A Simulation Model for the Separation of Dispersed Liquid-Liquid Systems in Hydrocyclones Based on the Coupling of CFD and Population Balances

Computational Fluid Dynamics in Chemical Reaction Engineering V
June 15th to 20th 2008, Whistler, British Columbia, Canada

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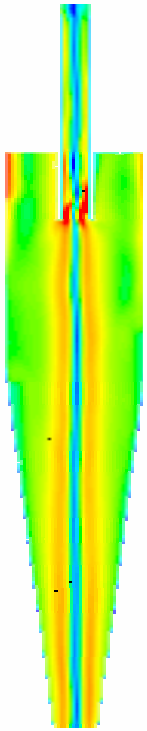
Institute of Mechanical Process Engineering IMVT
University of Stuttgart, Germany

Goals

Modelling of liquid-liquid separation with particle-particle interaction

CFD software (e.g. FLUENT™)



- ✓ Calculation of flow field
- ✓ Calculation of particle tracks
  (e. g. Euler-Lagrange)
- ✓ Interactions between phases
  (e. g. Euler-Euler)
- – Breakup / coalescence
  (Population balances)

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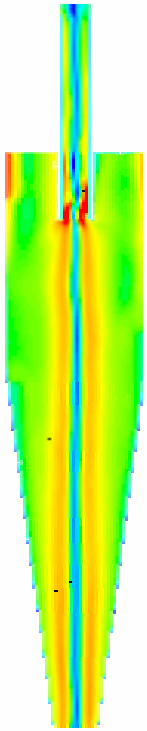

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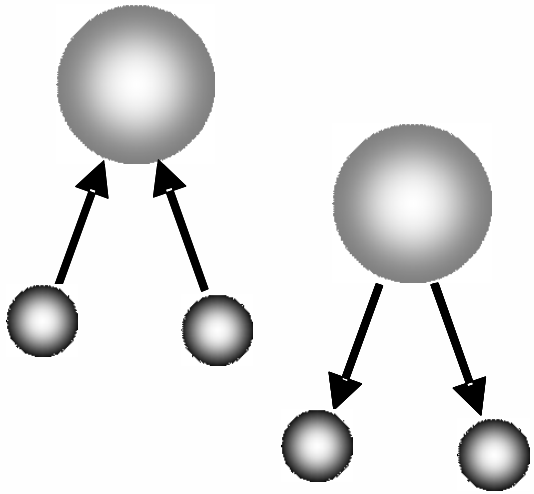
User defined functions (UDF)

- ✓ Breakup / coalescence (Population balances)
- – Separation process

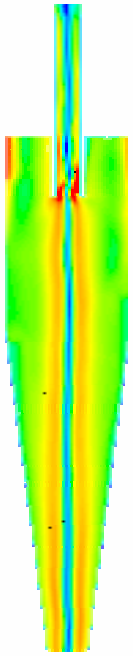


Goals

Modelling of liquid-liquid separation with droplet-droplet interaction in a hydrocyclone with direct impact of a non-homogeneous flow field

CFD software (e.g. FLUENT™) ⟷ User defined functions (UDF)

✓ Calculation of flow field



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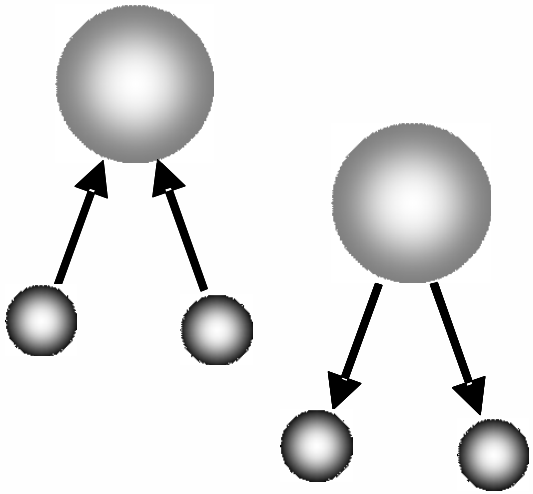


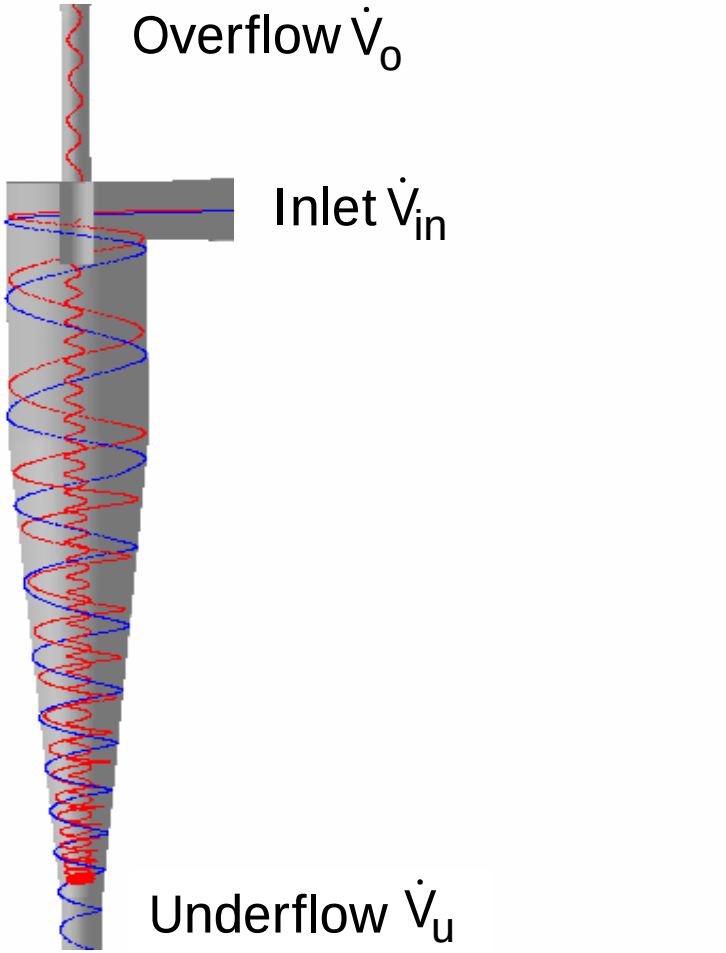
✓ Separation process

Outline

- Basics
- Population theory
- Solution strategy
- Results
- Summary and Outlook

Basics – Separation Processes in Hydrocyclones

- Continuous separators



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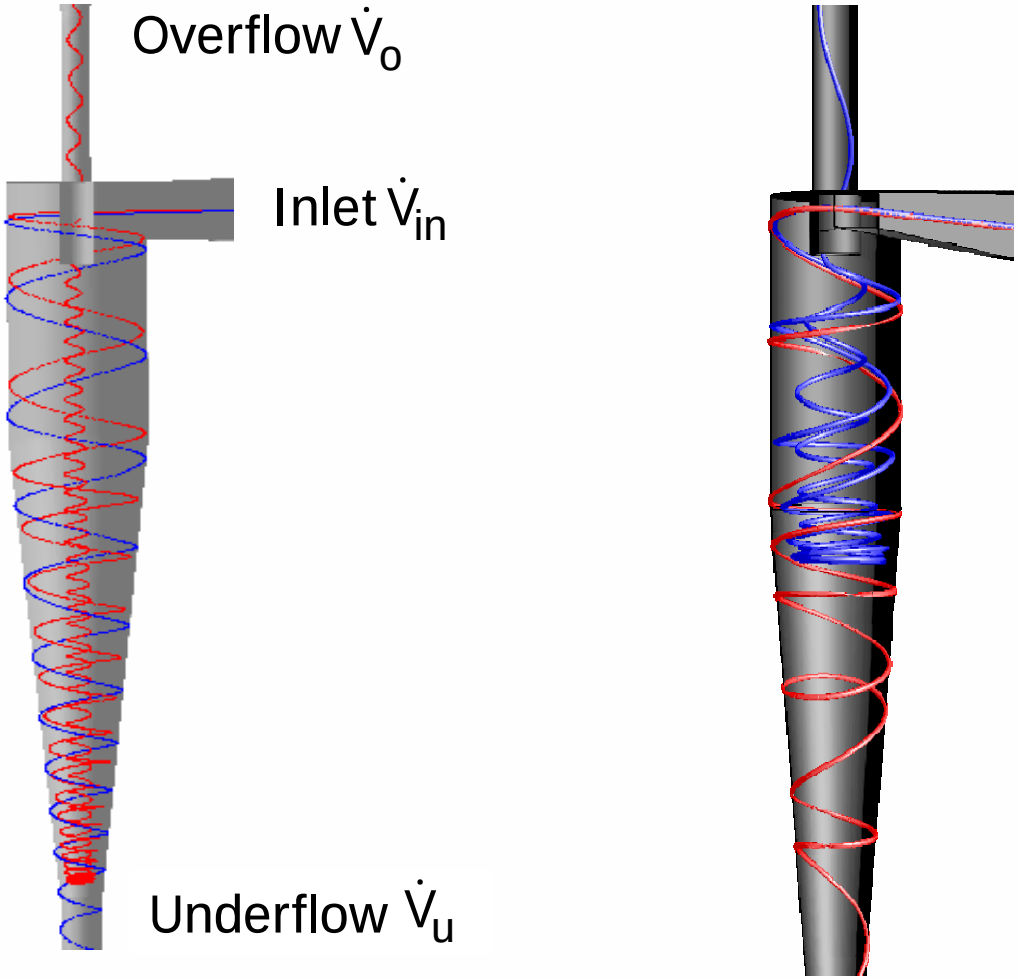


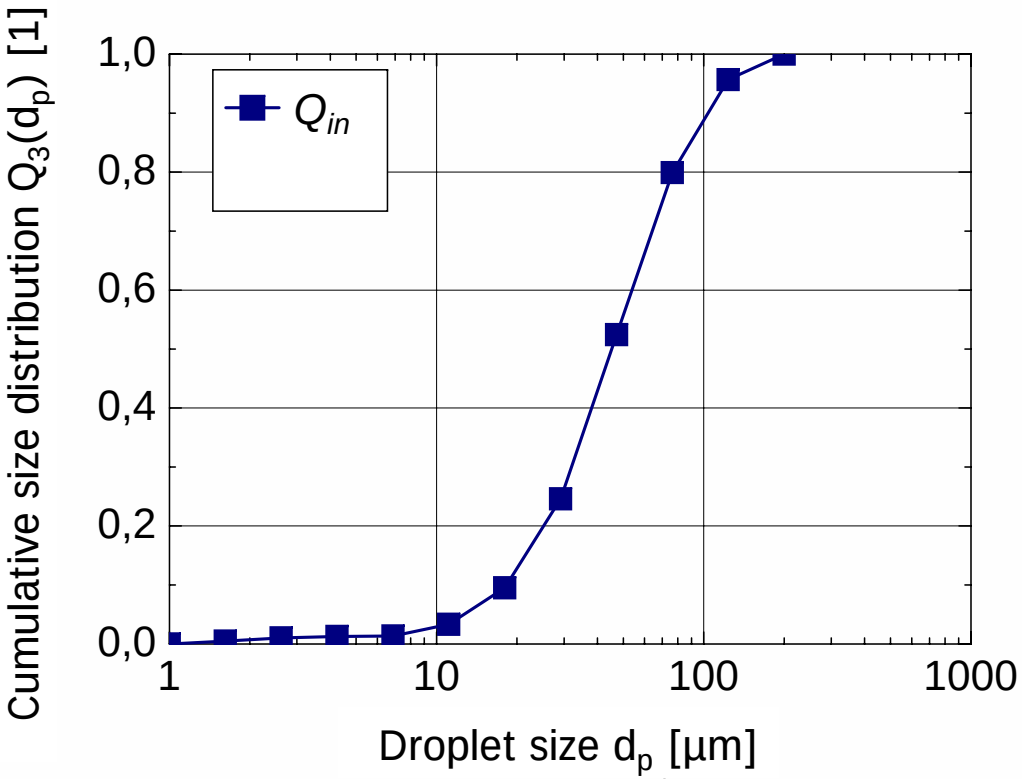
- Separation due to density difference
  - Phase with higher density: Accumulation to larger radii (here: dispersed water droplets)
  - Phase with lower density: Transport to smaller radii (here: continuous diesel fuel)

