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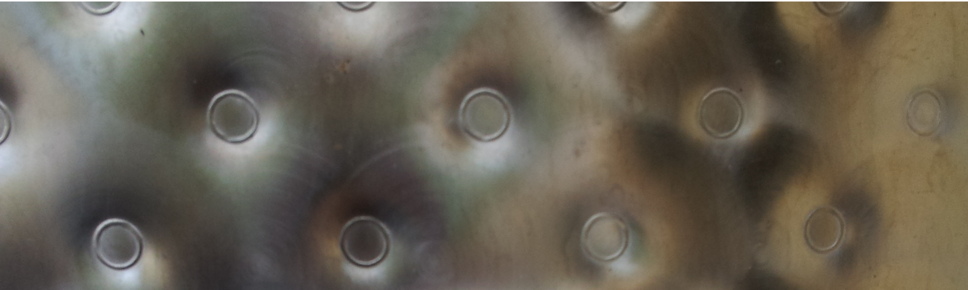
OFW11 11th OpenFOAM® Workshop Guimarães 2016

CFD Analysis of Nutrient Mixing during Wine Fermentation

Dominik Schmidt, Kai Velten

June 27, 2016

What happens behind these walls?



Goals

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- making use of computational science to analyze industrial scale wine fermentations

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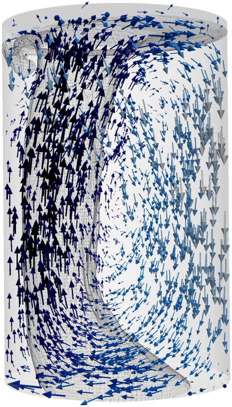
- making use of computational science to analyze industrial scale wine fermentations
  - set-up CFD model for fermentation flow simulations



Goals

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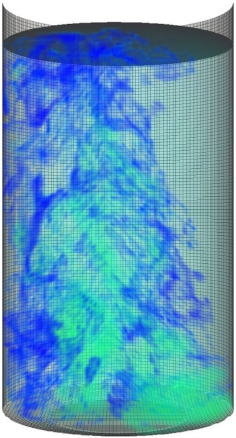
- making use of computational science to analyze industrial scale wine fermentations
  - set-up CFD model for fermentation flow simulations
  - analyze nutrient mixing



Winemaking . . . in short

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Harvest

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By John from UK (Harvesting the Grapes in Duras)[CC BY-SA 2.0, via Wikimedia Commons]

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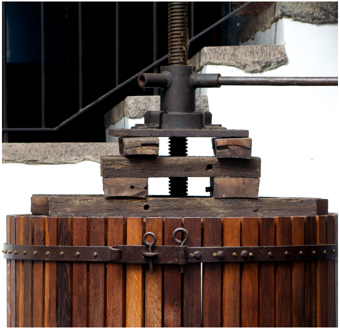
Harvest → Pressing



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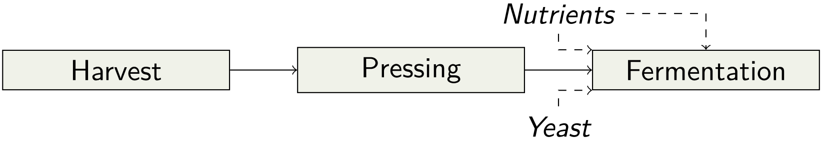

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Nutrient addition

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Di-Ammonium-Phosphate (DAP)

- Nitrogen source for yeast nutrition
- prevents stuck or sluggish fermentation
- two addition times recommended (Bely et al., 1990)
  1. during tank filling with yeast inoculation
  2. mid-fermentation

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Homogeneity?

