



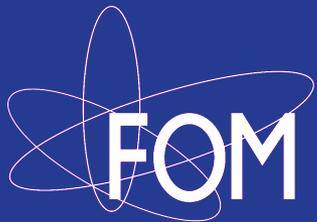
# University of Twente

Front Tracking simulations on liquid-liquid systems; an investigation of the drag force on droplets

Ivo Roghair, Wouter Dijkhuizen, Martin van Sint Annaland and Hans Kuipers

Fundamentals of Chemical Reaction Engineering

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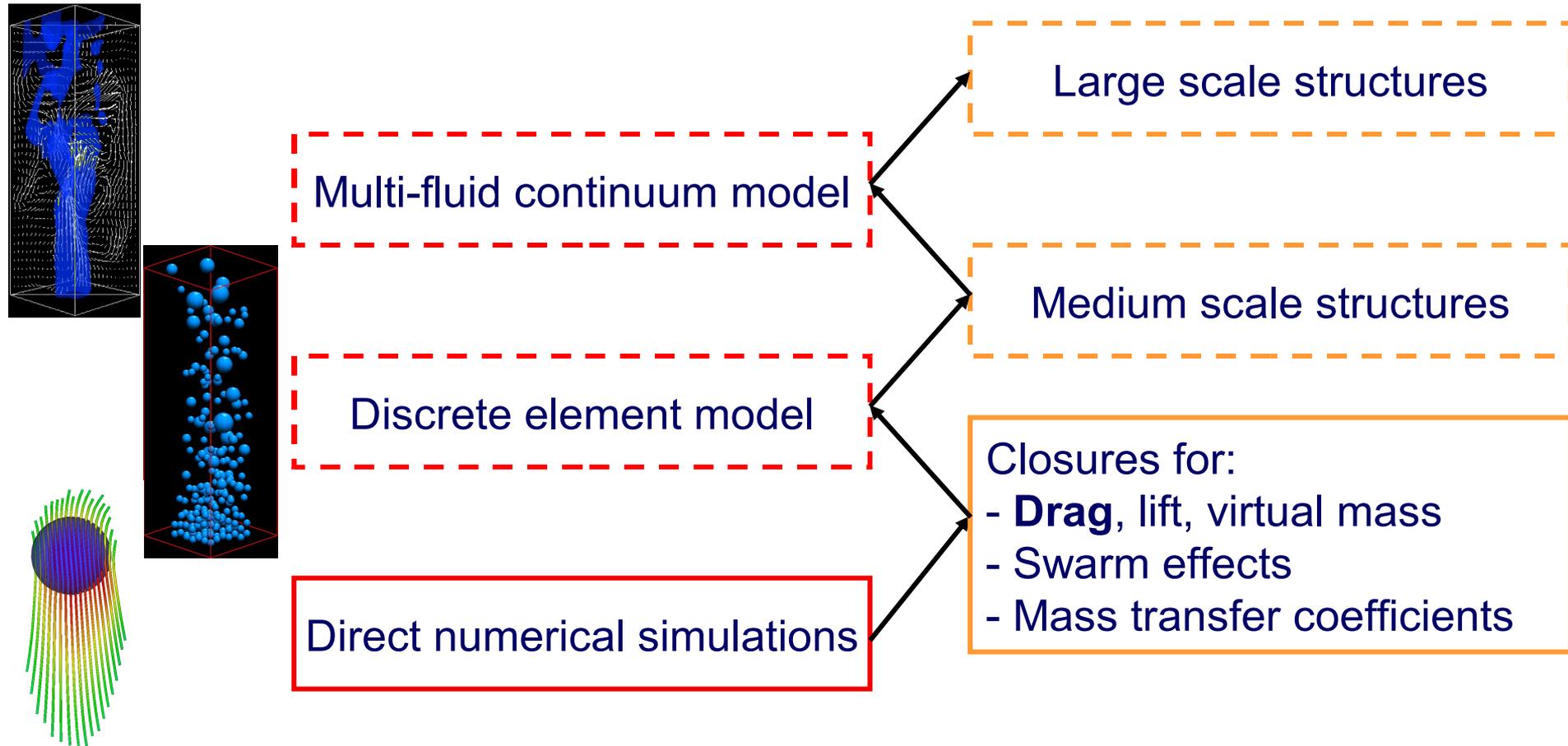


