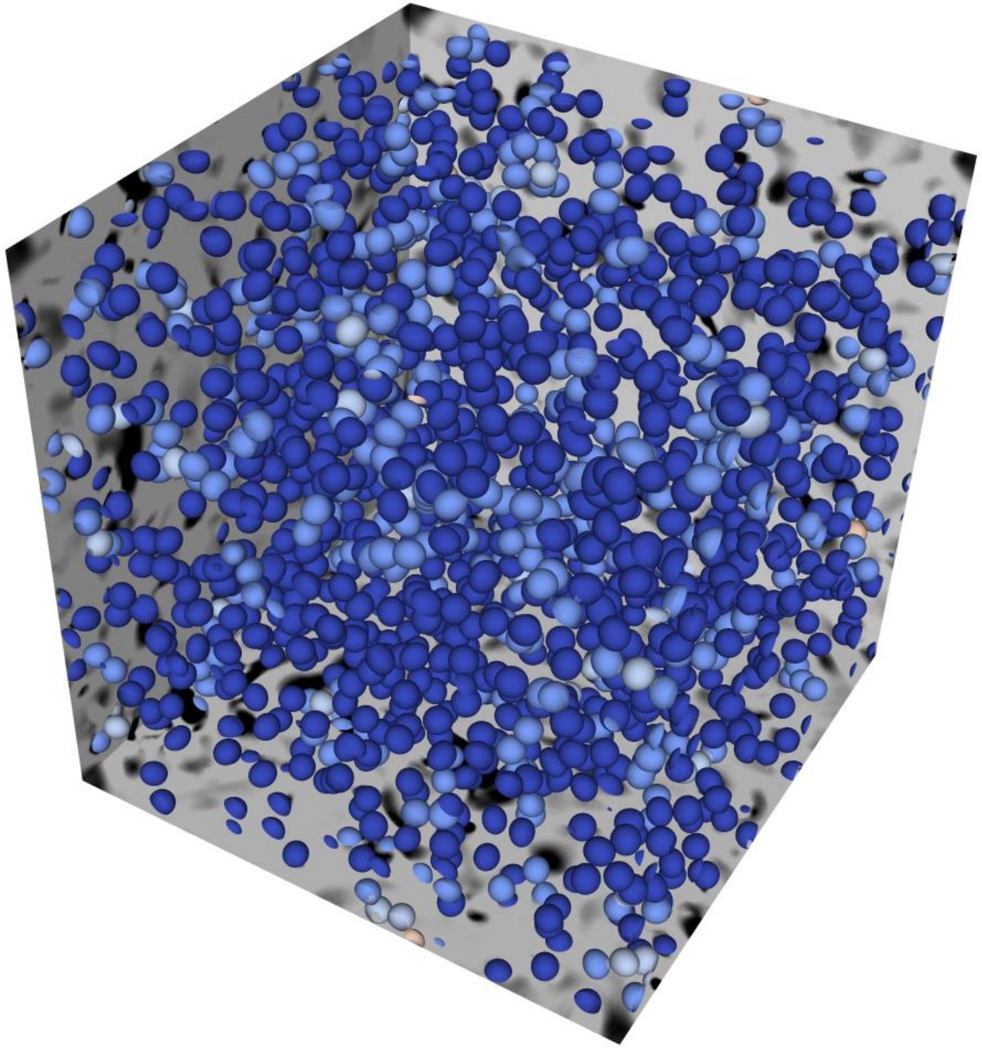
# ~~COLLISION~~ COALESCENCE RATE OF FINITE-SIZE MONODISPERSE DROPLETS IN HOMOGENEOUS ISOTROPIC TURBULENCE

*Victor Boniou*, Paul Rosener*
*Stéphane Jay, Jean-Lou Pierson,*
*Guillaume Vinay*