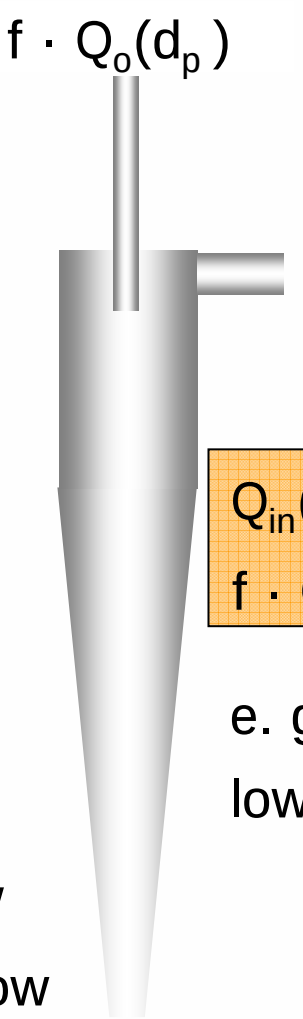
Calculation of particle tracks using Euler-Lagrange model

"big" particle/droplet

"small" particle/droplet

Basics – Separation Processes
Without Particle-Particle Interaction



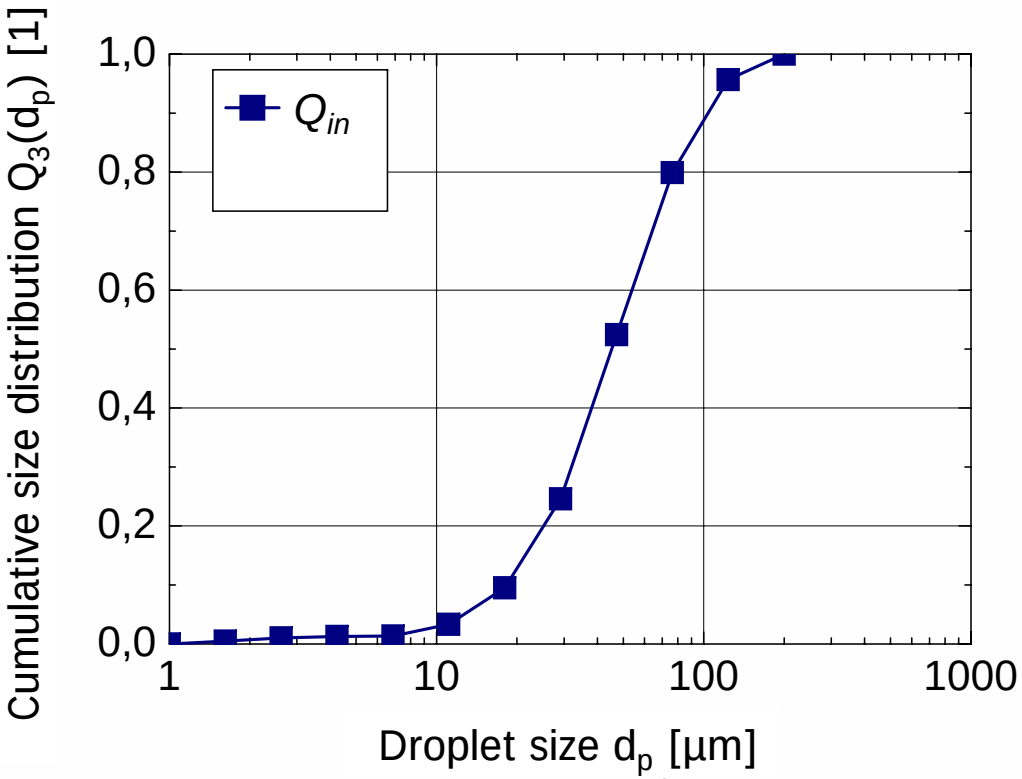


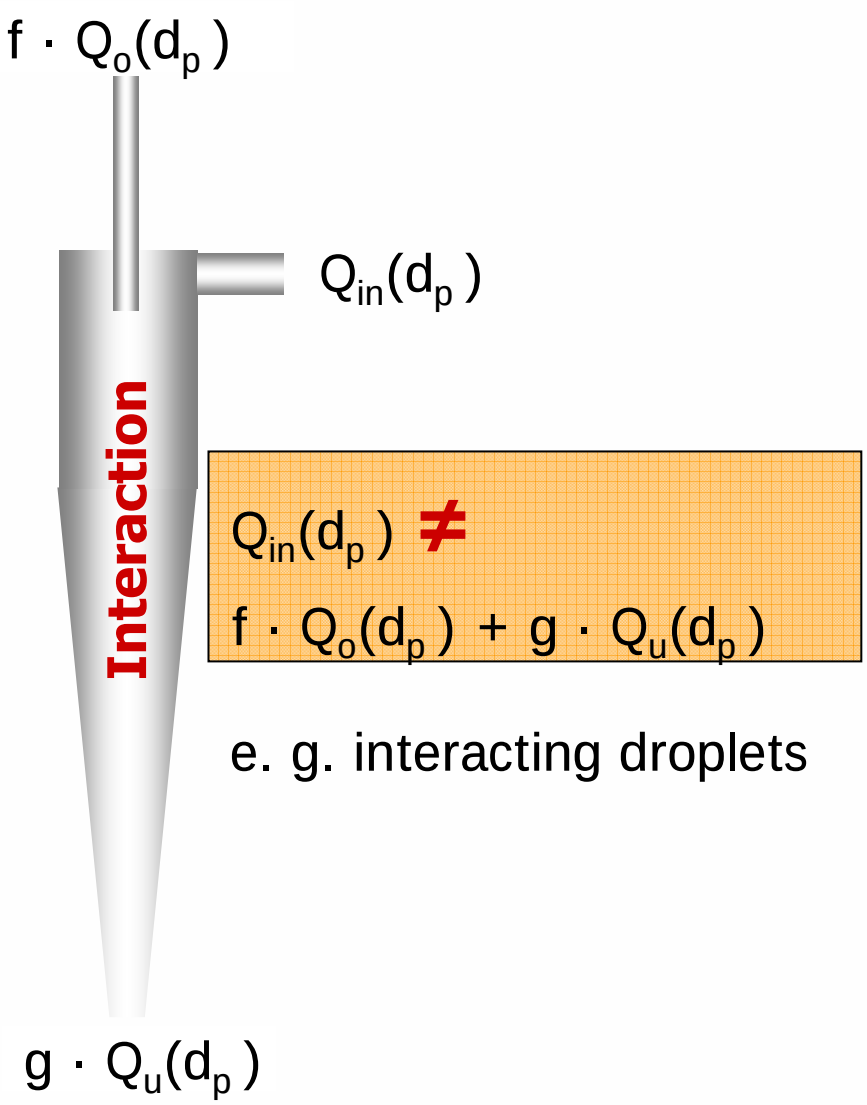
$$Q_{in}(d_p) = f \cdot Q_o(d_p) + g \cdot Q_u(d_p)$$

e. g. stable droplets at low concentrations

- f = integral droplet mass fraction overflow
- g = integral droplet mass fraction underflow

Basics – Separation Processes With Particle-Particle Interaction





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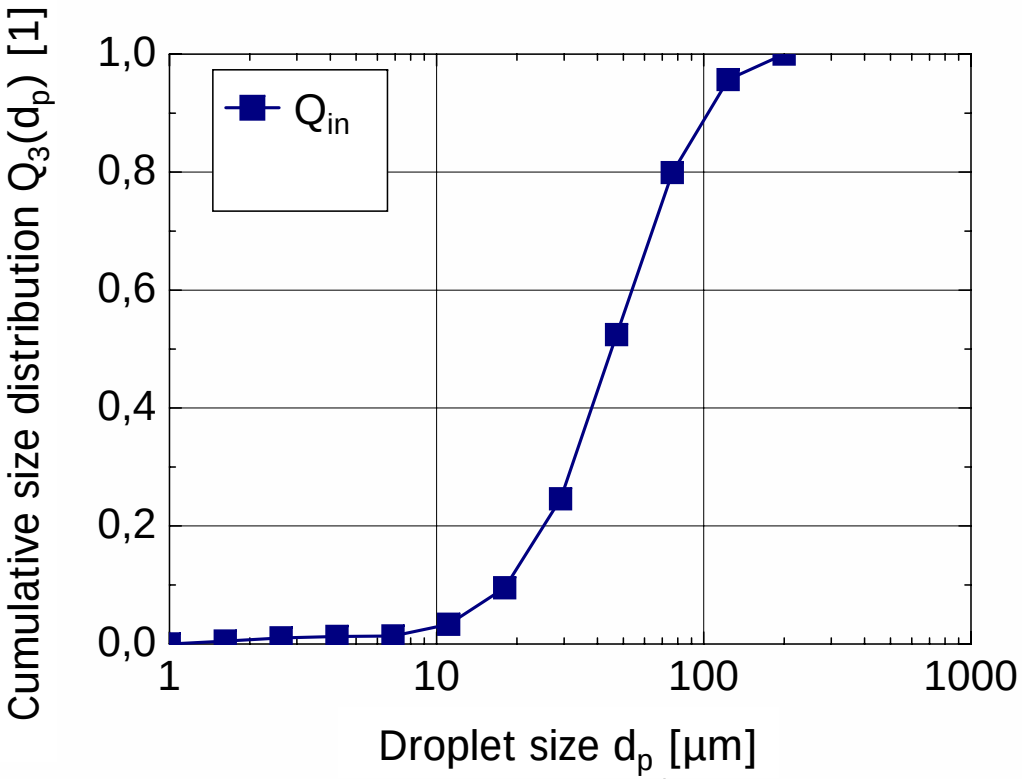