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- Introduction
- Objectives
- Numerical simulations
  - Grid dependency study
  - Drag force study
- Conclusions and outlook

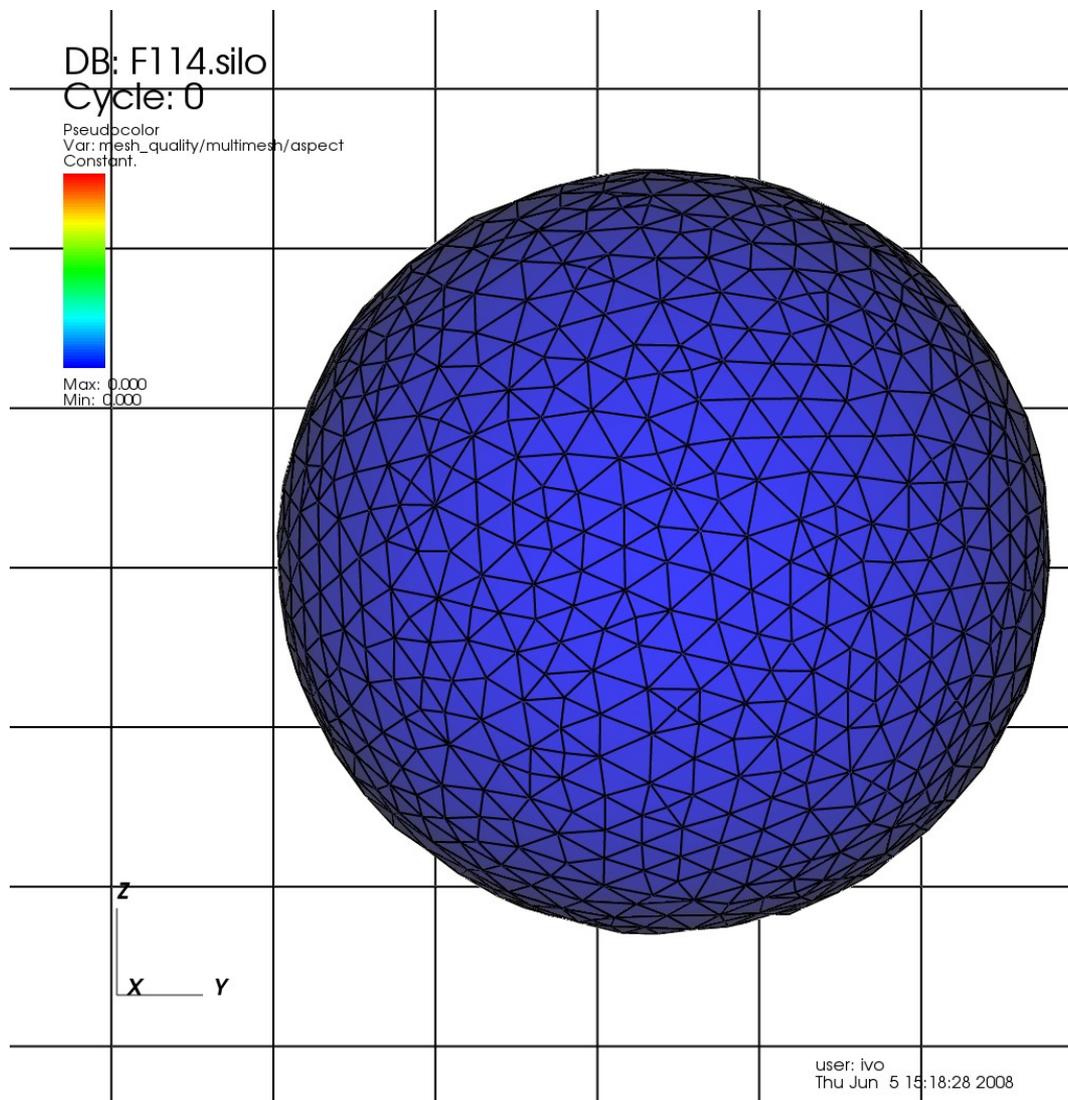
## Multi-level modelling strategy for multiphase flow