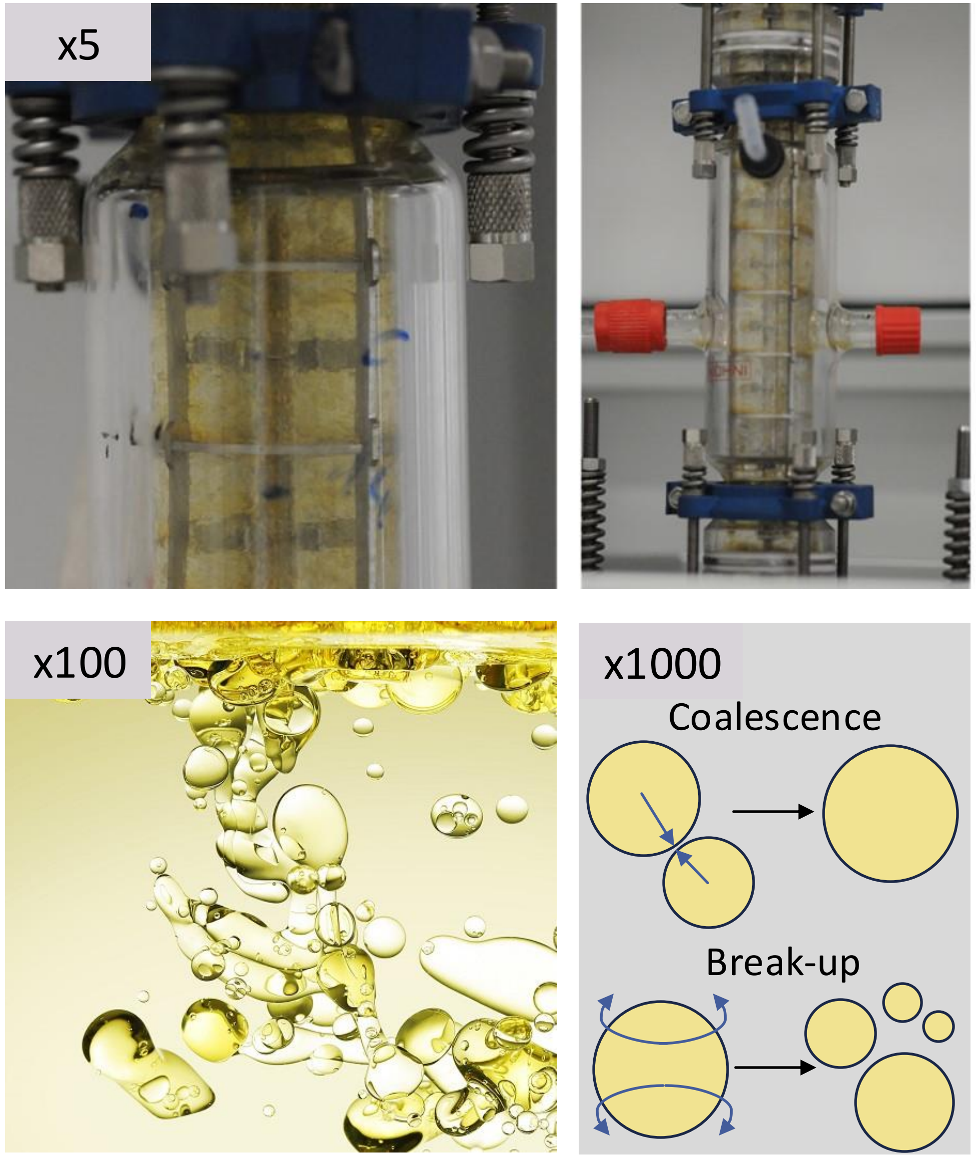
BGUM 2025



# Liquid-liquid extraction

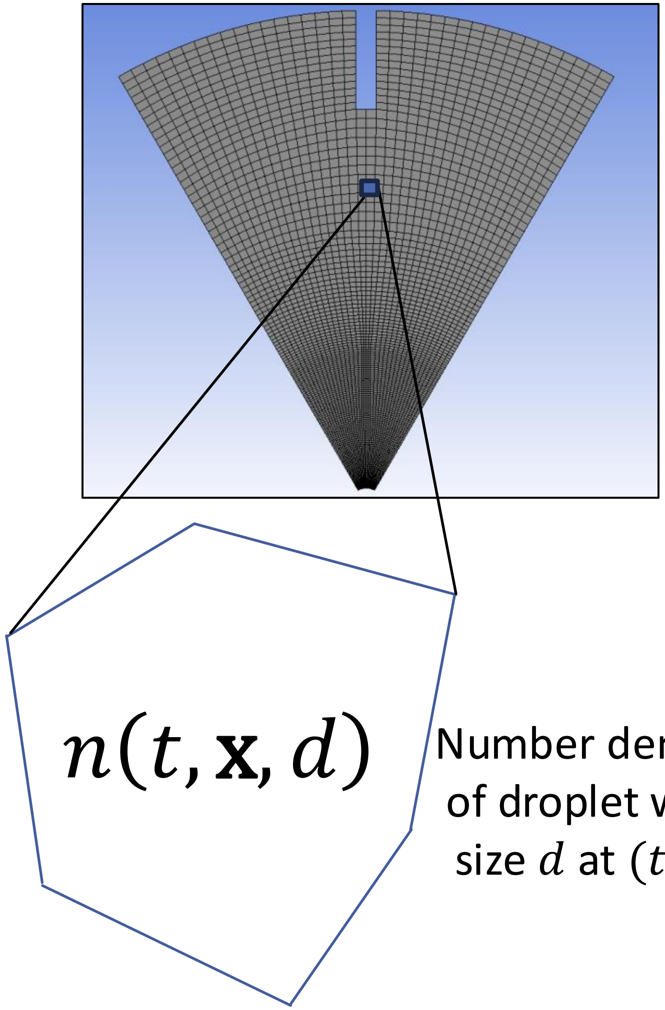
- Large range of length scales
  - Large domain: $L \sim 1$ m
  - Turbulent carrier phase: $\eta \sim 10$ µm
  - Polydisperse phase: $d_{min} \sim 100$ µm
- Droplets and turbulence highly coupled
  - Small-scale energy injection by droplet motion
  - Fragmentation and coalescence promoted by turbulence
- Multiphysics phenomenon
  - Mass transfer
  - Surfactant

**Predictive numerical tools for droplet size ?**



# Industrial scale CFD

## Euler-Euler



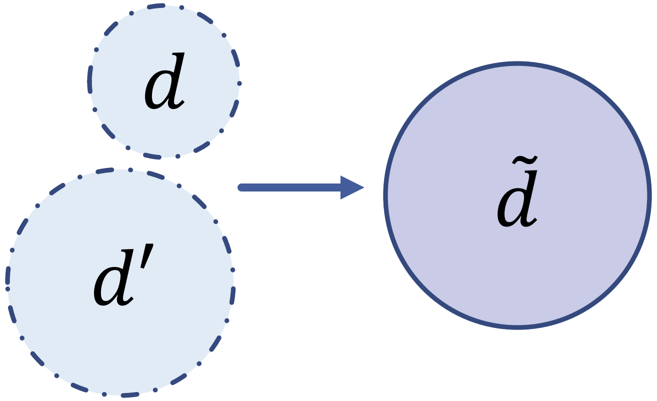

Number density of droplet with size $d$ at $(t, \mathbf{x})$

## Population Balance Equation

$$\frac{\partial n(t, \mathbf{x}, d)}{\partial t} + \underbrace{\boldsymbol{\nabla}_x . \left( n(t, \mathbf{x}, d) \mathbf{u}(t, \mathbf{x}, d) \right)}_{\text{Convective transport}} = \underbrace{S(t, \mathbf{x}, d)}_{\text{Break-up and Coalescence}}$$

Break-up not considered here… See related works with Basilisk[1,2]

## Coalescence frequency[3]




$$C(d, d') = \underbrace{\lambda(d, d')}_{\text{Coalescence efficiency}} \underbrace{\Gamma(d, d')}_{\text{Collision frequency}}$$

# Population balance equation: coalescence kernel

## Coalescence efficiency
$\lambda(\xi, \xi')$

$$\lambda(\xi, \xi') = \exp\left(-\frac{\bar{t}_d}{\bar{t}_c}\right)$$

From Coulaloglou & Tavlarides

Drainage time $\bar{t}_d = \frac{C_4 \mu_c \rho_c \epsilon^{2/3} d^{8/3}}{\sigma^2}$

Contact time $\bar{t}_c = C_5 \frac{d^{2/3}}{\epsilon^{1/3}}$

$$\lambda(d) = \exp\left(-\frac{C_4 \mu_c \rho_c \epsilon d^2}{C_5 \sigma^2}\right)$$

## Collision kernel
$\Gamma(\xi, \xi')$

$$\Gamma(\xi, \xi') = 2\pi d^2 g(d) \langle |w_r| \rangle$$

From Coulaloglou & Tavlarides

Radial distribution function $g(d) = 1$

Mean relative velocity $\langle |w_r| \rangle = C_3 d^{1/3} \epsilon^{1/3}$

$$\Gamma(d) = C_3 d^{7/3} \epsilon^{1/3}$$

Correct scaling in $\epsilon$ and $d$? $C_i$ could also depend on We, $\rho_r$, $\mu_r$ and $\Phi$!

## Scaling analysis

### Contact time

$$\bar{t}_c = \boldsymbol{C_4} \frac{d^{2/3}}{\epsilon^{1/3}}$$

### Collision kernel

$$\Gamma = \boldsymbol{C_3} d^{7/3} \epsilon^{1/3}$$

Augmented physics:

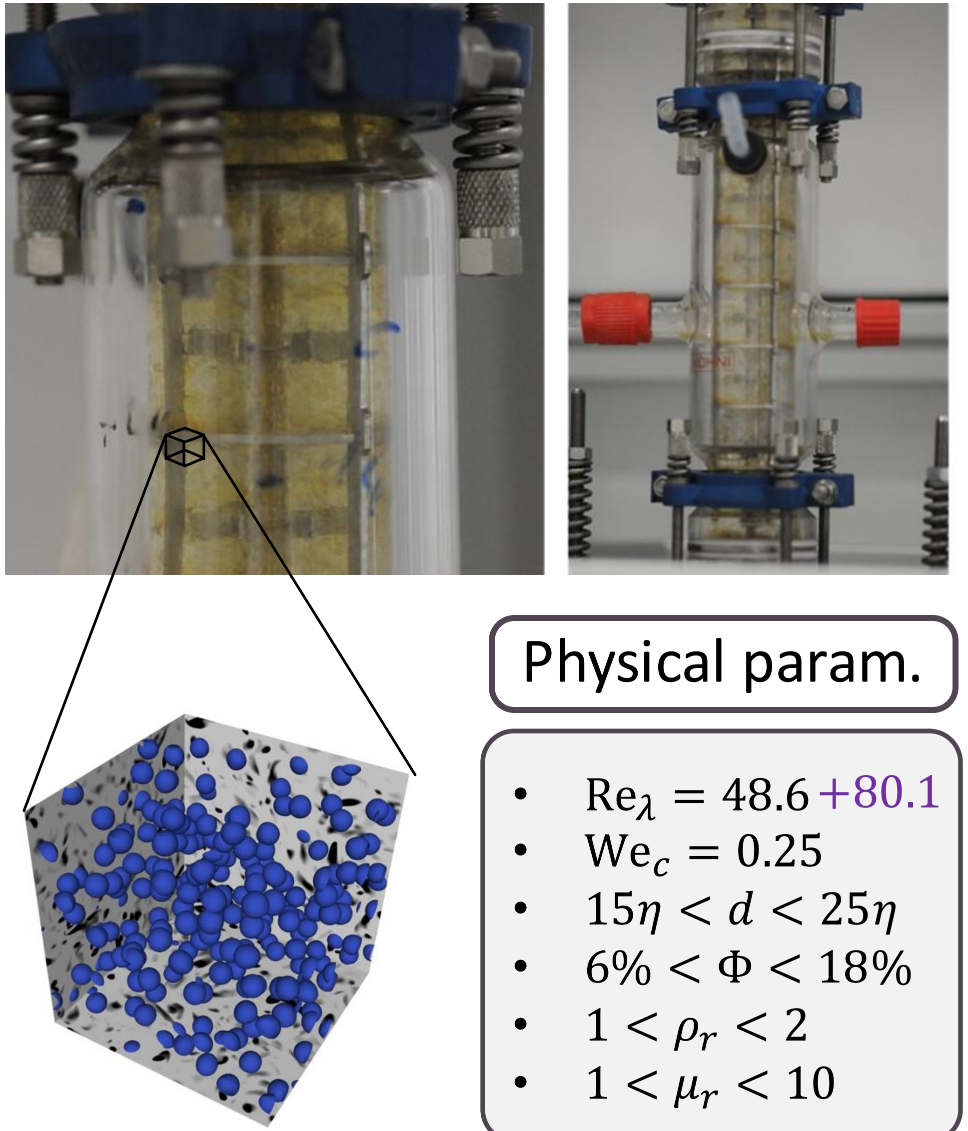
- Added mass effects (inertia of droplets is then included through density ratio $\rho_r$)
- Surface tension effects (with We scaling in contact time)
- Geometric effects of droplets included (depends on volume fraction $\Phi$)

$$\bar{t}_c = \sqrt{\frac{3}{64}\left(\rho_r + C_a^d\right) \mathrm{We}^{1/2}} \frac{d^{2/3}}{\epsilon^{1/3}}$$

$$\Gamma = \sqrt{8\pi C_k(\epsilon) \frac{\left(\rho_r + C_a^\infty\right)}{\left(\rho_r + C_a^d\right)}} d^{7/3} \epsilon^{1/3}$$

No viscous ratio $\mu_r$ effects included in these scaling laws

# Numerical set-up: setting the scene



Physical param.

