Minicourse in Industrial Mathematics

Segundo Enquentro Italo–Argentino

Third lecture: Dynamics of liquid–liquid dispersions

F. Rosso

www.math.unifi.it/~rosso/RICERCA/MinicorsoBA/minicorso-2.pdf

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Many processes in nature are described in terms of particle systems governed by coagulation fragmentation interaction. Among them

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Industrial interest of dispersions

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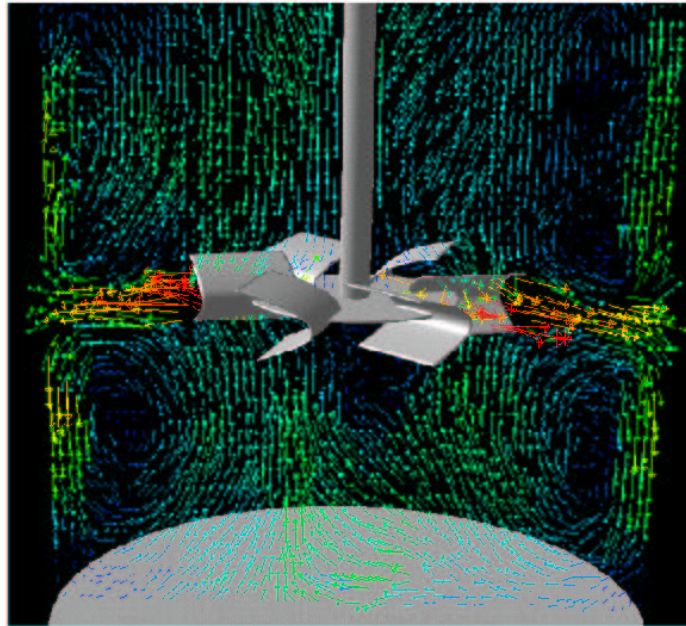- aerosol (liquid or solid particles suspended in a gas)

Baffle

Blade impeller

Sampling   Injection
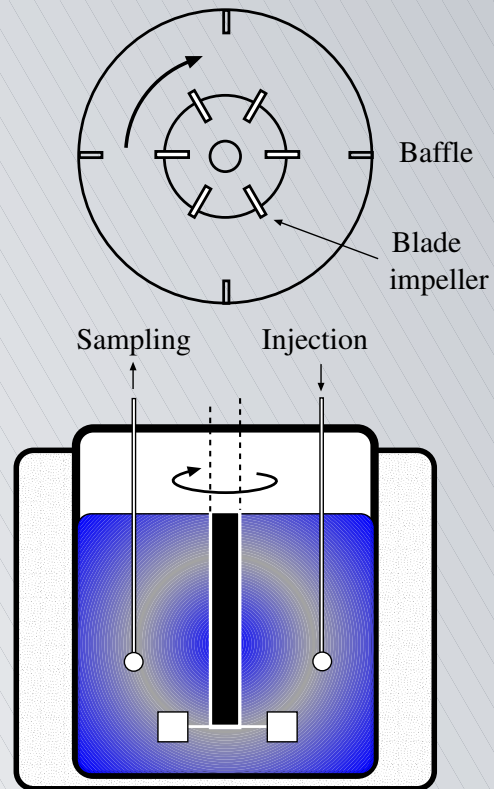
Costant temperature bath

Geometry of a batch reactor with blade impeller

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Motion pictures

Flow Pattern in Vessel

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Flow Around Impeller Blades

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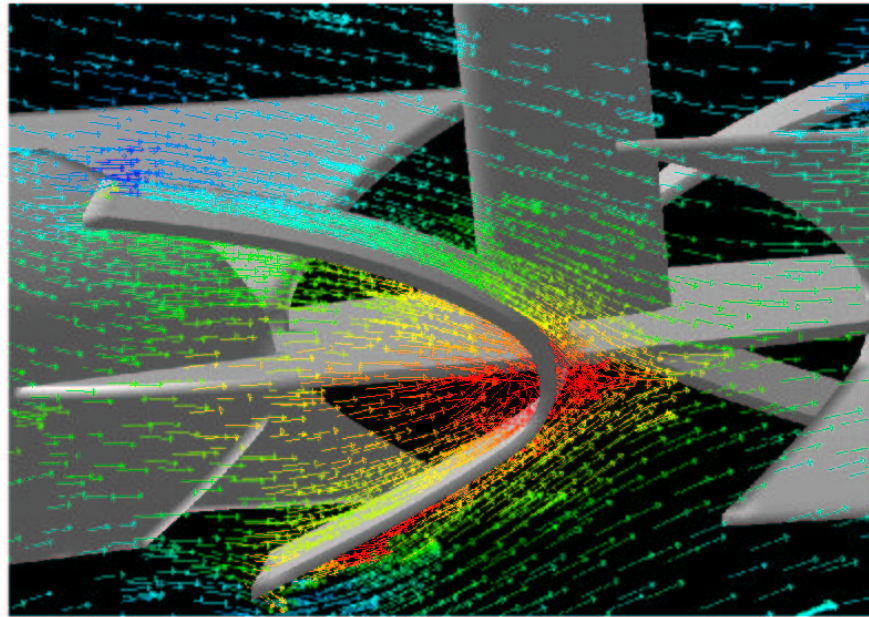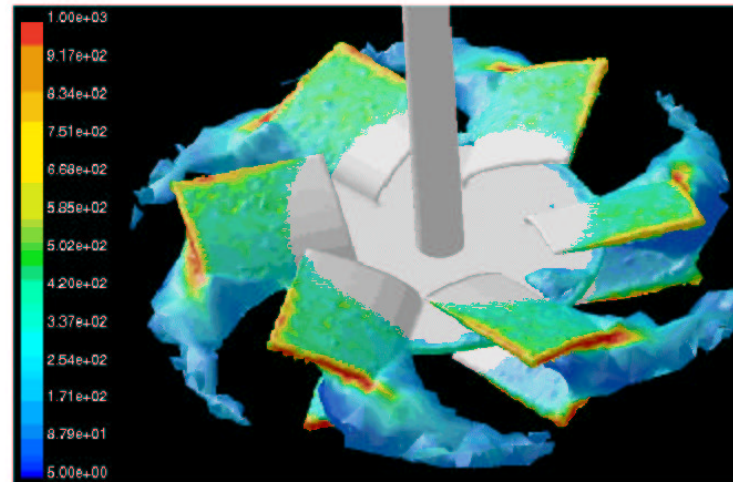
Motion pictures

