i^2 \tilde{f}(D_i) - \bar{D}_m^2$$

Another commonly used method to quantify particle size is the cumulative distribution, which is the sum of the frequency distribution. The cumulative number distribution associated with size D_k is:

$$\tilde{F}_n(D_k) = \sum_{i=1}^{D_k} \tilde{f}_n(D_i)$$

Continuous size distributions



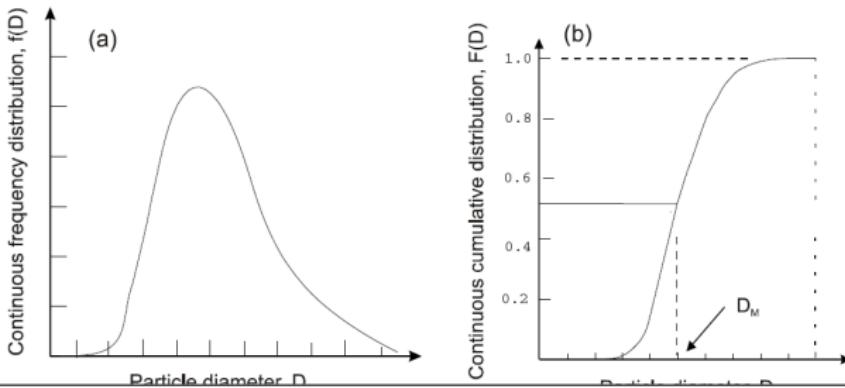
If the size intervals were made progressively smaller then, in the limit, as $\Delta D \rightarrow 0$, the continuous frequency function would be obtained

$$\int_0^{D_{\max}} f(D) dD = 1$$

where D_{\max} is the maximum particle size. The continuous cumulative distribution is obtained from the integral of the continuous frequency distribution,

$$F_n(D) = \int_0^D f_n(\lambda) d\lambda$$

Continuous size distributions



In general, size data are not available as a continuous distribution. It is common practice to consider the data obtained for a discrete distribution as values on a curve for a continuous distribution and to proceed accordingly to evaluate the appropriate statistical parameters.

$$\int_0^{D_{\max}} f(D) dD = 1$$

where D_{\max} is the maximum particle size. The continuous cumulative distribution is obtained from the integral of the continuous frequency distribution,

$$F_n(D) = \int_0^D f_n(\lambda) d\lambda$$

Statistical parameters

1) Mode

The mode corresponds to the point where the frequency function is a maximum;

2) Mean

The mean of a continuous distribution is analogous to the average of a discrete distribution. The mean is calculated from the frequency distribution by evaluating the integral:

$$F_n(D) = \int_0^D f_n(\lambda) d\lambda \rightarrow \mu = \int_0^{D_{max}} D f(D) dD$$

3) Variance

The variance of the distribution is calculated from

$$\sigma^2 = \int_0^{D_{max}} (D - \mu)^2 f(D) dD$$

or by the equivalent expression:

$$\sigma^2 = \int_0^{D_{max}} D^2 f(D) dD - \mu^2$$

The variance can be based on the number or mass distribution for particle size. **The variance is a measure of the spread of the distribution.**

Statistical parameters



1) Mode

The mode corresponds to the point where the frequency function is a maximum;

2) Mean

The mean of a continuous distribution is analogous to the average of a discrete distribution. The mean is calculated from the frequency distribution by evaluating the integral:

$$F_n(D) = \int_0^D f_n(\lambda) d\lambda$$

A distribution can be classified as monodisperse if:

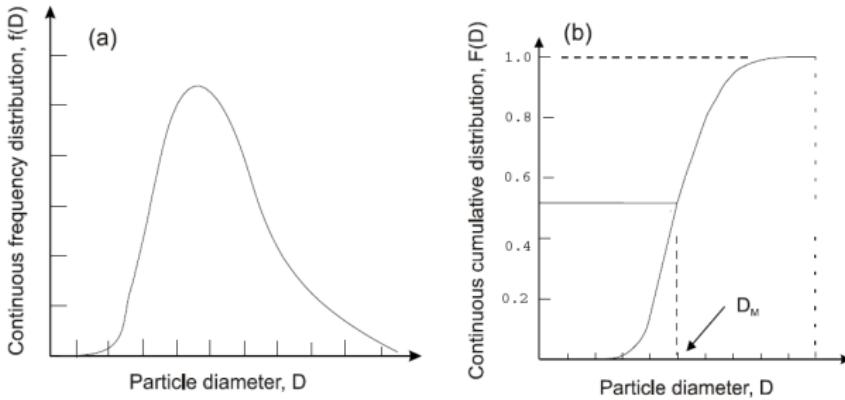
$$\frac{\sigma}{\mu} < 0.1$$

or by the equivalent expression:

$$\sigma^2 = \int_0^{D_{\max}} D^2 f(D) dD - \mu^2$$

The variance can be based on the number or mass distribution for particle size. **The variance is a measure of the spread of the distribution.**

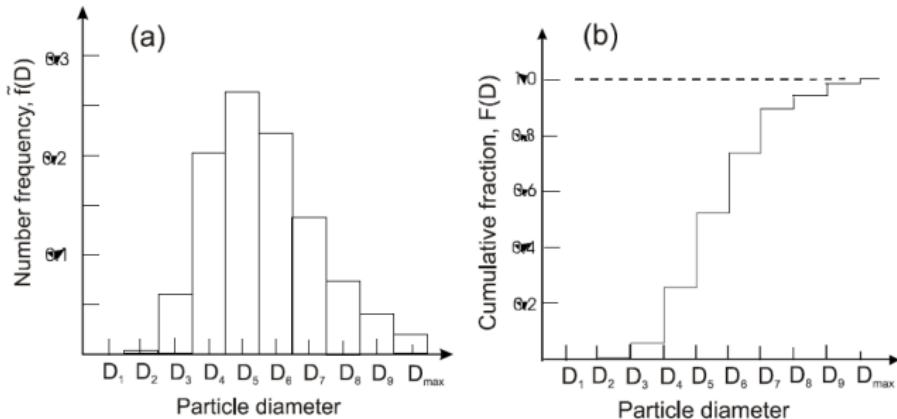
Diameter estimation



The **median diameter** D_M corresponds to the diameter for which the cumulative distribution is **0.5**.

- The median shown in figure corresponds to the number median diameter (D_{nM});
- the corresponding mass median diameter (D_{mM}) is determined from the cumulative mass distribution function.