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Flow modeling

Driving forces of the flow

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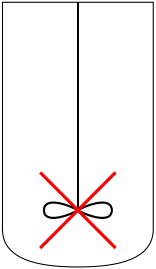

No mechanical agitation

Driving forces of the flow

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Alcoholic fermentation

$$\underbrace{C_6H_{12}O_6}_{\text{Sugar}} \xrightarrow{\triangledown} \underbrace{2\ C_2H_5OH}_{\text{Ethanol}} + \underbrace{2\ CO_2}_{\text{Carbon dioxide}} \qquad \Delta H_f^\circ = -23.5\,\mathrm{kcal\,mol^{-1}} \tag{1}$$

Driving forces of the flow

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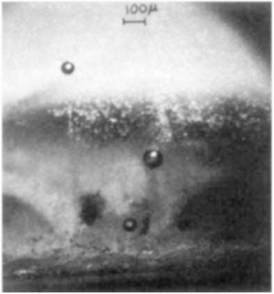
- approx. $50\,m^3$ CO_2 gas is released from $1\,m^3$ must
- CO_2 bubbling $\gg$ natural convection



(Delente et al., 1969)

Driving forces of the flow

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- approx. $50\,m^3$ CO_2 gas is released from $1\,m^3$ must
- CO_2 bubbling $\gg$ natural convection
- dispersed bubbly flow
  $\Longrightarrow$ **Euler-Euler model**

By Jim Champion (Flickr: Rising bubbles) [CC BY-SA 2.0], via Wikimedia Commons

Eulerian multiphase model

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- `multiphaseEulerFoam` (Wardle and Weller, 2013)
- interfacial forces: drag & lift

  (Dijkhuizen et al., 2010; Lau et al., 2011; Rastello et al., 2010; Roghair et al., 2013)

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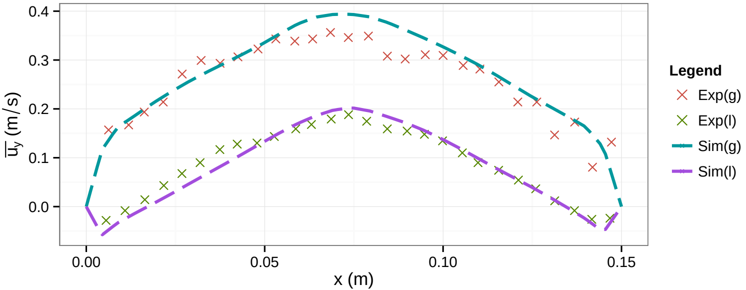

Validation against bubble column experiments from Deen et al. (2001) ($y = 0.25\,\text{m}$).

Example simulation szenario

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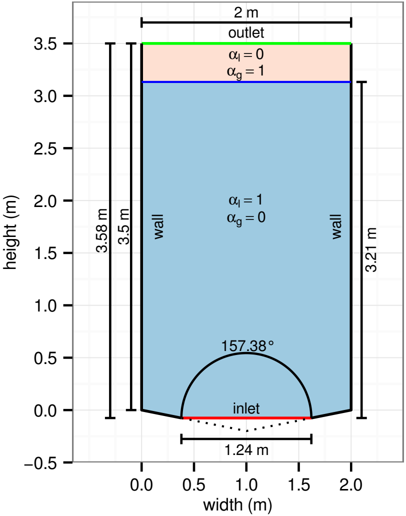
- Geometry
  - *Kloepper bottom*
  - $10\,m^3$ liquid volume



Example simulation szenario

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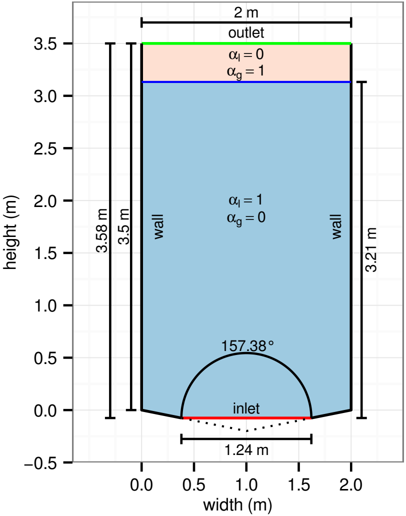
- Geometry
  - *Kloepper bottom*
  - $10\,m^3$ liquid volume
- Fermentation stage
  - peak fermentation
  - CO_2 formation: $1\,g\,L^{-1}\,h^{-1}$
  - $\dot{V}_{g,inlet} = 1.515 \times 10^{-3}\,m^3\,s^{-1}$