Vorticity magnitude on a surface of constant velocity (1.875 m/s).
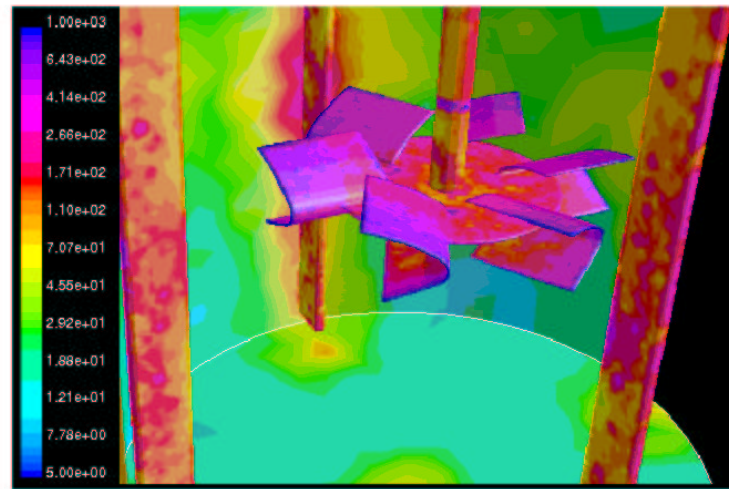
Motion pictures

Turbulence in Impeller Region

Velocity magnitude on a surface of constant turbulent kinetic energy (0.1 m²/s²).

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Motion pictures

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Discrete and continuous models

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— CHARACTERISTIC VARIABLE: cluster size (or volume or number of particles) which may be either a positive real number (continuous models) or a positive integer (discrete models) depending on the physical context

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$$\partial_t f + \mathscr{A}(x,t,v)f = r(x,t,v,f), \qquad x \in \mathbb{R}^n, \quad t > 0$$

$$f(x,0,v) = f_0(x,v), \qquad x \in \mathbb{R}^n$$

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- r describes the kinetic behaviour of the process

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where

- $\mathscr{A}$ is a convection–diffusion operator
- r describes the kinetic behaviour of the process
- f is the particle–size distribution function
- v is the volume (of the cluster)

Moreover

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Discrete and continuous models

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- 🔴 $\int_X \int_{v_0}^{v_1} f(x,t,v) \, \mathrm{d}v \, \mathrm{d}x$ is the total number of particles with volume belonging to the interval $[v_0, v_1] \subset \mathbb{R}^+$ and being at time t contained in the space region $X \subset \mathbb{R}^n$

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- 🔴   The measure $\mathrm{d}v$ is either the Lebesgue on $\mathrm{I\!R}^+$ (*continuous models*) or the counting measure on $\mathrm{I\!\dot{N}} := \{1, 2, 3, \dots\}$ (*discrete models*). In the latter case the integrals with respect to $\mathrm{d}v$ reduce to sums

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$$\mathscr{A}(x,t,v)f \quad := -\operatorname{div}\left(\mathbf{A}(x,t,v)\operatorname{grad} f + \vec{a}(x,t,v)f\right)$$

$$+\vec{b}(x,t,v)\cdot\operatorname{grad} f + a_0(x,t,v)f$$

Symbols:

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Symbols:

- $\mathbf{A}(x,t,v)$ —- diffusion matrix (depends in a known way by the temperature field $T(x,t)$ which may be unknown so it needs to be determined by coupling to the heat equation.)

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- a_0 —- adsorption rate

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Interesting problems

The whole system appears exceedingly complicated! However in many cases of physical interest T, $\vec{a}$, and $\vec{b}$ can be thought of as given.

For example if we assume that the suspended particles have no effect on the velocity distribution (as in low aerosol concentration) then we can solve the Navier–Stokes equation for $\vec{b}$ independently of the other equations.

Problems to be studied

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- to check the physical consistency of the model

State of the art I

Most of the mathematical research focuses on discrete models (basically without diffusion) (many papers since von Smoluchowski [1917], Chandrasekhar[1943],..., Ball &Carr [1990], Bénilan & Wrzosek [1997]). The main system reduces to an *infinite system of ordinary integro–differential equations*. Works with *diffusion* taken into account are very recent (Laurençot & Wrzosek [1998], Amann [2000]). In these papers $\mathscr{A}(x,t,v)f = -a(v)\nabla_2 f$ with $a(v)$ being non–negative constants for $v \in \dot{\mathbb{N}}$. Main interests are *existence, uniqueness, asymptotic behaviour under various functional hypotheses*

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State of the art II

Much less seems to be known for the case of continuous models (i.e. dv is the Lebesgue measure) without diffusion. Global existence and uniqueness proved by Melzak [1957] with kernels supposed to be symmetric, positive and bounded. Other results (with different methods) obtained by Aizenman & Bak [1979], McLaughlin, Lamb & McBride [1997–1998] Dubowski & Stewart [1996]

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State of the art III

All these papers allow v to run from 0 to $+\infty$ and claims that this — which is clearly a mathematical abstraction — is made for convenience and does not influence physical models since it can be always assumed that all the relevant kernels and coefficients vanish identically for sufficiently large or small values of v

Unbounded kernels and infinite domains of integration enhance the mathematical difficulties considerably

In all these models — unless suitable ad–hoc assumptions are made on the kernels and

the asymptotic decay of solutions — the conservation of volume may be violated, even for

isolated systems (Simons [1983])!

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State of the art IV

The failure of the volume conservation law does not occur if v is allowed to ran in a finite interval

To keep v in a finite interval we should need some new physical mechanism able to control

the growth of large particles. One could say (as Amann [2000]) that the coalescence ker-

nel cuts off to zero at a critical upper bound or that the breakage kernel becomes singular

there. However he former approach is quite unphysical, the latter destroys particles close

to criticality but it doesn't affect at all the coalescence of small drops leading to droplets

above criticality

What the physics says?