- $Re_\lambda = 48.6 + 80.1$
- $We_c = 0.25$
- $15\eta < d < 25\eta$
- $6\% < \Phi < 18\%$
- $1 < \rho_r < 2$
- $1 < \mu_r < 10$

Basilisk[1]

- Second-order in space and time finite volume method.
- Octree grids with AMR
- Centered velocity formulation
- VOF-PLIC interface capturing method of Weymouth and Yue
- Curvature from height function
- Well-balanced surface tension
- Linear forcing of turbulence[2]
- Multi-VOF to prevent coalescence of droplets[3]

[1] S. Popinet (JCP 2009) [2] V. Boniou et al. (PRF 2025) [3] N. Fintzi et al. (AM 2024)

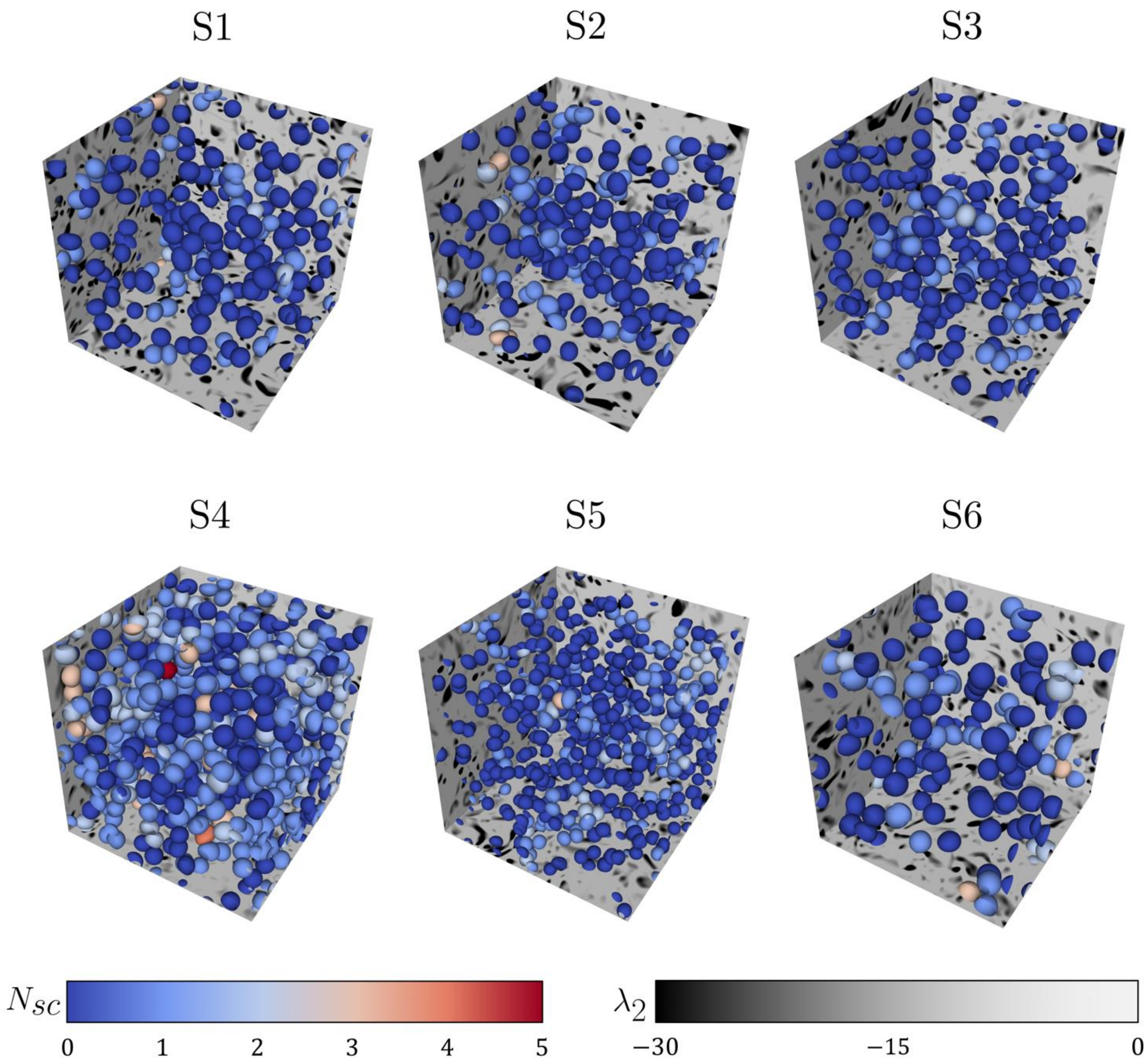
## Flow configuration

All simulations are run during 25 eddy turnovers with $N_{cells} = 512^3$ and:

- $\mathrm{Re}_\lambda = 48.6 \ +80.1$
- $\mathrm{We} = 0.25 \ \ +0.05$

Starting from a single-phase HIT simulation at steady-state (after 50 eddy turnovers)

| | $\mathrm{Re}_\lambda$ | We | $\rho_r$ | $\mu_r$ | $d/\eta$ | $\Phi/N_d$ |
|---|---|---|---|---|---|---|
| S1 | 48.6 | 0.25 | 1 | 1 | 20 | 6%/180 |
| S2 | 48.6 | 0.25 | 1 | 10 | 20 | 6%/180 |
| S3 | 48.6 | 0.25 | 2 | 1 | 20 | 6%/180 |
| S4 | 48.6 | 0.25 | 1 | 1 | 20 | 18%/540 |
| S5 | 48.6 | 0.25 | 1 | 1 | 15 | 6%/434 |
| S6 | 48.6 | 0.25 | 1 | 1 | 25 | 6%/94 |
| S6’ | 80.1 | 0.25 | 1 | 1 | 25 | 6%/94 |
| S7 | 48.6 | 0.05 | 1 | 1 | 20 | 18%/540 |