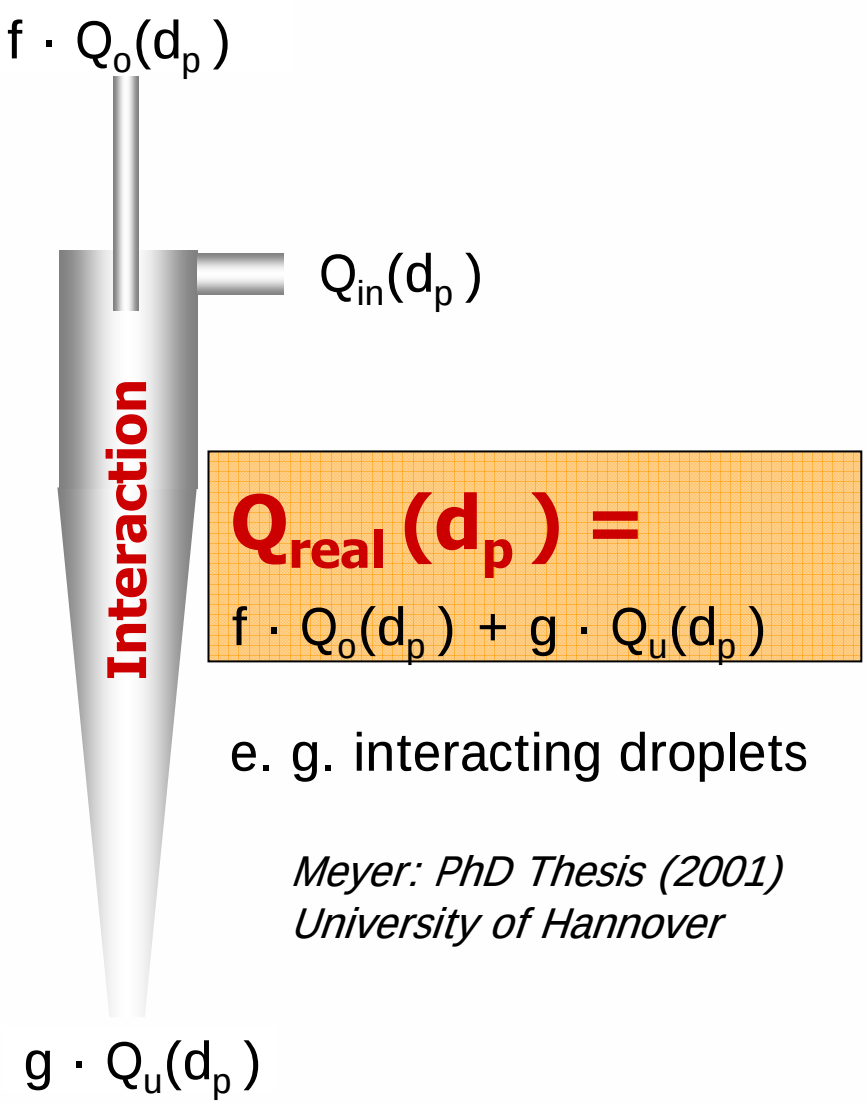

$$Q_{real}(d_p) = f \cdot Q_o(d_p) + g \cdot Q_u(d_p)$$

e. g. interacting droplets

Meyer: PhD Thesis (2001)
University of Hannover

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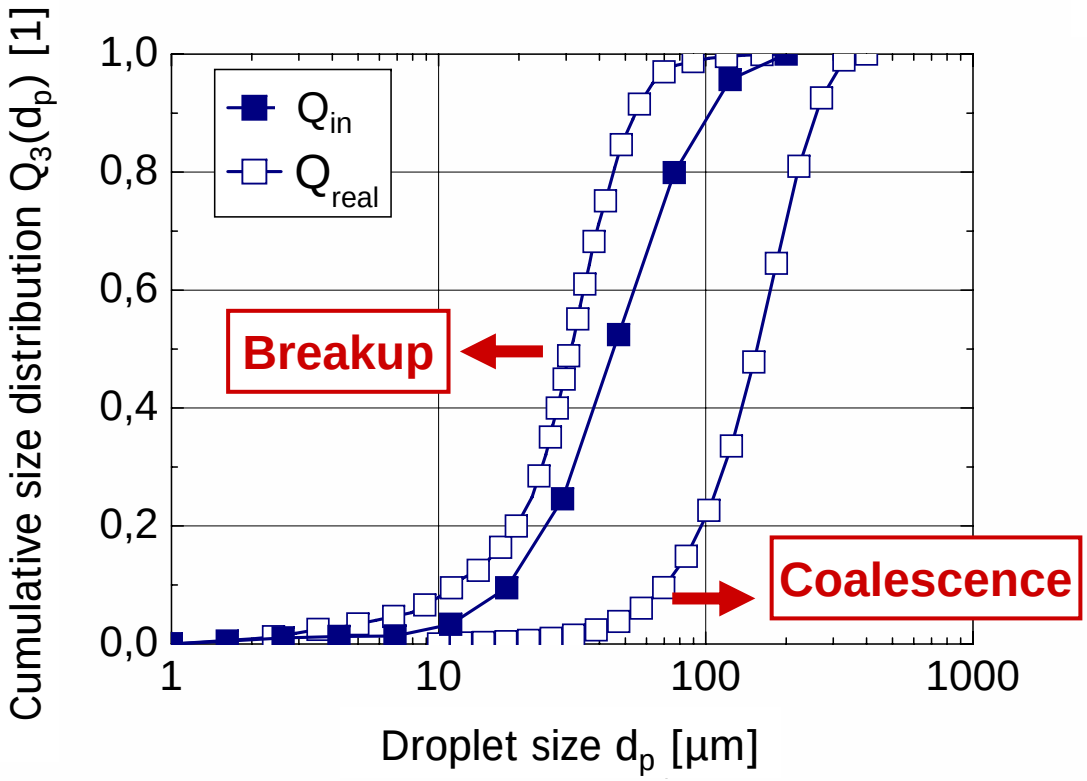

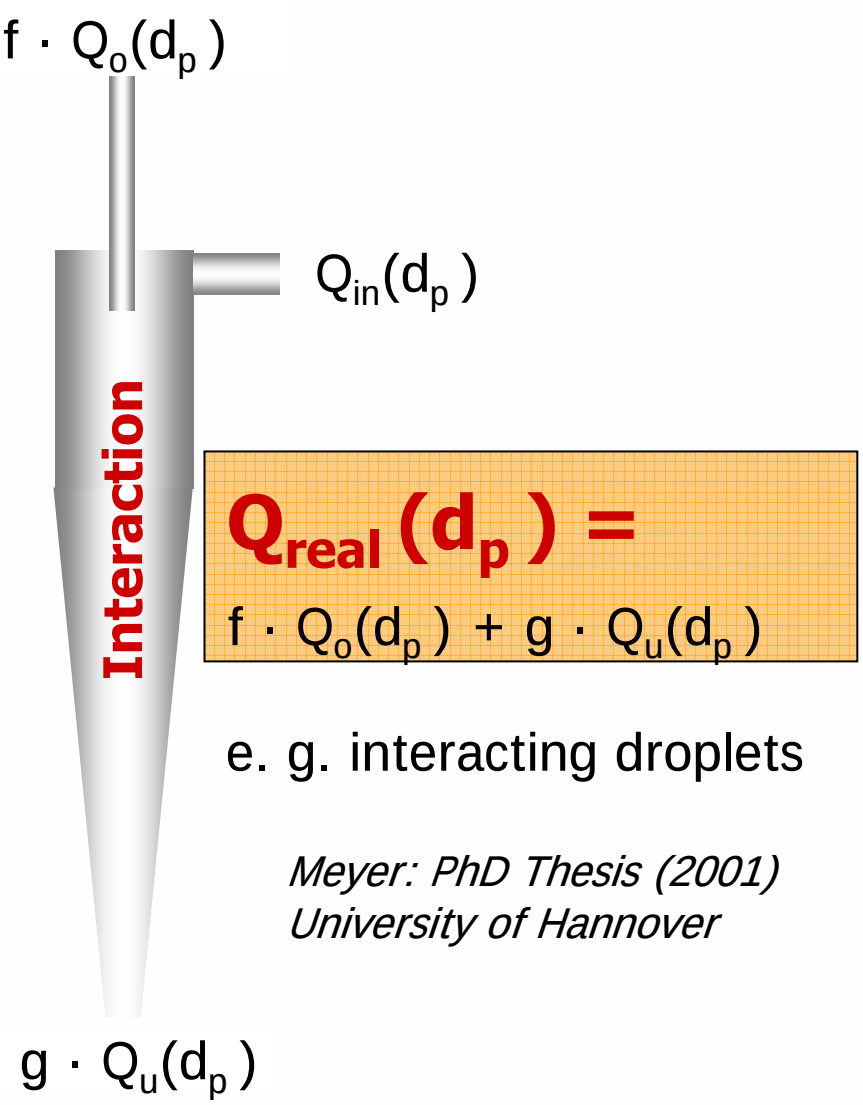

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Population Theory

- Shift of droplet size distribution with time and position is described by population balances
- Droplet mass as characteristic particle property
- Balancing of number density distribution F_i [1/m³] of each droplet size class i

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Chemical Engineering Science 19 (1964), 555-574

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$$\frac{\partial(\rho F_i)}{\partial t} + \nabla \cdot (\rho \vec{v}_i F_i) = \underbrace{B^+(F_i) - B^-(F_i)}_{\text{Birth Terms } B(F_i)\text{ Droplet Coalescence}} + \underbrace{D^+(F_i) - D^-(F_i)}_{\text{Death Terms } D(F_i)\text{ Droplet Breakup}}$$

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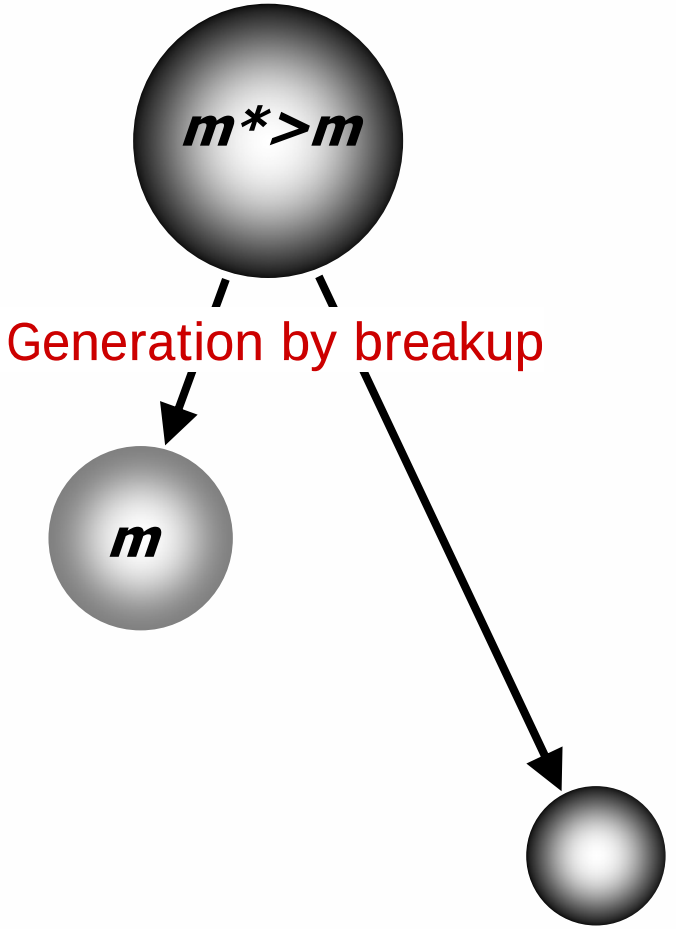