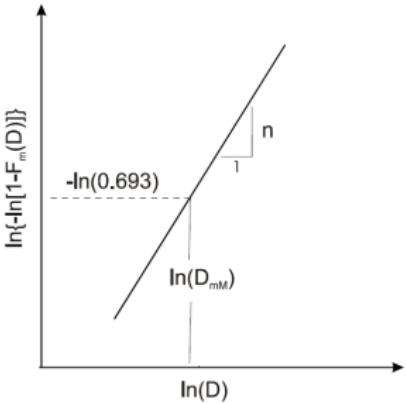
Sauter Mean Diameter (SMD)



There are several ways to estimate a characteristic diameter for a given distribution of parcels. In the spray and atomization, the **Sauter mean diameter (SMD)** is the most used. It is defined as:

$$D_{32} = \frac{\int_0^{D_{\max}} D^3 f_n(D) dD}{\int_0^{D_{\max}} D^2 f_n(D) dD}$$

Frequently used size distributions



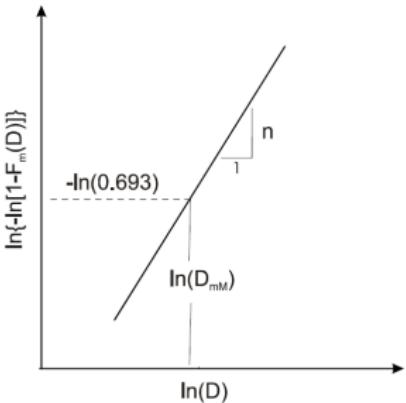
- The Rosin-Rammler distribution

The Rosin-Rammler distribution (Mugele & Evans, 1951) is frequently used for representing droplet size distributions in sprays. It is expressed in terms of the cumulative mass distribution in the form:

$$F_m(D) = 1 - e^{-\left(\frac{D}{\delta}\right)^n}$$

where δ and n are two empirical constants. One notes that $F_m(0) = 0$ and $F_m(\infty) \rightarrow 1$. The empirical constants can be determined by plotting the cumulative distribution on log-log coordinates.

Rosin-Rammler distribution



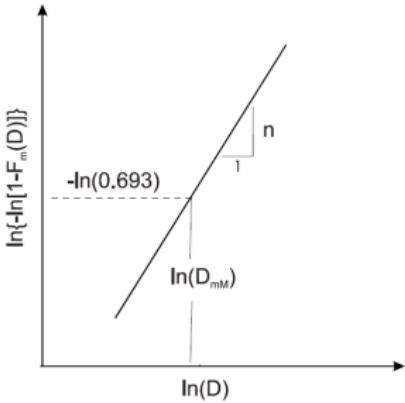
If we take the logarithm of the distribution twice, it follows:

$$\ln[-\ln(1 - F_m(D))] = n \ln(D) - n \ln \delta$$

Thus the slope of the line obtained by plotting $-\ln(1 - F_m(D))$ versus diameter on a log-log paper provides n . The parameter δ can be obtained using n and the mass median diameter with

$$\delta = \frac{D_{mM}}{0.693^{\frac{1}{n}}}$$

Rosin-Rammler distribution



The mass frequency distribution is obtained by taking the derivative of the cumulative distribution

$$f_m(D) = \frac{dF_m}{dD} = e^{-(\frac{D}{\delta})^n} \frac{n}{\delta} \left(\frac{D}{\delta}\right)^{n-1}$$

Rosin-Rammler distribution



A very useful function for evaluating the statistical parameters for the Rosin-Rammler distribution is the **gamma function** which is defined as:

$$\Gamma(r) = \int_0^{\infty} e^{-\lambda} \lambda^{t-1} d\lambda$$

It can be shown that:

$$\int_0^{\infty} n D^{\alpha} \left(\frac{D}{\delta}\right)^{n-1} \exp\left[-\left(\frac{D}{\delta}\right)^n\right] d\left(\frac{D}{\delta}\right) = \delta^{\alpha} \Gamma\left(\frac{\alpha}{n} + 1\right)$$

so, it follows:

$$\delta^{\alpha} \Gamma\left(\frac{\alpha}{n} + 1\right) = \int_0^{\infty} D^{\alpha} f_m(D) dD$$

Rosin-Rammler distribution



An example application of this equation is evaluating the mass mean diameter which is given by

$$\mu_m = \int_0^\infty D f_m(D) dD = \int_0^\infty D e^{-\left(\frac{D}{\delta}\right)^n} \frac{n}{\delta} \left(\frac{D}{\delta}\right)^{n-1} dD$$

Setting $\alpha = 1$ in the previous equations, it follows:

$$\mu_m = \delta \Gamma \left(\frac{1}{n} + 1 \right)$$

Rosin-Rammler: an example



Example: A Rosin-Rammler distribution has a mass median diameter of 120 microns with a δ -value of 2.0. Please find the mass mean of the distribution.

Solution: First we must evaluate δ from

$$\delta = \frac{D_{mM}}{0.693^{\frac{1}{n}}} = \frac{120}{0.693^{\frac{1}{2}}} = 144 \mu m$$

The mass mean is:

$$\mu_m = \delta \Gamma \left(\frac{1}{n} + 1 \right) = 144 \Gamma \left(\frac{3}{2} \right) = 128 \mu m$$

→ The Rosin-Rammler distribution is a special case of the more general Nukiyama-Tanasawa distributions.

Particles Vs Parcels



For applications involving tracking of discrete particles, **it is not practical to track all physically existing particles**. Instead, **representative particles, or parcels**, are used to track these discrete particles.

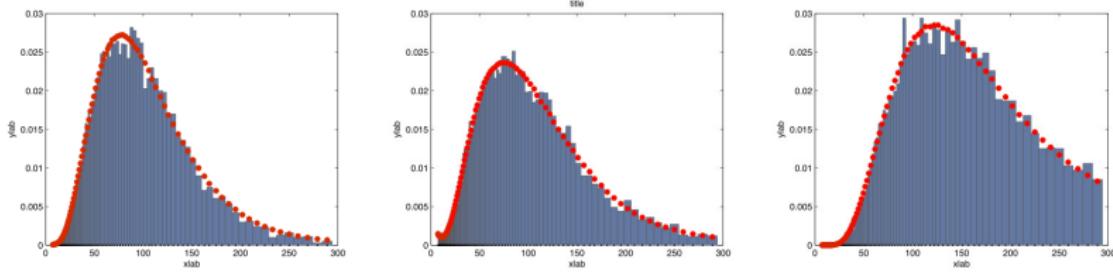
- Each representative particle characterizes a certain number of actual particles.
- The actual number of particles represented by the representative particle is called the Particle Number Rate. The Particle Number Rate is determined from the mass flow rate assigned to the representative particle divided by the mass of an actual particle.

Lagrangian Particle Tracking

Lagrangian Particle Tracking

PARCELS vs PARTICLES

The mathematical concept behind the Lagrangian Particle Tracking is closely related to the description of fluid motion - its kinematics and dynamics - in a Lagrangian frame of reference. In this reference frame, fluid parcels are labelled and followed through space and time.



- Evaporating liquid sprays are represented by a **DISCRETE PARTICLE TECHNIQUE**, in which each computational particle represents a number of droplets of identical size, velocity and temperature.
- Probability distributions often govern the assignment of droplet properties at injection or the changes in drop properties at downstream locations. When this is the case, droplet properties are determined by using a **Monte Carlo sampling technique**.