The two key processes are coalescence and breakage

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🔴 COALESCENCE

a) collision *does not imply* coalescence

b) usually *binary*

c) evidence of a *critical size* v_{max} *for merging* droplets (droplets with $v > v_{max}$ are *unstable* at any time)

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🔴 BREAKAGE

    a) *several different mechanisms* (by elongation, pressure fluctuation, drop–eddy collision, erosion)

    b) usually *multiple*

    c) experimental evidence of a *critical size v_{min} for breaking* droplets (droplets with $0 < v < v_{min}$ are *stable* at any time)

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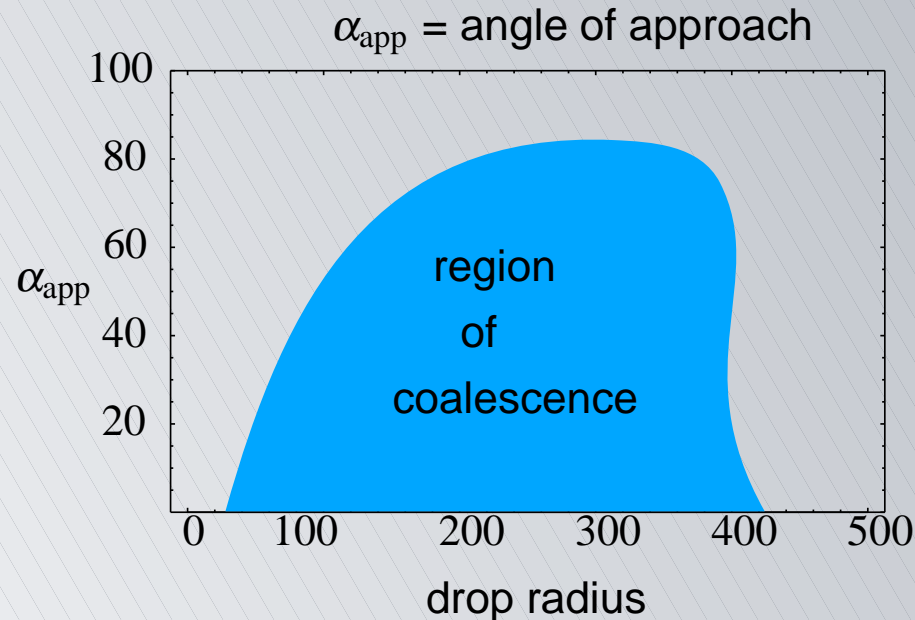
Facts about coalescence

Coalescence modes:

— by embedding and squeezing in one eddy

— drops drawn together by asymmetric bombardment by small eddies

— by shear coalescence (relatively slow motion)

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Facts about coalescence

• Kumar, Kumar, Ghandi [1993]

α_{app} = angle of approach

drop radius
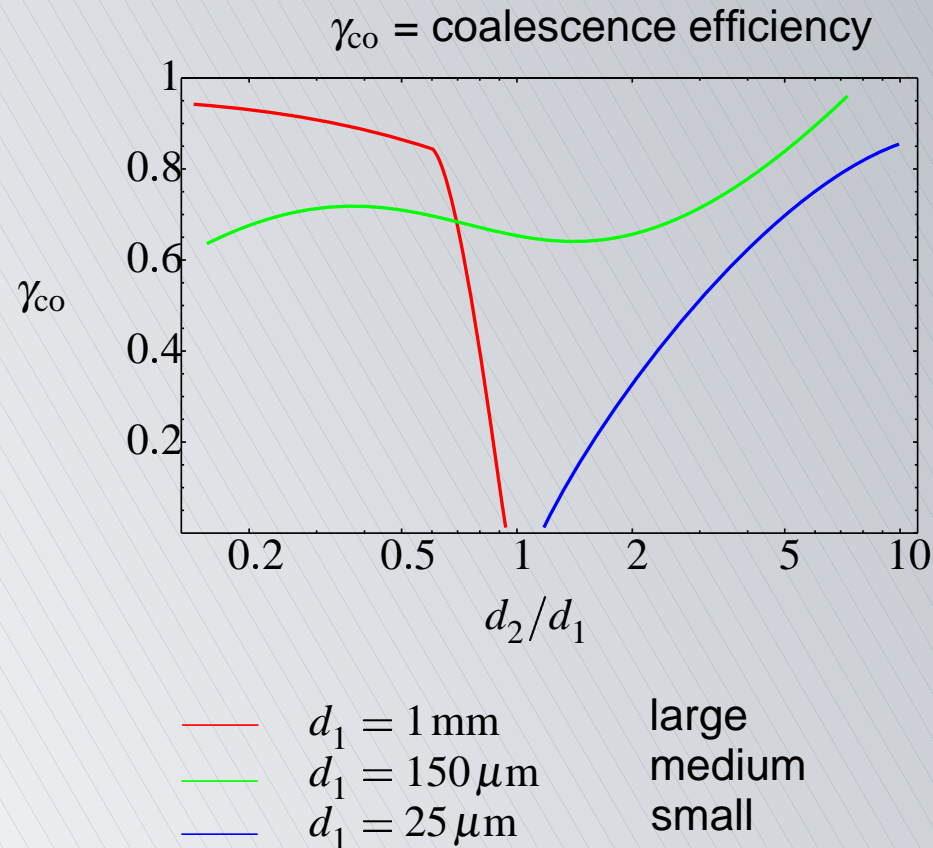
Coalescence region for drops of equal size. Very large and very small droplets do not coalesce regardless of the mutual angle of approach ($\alpha_{app} = 0°$ means "head-on collision", $\alpha_{app} = 90°$ means "grazing droplets")

Physical interpretation: coalescence occurs by drainage and rupture of the interposed protective film.