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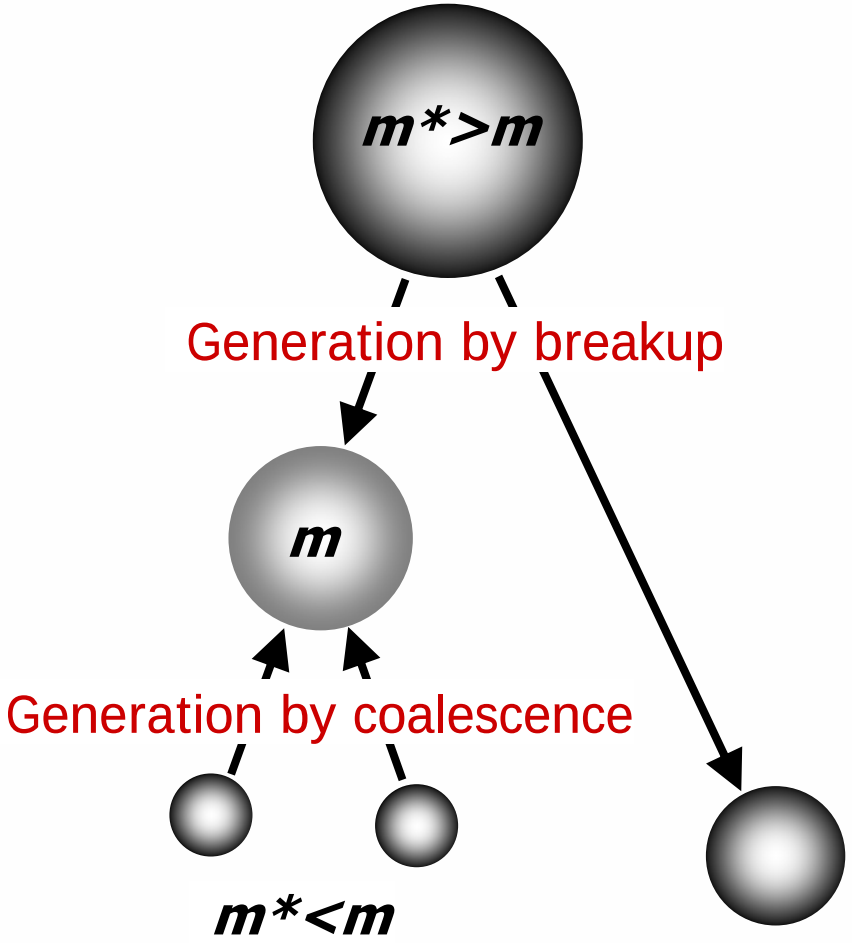

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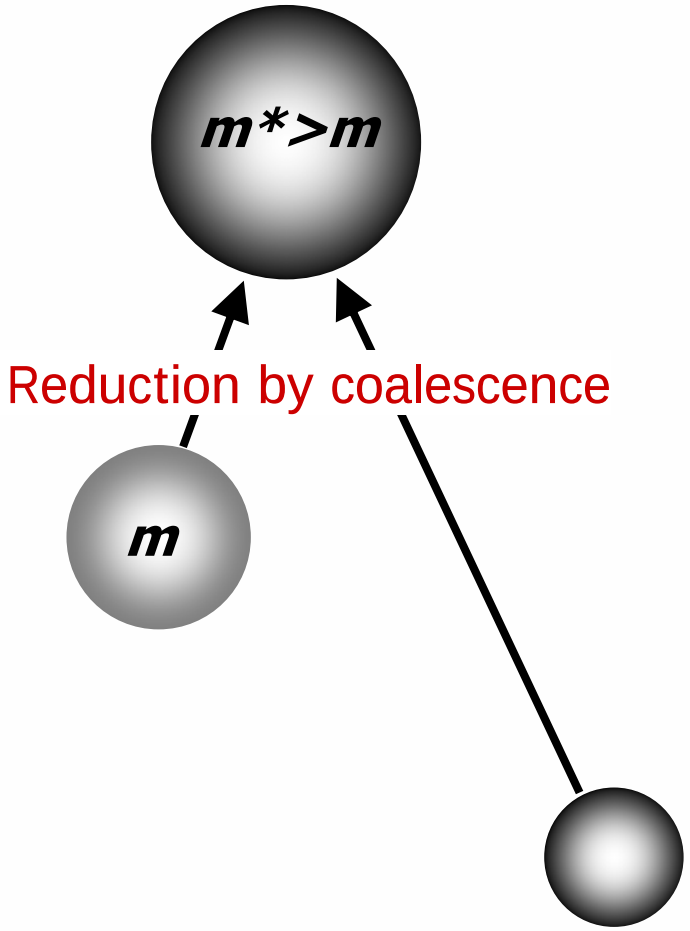

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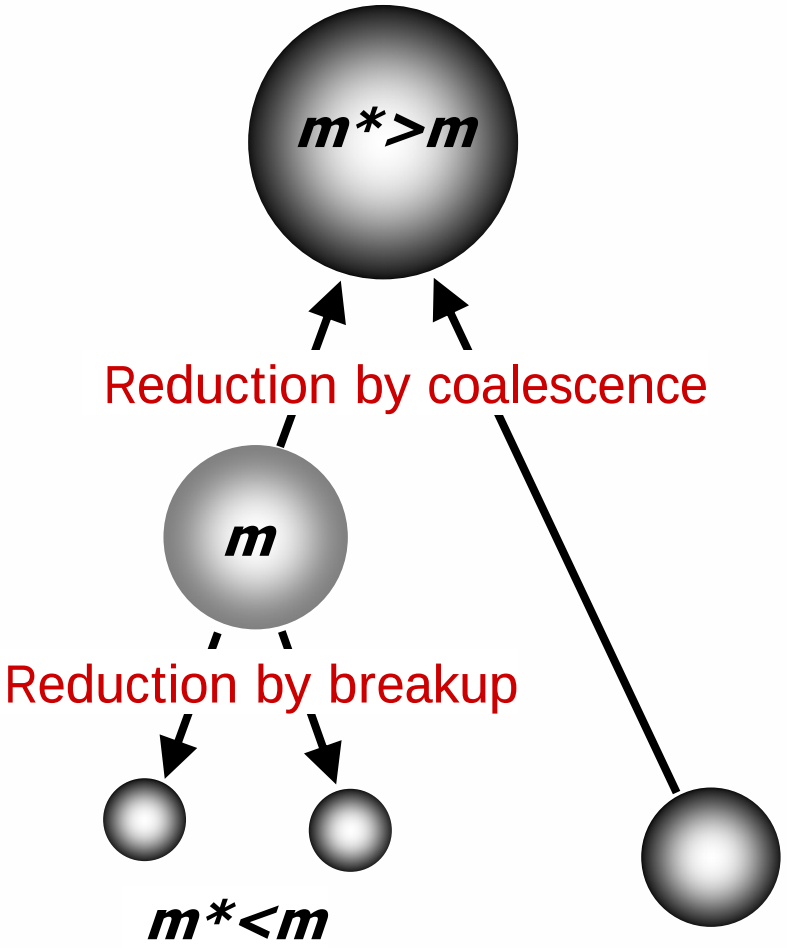

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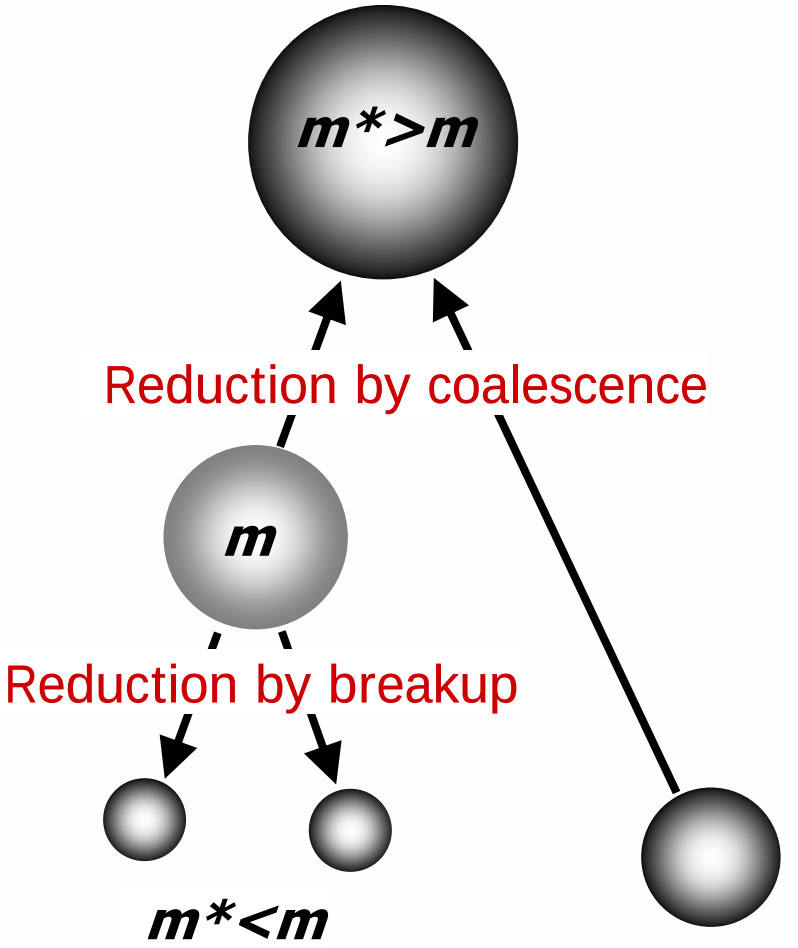

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Description by interaction kinetics

Population Theory

$$B^+\left(F_i(m,t)\right) - B^-\left(F_i(m,t)\right) + D^+\left(F_i(m,t)\right) - D^-\left(F_i(m,t)\right) =$$

$$+\frac{1}{2}\int_0^m \lambda(m-m^*,m^*)\, g_{coll}(m-m^*,m^*)\, F_i(m-m^*,t)\, F_i(m^*,t)\, dm^*$$

Generation by coalescence

$$-\int_0^{m_{max}-m} \lambda(m,m^*)\, g_{coll}(m,m^*)\, F_i(m,t)\, F_i(m^*,t)\, dm^*$$

Reduction by coalescence

$$+\int_m^{m_{max}} \upsilon(m^*)\,\beta(m,m^*)\, g_{br}(m^*)\, F_i(m^*,t)\, dm^*$$

Generation by breakup

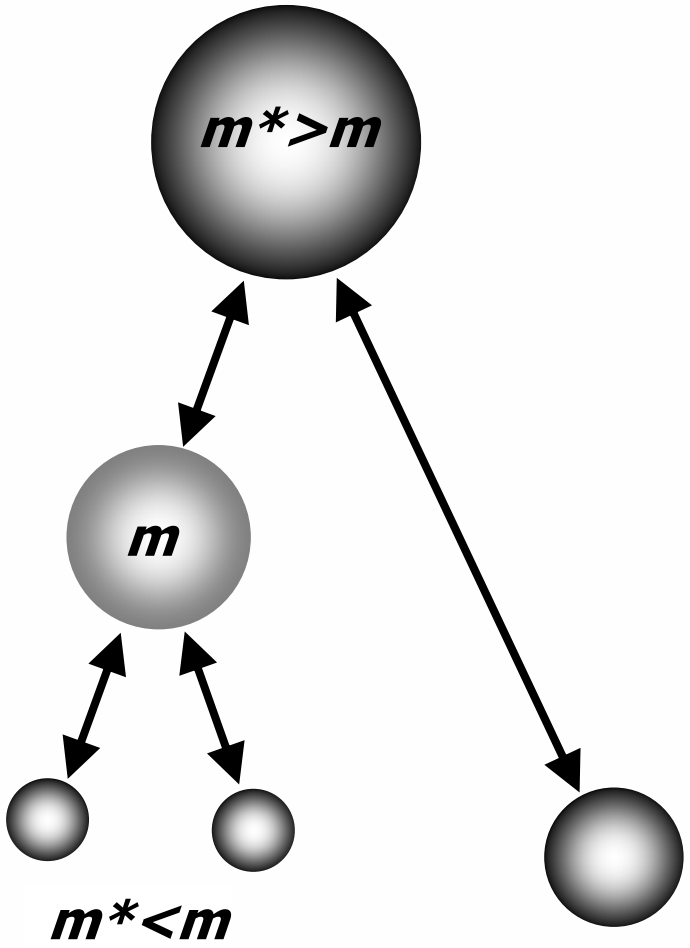
$$-g_{br}(m)\, F_i(m,t)$$

Reduction by breakup

Population Theory

- Kinetic approach of Coulaloglou/Tavlarides
  Chemical Engineering Science 32 (1977), 1289-1297
  - Strongly empirical
  - Influence of turbulence on droplet breakup is not considered