Example simulation szenario

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Geometry

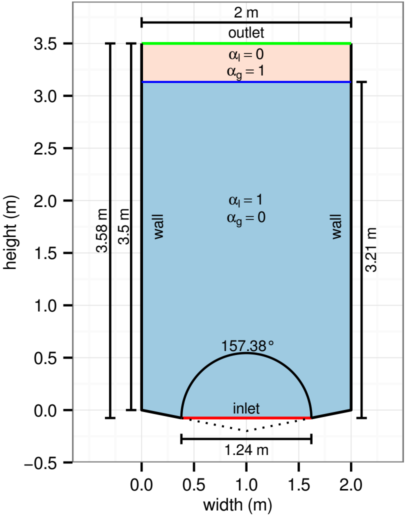
- *Kloepper bottom*
- $10\,m^3$ liquid volume

Fermentation stage

- peak fermentation
- CO_2 formation: $1\,g\,L^{-1}\,h^{-1}$
- $\dot{V}_{g,inlet} = 1.515 \times 10^{-3}\,m^3\,s^{-1}$

Assumptions

- bubble formation predominantly at vessel bottom (Delente et al., 1969)
- constant bubble diameter (1 mm)



Flow pattern initialization

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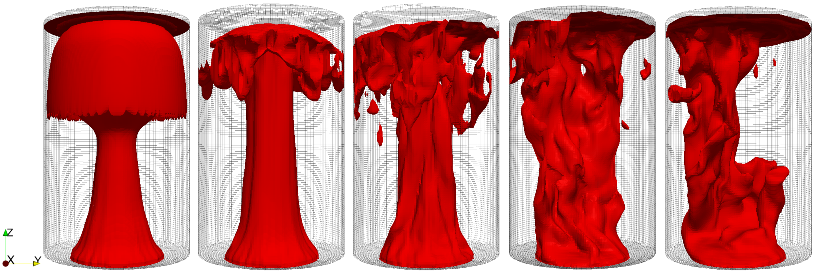

Bubble plume development with snapshots of the isosurface $\alpha_g = 0.003$ after 10, 30 60, 90 and 120 s of real time.

Fully developed flow

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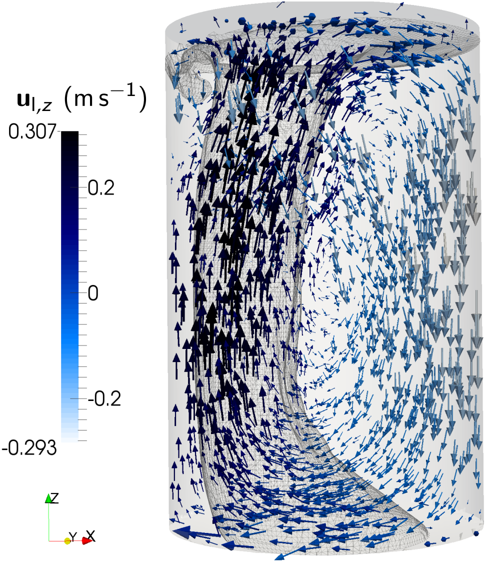

Time averaged liquid flow pattern and bubble plume dimensions (isosurface $\alpha_g = 0.003$, $120\,s \leq t \leq 300\,s$).