Lagrangian Particle Tracking



- As it moves, the mass of a fluid parcel remains constant, while in a compressible flow its volume may change, as well as its shape changes due to the distortion by the flow. The particles and the fluid interact by exchanging mass, momentum and energy.
- The **momentum exchange** is treated by a coupling procedures to the governing equations. Calculation of mass and energy exchange is ensured by automatic reductions in the timestep when the exchange rates become large.
- **Turbulence effects** on the droplets may be accounted for in one of two ways. When the timestep is smaller than the droplet turbulence correlation time, a fluctuating component is added to the local mean gas velocity when calculating each particle's mass, momentum, and energy exchange with the gas.
- **Droplet collisions** and coalescence are accounted for and a new model for droplet aerodynamic breakup has been installed.

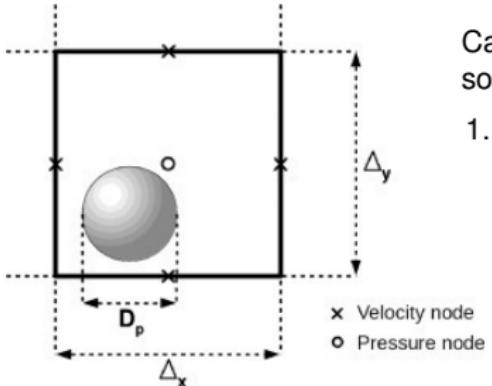
Lagrangian Particle Tracking



Coupling can take place through **mass**, **momentum** and **energy** transfer between phases:

- **MASS COUPLING** is the addition of mass through evaporation or the removal of mass from the carrier stream by condensation.
- **MOMENTUM COUPLING** is the result of the drag force on the dispersed and continuous phase; momentum coupling can also occur with momentum addition or depletion due to mass transfer.
- **ENERGY COUPLING** occurs through heat transfer between phases. Thermal and kinetic energy can also be transferred between phases owing to mass transfer.

Lagrangian Tracking: Governing Equations



Calculation of lagrangian particle motion requires the solution of:

1. a **continuous phase (Eulerian fluid)**:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \mathbf{u} \, d\Omega + \int_S \rho \mathbf{u} \cdot (\mathbf{u} - \mathbf{u}_b) \cdot \mathbf{n} dS = \sum f$$

2. A **dispersed phase (lagrangian particles)**. In Eulerian–Lagrangian simulations the bubbles are represented by volumeless Lagrangian points/markers. The physical effect of the inter-phase liquid-gas is modelled through acting forces. Bubbles are assumed to be rigid and spherical; there can be direct interaction between them. The motion of particles is computed by **Newton's second law**:

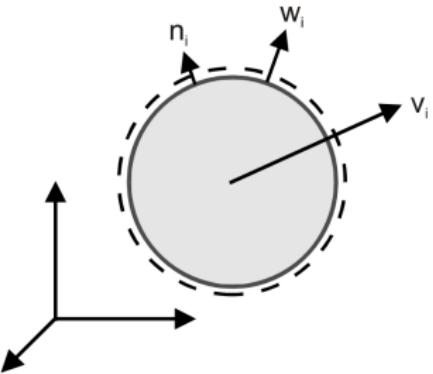
$$\frac{d\mathbf{x}_P}{dt} = \mathbf{u}_P$$

$$m_p \frac{d\mathbf{u}_P}{dt} = \sum_i \mathbf{F}_i$$

$$\mathbf{I}_p \frac{d\omega_P}{dt} = \sum_i \mathbf{T}$$

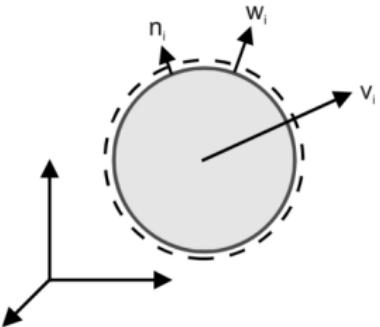
Particle-Fluid interaction

Previous equations would suffice to calculate the properties of a system with a constant mass, however, they are not appropriate for a droplet which may be evaporating or condensing or a coal particle which is undergoing devolatilization. In those cases, the Reynolds transport theorem is needed to account for the change in mass.



Consider a droplet which has a mass m and whose center of mass is moving with a velocity v_i with respect to an inertial reference frame. A control surface surrounds the droplet and is adjacent to the surface of the droplet so it assumes the instantaneous surface area of the droplet. The unit vector n_i is the unit outward normal vector from the control surface. The velocity of the gases through the control surface with respect to the control surface is w_i .

Governing Equations: continuity



The droplet continuity equation simply states that the rate of change of droplet mass is the negative value of the mass efflux through the droplet surface

$$\frac{dm}{dt} = -\rho_s w S$$

where S is the area of the control (droplet) surface and $\rho_s w$ is the average mass flux over the surface due to evaporation or condensation. It is clear that if no phase change is accounted the equation simplifies in the conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

Translational momentum

The formal statement of the momentum equation is that the rate of change of momentum within the control volume plus the net efflux of momentum through the control surface is equal to the forces acting on the system (surface and/or body forces), thus obtaining

$$F_i = m \frac{du_i}{dt} + \int_S \rho_s (\dot{r} n_i + w_i) w_i n_i dS$$

in which the regression rate of the surface \dot{r} must be discussed. The last term represents the thrust on the droplet due to momentum mass flux from the drop surface itself but, if this momentum flux is uniform over the droplet surface S , which is usually a good approximation, then

$$\dot{r} n_i + w_i = (\dot{r} + w) n_i = w' n_i$$

and the thrust becomes zero

$$\int_S \rho_s (\dot{r} n_i + w_i) w_i n_i dS = w' w \rho_s \int_S n_i dS = 0$$

so the droplet momentum equation simplifies to

$$F_i = m \frac{du_i}{dt}$$

The forces acting on the droplet are subdivided into body forces and surface force. The body force is the one acting on the mass of the droplet, such as gravity, and the surface force is commonly due to drag and lift which represent a momentum coupling between two phases.

Translational momentum



In the momentum equation all relevant forces acting on the particle, ie drag, gravitational and buoyancy forces, pressure forces are considered:

$$m_P \frac{\mathbf{u}_P}{dt} = \sum_i \mathbf{F}_i = \mathbf{F}_D + \mathbf{F}_G + \mathbf{F}_P + \dots$$

DRAG FORCE (\mathbf{F}_D)

$$\mathbf{F}_D = C_D \frac{\pi D_P^2}{8} \rho_f (\mathbf{u}_f - \mathbf{u}_P) |\mathbf{u}_f - \mathbf{u}_P|$$

where the drag coefficient C_d is estimated by empirical correlations:

- Schiller-Naumann (1935)

$$C_D = \begin{cases} \frac{24}{Re_P} (1 + 0.15 Re_P^0.687), & \text{if } Re_P \leq 1000 \\ 0.44, & \text{otherwise} \end{cases}$$

- Putnam (1961)

$$C_D = \begin{cases} \frac{24}{Re_P} (1 + \frac{1}{6} Re_P^{2/3}), & \text{if } Re_P \leq 1000 \\ 0.424, & \text{otherwise} \end{cases}$$