- Kinetic approach of Lehr
  (PhD Thesis (2001) University of Hannover, Germany)
  - Definition of critical velocity (only dependent of disperse phase)
  - Influence of turbulence on droplet breakup is considered



Droplet Reduction by Separation

- Relative transport of droplets with respect to mean flux driven by centrifugal forces results in droplet separation at the cyclone walls and at the underflow

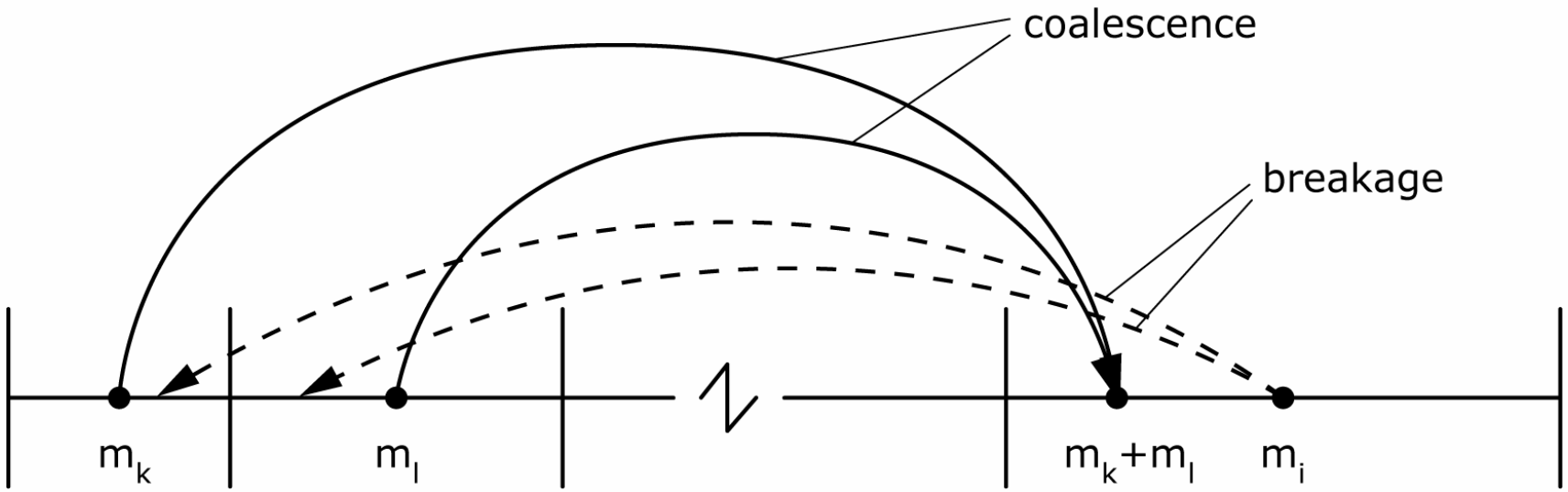
→ “Drift flux” described by transport laws for drag force

$$\vec{v}_{rel,i} = \frac{1}{18 c_D} \frac{\rho_d d_{p,i}}{\mu_m} \frac{\rho_d - \rho_m}{\rho_d} \vec{a}_i - \frac{\nu_{t,m}}{\alpha_{d,i} D_t} \nabla^x \alpha_c$$

→ Droplet separation as further contribution to the death term $D^-(F_i)$

Droplet Size Discretization

- Non-equidistant droplet size discretization with discrete droplet size classes
- Close size intervals with small droplets due to their high number concentration
- Numerical correction to keep the droplet mass constant



Solution Strategy

Flow field simulation with multiphase mixture model in FLUENT™

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- Solution of transport equation for volume phase fraction α_i of each phase i

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$$F_i = \frac{\alpha_i}{V_{p,i}}$$ Droplet volume $V_{p,i}$

Coupling condition

Solution Strategy

Calculation of droplet interaction kinetics

and droplet separation

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Implementation into

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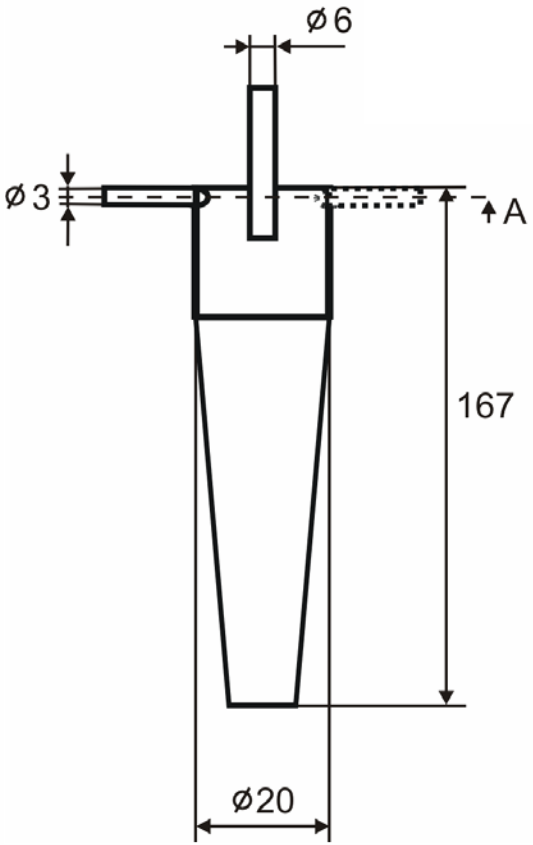
Coupled solution

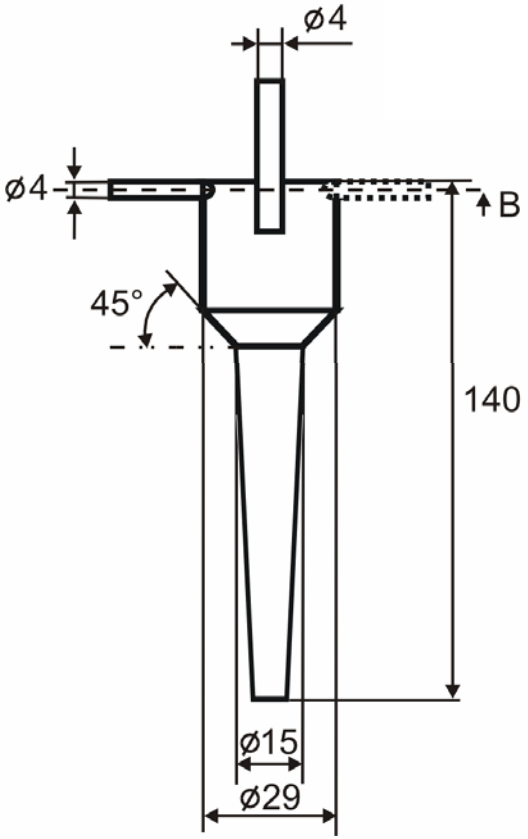
of the flow field with

population balances in FLUENT™

Results – Cyclone Geometries



Conventional geometry

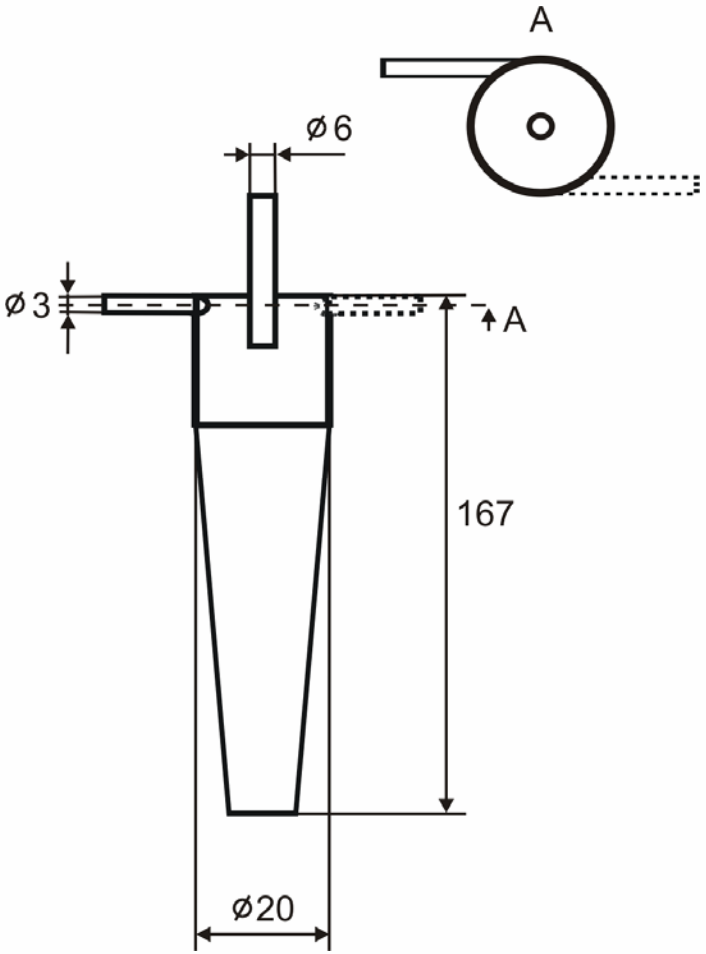


Geometry with double cone (Smyth)