## Direct Numerical Simulations (DNS)

- Fully resolved
  - Based only on fundamental equations for fluid flow
    - Navier-Stokes + continuity equation for incompressible flow
  - Can be used to derive closures for forces on
    - Bubbles
    - **Droplets**
    - Particles
- Only valid when grid independence can be shown!

- Incompressible fluids
- Fixed Eulerian grid
- Interface consists of Lagrangian marker points that build up a triangular mesh
  - Points are moved with the interpolated fluid flow
  - Straightforward surface tension force calculation
- Advantages
  - Calculation of surface tension force with sub-grid accuracy.
  - No numerical coalescence of dispersed phase elements



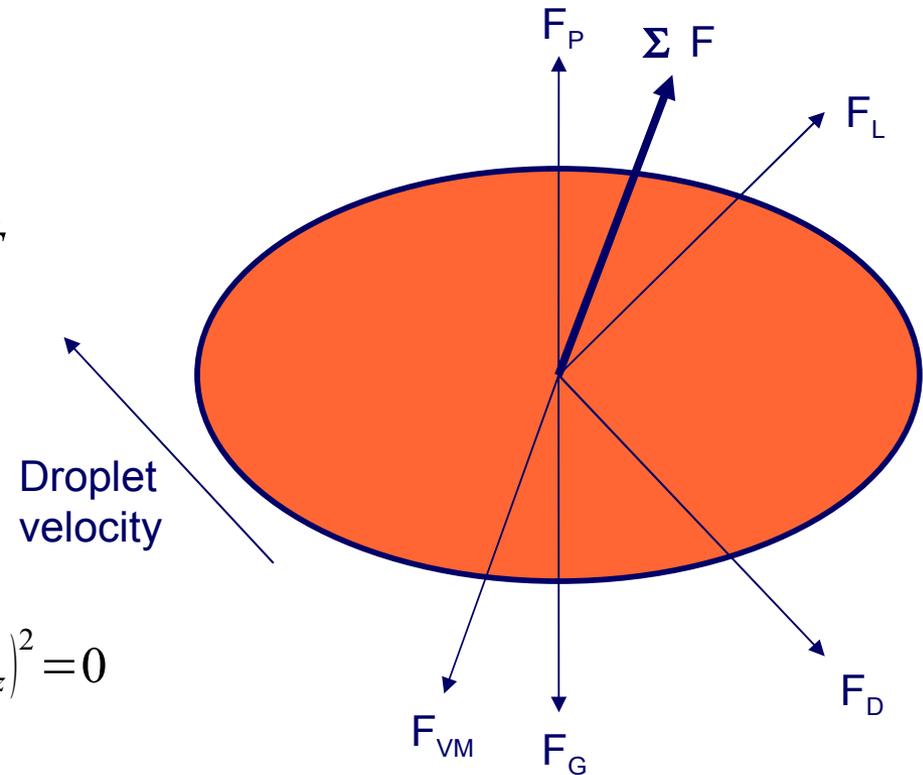
## Forces acting on a droplet

$$m_b \frac{d\vec{v}_b}{dt} = \vec{F}_G + \vec{F}_P + \vec{F}_D + \vec{F}_L + \vec{F}_{VM} = \sum \vec{F}$$