Unsteadiness

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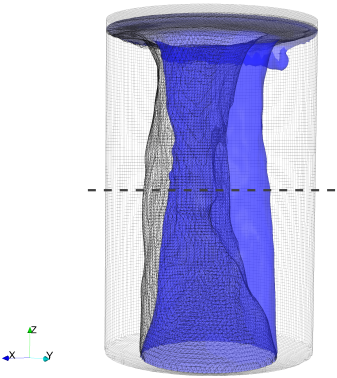
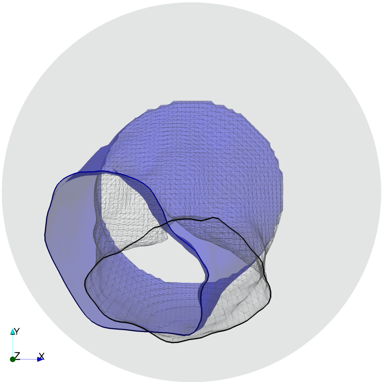


(a) front



(b) top, cut at $z = 0.5H$

Time averaged bubble plume isosurface ($\alpha_g = 0.003$)
blue: $120\,s \leq t \leq 300\,s$, wireframe: $300\,s \leq t \leq 480\,s$.

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Mixing evaluation

Nutrient addition

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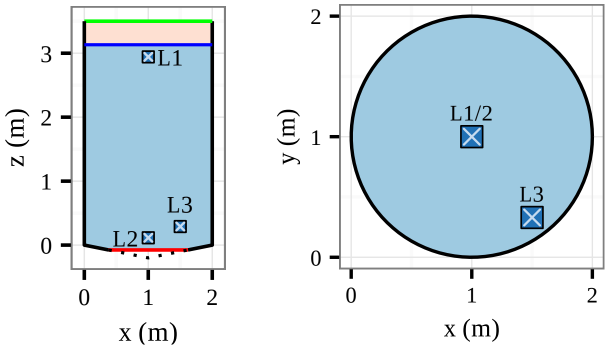
Passive scalar transport

$$\frac{\partial \alpha_l N}{\partial t} + \nabla \cdot (\alpha_l \vec{u}_l N) = \nabla \cdot (\alpha_l \Gamma_{\text{eff}} \nabla N) \quad (2)$$



Tracer dosage locations L1-L3 inside GK

Locations

- L1 top
- L2 bottom
- L3 racking port

Mixing scenarios

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#	Fermentation stage	CO_2 formation	Flow initialization
T1	peak fermentation	$1.0\,g\,L^{-1}\,h^{-1}$	120 s
T1r	peak fermentation	$1.0\,g\,L^{-1}\,h^{-1}$	300 s
T2	early fermentation	$0.1\,g\,L^{-1}\,h^{-1}$	120 s

Mixing scenarios

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Mixing time

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Definition

"the time in which the concentration of the tracer reaches within 95–98% of the final concentration" (Sahu et al., 1999)

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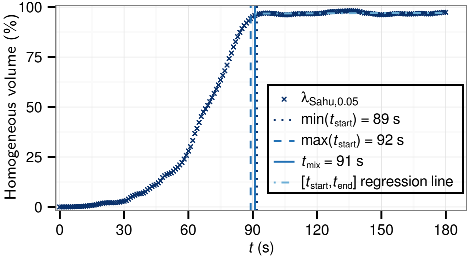
CFD adaption

- usually based on experimental measurements
  $\longrightarrow$ limited locations
- here: evaluation in each cell
  $\longrightarrow$ measuring total homogeneous volume
- t_{mix} at almost steady state

Example: T1 - GK - L1



Mixing simulation

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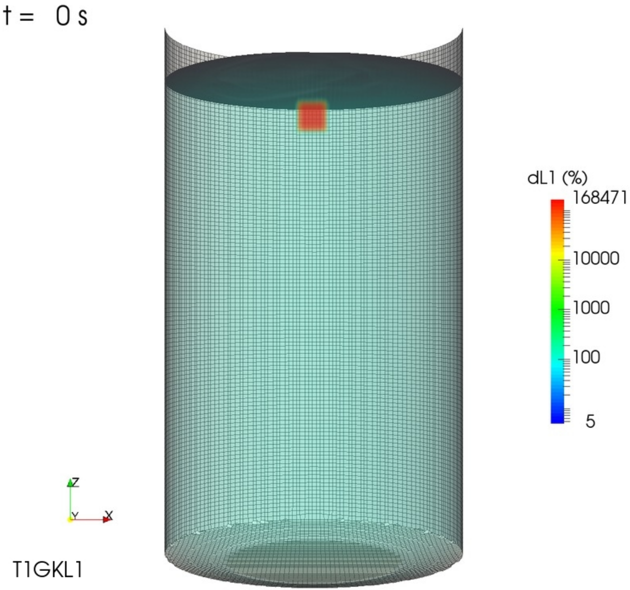