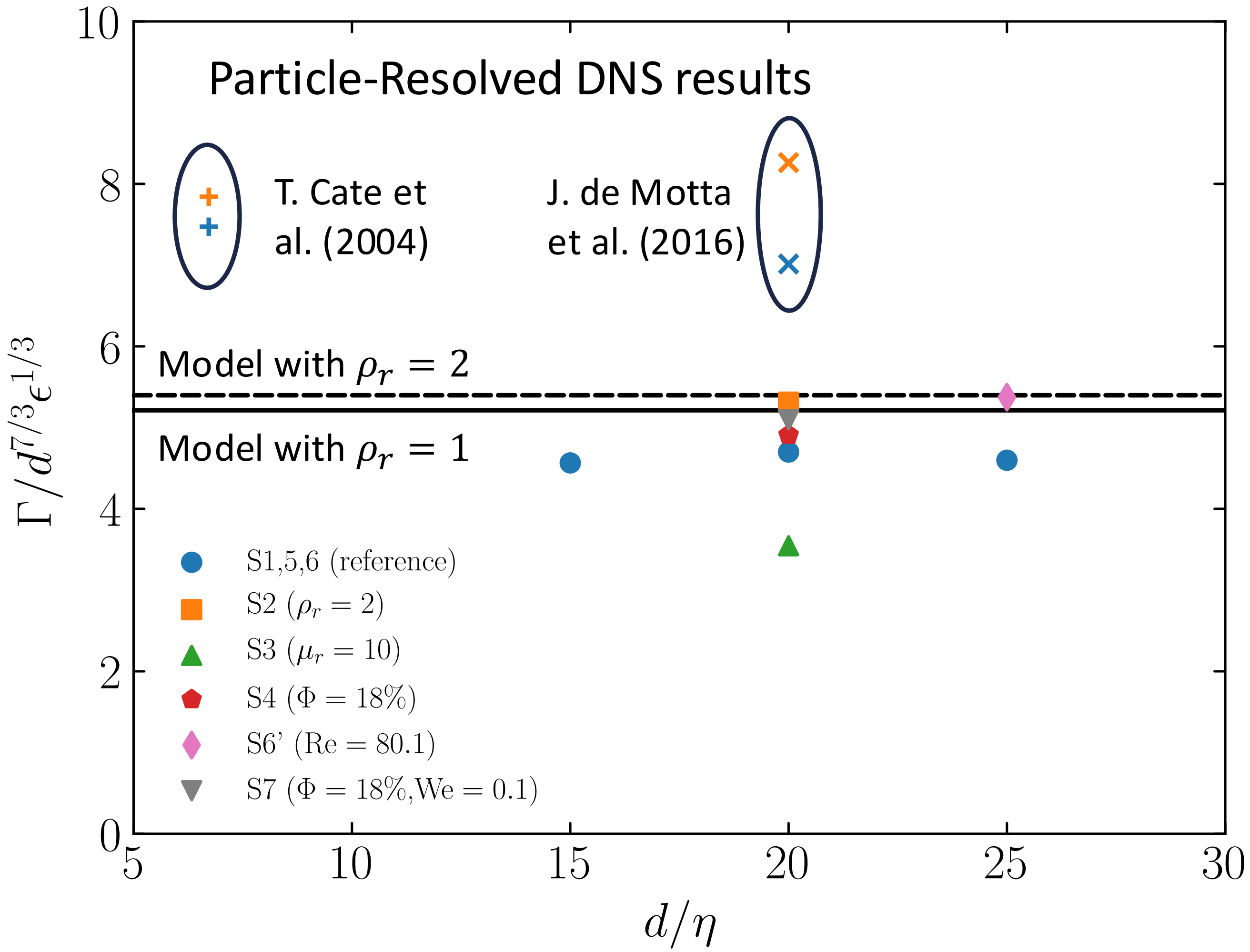
## Collision kernel

From study of $g(r)$ and $\langle|w_r(r)|\rangle$:

$$\Gamma = f(\mu_r) = 1 \sqrt{8\pi C_k \frac{(\rho_r + C_a^\infty)}{(\rho_r + C_a^d)}} d^{7/3}\epsilon^{1/3}$$

Conclusions on the model:

- Particle-Resolved DNS predicts higher collision rates which is expected
- Correct scaling for $d$
- Correct behavior for $\rho_r$
- Small increase due to $\Phi$ not included
- Huge decrease due to $\mu_r$ should be included through a correction $f(\mu_r)$




Boniou, V., Jay, S., Vinay, G., & Pierson, J. L. *Collision statistics of finite-size monodisperse droplets in homogeneous isotropic turbulence*. Journal of Fluid Mechanics (In review 2025).

# Contact time

$$\lambda(\xi, \xi') = \exp\left(-\frac{\bar{t}_d}{\bar{t}_c}\right)$$

$\bar{t}_c$: Mean contact time

- Do we retrieve the correct scalings?
- Does it depend on $\rho_r$? On $\mu_r$? On We?
- Is the pdf really exponential?

$$\bar{t}_c = \sqrt{\frac{3}{64}(\rho_r + C_a^d)\mathrm{We}^{1/2}}\,\frac{d^{2/3}}{\epsilon^{1/3}}$$

# Contact time pdf

Coalescence efficiency

From Ross work:

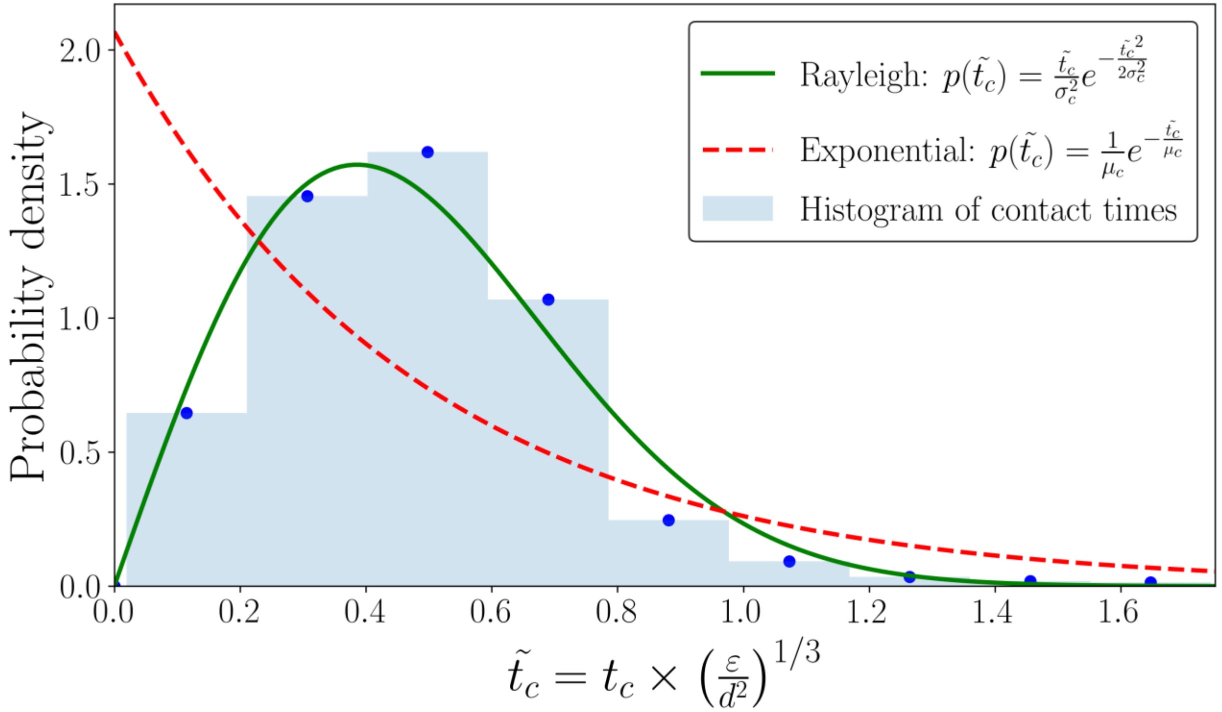
$$p(t_c) = \frac{1}{\overline{t_c}} \exp(-\frac{t_c}{\overline{t_c}})$$

Contact time does not follow an exponential distribution in DNS:

$$p(t_c) = \frac{t_c}{\sigma_{tc}^2} \exp(-\frac{t_c^2}{2\sigma_{tc}^2})$$

with $\sigma_{tc} = \sqrt{2/\pi}\,\overline{t}_c$

$$\lambda(\xi,\xi') = \exp\left(-\frac{1}{\pi}\frac{\overline{t}_d^2}{\overline{t}_c^2}\right)$$