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Facts about coalescence

- Kumar, Kumar, Ghandi [1993]

γ_{co} = coalescence efficiency

$d_1 = 1\,\text{mm}$ large
$d_1 = 150\,\mu\text{m}$ medium
$d_1 = 25\,\mu\text{m}$ small

Coalescence efficiency *vs.* droplets ratio

Coalescence rate

• Tsouris and Tavlarides [1994]

Coalescence rate $= n_m n_j R(d_m, d_j) \lambda(d_m, d_j)$

$$R \quad = \text{collision frequency}$$

$$= \kappa_1 \frac{\varepsilon^{1/3}}{1+\varphi} (d_m + d_j)^2 \left(d_m^{2/3} + d_j^{2/3} \right)^{1/2}$$

$$\lambda \quad = \text{coalescence efficiency}$$

$$= \exp\left[-\kappa_2 \frac{\mu_c \rho_c \varepsilon}{\sigma^2 (1+\varphi)^3} \left(\frac{d_m d_j}{d_m + d_j} \right)^4 \right]$$

Remark. Even if $\lambda \to 0$ as $\dfrac{d_m d_j}{d_m + d_j} \to +\infty$, we can *fix* the product $d_m d_j$ letting d_m become

large and d_j become *small* (large droplets can grow at the expense of small ones).

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Some Remarks About Breakage

- Tsouris and Tavlarides [1994]

Possible breakage mechanisms:

- Elongation in a shear flow field (Taylor [1934])

- Pressure fluctuations in turbulence (Hinze [1955])

- Drop–Eddy collisions (Coulaloglou and Tavlarides [1977])

- Erosive Breakage (stripping by turbulence)

MOVIE 1   MOVIE 2   MOVIE 3

Breakage can be either *binary* or *multiple*. Erosive breakage generates a large number

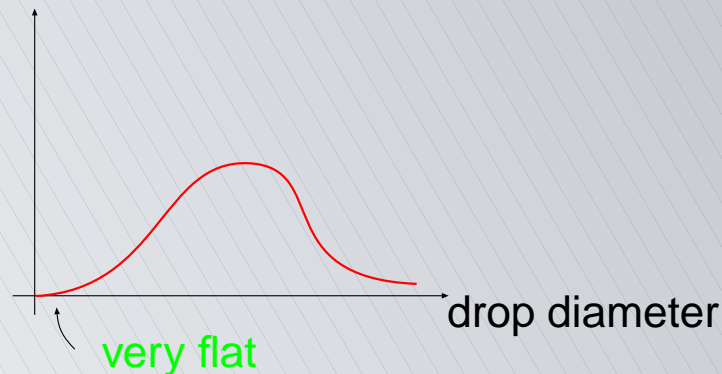of very small droplets. Breakage rate is always an *average*.

Some breakage rate formulas

- Coulaloglou and Tavlarides 1977

$$\text{break. rate} = \kappa_1 \frac{\varepsilon^{1/3}}{(1+\varphi_d)d^{2/3}} \exp\left[-\kappa_2 \frac{\sigma(1+\varphi)^2}{\rho_d \varepsilon^{2/3} d^{5/3}}\right]$$

(independent of the breakage mode) where d = drop diameter σ = inter-facial tension ρ_d = density of dispersed phase ε = energy dissipation rate φ_d = volume fraction of dispersed phase (*hold–up*) κ_1, κ_2 = constants

Breakage rate *vs.* drop size according Coulaloglou and Tavlarides

Disadvantages: existence of a maximum, positive for all d (even very small drops could break against experimental evidence)

Some breakage rate formulas

- Narsimhan *et al.* (1980,1984)

$$\text{break. rate} = 5.75 \left(\frac{\sigma}{\rho v} \right)^{1/2} \text{We}^{3.2} \left(\frac{v}{D_i^3} \right)^{1.78}$$

where $v =$ drop volume $D_i =$ impeller diameter $\text{We} = \Theta^2 \rho D_i^3 \sigma^{-1}$ Weber number $\Theta =$ agitation speed

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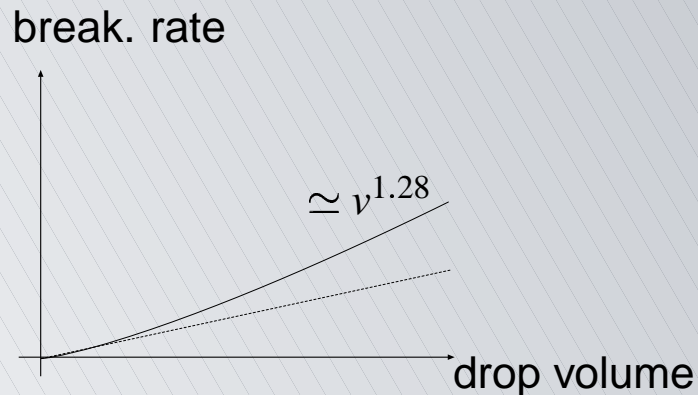Math. Dept. "U.Dini" Univ. of Firenze – 13th December 2002

Some breakage rate formulas

Disadvantage: not easy to define the size of the largest stable drop (that we called $v_{\min}$)

Diameter of the largest stable drop (Shinnar [1961])

$$d_{\text{stable}} = c\,\text{We}^{-0.6} D_i \frac{\mu^*}{\mu_c}$$

where $\mu^* = \mu_c \left[1 + 2.5\varphi \left(\dfrac{\mu_d + 0.4\mu_c}{\mu_d + \mu_c} \right) \right]$ (Taylor [1932]) ($\bullet_c =$ *continuous phase,*

$\bullet_d =$ *dispersed phase* $\bullet^* =$ *dispersion*

break. rate

$\simeq v^{1.28}$

drop volume

Breakage rate *vs.* drop size according to Narsimhan *et al.* [1980,1984]

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Heuristic conclusions

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what is the maximum size of the drops in a dispersion?

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Experimental evidence: there is a maximum size depending on the agitation speed

Heuristic conclusions

In any case we have to answer the question:

what is the maximum size of the drops in a dispersion?