## Stationary force balance in the rise direction

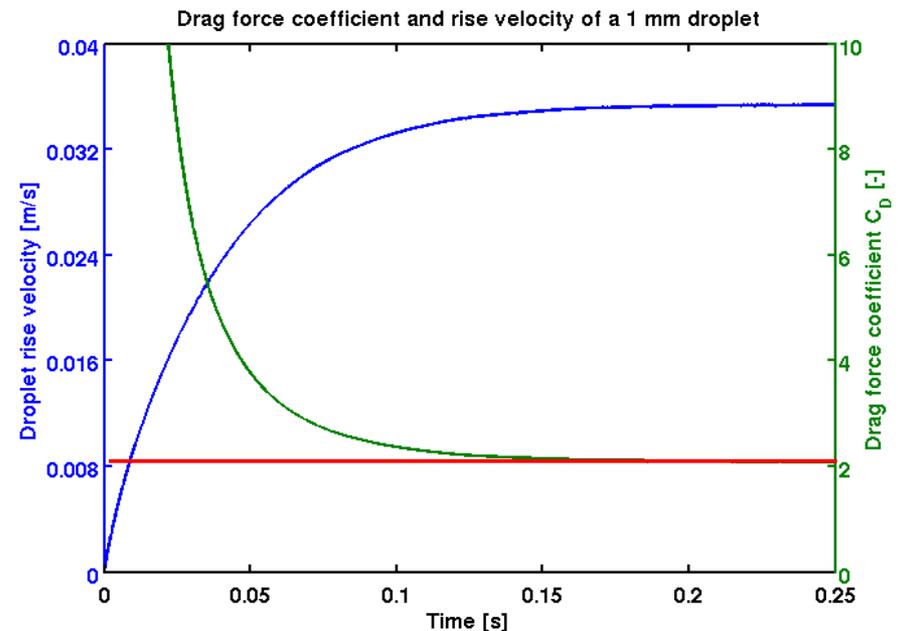
$$(\rho_c - \rho_d) g \frac{\pi}{6} d_{eq}^3 - \frac{1}{2} C_D \rho_c \frac{\pi}{4} d_{eq}^2 (u_{d,z}^{\vec{}} - u_{c,z}^{\vec{}})^2 = 0$$

$$C_D = \frac{4(\rho_c - \rho_d) g d_{eq}}{3 \rho_c (u_{d,z}^{\vec{}} - u_{c,z}^{\vec{}})}$$



- Determine drag force coefficient by different averaging procedures
  - Average rise velocity, then determine  $C_D$
  - Determine  $C_D$  as a function of time, average this value

→ No difference



## Correlations from literature (bubbly flow)

- Rigid sphere:

$$C_D = \frac{24}{Re}$$

- Mei et al. (1994):

$$C_D = \frac{16}{Re} \left( 1 + \frac{2}{1 + \frac{16}{Re} + \frac{3.315}{Re^{0.5}}} \right)$$

- Tomiyama (1998):