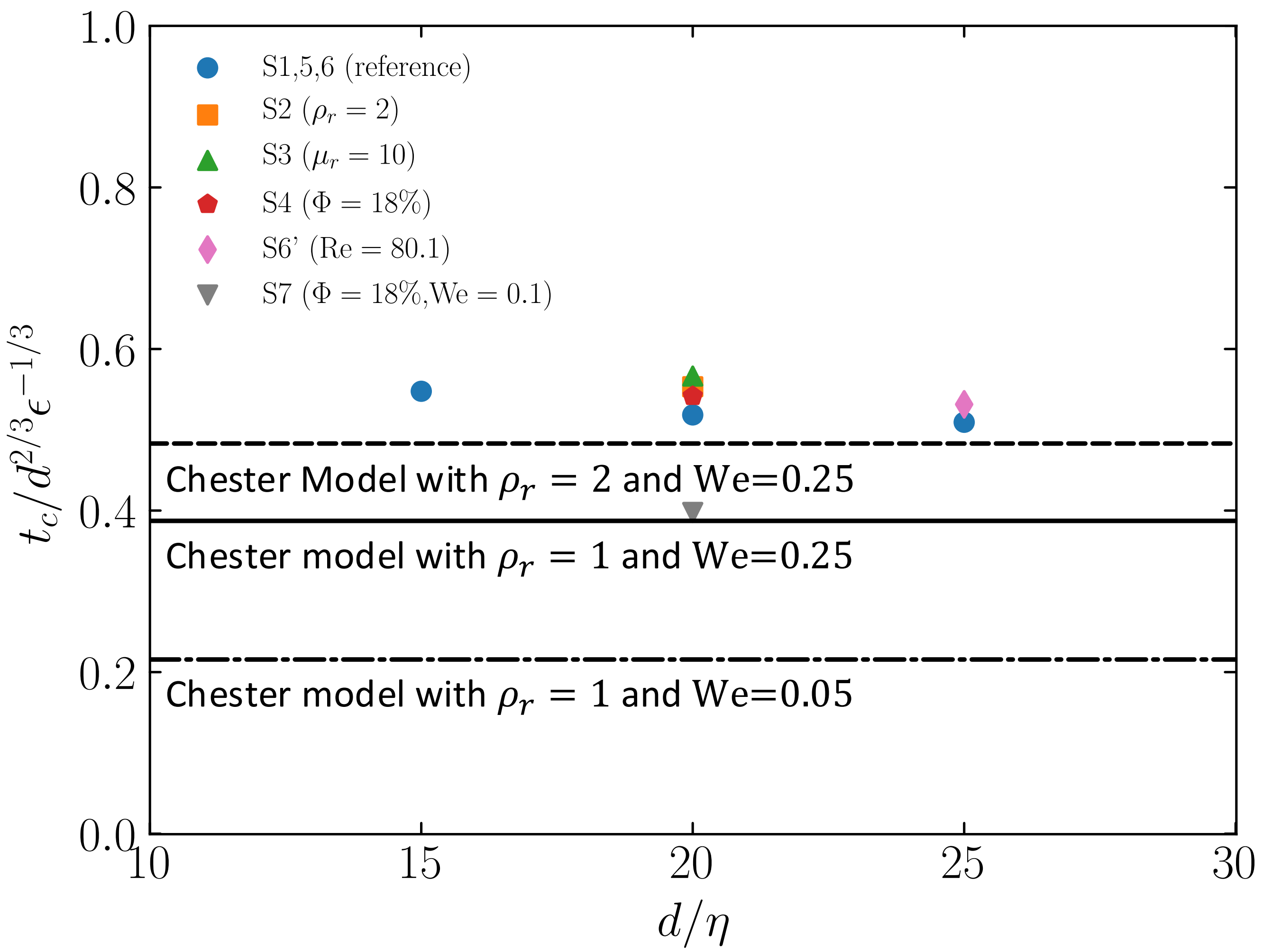
## Mean contact time

From Chester work (inviscid):

$$\bar{t}_c = \sqrt{\frac{3}{64}\left(\rho_r + C_a^d\right)\mathrm{We}^{1/2} d^{2/3} \epsilon^{1/3}}$$

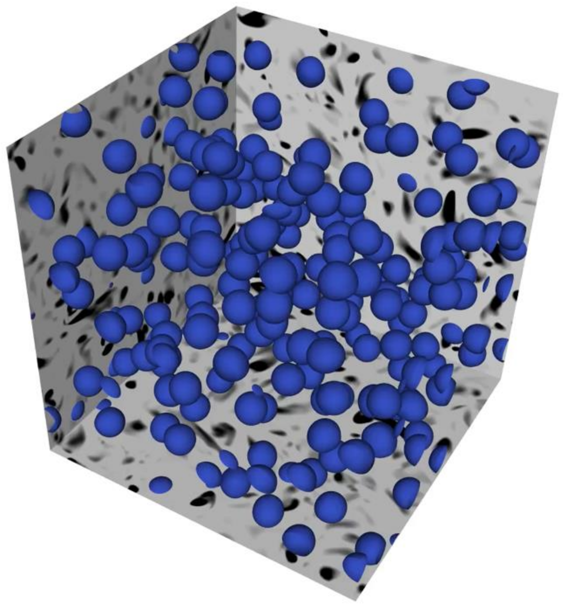
- Scaling with $d$ is verified
- Contact time weakly depends $\Phi$ but $\mu_r$ should be included
- We and $\rho_r$ might be reevaluated

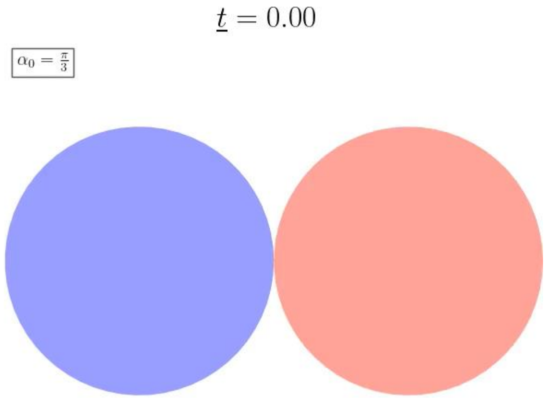
Not a lot of points in We and $\rho_r$ to confirm scaling!!



# An intermediate approach to compute contact time

| Quasi-DNS | System of ODE | Scaling analysis |
| --- | --- | --- |






$$\bar{t}_c = \sqrt{\frac{3}{64}\left(\rho_r + C_a^d\right)\mathrm{We}^{1/2} d^{2/3} \epsilon^{1/3}}$$

Direct solution of Navier-Stokes **but only few points in param matrix!**

Relative equations of motion of two bubbles from Kok + Denkov

Chester's scaling law for **non-dissipative head-on** collisions of **bubbles**

## Model reduction of collision

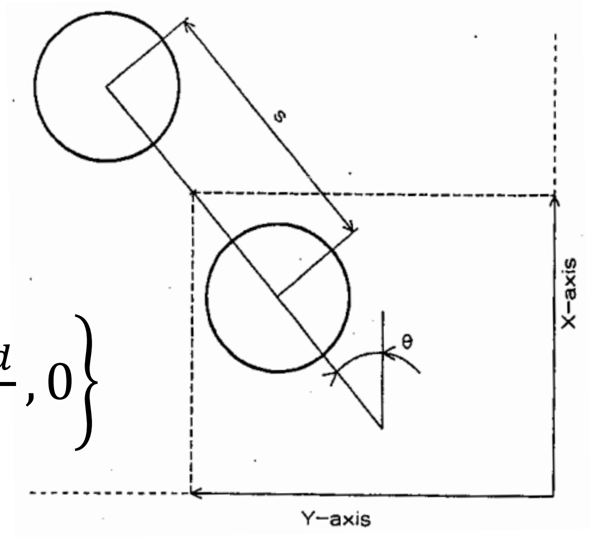
Collision discribed by an ODE system of $4$ variables $(x, y, s, \theta)$ such that:

- Collision on a 2D plane (still 3D collisions)
- External flow (Kok)
- Capillary forces (Denkov)
- Droplet inertia

$$\mathbf{q} = \{x, y, r, \theta\}$$

$$\dot{\mathbf{q}} = \{u, v, w_r, \omega\}$$

$$\mathbf{f} = \left\{0,0,-2\sigma\frac{\partial S_d}{\partial r}, 0\right\}$$

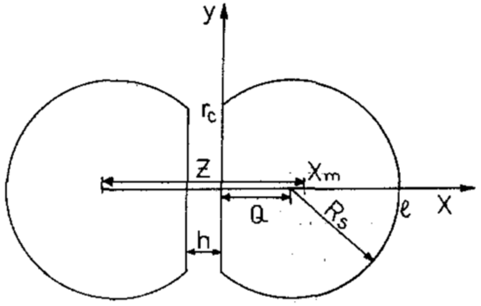



Lagrange's equations on kinetic energy:

$$\frac{d}{dt}\left(\frac{\partial K}{\partial \dot{q}_i}\right) - \frac{\partial K}{\partial q_i} = f_i$$