Proc. 2nd Int. Conf. on Hydrocyclones (1984), 177-190, Bath, UK

Results – Cyclone Geometries

Cyclone separators
with one or two inlets



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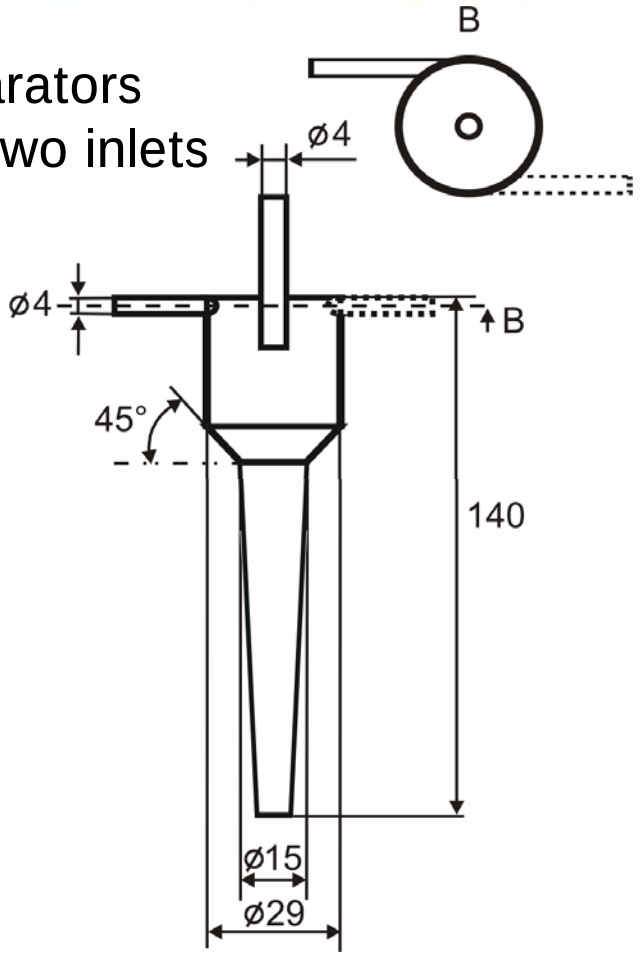

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Results – Phase Properties

Separation of water droplets from diesel fuel

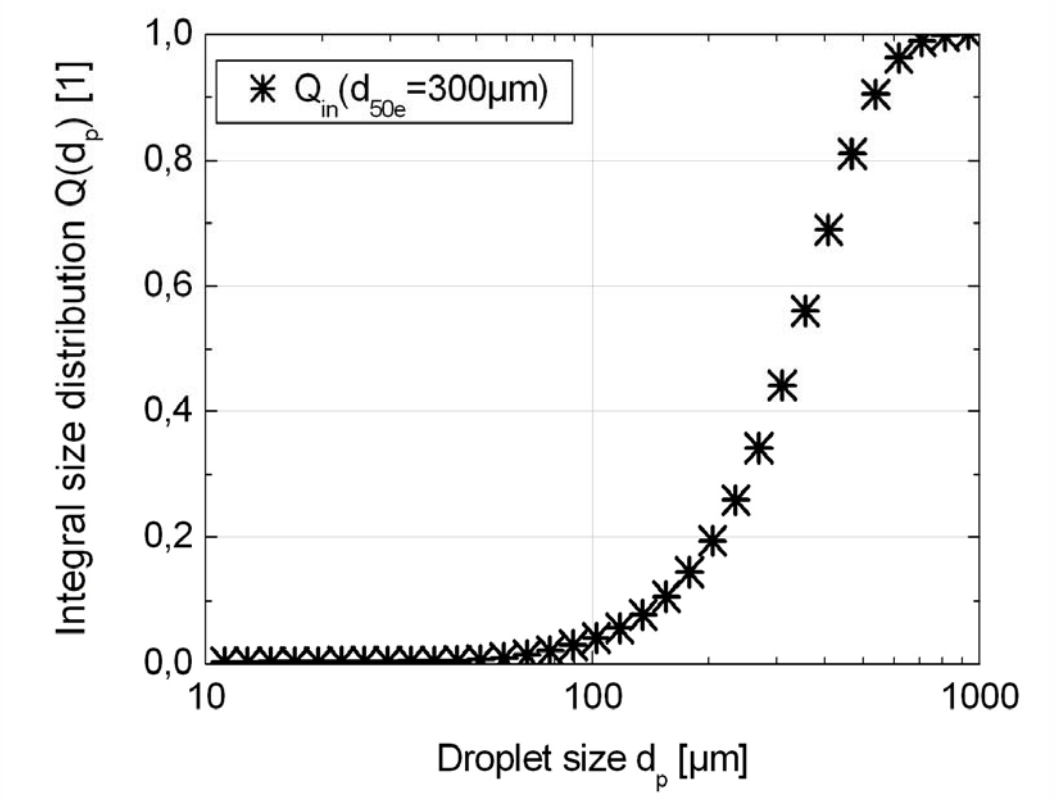
Density difference $\Delta\rho$=170 kg/m³, interfacial tension σ=0.015 N/m

Droplet size distribution inlet:

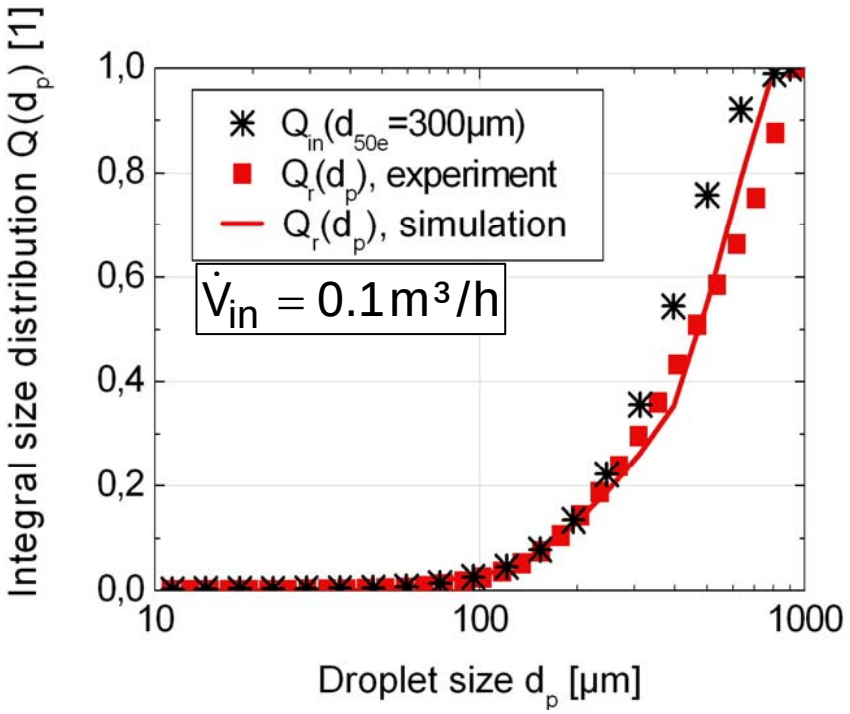
Mean diameter d_{50e}=300µm

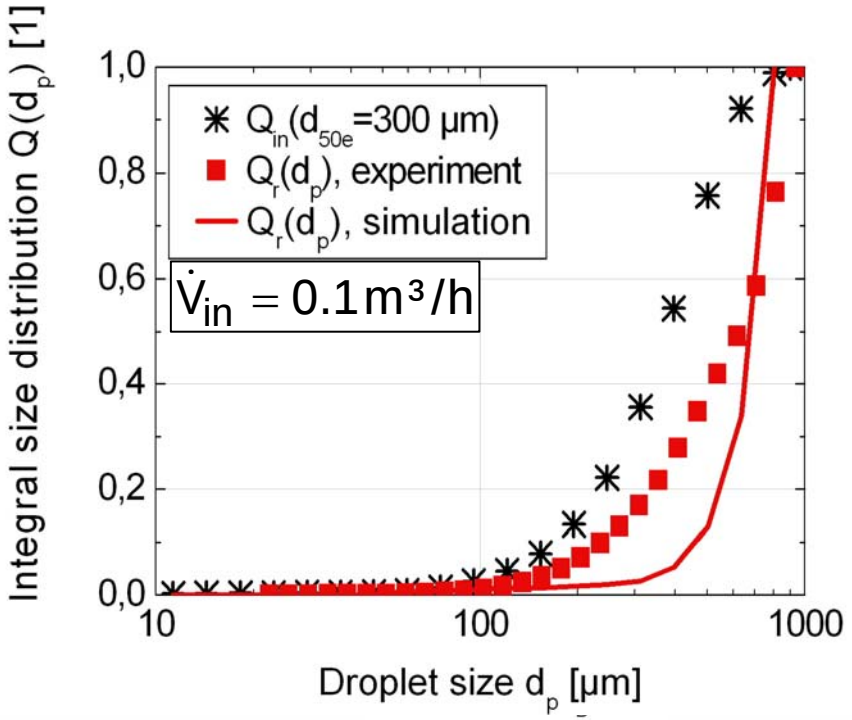
Logarithmical discretization

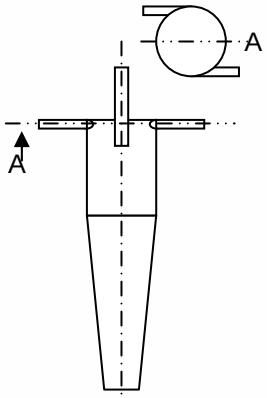
into n=19 droplet size classes



Results –
Two Different Cyclone Geometries

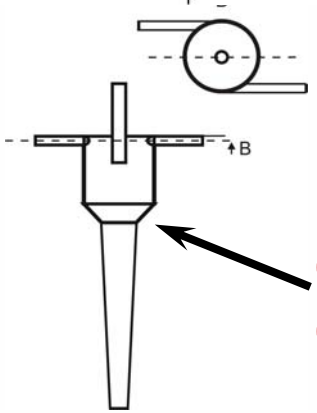






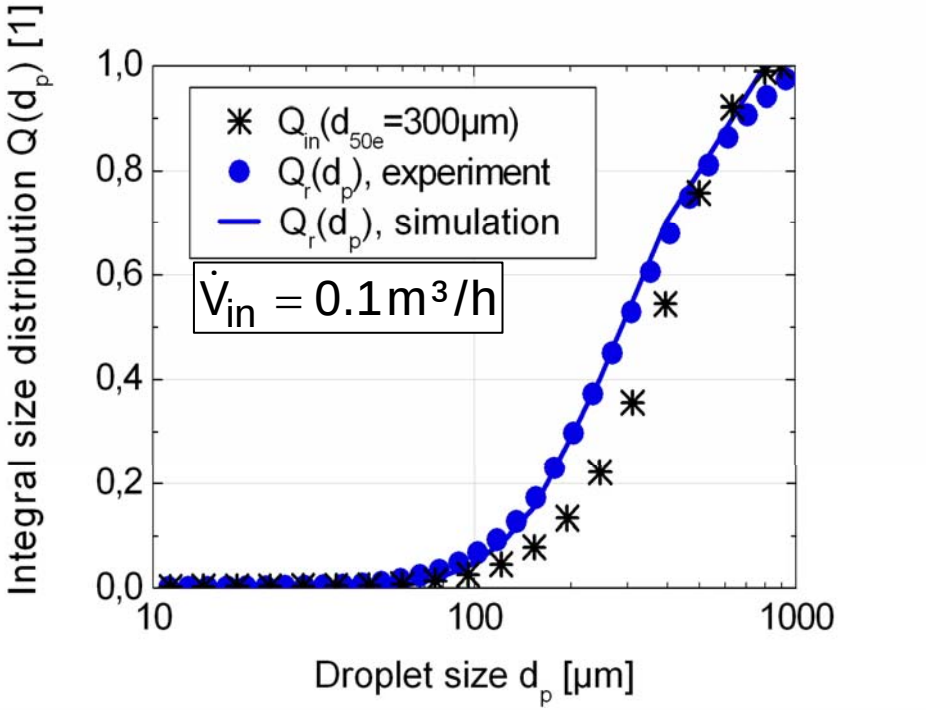
Reduced droplet breakup

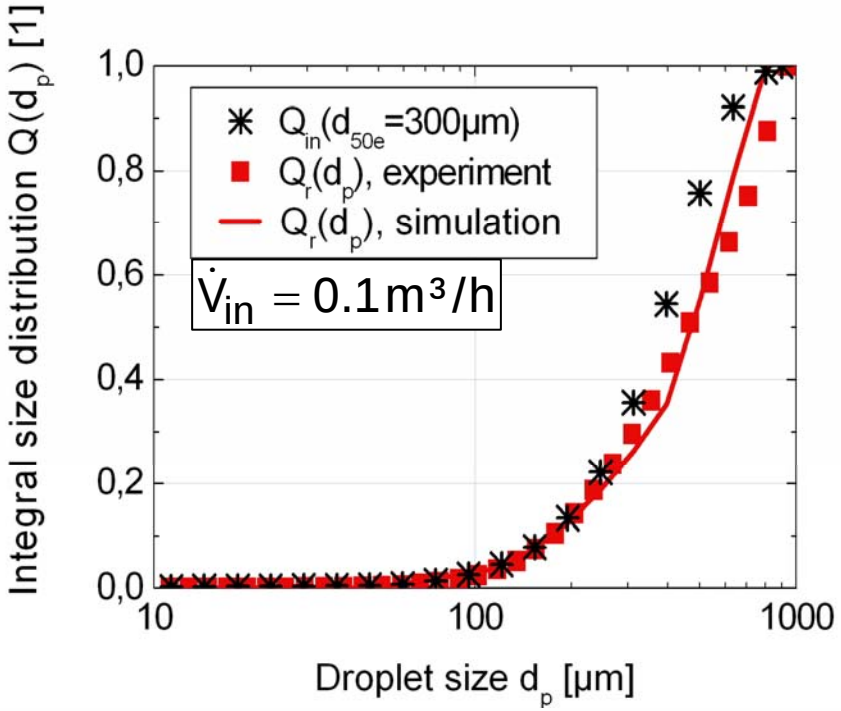
Increased droplet coalescence

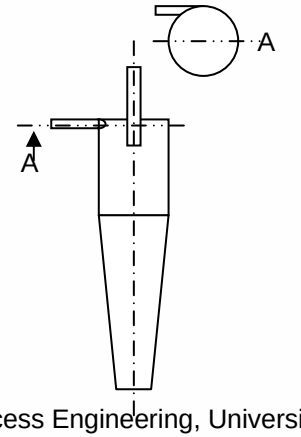


double cone geometry

Results –
One and Two Cyclone Inlets







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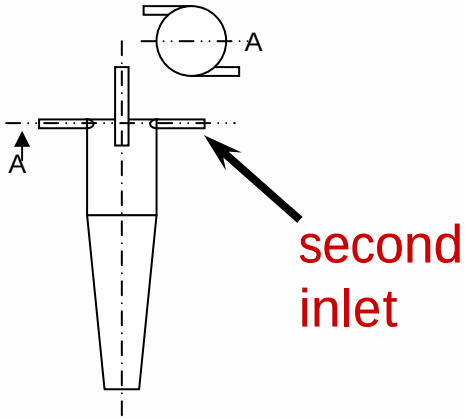
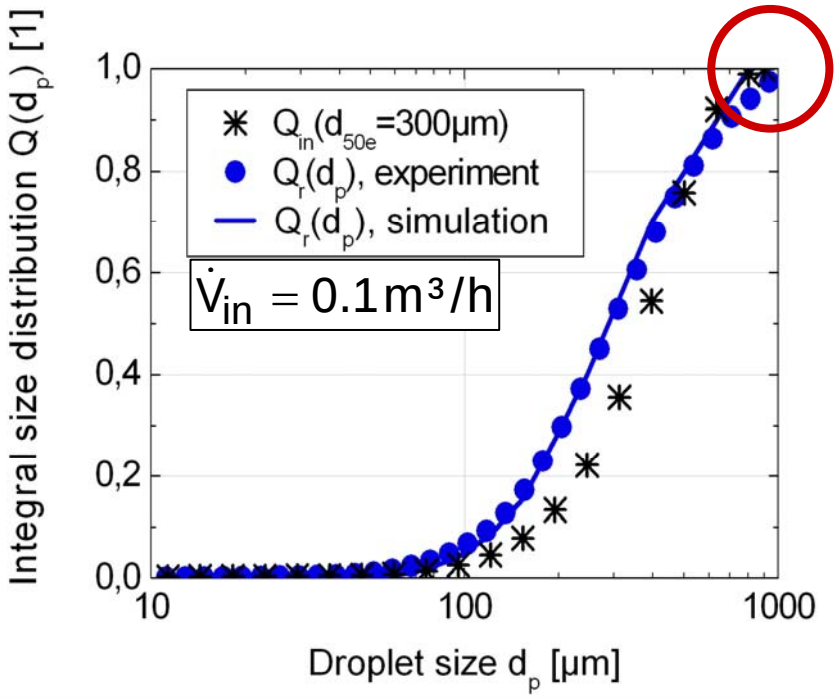
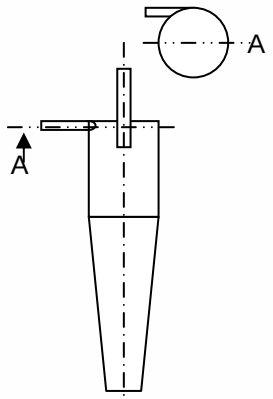
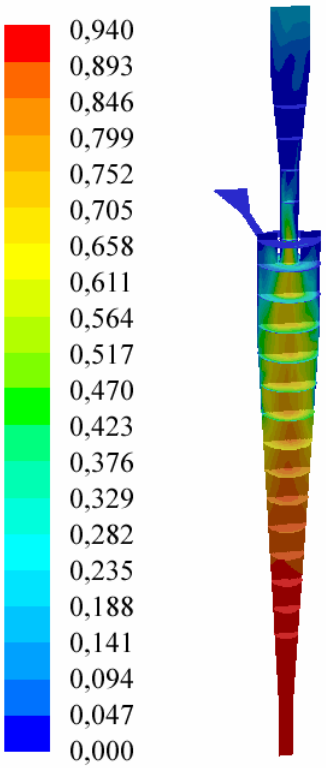


Results – Phase Distribution



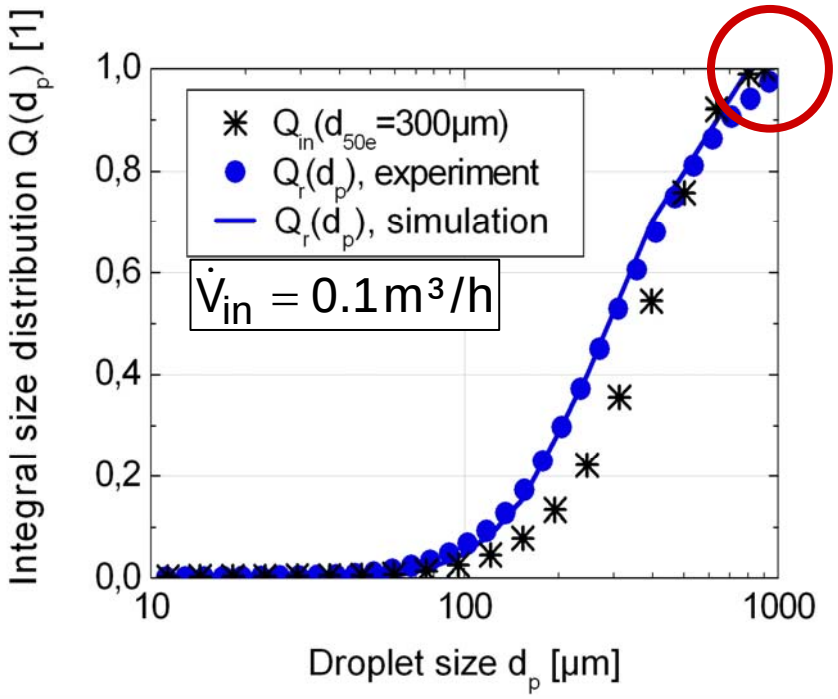


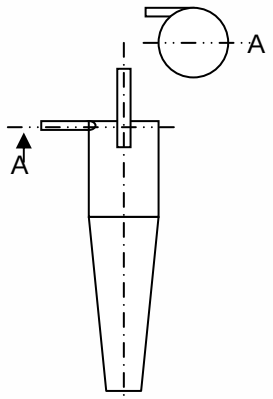
phase 19, $\bar{d}_p = 805\,\mu m$



phase fraction

Results – Phase Distribution





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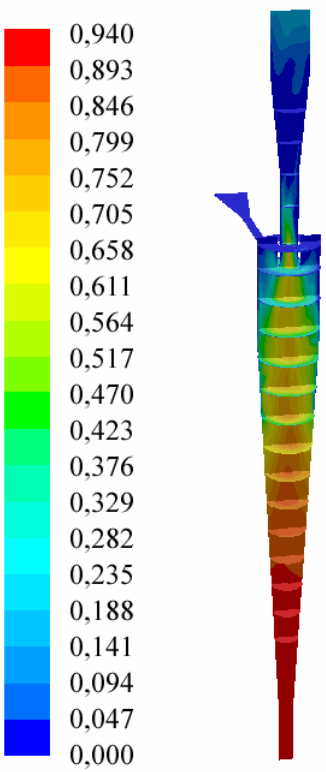

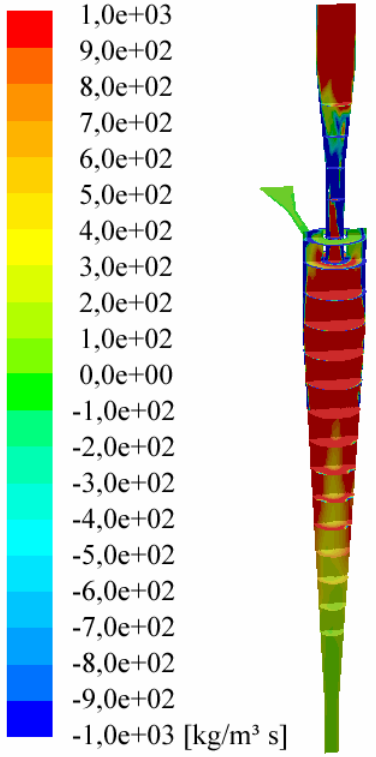

phase fraction $(B_i^+ - D_i^-) \cdot \rho_d \cdot V_{P,i} \cdot \Delta m_i$

Summary and Outlook

- Development of new method for coupled solution of population balances with flow field
  - Modelling of droplet breakup and coalescence
  - Describing impact of droplet interactions on separation process
  - Good agreement between simulation and experiment

Summary and Outlook

- Development of new method for coupled solution of population balances with flow field
  - Modelling of droplet breakup and coalescence
  - Describing impact of droplet interactions on separation process
  - Good agreement between simulation and experiment

- Further activities

  Direct numerical simulation (DNS) of droplet-droplet interactions for definition of kinetics (Empirical assumptions are no longer required for the solution of population balances)

A Simulation Model for the Separation of Dispersed Liquid-Liquid Systems in Hydrocyclones Based on the Coupling of CFD and Population Balances

Computational Fluid Dynamics in Chemical Reaction Engineering V
June 15th to 20th 2008, Whistler, British Columbia, Canada