- Pure

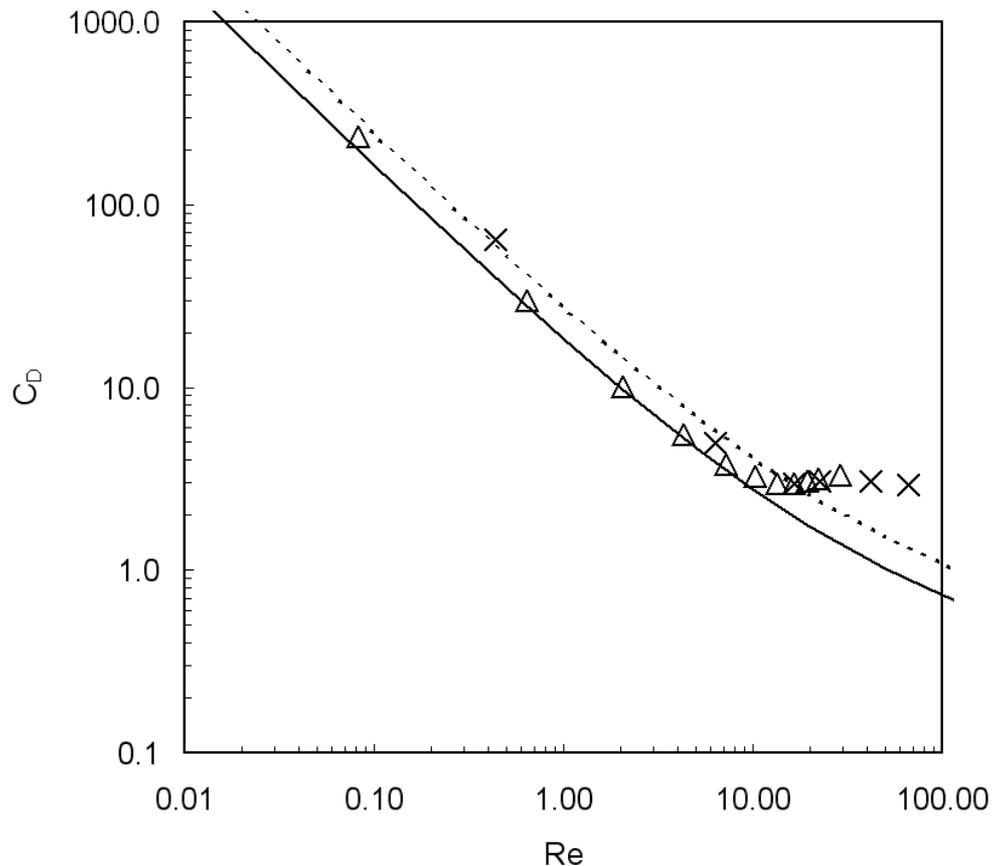
$$C_D = \max \left[ \min \left[ \frac{16}{Re} (1 + 0.15 Re^{0.687}), \frac{48}{Re} \right], \frac{8}{3} \frac{Eo}{Eo + 4} \right]$$

- Contaminated

$$C_D = \max \left[ \frac{24}{Re} (1 + 0.15 Re^{0.687}), \frac{8}{3} \frac{Eo}{Eo + 4} \right]$$

$$Re = \frac{\rho_c \vec{u}_d d_{eq}}{\mu_c} \quad Eo = \frac{(\rho_c - \rho_d) g d_{eq}^2}{\sigma}$$

- Experiments and simulations on drag force for bubbly flow



From:  
Wouter Dijkhuizen, PhD thesis,  
University of Twente, 2008

- Investigate the behavior of the Front Tracking model for liquid-liquid systems
- Simulate droplets in an infinite quiescent liquid to derive drag force closures
- Investigate the relation between gas-liquid and liquid-liquid drag force and their dependencies

- Vary resolution in droplet, domain 5 times droplet size
- Vary resolution in droplet, keep domain at  $100^3$  cells
- Keep resolution in droplet at 20 cells, vary domain size

## Simulation parameters:

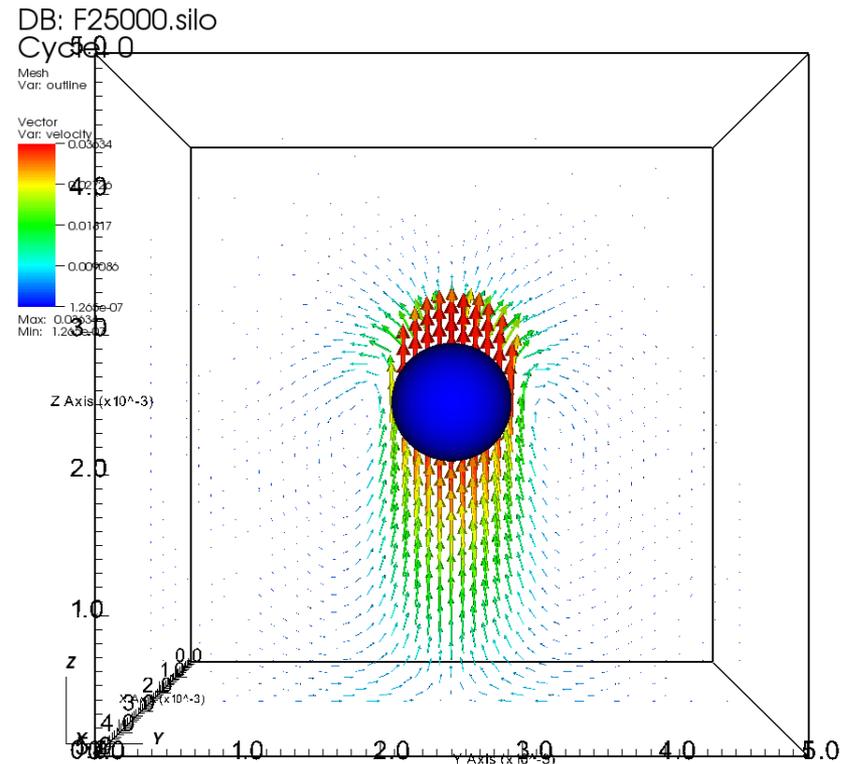
$$\rho_c = 1000 \text{ kg/m}^3, \quad \mu_c = 10^{-3} \text{ Pa}\cdot\text{s}$$