Mixing simulation

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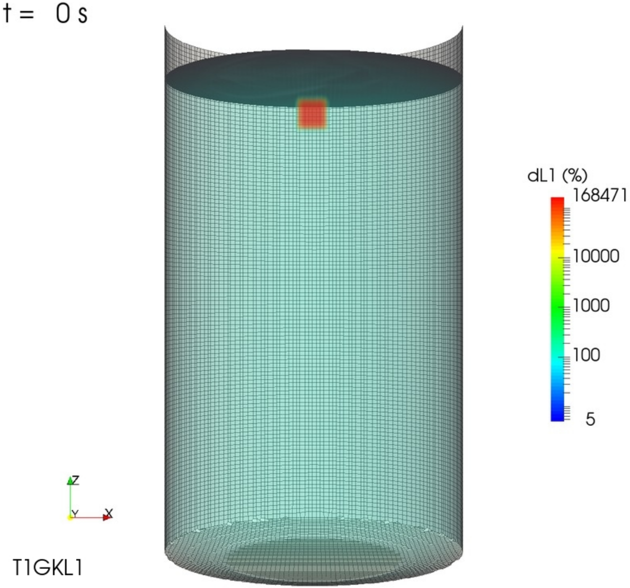

Results

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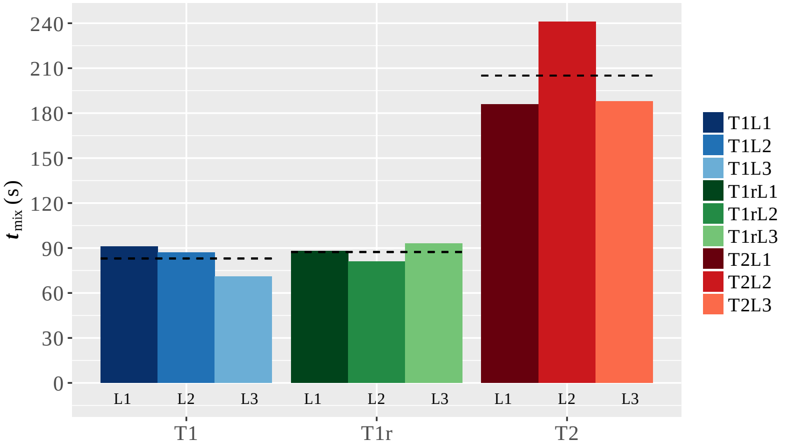

Comparison with empirical correlations

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Mixing time correlations for bubble columns

$$t_{m,\mathrm{Riet}} = 11\frac{H_T}{D_T}\left(g u_{gs} D_T^{-2}\right)^{-0.33} \tag{3}$$

(Van't Riet and Tramper, 1991)

$$t_{m,\mathrm{Sweere}} = \frac{H_T^2}{\mathbb{D}_z} \tag{4}$$

$$\mathbb{D}_z = 0.36(g D_T^4 u_{gs})^{\frac{1}{3}} \tag{5}$$

(Sweere et al., 1987)

D_T: tank diameter (2 m)

H_T: tank height (m), here: $H_T = \frac{V_T}{\pi R_T^2} \approx 3.14\,\mathrm{m}$ ($R_T = 1\,\mathrm{m}$)

u_{gs}: superficial gas velocity ($u_{gs} = \frac{\dot{V}_{g,\mathrm{inlet}}}{\pi R_T^2}$, $\mathrm{m\,s^{-1}}$)

V_T: tank volume ($10\,\mathrm{m^3}$)

g: gravitational acceleration ($9.81\,\mathrm{m\,s^{-2}}$)