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Not much attention has been devoted to explaining the maximum size (the practical
relevant quantity is d_{stable}, that is the size of unbreakable drops)

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Thus we need one more mechanism (in addition to coalescence and breakage)

This leads naturally to a new mechanism that we called volume scattering (Fasano & Rosso [1998,2000,2001,2002], Mancini & Rosso (num. simulations) [2002], Borsi (generalizes our model [2000]), Walker (generalizes our model [2001]))

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Mathematical set–up

- THE KINETIC TERM ACCORDING WITH THE CLASSICAL THEORY

We neglect — for simplicity — diffusion and refer directly to continuous models for liquid–liquid dispersions in a batch reactor so the basic reactions (classically) are "coalescence" and "breakage"

We assume

— droplets uniformly distributed in the reactor (thus $f(v,t)$ does not depend on spatial coordinates) (thus no diffusion!).

— whole system isolated (thus no heat or mass exchange!).

Classical model for the distribution function $f(v,t)$ (*per unit volume*), with no diffusion and mass or heat exchange

$$\frac{\partial f}{\partial t} = L_{\text{coal}} f + L_{\text{break}} f \qquad (0)$$

where

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Mathematical set–up

— coagulation (or coalescence) operator (τ_c coal. kernel, symmetric:
$\tau_c(\cdot, a, b) = \tau_c(\cdot, b, a)$)

$$L_{\text{coal}} f := \underbrace{\frac{1}{2} \int_0^v \tau_c(t, w, v - w) f(w, t) f(v - w, t) \, dw}_{\text{gain}}$$

$$\underbrace{- f(v, t) \int_0^{+\infty} \tau_c(t, v, w) f(w, t) \, dw}_{\text{loss}}$$

— fragmentation (or breakage) operator (α breakage frequency, β probability density
of splitting $w \to (v, w - v)$)

$$L_{\text{break}} f := \underbrace{\int_v^{+\infty} \alpha(t, w) \beta(t, w, v) f(w, t) \, dw}_{\text{gain}} - \underbrace{\alpha(t, v) f(v, t)}_{\text{loss}}$$

— notice: $v \in [0, +\infty)$!

Drawbacks of the classical model

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—> In a practical experiment we deal with systems of finite volume. Thus drops with arbitrarily large size are physically meaningless!

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—>   This point of view looks reasonable within the mathematical community and commonly accepted

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—> Also recall that Simons' counterexample works only if $v \in [0, +\infty)$ and if this is the case also the steady–state equations leads to unacceptable conclusions!

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Our suggestion

It seems more physical to admit that when two droplets coalesce to form a drop above the critical size, the result is a *virtual drop* that is totally unstable and breaks immediately into two or more daughters, each with volume within the admissible range. The stabilizing interaction must be a *combination* of the two well established mechanisms (coalescence+breakage). By analogy with kinetic theory we called this phenomenon *volume scattering*. This is meant as a *third mechanism* regulating the evolution of f

$$\frac{\partial}{\partial t} f = L_{\text{coal}} f + L_{\text{break}} f + L_{\text{scatt}} f \tag{1}$$

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$$\frac{\partial}{\partial t}f = L_{\text{coal}}f + L_{\text{break}}f + \boxed{L_{\text{scatt}}f} \qquad (1)$$

where $L_{\text{scatt}}f$ also consists of one production and one loss term.

Consistently with this picture, in equation (1) v varies in a *bounded interval*.

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A general comment

The many models proposed (all based on (**??**) but with different choices of breakage and coalescence kernels) have all been claimed to be consistent with experimental data

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Moreover – as we shall see – this new model DOES NOT INTRODUCE ANY NEW PARAMETER

Indeed the scattering operator is formed with a suitable combination of coalescence and

breakage, just following its physical interpretation

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Volume scattering (a necessary interaction!)
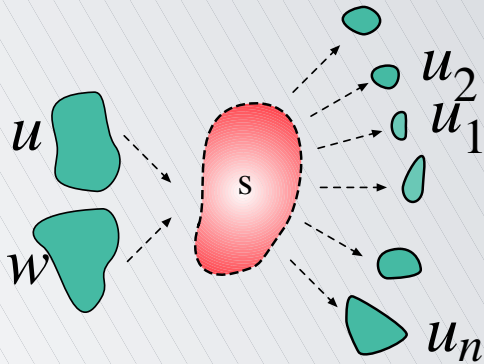
Scattering mechanism: droplet $s = u + w > v_{\max}$ (resulting from coalescence of u and w) is unstable and decays immediately into n "daughters" with volume $< v_{\max}$

Notice: without volume scattering there is no natural mechanism in the classical model to

prevent the appearance of "large droplets"!

Our model

— balance population equation (for binary breakage, but we recently extended that to include multiple breakage) with an "efficiency" factor

$$\frac{\partial}{\partial t} f = \varphi(t) \left(L_{\text{coal}} f + L_{\text{break}} f + L_{\text{scatt}} f \right)$$

with

$$\varphi(t) = \varphi \left[\mathfrak{N}(t), \mathfrak{S}(t) \right], \qquad (\text{ efficiency factor})$$

$$\mathfrak{N}(t) = \int_0^{v_{\max}} f(v,t) \, dv, \qquad (\text{# of drops p.u.v.})$$

$$\mathfrak{S}(t) = \int_0^{v_{\max}} v^{(2/3)} f(v,t) \, dv, \qquad (\text{interfacial area p.u.v.})$$

Our model

— coalescence operator

$$L_{\text{coal}}f := \int_0^{v/2} \tau_c(w, v-w) f(w,t) f(v-w,t)\, dw$$

$$-f(v,t) \int_0^{v_{\max}-v} \tau_c(v,w) f(w,t)\, dw$$

— breakage operator

$$L_{break}f := \int_v^{v_{\max}} \alpha(w)\beta(w,v) f(w,t)\, dw - \alpha(v) f(v,t)$$

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Our model

— scattering operator

$$L_{scatt} f := \int_{v_{max}-v}^{v_{max}} dw \int_{v+w-v_{max}}^{(v+w)/2} \tau_c(u, v+w-u) \beta(v+w, v) f(u,t)$$

$$\times f(v+w-u, t)\, du - f(v,t) \int_{v_{max}-v}^{v_{max}} \tau_c(v,w) f(w,t)\, dw \ .$$