Response times

The response time of a particle or droplet to changes in flow velocity or temperature are important in establishing non-dimensional parameters to characterize the flow. **The momentum response time relates to the time required for a particle or droplet to respond to a change in velocity.** The equation of motion for a spherical particle in a gas is given by:

$$m \frac{dv}{dt} = \frac{1}{2} C_D \frac{\pi D_p^2}{4} \rho_f (u - v) |u - v|$$

Defining the disperse phase Reynolds number (relative Reynolds number) as:

$$Re_p = \frac{\rho_f D_p |u - v|}{\mu_f}$$

and dividing through by the particle mass gives

$$\frac{dv}{dt} = \underbrace{\frac{18\mu_f}{\rho_d D^2}}_{\frac{1}{\tau_p} = [\frac{1}{s}] \atop \simeq 1 \text{ at low Re} \text{ (Stokes flow)}} \underbrace{\frac{C_D Re_p}{24}}_{\simeq 1 \text{ at low Re} \text{ (Stokes flow)}} (u - v)$$

where μ_c is the viscosity of the continuous phase and τ_p defines the **momentum (velocity) response time.**

Governing Equations: translational momentum



GRAVITATIONAL AND BUOYANCY FORCE (F_G):

$$\mathbf{F}_G = m_P \mathbf{g} \left(1 - \frac{\rho_f}{\rho_P} \right)$$

LOCAL PRESSURE GRADIENT (F_P):

$$\mathbf{F}_P = -\frac{\pi D_P^3}{6} \nabla p = -\frac{\pi D_P^3}{6} \underbrace{\rho_f \left[\frac{D\mathbf{u}_f}{Dt} - \nabla \cdot \nu (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T) \right]}_{\text{momentum equation for the (incompressible) fluid}}$$

OTHER FORCES:

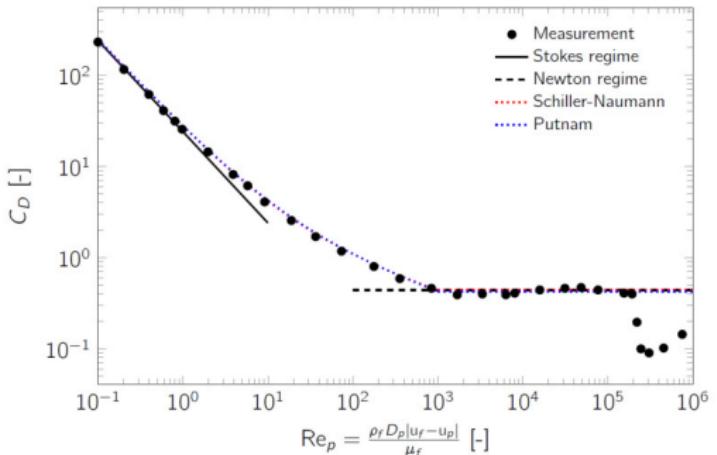
- **Added mass force:** particle acceleration or deceleration in a fluid requires also an accelerating or decelerating of a certain amount of the fluid surrounding the particle (important for liquid-particle flows)
- **Slip-shear lift force:** particles moving in a shear layer experience a transverse lift force due to the nonuniform relative velocity over the particle and the resulting nonuniform pressure distribution
- **Slip-rotation lift force:** particles, which are freely rotating in a flow, may also experience a lift force due to their rotation (Magnus force)
- **Thermophoretic force:** a thermal force moves fine particles in the direction of negative temperature gradients (important for gas-particle flows)

Translational momentum

One possible example of general form of the forcing term F is given by the **drag and gravitational force** for simplicity

$$F = \frac{\pi d^2}{8} \rho c_D |\mathbf{u}_d - \mathbf{u}| (\mathbf{u}_d - \mathbf{u}) + m_d \mathbf{g}$$

even though the latter can be neglected sometimes in Diesel sprays.



Drag coefficient as a function of particle Reynolds number, comparison of experimental data with correlations of Schiller-Naumann (1935) and Putnam (1961).

Governing Equations: angular momentum



The conservation equation for angular momentum states that the rate of change of angular momentum within the control volume plus the net efflux of angular momentum through the control surface is equal to the torque acting on the particle. If the particle is spherical, the mass efflux from the surface contributes no torque so the equation for rotation becomes

$$\mathbf{I}_p \frac{d\omega_p}{dt} = \sum_i \mathbf{T}$$

In which I is the **instantaneous momentum of inertia** about an axis of symmetry and $\omega_{d,i}$ is the particle rotation vector.

Moreover, mind the **Energy equation**: the energy of a droplet consists of the Kinetic (external) and the Internal Energy, plus the energy linked to the surface tension. Also, the heat transfer term includes both the convective and radiative heat transfer. The work therm includes the flow work due to the efflux of fluid through the control surface as well as the work associated with the forces on the droplet.

$$mc_d \frac{dT_d}{dt} = \dot{Q} + \dot{m} \left(h_S - h_d + \frac{w' w'}{2} \right)$$

where \dot{m} is the rate of mass change of the droplet, h_S is the enthalpy of the vapor at the control surface, and w' is the efflux velocity through the droplet surface with respect to the droplet center.

Governing Equations: angular momentum

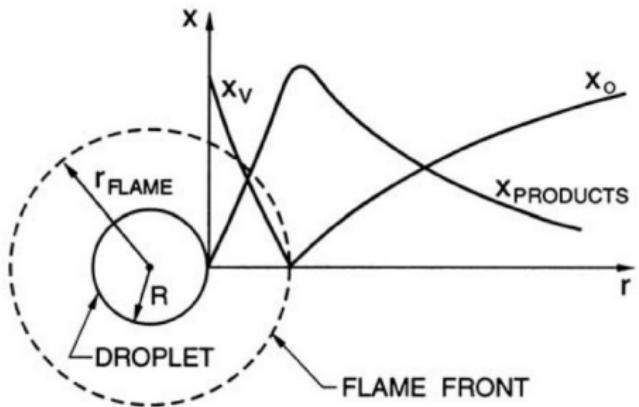


The kinetic energy associated with the efflux velocity is typically very small compared to the enthalpy change so it can be neglected, making the final form of the energy equation as follows

$$mc_d \frac{dT_d}{dt} = \dot{Q} + \dot{m}h_l$$

During a change in phase, when the droplet temperature remains constant at the saturation temperature, the heat transfer is just sufficient to balance the energy required for the change of phase.

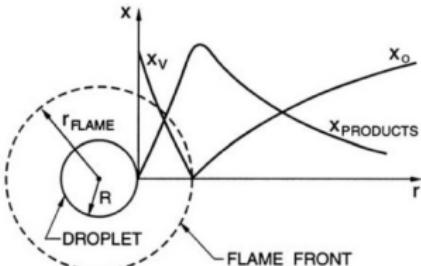
Droplet analysis



Fundamentals of multiphase flows, C.E. Brennen, Caltech, 2005

Let's consider a stationary spherical droplet which volume, and therefore diameter, is not reducing while it's burning, but is continuously fed with fuel. Then the problem can be studied by means of just one spatial parameter, ie the distance from the center of the drop, its radius. Commonly the description is performed by means of a double-film model approach, for which one film lays between the droplet surface and the front of the flame, and the second one is linking the front with the oxidizer.