$$\rho_d = 800 \text{ kg/m}^3, \quad \mu_d = 10^{-1} \text{ Pa}\cdot\text{s}$$

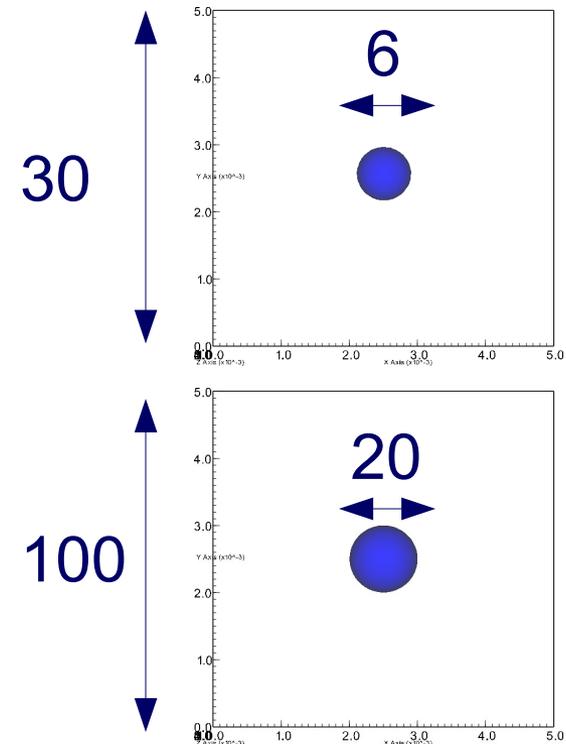
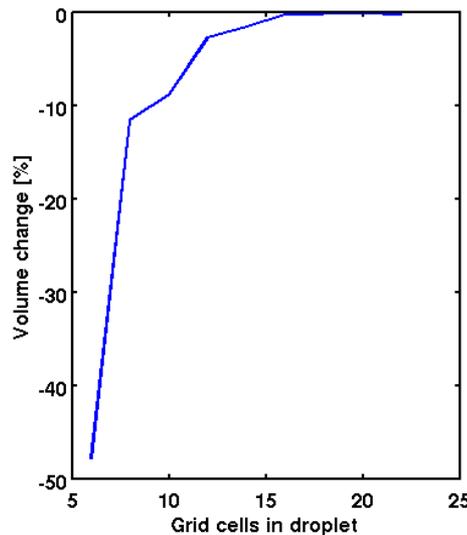
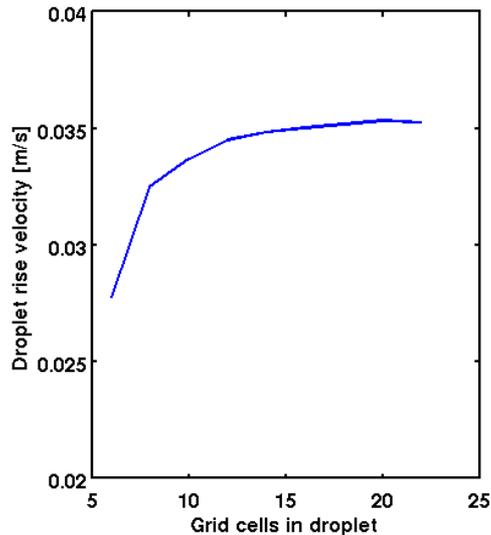
$$\sigma = 52.9 \text{ mN/m}, \quad d_{eq} = 1 \text{ mm}$$