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Our model

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$$L_{scatt}\, f := \int_{v_{\max}-v}^{v_{\max}} \mathrm{d}w \int_{v+w-v_{\max}}^{(v+w)/2} \tau_{\mathrm{c}}\,(u,v+w-u)\beta\,(v+w,v)f(u,t)$$

$$\times f(v+w-u,t)\ \mathrm{d}u - f(v,t)\int_{v_{\max}-v}^{v_{\max}} \tau_{\mathrm{c}}(v,w)f(w,t)\ \mathrm{d}w\ \ .$$

gain scatt. kernel

$(u,v+w-u) \rightarrow$

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$$(u, v+w-u) \rightarrow \boxed{w+v}$$

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$$(u, v+w-u) \to \boxed{w+v} \to (v,w) \qquad \tau_{s,gain} := \tau_c(u,v+w-u)\beta(v+w,v)$$

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loss scatt. kernel

$(v,w) \rightarrow$

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— NOTICE: in this model $v \in [0, v_{max}]$ (physically meaningful). A lower critical size v_{min} can

be easily included

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Main theorems

Theorem — The scattering operator is volume preserving (The model is consistent!)

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Assume reasonable regularity conditions on β, α, τ_c (such as continuity, boundedness,...).

Main Theorem — Let f_0 be a Lipschitz continuous initial size distribution on $[0, v_{\max}]$. Then the Cauchy problem for the mathematical model

$$\frac{\partial}{\partial t} f = \varphi(t) \left(L_{\text{coal}} f + L_{\text{break}} f + L_{\text{scatt}} f \right)$$

(with both binary and multiple modes) is well posed. The unique solution f is non–negative, exists for all times, continuously differentiable with respect to time and Lipschitz continuous with respect to v

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(with both binary and multiple modes) is well posed. The unique solution f is non–negative, exists for all times, continuously differentiable with respect to time and Lipschitz continuous with respect to v

The extension to *higher order modes* is only a matter of increasing mathematical complication but the strategy remains the same.

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Existence and uniqueness

sketch of the proof

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Numerical simulations

PRELIMINARY REMARKS

— Simulations consider the binary mode only (the addition of the sole ternary mode increases considerably the computational time!)

— Our model applies to any kind of fluid–fluid dispersion (with no chemical reactions) since it is just based on the *mechanics* of breakage and coalescence. However the selection of the parameters of the model (the *coalescence kernel* τ_c, the *breakage-frequency* α and the probability distribution β), able to fit the effective behavior of a real dispersion, is really a hard problem.

— We used the simplest possible equations for the kernels based just on geometrical and mechanical considerations (with an eye also towards technical papers...!)

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Remarks about the integration domain

— Mathematically v_{max} is a *fixed* upper bound for the volume size of droplets independent of time.

— In practice characteristic length scales for f_{o} and $f(v, \infty)$ may differ even by two or three orders of magnitude. Define $v^\star(t) = \sup \mathrm{supp}\, f(v, t)$; clearly $v^\star$ depends, besides t, on the rotational speed Θ, the geometry of the container and impeller, the hold-up λ, the temperature and many other rheological parameters

— Mathematically we put the lower bound for the volume of breakable drops $v_{\mathrm{min}} = 0$ in all simulations.

— In practice v_{min} is given by (Weber relation)

$$v_{\mathrm{min}} = 10^{-4} \pi D^3 We^{-1.8}, \qquad \left(We := \frac{\Theta D^3 \rho_{\mathrm{c}}}{\sigma} \right) \text{ where } \sigma, \rho_{\mathrm{c}} \text{ and } D \text{ are the surface}$$

tension, the density of the dispersed phase and the impeller diameter respectively.

Example of stable diameters

Example: for $\sigma = 29$ dyne/cm, $\rho \simeq 1$ gr/cm^3 and $D = 15$ cm

Θ (in r.p.m.)	$v_{\min}$ (in cm^3)
1000	$8.094 \, 10^{-9}$
2000	$6.675 \, 10^{-10}$
3000	$1.550 \, 10^{-10}$
4000	$5.505 \, 10^{-11}$
5000	$2.465 \, 10^{-11}$
6000	$1.278 \, 10^{-11}$
7000	$7.342 \, 10^{-12}$
8000	$4.540 \, 10^{-12}$

Consequence

$v^{\star}(\infty)/v_{\min} \simeq 10^4$ for $\Theta \simeq 4000 \div 6000$ r.p.m. (which is a rather standard rotational speed in industrial applications). This means that only with a very large sampling in the v axis (something like 10^5 or more nodes in the v direction) the numerical code is able to appreciate the effect of $v_{\min} \neq 0$. Being all the simulations done with nodes on the v axis spaced not less than .01 units, we consistently set $v_{\min} = 0$.

Asymptotic diameter

Example: for a water–in–oil dispersion, temperature $\simeq 60\ ^\circ C$, high rotational speeds ($\simeq 4000 - -6000$ r.p.m.), hold-up $\simeq 60\%$, and an agitation time of about 15 minutes, the top size diameter is $\simeq 60 \div 70\ \mu$m. This can be identified with the asymptotic value since there is practically no change for $t > 15$ minutes. This means, for this case, that we can set $v^\star(\infty) \simeq 10^{-7}\,\mathrm{cm}^3$; since typical values of the maximum diameter at the very early stages of agitation is about ten times larger than the initial ones, we have

$$\frac{v^\star(\infty)}{v^\star(0)} \simeq 10^{-3}.$$

Further consequence

Thus, in cases like the above, it is quite difficult to show graphically the evolution of f from f_{o} using the same length scale $v_{\max}$. In these cases we did not use the effective initial data but rather an intermediate configuration with a characteristic length much closer to that of the expected asymptotic distribution. Physically this corresponds to a *pre–mixing* period before examining the evolution.