Droplet analysis



Then, by assuming:

- quiescent atmosphere;
- constant continuous phase c_p ;
- uniform droplet temperature, knowing the surface one;
- infinitely fast chemical reaction (see reaction) so that oxidizer and fuel can't co-exist;
- molecular diffusion coefficient equal to the diffusivity (\mathcal{D}) both for fuel and oxidizer;

the **mass consumption rate, or the regression rate**, has to be computed by means of a study on the liquid droplet under consideration. and it must be referred to the amount of mass which has gasified. In return, the latter must be linked to the amount of energy which was necessary to gasify a portion of the liquid mass. The **surface heat flux** is

$$q_s = r \rho_l Q$$

in which Q contains the summation of the heat of vaporization, sublimation and/or gasification plus the enthalpy required to reach the vaporization temperature.

Droplet analysis



Last equation is relevant as if one is interested in the rate of consumption in the mass, no coefficient can be derived from the gasous surrounding continuous phase, while a parameter can be obtained checking the evolution of the liquid phase droplet under consideration.

Moreover, the **overall vaporization energy** is computed as

$$Q = \Delta h_v + c_l (T_s - T_0)$$

At the same time the **evaporation coefficient** is defined by the *experimental evaporation law* (d^2), starting from the initial diameter d_0 :

$$d^2 = d_0^2 - \beta_0 t$$

Now, be aware that if no radiation is present, the heat flux on the droplet surface follows the common form

$$q_s = -\lambda_g \left(\frac{\partial T}{\partial y} \right)$$

while in other cases, for which convection is relevant (when the droplet is not in a quiescent atmosphere), the surface heat flux is expressed by means of the heat transfer coefficient \bar{h}_c , computed as average on the entire external droplet surface.

$$q_s = \bar{h}_c (T_{\text{inf}} - T_s)$$

Droplet analysis



Combining the two equations, one obtains the **Nusselt number**, useful for the description of the heat-transfer coefficient, and formally dependant on the Reynolds and Prantl number:

$$\bar{N}u = f(Re, Pr) = \frac{\bar{h}_c d_0}{\lambda_g}$$

Finally, by following the initial assumptions, and a so-called **Spalding approach**, by performing a double integration, the **fuel evaporation rate** is rearranged to obtain

$$G_f = \frac{\dot{m}_f}{4\pi r_s^2} = \rho_s D_s \frac{\ln(1+B)}{r_s}$$

in which B is the **Spalding transfer number**, depending on the *Spalding number* (b) that is dependant on the fuel mass fraction in the location considered (b_∞ considers $r = \infty$)

$$B = b_\infty - b = \frac{Y_{F_\infty}}{Y_{F_s} - 1} - \frac{Y_F}{Y_{F_s} - 1}$$

In order to calculate the **mass evaporation rate** it is necessary to know the value of the Spalding transfer number (B), which requires the knowledge of the Spalding numbers (b and b_∞). And by **assuming that the surrounding gas is saturated by the liquid vapor of the fuel droplet, the latter has a surface temperature T_s**

Droplet analysis

The problem evolves then in the research of the droplet surface temperature. Thus, a detailed process begins to compute that.

Starting from the energy equation from the droplet point of view

$$r^2 \rho u \frac{d(c_p T)}{dr} = \frac{d}{dr} \left(\frac{\lambda}{c_p} r^2 \frac{d(c_p T)}{dr} \right) + r^2 \dot{Q}$$

and knowing that the temperature is balanced within the drop with the superficial one, so that the analysis can focus on the internal part of the drop, in order to neglect the superficial \dot{Q} , as well as the c_p which is constant in space, one obtains

$$r^2 \rho u \frac{dT}{dr} = \frac{d}{dr} \left(\frac{\lambda}{c_p} r^2 \frac{dT}{dr} \right)$$

The latter can be rearranged in the following way, knowing that c_p is constant

$$r^2 \rho c_p u \frac{dT}{dr} = \frac{d}{dr} \left(\lambda r^2 \frac{dT}{dr} \right)$$

Integration can be performed

$$r^2 \rho c_p u T = \lambda r^2 \frac{dT}{dr} + c$$

and boundary conditions are necessary: $T(r = s) = T_s$, and $\lambda \frac{\partial T}{\partial r}|_s = \rho_s u_s \Delta h$. Do not forget that T_s is unknown and has to be computed.

Droplet analysis

Therefore, by applying B.C.,

$$r_s^2 \rho_s c_p \mathbf{u}_s \left(T - T_s + \frac{\Delta h_v}{c_p} \right) = \lambda r^2 \frac{dT}{dr}$$

Separate variables for by part integration, to obtain

$$-\frac{r_s^2 \rho_s c_p \mathbf{u}_s}{r \lambda} = \ln \left(T - T_s + \frac{\Delta h_v}{c_p} \right) + c'$$

Now, don't forget that it assumed ad known the temperature at ∞ distance $T(r = \infty) = T_\infty$, thus

$$\frac{r_s \rho_s c_p \mathbf{u}_s}{\lambda} = \ln \left(\frac{c_p(T_\infty - T_s)}{\Delta h_v} + 1 \right)$$

By defining $\alpha = \frac{\lambda}{\rho c_p}$ and $B_T = \frac{c_p(T_\infty - T_s)}{\Delta h_v}$, the equation is rearranged in the following way

$$r_s \mathbf{u}_s = \alpha_s \ln(1 + B_T)$$

BUT, being the left term also linked to the mass conservation, so that $r_s \mathbf{u}_s = \mathcal{D} \ln(1 + B_M)$, and **IF** $\alpha = \mathcal{D}$, so that $Le = 1$, then $B_T = B_M$, which means

$$\frac{c_p(T_\infty - T_s)}{\Delta h_v} = \frac{Y_{F_\infty} - Y_F}{Y_F - 1}$$

Droplet analysis



Problem now has two unknown terms, ie Y_F and T_s , therefore a second equation is needed: a link between Y_F and the partial pressure p_F

$$Y_F = \frac{\rho_F}{\rho} = \frac{n_F W_F}{nW} = \frac{p_F W_F}{pW}$$

Thus, the p_F term has been introduced, and while it is increasing the number of unknown terms, this last value can be linked (or neglected by substitution) by including the **Clausius-Clapeyron vapor pressure equation** so that

$$\frac{d \ln(p_F)}{dT} = \frac{\Delta h_v}{RT_s}$$

Finally, from these 3 equations the 3 unknowns can be found, so that the initial request, T_s , is computed.