$\mathbb{D}_z$: axial dispersion coefficient ($\mathrm{m^2\,s^{-1}}$)

Comparison with empirical correlations

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Simulations & correlations

#	u_{gs}	$\bar{t}_{mix}$	$t_{m,\text{Riet}}$	$t_{m,\text{Sweere}}$
T1	$4.8 \times 10^{-4}\,\text{m}\,\text{s}^{-1}$	83 s	158 s	65 s
T1r	$4.8 \times 10^{-4}\,\text{m}\,\text{s}^{-1}$	87 s	158 s	65 s
T2	$4.8 \times 10^{-5}\,\text{m}\,\text{s}^{-1}$	205 s	341 s	139 s
T2/T1		2.47/2.35	2.15	2.14

Summary: Mixing evaluation

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- repeatable average mixing time
- $\bar{t}_{mix,\mathbf{T2}} \approx 2 \times \bar{t}_{mix,\mathbf{T1}}$

≫ time scale of mixing should not affect yeast metabolism in phases of sufficient bubble formation

Outlook

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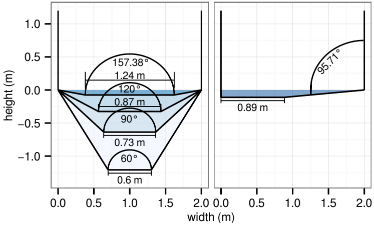
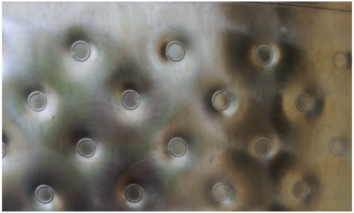
Mixing analysis

- different tank geometries
- inlet definition





Jacketed cooling

- temperature distribution
- optimal jacket dimensions

CFD Analysis of Nutrient Mixing during Wine Fermentation

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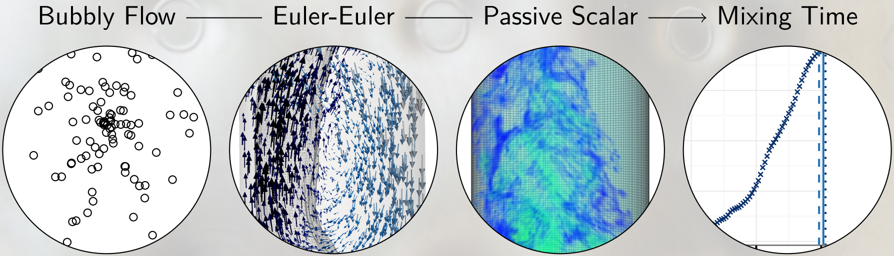

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Drag & Lift Coefficient

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Drag Coefficient

(Dijkhuizen et al., 2010; Lau et al., 2011; Roghair et al., 2013)

$$C_{\mathrm{D}} = Y_{\mathrm{swarm}} \sqrt{C_{\mathrm{D}}(\mathrm{Re_B})^2 + C_{\mathrm{D}}(\mathrm{Eo})^2} \tag{6}$$

$$C_{\mathrm{D}}(\mathrm{Re_B}) = \frac{16}{\mathrm{Re_B}} \cdot \left(1 + \frac{2}{1 + \frac{16}{\mathrm{Re_B}} + \frac{3.315}{\sqrt{\mathrm{Re_B}}}}\right) \tag{7}$$

$$C_{\mathrm{D}}(\mathrm{Eo}) = \frac{4\mathrm{Eo}}{\mathrm{Eo} + 9.5} \tag{8}$$

$$Y_{\mathrm{swarm}} = 1 + \left(\frac{22}{\mathrm{Eo} + 0.4}\right) \alpha_{\mathrm{g}} \tag{9}$$

Lift Coefficient

(Rastello et al., 2010)

$$C_{\mathrm{L}} = 0.5 + 4.0 \left(1 - \frac{6}{5\mathrm{Re_B}}\right) \exp\left(-\mathrm{Re_B}^{1/6}\right) \tag{10}$$