$$S_d = \frac{\pi}{3}\left(\ell^2 + 16\frac{r}{\ell}\right)$$

$$\ell^4 + 16\ell - 24r = 0$$



## Final system of ODE

$$
\begin{cases}
(A_1 + 2\rho_r - A_2\cos(2\theta))\ddot{x} + 2A_2\sin(2\theta)\dot{\theta}\,\dot{x} - A_2\sin(2\theta)\,\ddot{y} - 2A_2\cos(2\theta)\dot{\theta}\,\dot{y} = 0 \\
(A_1 + 2\rho_r + A_2\sin(2\theta))\ddot{x} - 2A_2\cos(2\theta)\dot{\theta}\,\dot{x} + A_2\cos(2\theta)\,\ddot{y} - 2A_2\sin(2\theta)\dot{\theta}\,\dot{y} = 0 \\
(2A_3 + \rho_r)\ddot{s} - \rho_r s\dot{\theta}^2 = -\dfrac{192}{\mathrm{We}}\left(\ell - \dfrac{8}{\ell^2}\right)/(4 + \ell^3) \\
(2A_4 + \rho_r s^2)\ddot{\theta} + 2\rho_r s\dot{\theta}\dot{s} - 2A_2\sin(2\theta)\,\dot{x}^2 + 2A_2\sin(2\theta)\,\dot{y}^2 - 2\dot{x}\dot{y}\cos(2\theta) = 0
\end{cases}
$$

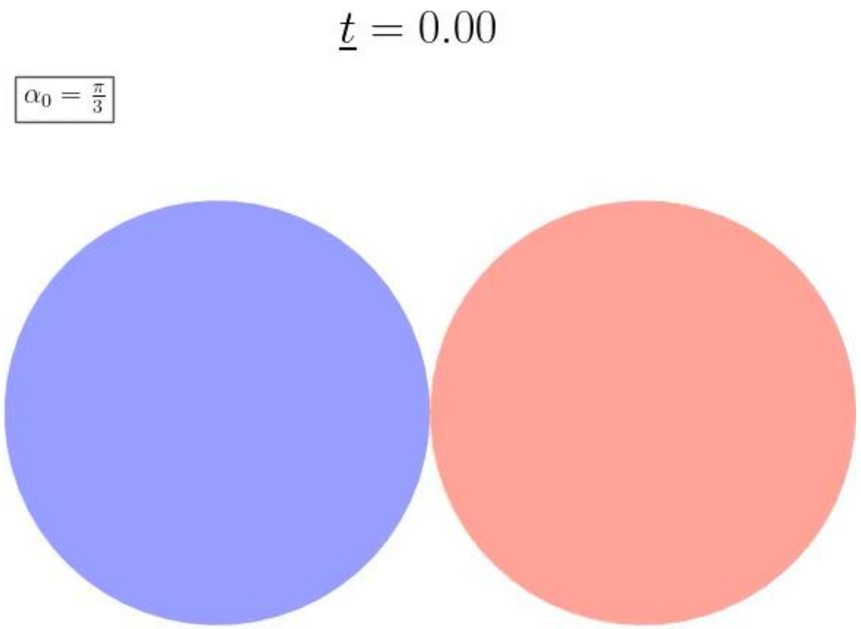
With $\rho_r$ and $\mathrm{We}$ parameters of the system

## Contact time from the model

1. Initial conditions of the collision:

$$\mathbf{q}_0 = \left\{\frac{d}{2}, 0, d, 0\right\} \quad \dot{\mathbf{q}}_0 = \left\{\frac{w_{r,0}}{2}, \frac{w_{\theta,0}}{2}, w_{r,0}, \frac{w_{\theta,0}}{d}\right\}$$

$$w_{r,0} = -\sqrt{8\pi C_k \frac{(\rho_r + C_a^{\infty})}{(\rho_r + C_a^{d})}} \quad w_{\theta,0} = -w_{r,0}\tan(\alpha_0)$$



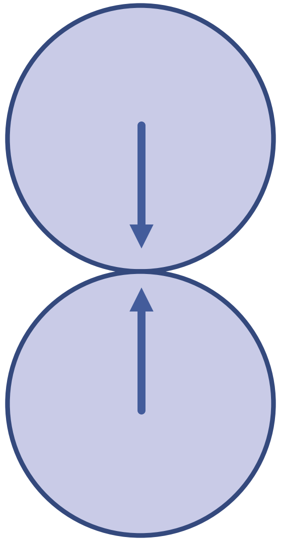

2. Choice of $\rho_r$ and We
3. ODE solved until $r > d$ to get contact time from the resolved system

# Model reduction of collision: parameter study

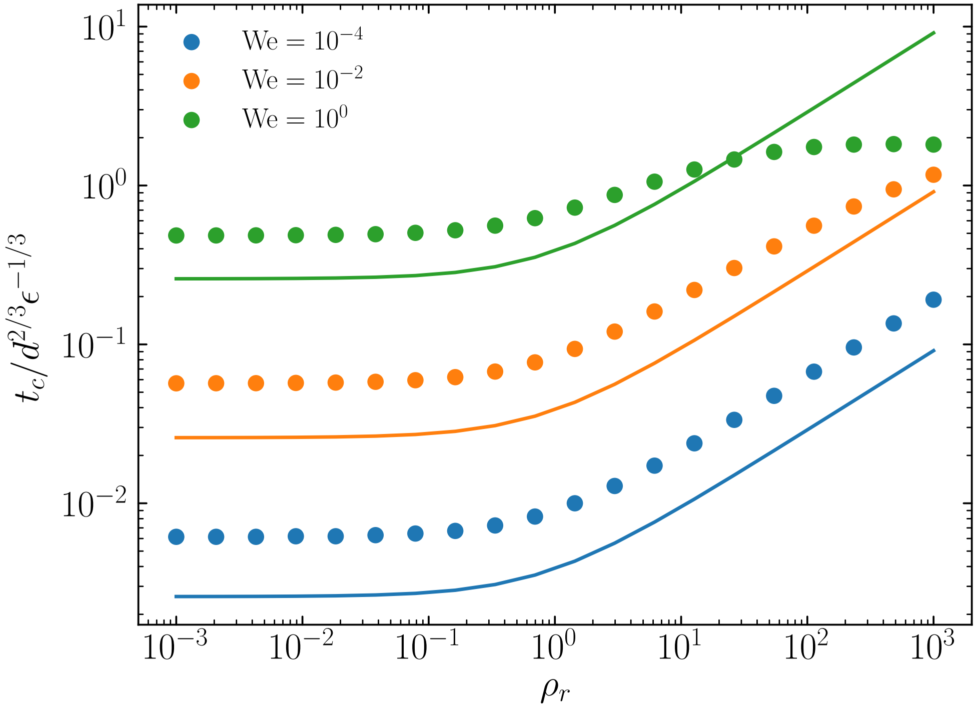
$$\bar{t}_c = \sqrt{\frac{3}{64}\left(\rho_r + C_a^d\right)\mathrm{We}^{1/2} d^{2/3} \epsilon^{1/3}}$$