Droplet analysis: evaporation time

Also, another important parameter is the **Evaporation Time**, which is of predominant relevance in combustion chamber design due to the fact that it must be investigated the largest droplet lifetime so as to predict the MINIMUM time a droplet has to remain in the chamber itself. By looking at mass continuity on droplet surface

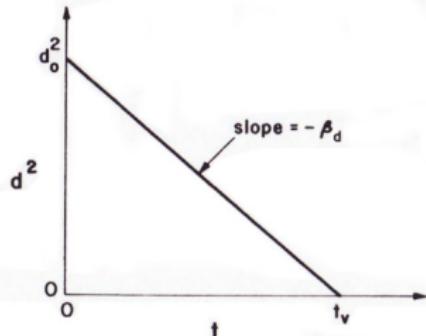
$$\frac{dr}{dt} = -\frac{\rho_s \mathcal{D}}{\rho_l r_s} \ln(1 + B)$$

so that, by performing by part integration

$$\Delta r = r - r_0 = -\frac{\rho_s \mathcal{D}}{\rho_l r_s} \ln(1 + B)t \quad \text{since } t_0 = 0$$

The last equation becomes $r = r_0 - \beta_d t$, which follows the d^2 rule.

It is important to note that the estimation done is valid overall, but it becomes more accurate as droplets considered are larger, thus when the evaporation time gets longer. Moreover the flame diameter does NOT decrease in the same way of the droplet one, instead, it is known to initially increase as the flame arises around the droplet.



Droplet analysis: observations



Regarding the shape of the droplets, an assumption of perfect sphericity was presented, but it is well known that the latter is valid only if the collision and/or agglomeration effects are small, ie if the volume of the condensed phase is much less than the total one, and the Weber number $We \ll 20$.

Remind the Weber number as the ratio between dynamic forces and surface tension ones:

$$We = \frac{2r\rho_g(\mathbf{u}_d - \mathbf{u}_g)^2}{\sigma_s}$$

Thus, if $We \ll 20$ is not satisfied, droplets are no longer spherical, they deform, and subsequently break up by progressively increasing this number.

Also, whenever combustion of fuel droplets is considered, not only the size, but also the volatility of the drop has to be accounted. Indeed, if small particles are considered, their high level of volatility is such that the evaporation can occur completely during the heating process, consuming the drop itself.

It is also important to note that whenever there is an increase in the initial drop size, which refers to a longer time taken to complete the evaporation process, the flame speed decreases.

Response times

The response time of a particle or droplet to changes in flow velocity or temperature are important in establishing non-dimensional parameters to characterize the flow. **The momentum response time relates to the time required for a particle or droplet to respond to a change in velocity.** The equation of motion for a spherical particle in a gas is given by:

$$m \frac{dv}{dt} = \frac{1}{2} C_D \frac{\pi D_p^2}{4} \rho_f (u - v) |u - v|$$

Defining the disperse phase Reynolds number (relative Reynolds number) as:

$$Re_p = \frac{\rho_f D_p |u - v|}{\mu_f}$$

and dividing through by the particle mass gives

$$\frac{dv}{dt} = \underbrace{\frac{18\mu_f}{\rho_d D^2}}_{\frac{1}{\tau_p} = [\frac{1}{s}] \atop \text{s} \approx 1 \text{ at low Re} \atop \text{(Stokes flow)}} \underbrace{\frac{C_D Re_p}{24}}_{\simeq 1 \text{ at low Re}} (u - v)$$

where μ_c is the viscosity of the continuous phase and τ_p defines the **momentum (velocity) response time.**

Response times

The response time of a particle or droplet to changes in flow velocity or temperature are important in establishing non-dimensional parameters to characterize the flow. **The momentum response time relates to the time required for a particle or droplet to respond to a change in velocity.** The equation of motion for a spherical particle in a gas is given by:

$$m \frac{dv}{dt} = \frac{1}{2} C_D \frac{\pi D_p^2}{4} \rho_f (u - u_p) |u - u_p|$$

where:

- u_p and u are namely the particle and the flow velocity;
- ρ_f and μ_f are namely the density and the viscosity of the continuous phase;
- C_D is the particle drag coefficient;
- Re_p is the disperse phase Reynolds number (relative Reynolds number) defined as:

$$Re_p = \frac{\rho_f D_p |u - u_p|}{\mu_f}$$

and dividing through by the particle mass gives

$$\frac{dv}{dt} = \underbrace{\frac{18\mu_f}{\rho_d D_p^2}}_{\frac{1}{\tau_p} = [\frac{1}{s}]} \underbrace{\frac{C_D Re_p}{24}}_{\simeq 1 \text{ at low } Re} (u - u_p) \simeq \frac{1}{\tau_p} (u - u_p)$$

(Stokes flow)

Response times

In the equation of motion a the spherical particle in a gas:

$$\frac{du_p}{dt} = \underbrace{\frac{18\mu_f}{\rho_p D^2}}_{\frac{1}{\tau_p} = \left[\frac{1}{s} \right]} \underbrace{\frac{C_D Rep}{24}}_{\simeq 1 \text{ at low Re} \text{ (Stokes flow)}} (u - u_p) \simeq \frac{1}{\tau_p} (u - u_p)$$

τ_p defines the **momentum (velocity) response time**:

$$\tau_p = \frac{\rho_p D^2}{18\mu_f}$$

The solution to the equation

$$\frac{du_p}{dt} = \frac{1}{\tau_p} (u - u_p)$$

for constant u and an initial particle velocity of zero ($u_p^0 = 0$) is:

$$u_p = u (1 - e^{-t/\tau_p})$$

Thus the momentum response time is the time required for a particle released from rest to achieve 63% of the free stream velocity.

Thermal Response Time 1/2



The thermal response time relates to the responsiveness of a particle or droplet to changes in temperature in the carrier fluid. The equation for particle temperature, assuming the temperature is uniform throughout the particle and negligible radiative effects is:

$$m c_{d,p} \frac{\partial T_p}{\partial t} = Nu \pi k_c D (T_c - T_p) \rightarrow \frac{\partial T_p}{\partial t} = \underbrace{\frac{Nu}{2}}_{\substack{\approx 1 \\ \text{low Re}}} \underbrace{\frac{12k'_c}{\rho_p c_p D^2}}_{\frac{1}{\tau_T}} (T_c - T_p) = \frac{1}{\tau_T} (T_c - T_p)$$

where

- Nu is the Nusselt number;
- $c_{d,p}$ is the specific heat of the particle material;
- k'_c is the thermal conductivity of the continuous phase.

Thermal Response Time 2/2



The momentum and thermal response times are related through the properties of the fluid and the particles.

$$\frac{\tau_p}{\tau_T} = \frac{\rho_d D^2}{18\mu_c} \frac{12k'_c}{\rho_d c_d D^2} = \frac{2}{3} \frac{k'_c}{\mu_c c_d} = \frac{2}{3} \frac{c_c}{c_d} \frac{k'_c}{\mu_c c_c}$$

Being $Pr = \frac{\mu_c c_c}{k'_c}$, it follows:

$$\frac{\tau_p}{\tau_T} = \frac{2}{3} \frac{c_c}{c_d} \frac{1}{Pr}$$

where Pr is the Prandtl number.

- For **gases**, the Prandtl number is on the order of unity so the response times are of the same order of magnitude.
- For **liquids**, Pr can be the order of 10^2 which means that velocity equilibrium is achieved much more rapidly than thermal equilibrium in a liquid.