Steffen Schütz, Gabriele Gorbach, Christian Winkler and Manfred Piesche

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Additional Slides

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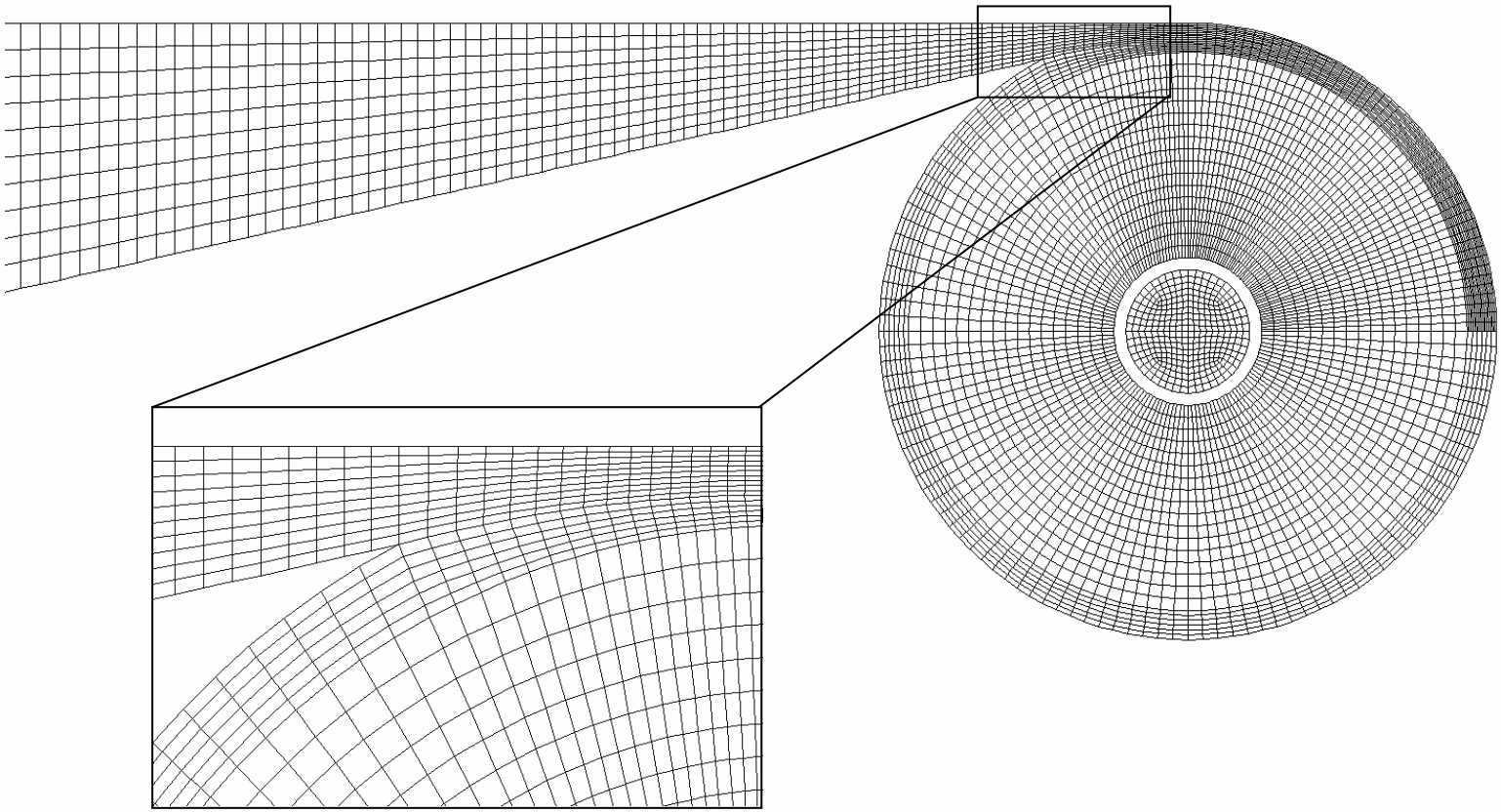
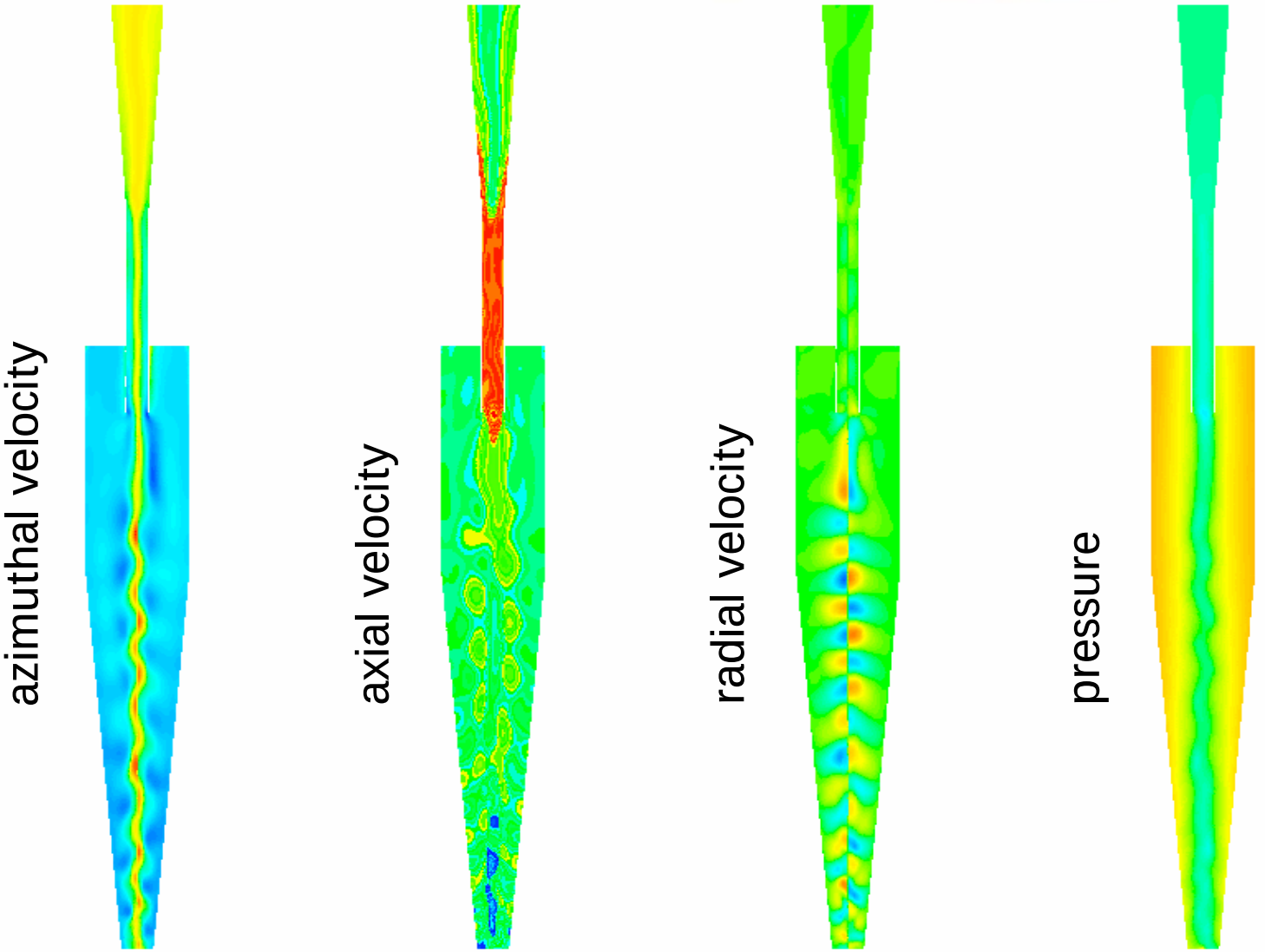
Discretization – 3D

- Partially structured grid – cross-section at the inlet region



Results
Velocity and Pressure Distribution



Kinetic Approaches

- Daughter droplet distribution according to Chatzi

$$\beta(m, m^*) = \frac{6}{m^* (2\pi)^{1/2}} \exp\left[-18 \frac{\left(m - \frac{m^*}{2} \right)^2}{(m^*)^2} \right].$$

- Daughter droplet distribution according to Lehr

$$ß(m, m^*) = \frac{6}{\pi^{2/3} (d^*)^3 \rho_d} \frac{\exp\left[-\frac{9}{4} \left(\ln\left[2^{2/5} d \left(\frac{\rho_c}{\sigma} \right)^{3/5} \varepsilon^{2/5} \right]^2 \right) \right]}{\left(1 + \mathrm{erf}\left[\frac{3}{2} \ln\left[2^{1/15} d^* \left(\frac{\rho_c}{\sigma} \right)^{3/5} \varepsilon^{2/5} \right] \right] \right)}$$

Kinetic Approaches – Coulaloglou and Tavlarides

- Breakup frequency

$$g_{br}(d) = C_1 \frac{\varepsilon^{1/3}}{d^{2/3}(1+\alpha)} \exp\left[-C_2 \frac{\sigma(1+\alpha)^2}{\rho_d d^5 \varepsilon^{2/3}}\right]$$

- Collision frequency

$$g_{coll}(d, d^*) = C_3 \frac{\varepsilon^{1/3}}{1+\alpha}\left(d^2 + (d^*)^2\right)\left(d^{2/3} + (d^*)^{2/3}\right)^{1/2}$$

- Coalescence efficiency

$$\lambda(d, d^*) = \exp\left[-C_4 \frac{\eta_c \rho_c \varepsilon}{\sigma^2 (1+\alpha)^3}\left(\frac{d \cdot d^*}{d + d^*}\right)^4\right]$$

Kinetic Approaches – Lehr

- Breakup frequency

$$g_{br}(d) = 0.5 \cdot d^{5/3} \left(\frac{\rho_c}{\sigma}\right)^{7/5} \varepsilon^{19/15} \exp\left(-\frac{\sqrt{2}}{d^3}\left(\frac{\sigma}{\rho_c}\right)^{9/5} \frac{1}{\varepsilon^{6/5}}\right)$$

- Coalescence function

$$\Omega(d, d^*) = \lambda\left(d, d^*\right) \cdot g_{coll}\left(d, d^*\right)$$

$$= \frac{\pi}{4}(d + d^*)^2 \min(v_c, v_{crit}) \exp\left(-\left(\frac{\alpha_{max}^{1/3}}{\alpha^{1/3}} - 1\right)^2\right)$$

Kinetic Approaches – Lehr

- Characteristic and critical velocity

$$v_c = \max\left(\underbrace{\sqrt{2}\varepsilon^{1/3}\sqrt{d^{2/3} + (d^*)^{2/3}}}_{\text{turbulent fluctuation velocity}} , \underbrace{|\underline{v} - \underline{v}^*|}_{\text{relative velocity}} \right)$$

$v_{crit} = 0.05\,m/s$ parameter, dependent on material data

- Coalescence close to walls and in the overflow/underflow region
- With high energy dissipation rate close to walls
  characteristic velocity > critical velocity
  → coalescence function only dependent on material data

Non-equidistant Droplet Size Discretization

- Coalescence correction term

$$K_{ikl}^{coal} = \frac{m_k + m_l}{m_i}$$

- Breakup correction term

$$K_i^{br} = \frac{m_i}{\sum_{k=1}^{i} \nu \ \beta(m_k, m_i) \ \Delta m_k \ m_k}$$