Head-on

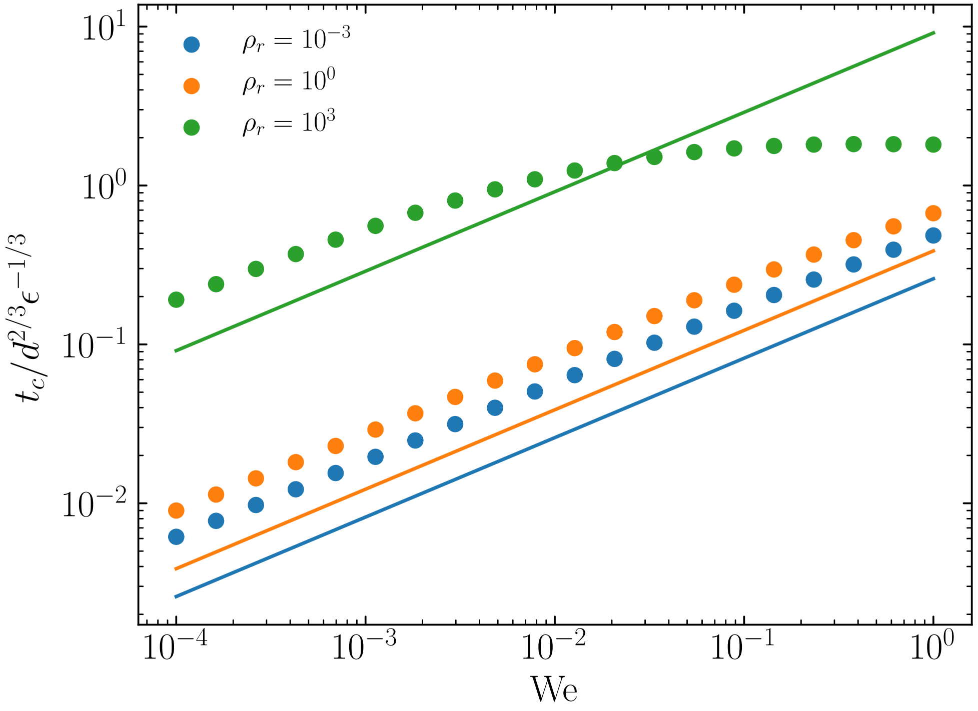
$\alpha_0 = 0$



Scaling in $\rho_r$

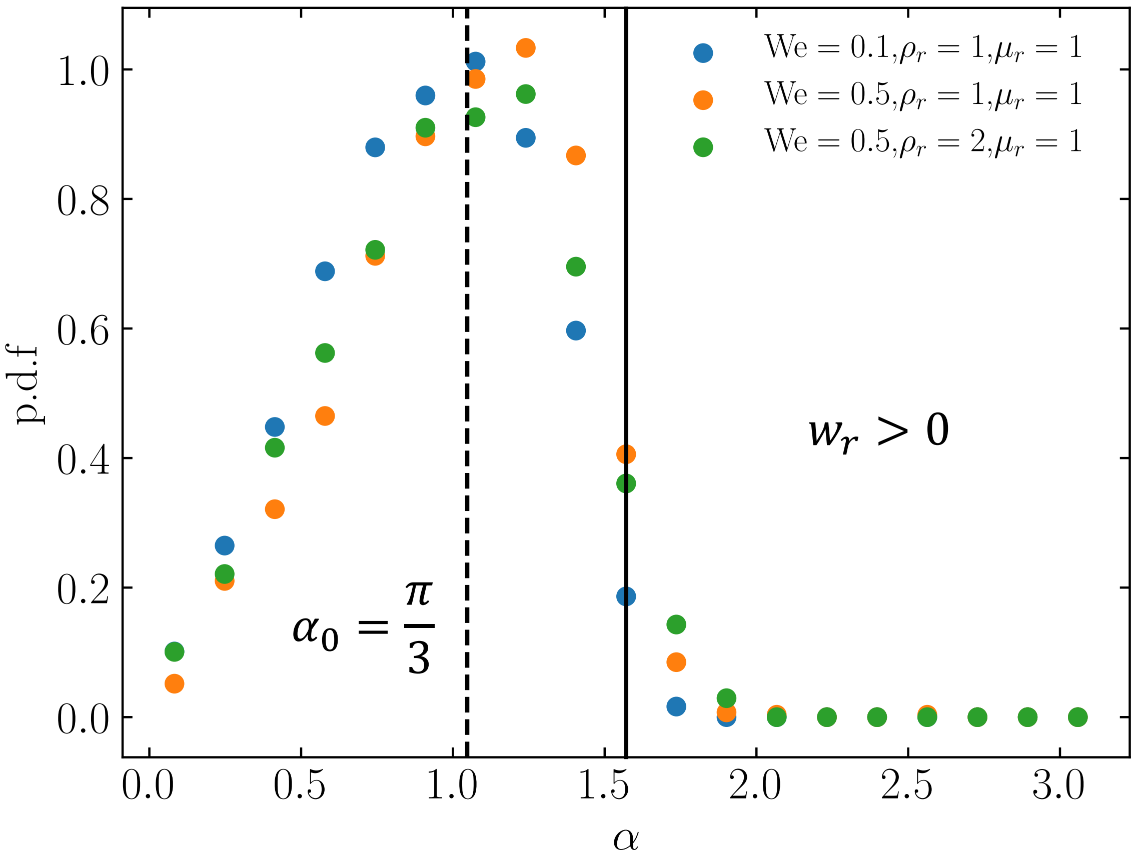


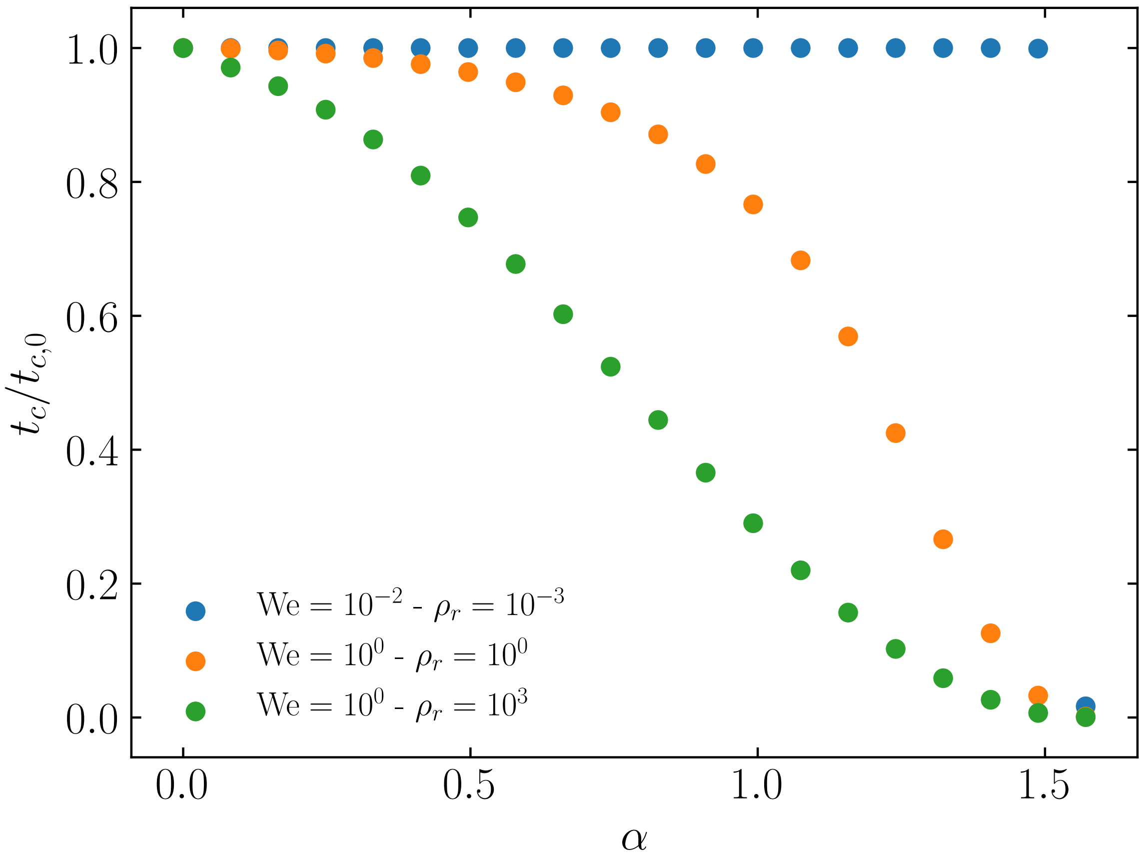

Scaling in We




Scalings of Chester is retreived for all points apart from high We droplets in gas!

# Model reduction of collision: parameter study




$\alpha_0 = \frac{\pi}{3} \approx \tan^{-1}\sqrt{\frac{8}{3}}$ in agreement with Kolmogorov theory!!