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Initial distribution and kernels

Initial distributions $f_o(v)$ we considered:

- 🔴 a *a Gaussian distribution function* centered somewhere about the middle of the normalized droplet size interval
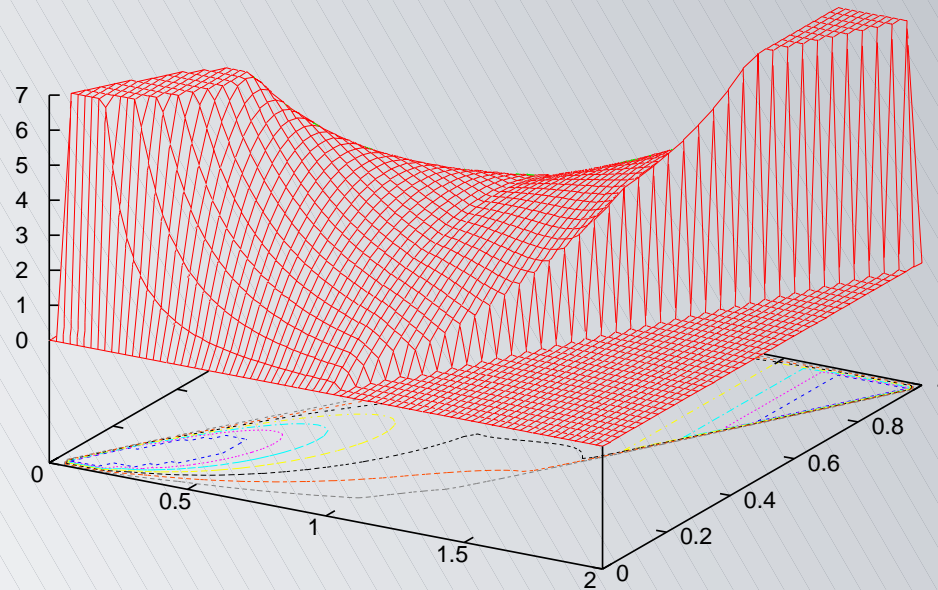
$$f_o(v) = k\exp(-(v-\mu)^2/2\sigma^2)$$

- 🔴 a *piecewise constant function*

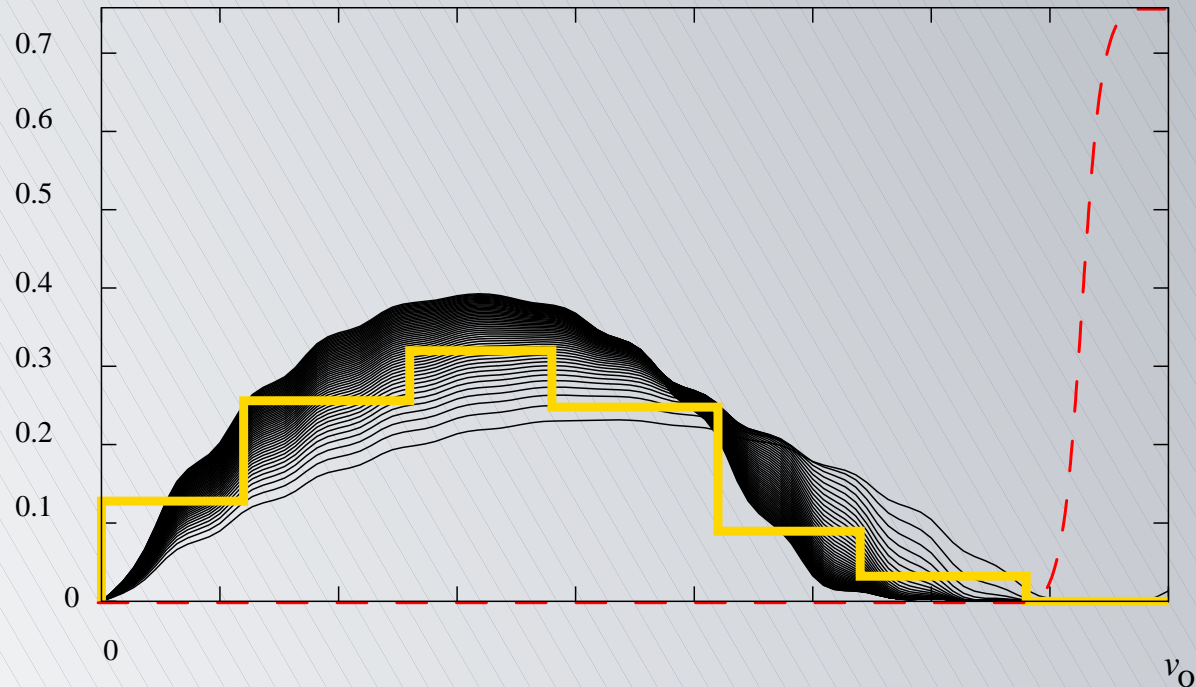$$f_o(v) = \begin{cases} k & \text{if} \quad v \in [0.2, 0.6], \\ 0 & \text{otherwise,} \end{cases}$$

$$\lambda = \int_0^1 v f_o(v)\, dv \in (0,1) \qquad (given\ hold\text{-}up)$$

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Distribution density β

Evolution from a stepwise initial data (dashed) towards a final distribution (solid lines). The asymptotic shape fits one of the experimental curves (histogram) and obtained with a high-speed rotational impeller (ultra-Turrax at 8000 r.p.m.); v_{max} is about 70 μm

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Model kernel and frequency

Breakage frequency

$$\alpha(w) = A_{\min} w^q, \qquad q > 0, \tag{-8}$$

Coalescence kernel

$$\tau_c(v,w) \quad = A_c \left(v^{\frac{1}{3}} + w^{\frac{1}{3}} \right)^2 \exp\left[-\left(\frac{v^{1/3} + w^{1/3}}{v^{1/3} w^{1/3}} \right)^4 \right], \tag{-8}$$

Proportionality factors depend on the rotational speed: we set $A_{\min}(\Theta) = \overline{A}_{\min} \Theta$, $A_c(\Theta) = \overline{A}_c (\overline{\Theta} - \Theta) \Theta$, where $\overline{A}_{\min}, \overline{A}_c, \overline{\Theta}$ are constants which typically depend on the rheology, geometry and the hold-up λ.

The expression for A_c is suggested by the fact that in most cases the coalescence efficiency increases with Θ up to a maximum and then reduces drastically for high rotational speeds.