Even though the above relations for the ratio of response times have been derived for low Reynolds number (Stokes flow), the ratio changes little for higher Reynolds numbers.

Stokes number

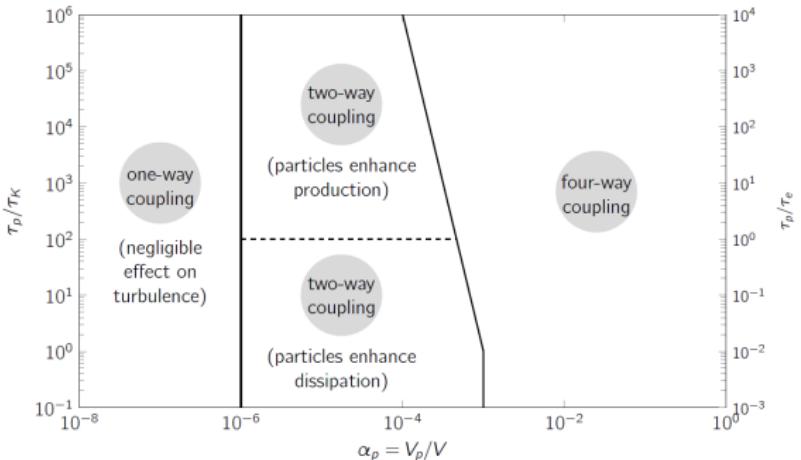


The **Stokes number related to the particle velocity** is a very important parameter in fluid-particle flows and it is defined as:

$$St_v = \frac{\tau_v}{\tau_T}$$

- If $St_v \ll 1$, the response time of the particles is much less than the characteristic time associated with the flow field. Thus the particles will have ample time to respond to changes in flow velocity, so the particle and fluid velocities will be nearly equal (velocity equilibrium).
- If $St_v \gg 1$, then the particle will have essentially no time to respond to the fluid velocity changes and the particle velocity will be little affected by the flow velocity.

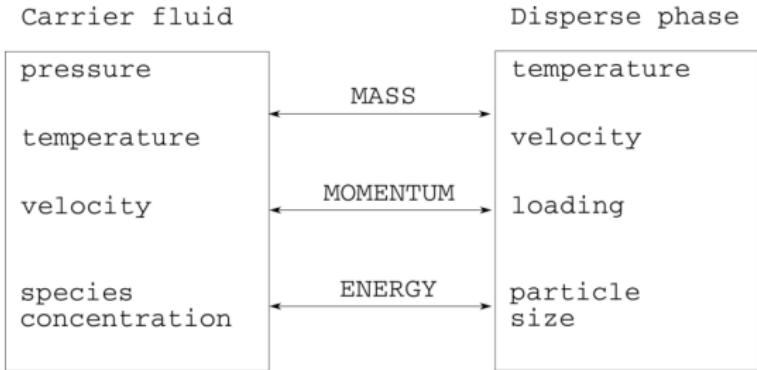
Lagrangian-Eulerian coupling



To simulate particle-laden flows, an appropriate coupling of dispersed and continuous phases must be defined:

- the decision about the **coupling scheme is reliant on the volume fraction** of the particles (→ Elghobashi). The particle motion in diluted flows is primarily influenced by the aerodynamic forces acting on the particles;
- furthermore, **if interactions between particles have to be considered, a four-way coupling must be enabled**, at which point particle collisions are resolved within the Lagrangian solver.

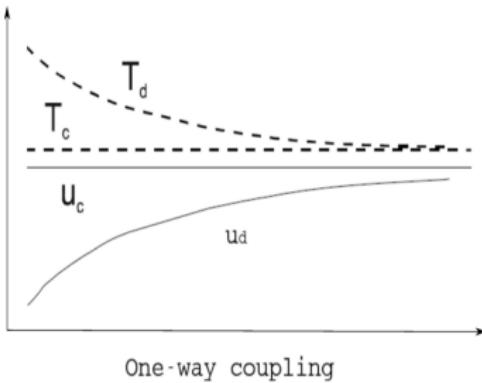
Phase coupling



Phase-coupling mechanisms strongly influences the behavior of the continuous and dispersed phase:

- **One-way coupling:** fluid \rightarrow particles
 - fluid phase influences the motion of the parcels via drag and turbulence;
 - Parcels (liquid phase) have no influence on the gas phase.
- **Two-way coupling:** fluid \rightleftharpoons particles
 - fluid phase influences the motion of the parcels via drag and turbulence;
 - parcels influence the Eulerian phase via source terms of mass, momentum and energy.
- **Four-way coupling:** fluid \rightleftharpoons particles + particle collisions

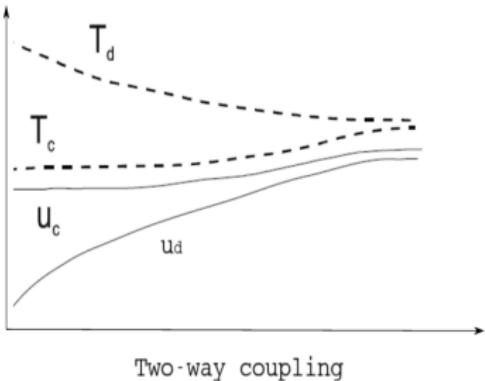
One-way coupling



EXAMPLE.

- Assume that hot particles were injected into a cool gas flowing in a pipe. Also assume that the void fraction is near unity. One can calculate the trajectory and the corresponding thermal history of the particles by using the local velocity and temperature of the gas. Thus particle temperature will decrease toward the gas temperature while the particle velocity will increase toward the gas velocity. **One-way coupling implies that the presence of the particles does not affect the gas flow field** while the gas flow field is responsible for the change in particle temperature and velocity.

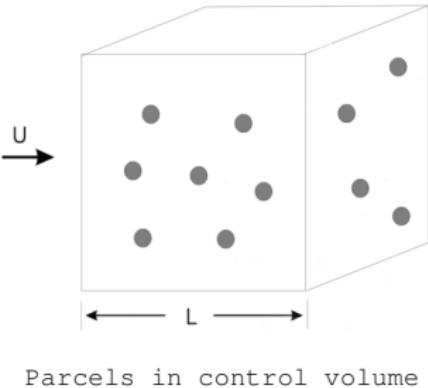
Two-way coupling



EXAMPLE.

- If the effect of the particles on the gas were included (two-way coupling), the temperature of the gas would increase and the gas density would decrease. This, in turn, would lead to an increased gas velocity to satisfy mass conservation. Thus the particle cooling rate would be reduced (smaller temperature difference) and the particles would be accelerated to a higher velocity. The acceleration of the particles together with the increased gas velocity would lead to a more negative pressure gradient.

Mass coupling



Parcels in control volume

Mass coupling can occur through a variety of mechanisms such as evaporation, condensation, or chemical reaction.