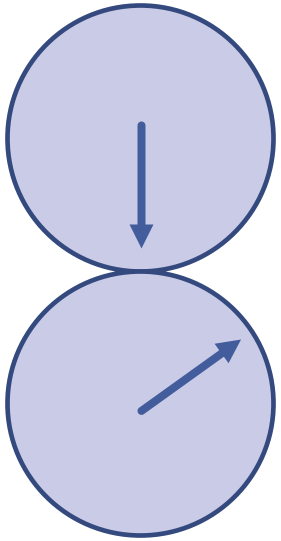
For bubbles: $\alpha_0$ does not matter
For droplet in liquid or gas, huge decrease of $t_c$ when not head-on

# Internship P.Rosener: model reduction of collisions

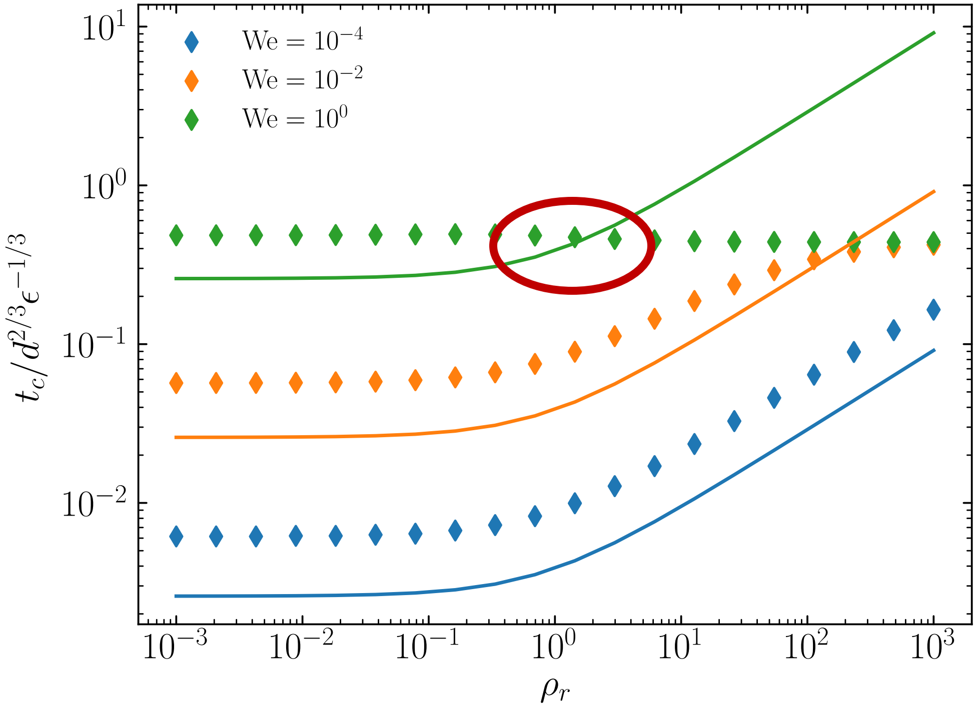
$$\bar{t}_c = \sqrt{\frac{3}{64}(\rho_r + C_a^d)\mathrm{We}^{1/2} d^{2/3} \epsilon^{1/3}}$$

Head-on

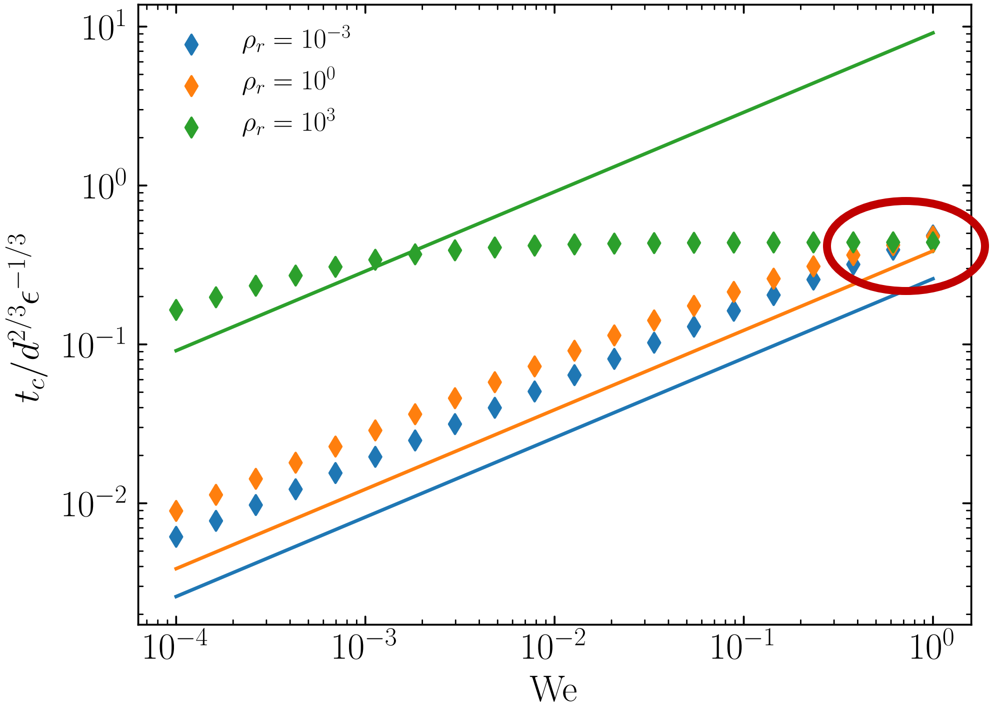
$$\alpha_0 = \frac{\pi}{3}$$



**Scaling in $\rho_r$**




**Scaling in We**




Scalings of Chester are not retreived for We around 1 for not head-on collisions!

$$\lambda(\xi, \xi') = \exp\left(-\frac{\bar{t}_d}{\bar{t}_c}\right)$$

$\bar{t}_d$: Mean drainage time

- Here we just consider that the pdf $p(t_d)$ is a Dirac to

$$\bar{t}_d = \frac{\mu_c \rho_c \epsilon^{2/3} d^{8/3}}{\sigma^2}$$

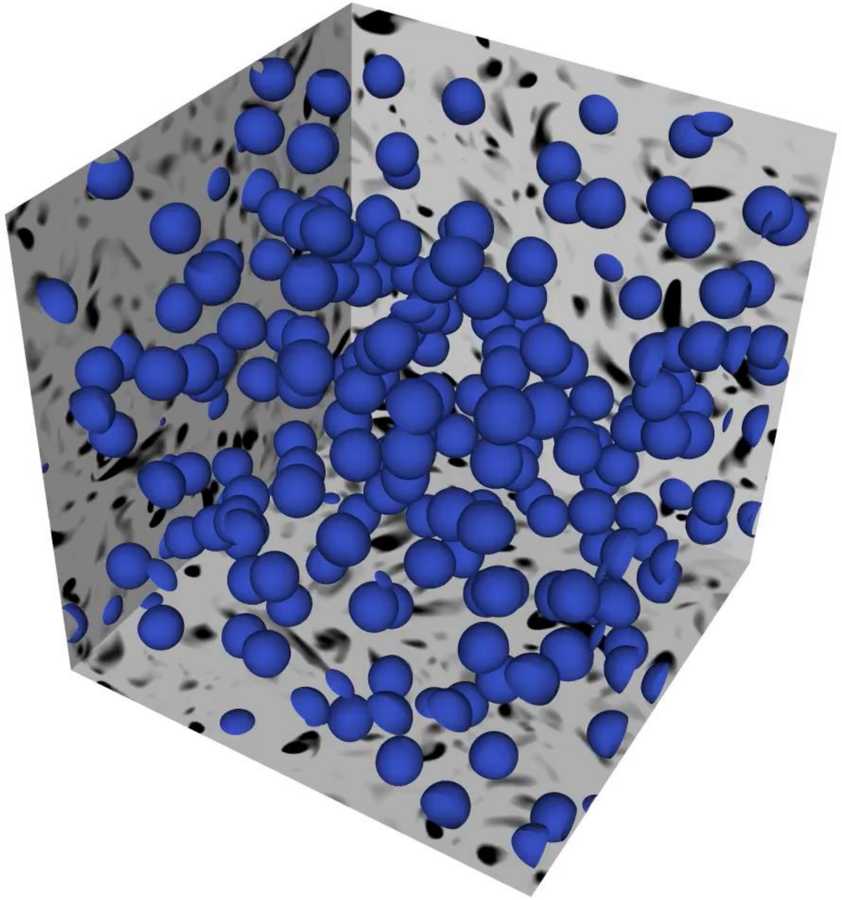
See presentation of Paul-Peter tomorrow! (With Multilayer solver!!)

## Conclusions

1. DNS to study the collision statistics of population of droplets using multi-VOF interface capturing.

2. Data thoroughlty validated on collision rate and leading to a new formula for the coalescence rate.

3. New reduced model for binary collisions useful to study the scaling law and to compare with DNS



Try it yourself!
http://basilisk.fr/sandbox/boniouv