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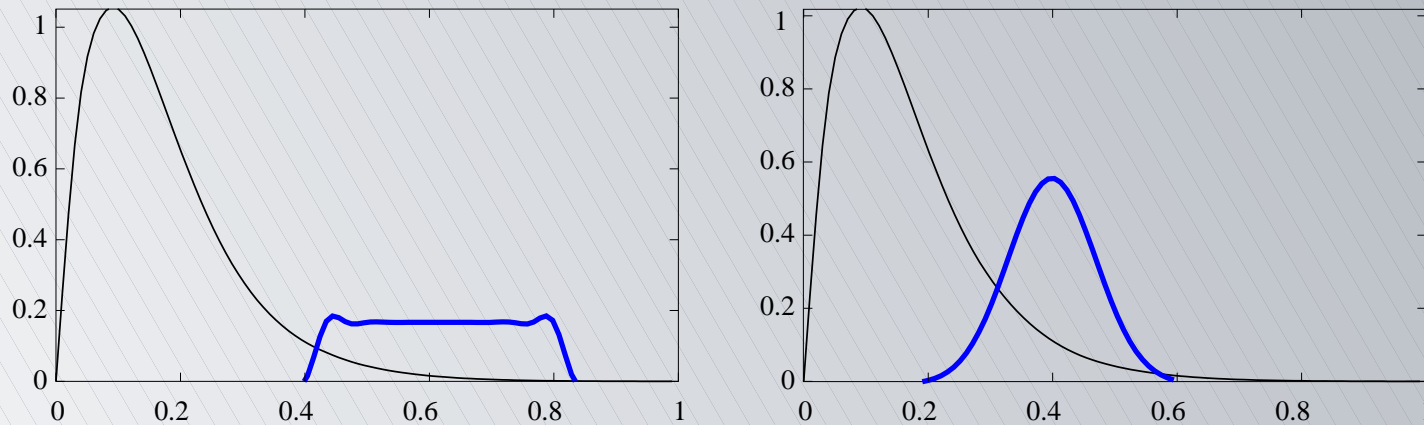Math. Dept. "U.Dini" Univ. of Firenze – 13th December 2002

Mutual importance of all effects
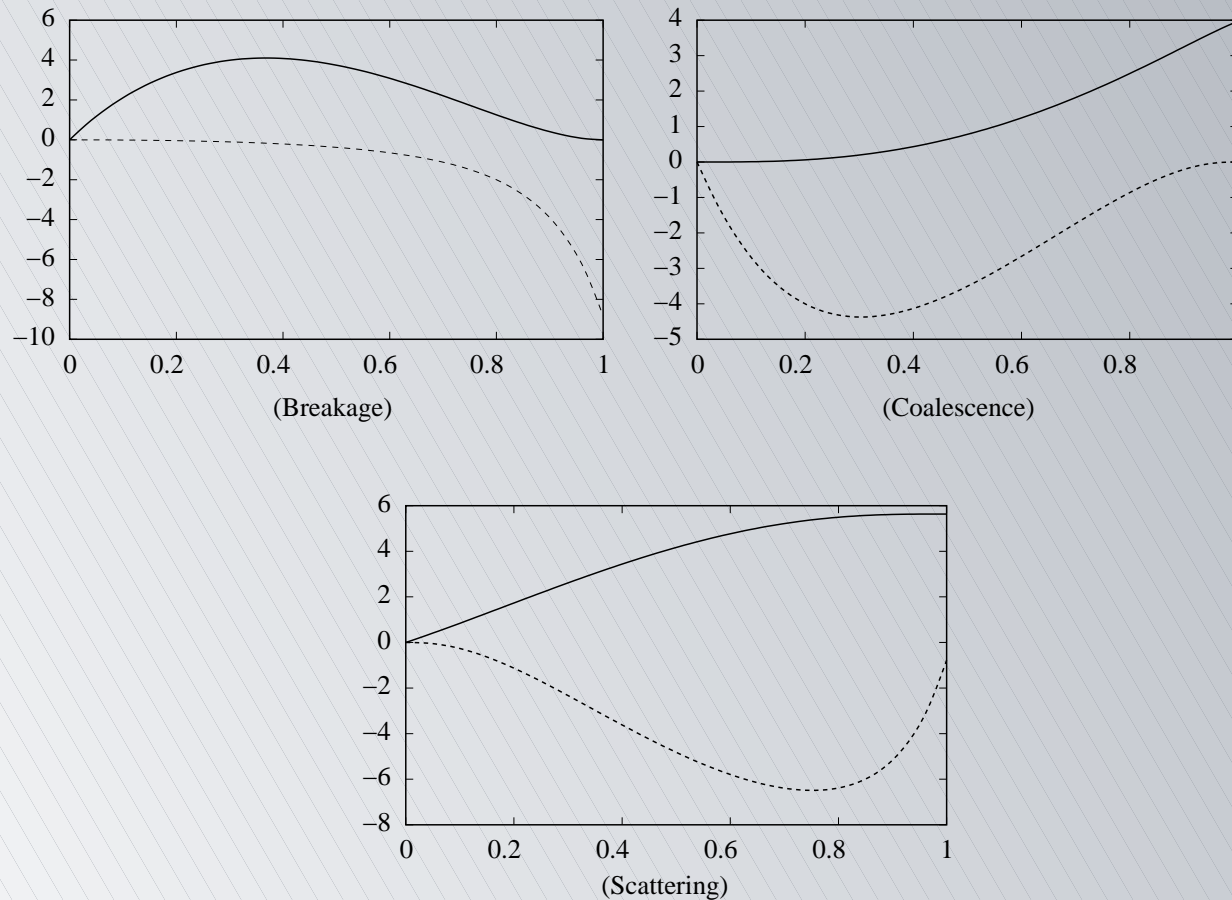
Mutual importance at equilibrium (large t) of breakage, coalescence and scattering terms at low rotational speed; the dashed line represents the loss term, the solid one the gain term

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Invariance of the asymptotic configuration with respect to $f_o(v)$: in the two cases considered the volume of dispersed phase (*hold–up*) is the same but the shape of the initial distribution is totally different

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