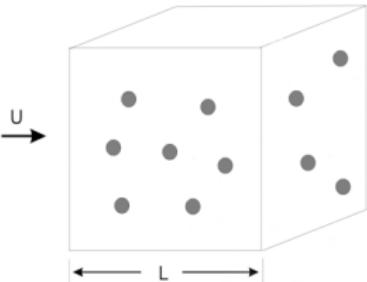
Suppose there are n droplets per unit volume V in a box with side L , and that each droplet is evaporating at a rate \dot{m} . Thus the **mass generated by the dispersed phase per unit time due to evaporation** is

$$\dot{M}_d = n L^3 \dot{m}$$

while the **mass flux of the continuous phase** passing through this control volume is

$$\dot{M}_c = \bar{\rho}_c \mathbf{u} L^2$$

Mass coupling



A **mass coupling parameter** is defined as

$$\Pi_m = \frac{\dot{M}_d}{\dot{M}_c}$$

If $\Pi_m \ll 1$ then the effect of mass addition to the continuous phase would be insignificant and mass coupling could be neglected. This ratio can be expressed as

$$\Pi_m = \frac{\dot{M}_d}{\dot{M}_c} \sim \frac{\bar{\rho}_d}{\bar{\rho}_c} \frac{L \dot{m}}{u m}$$

The ratio $\frac{\dot{m}}{m}$ scales as the reciprocal of characteristic evaporation, burning or condensation time, τ_m .

Momentum coupling

The importance of momentum coupling can be assessed by **comparing the drag force due to the dispersed phase with the momentum flux of the continuous phase.**

A momentum coupling parameter can be defined as

$$\Pi_M = \frac{F_D}{\mathcal{M}_c}$$

in which F_d is the drag force due to the particles in the volume and \mathcal{M}_c is the momentum flux through the volume.

The drag associated with droplets in volume with side L is

$$F_d = nL^3 3\pi\mu_c D(u - v)$$

The momentum flux of the continuous phase is given by

$$\mathcal{M}_c = \bar{\rho}_c u^2 L^2$$

The momentum coupling parameter can be expressed as

$$\Pi_M = \frac{F_D}{\mathcal{M}_c} = \frac{nmL}{\bar{\rho}_c u \tau_v} \left(1 - \frac{v}{u}\right)$$

Momentum coupling



If one considers the ratio $\tau_v \mathbf{u} / L$ as the ratio of the time associated with momentum transfer to a time characteristic of the flow or the Stokes number for momentum transfer, such as

$$St_M = \frac{\tau_v \mathbf{u}}{L}$$

then as the Stokes number approaches zero, the velocity of the dispersed phase approaches that of the continuous phase so the above equation develops an indeterminacy (0/0).

Momentum coupling effects become less important for small concentrations (loadings) and large Stokes numbers.

Energy coupling

Energy coupling follows the same model as used for mass and momentum coupling. The significance of energy coupling can be assessed by comparing the heat transfer to (or from) the dispersed phase and the energy flux of the continuous phase.

The energy coupling parameter is defined as

$$\Pi_e = \frac{\dot{Q}_d}{\dot{E}_c}$$

Obviously if $\Pi_e \ll 1$ then energy coupling is unimportant.

The heat transfer associated with the dispersed phase elements in volume (L^3) is

$$\dot{Q}_d = nL^3\pi Nu k'_c D (T_d - T_c)$$

in which the Nusselt number (Nu) and the thermal conductivity of the continuous phase (k'_c) are accounted.

The energy flux of the continuous phase is

$$\dot{E}_c = \bar{\rho}_c u c_p T_c L^2$$

For gaseous flows, the momentum and thermal response times are of the same order ($\Pi_M \sim \Pi_e$), and if one-way coupling is chosen for momentum, this assumption justifies the choice for one-way coupling also for energy transfer.

Energy coupling



If most of the energy transfer in a system is associated with latent heat in the dispersed phase (h_L), there is another form of the energy coupling parameter which may be appropriate.

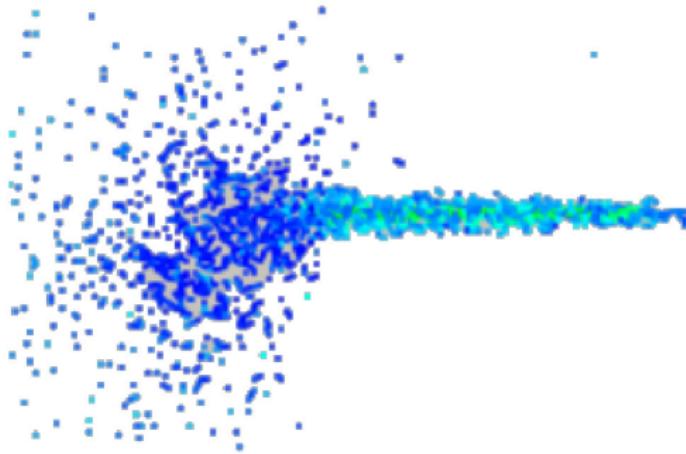
The energy associated with change of phase in a volume L^3 is

$$\dot{E}_d = nL^3\dot{m}h_L$$

The Energy factor can be large, causing energy transfer due to phase change to be important even though mass transfer itself is unimportant.

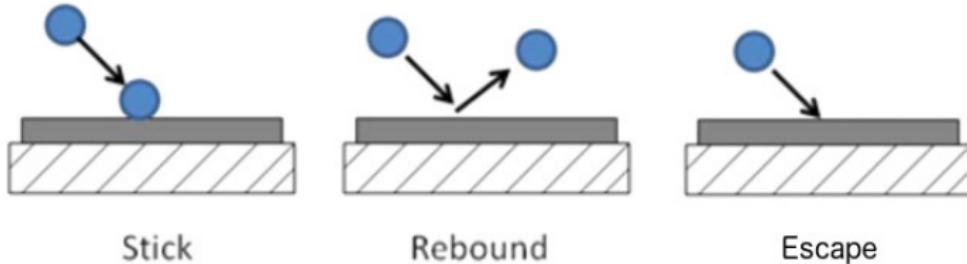
In many spray problems, the energy coupling due to phase change may be the only two-way coupling which must be included in developing an analysis for a gas-droplet flow.

Wall Interaction in Lagrangian Modeling



- The behavior of various droplets within different regimes of a spray is quite different. Obviously, droplet-droplet interactions such as collision and coalescence can be significant close to the nozzle orifice.
- Moreover, when the droplet spacing is small, the motion of a droplet is affected by an adjacent droplet: consequently, it can no longer be assumed that there is an undisturbed gas phase around the droplet in order to calculate the exchange processes between liquid and gas.

Wall Interaction in Lagrangian Modeling



Wall Interaction in Lagrangian modeling involves several submodels to simulate parcels' behavior at the walls. We can classify two different kind kind of boundary treatments:

- standard wall treatment, usually applied to standard DPM methods includes:
 - Sticking of the particles at the walls
 - Rebound of the particles at the walls
 - Escape of the particles through open boundaries (processor, patch boundaries, open boundaries etc.)
- wall-film modeling at the solid walls

Depending on the modeling adopted at the walls, the complexity of the simulation may significantly change.

Thank you for your attention!

contact: federico.piscaglia@polimi.it