$$t_{end} = 1 \text{ s}$$

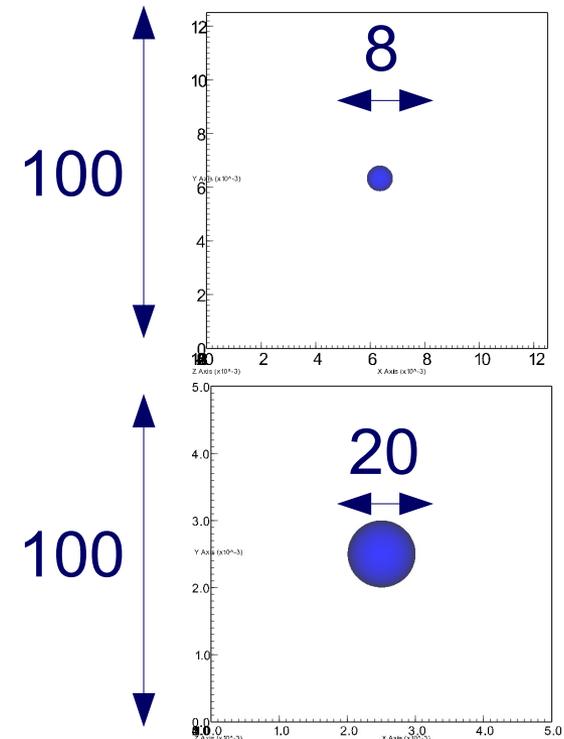
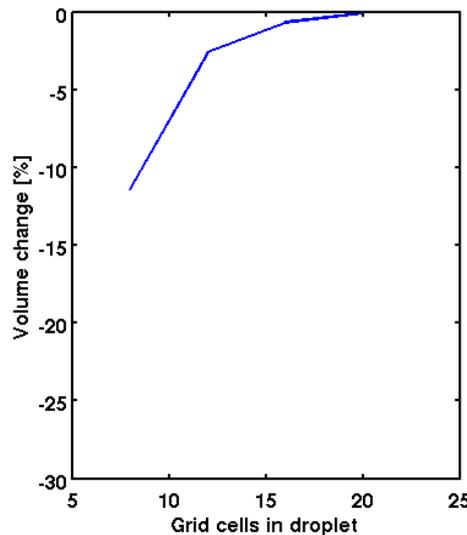
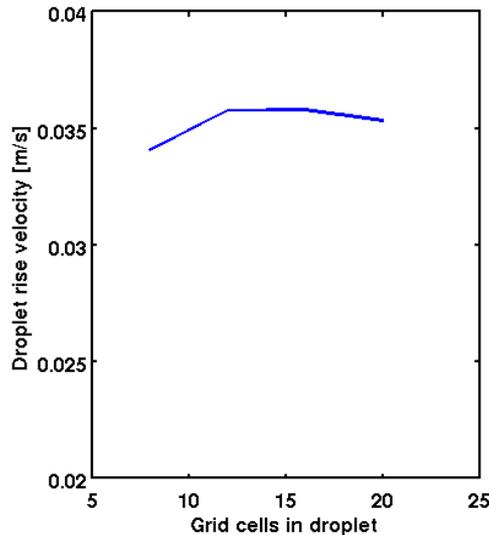
$$dt = 10^{-5} \text{ s}$$



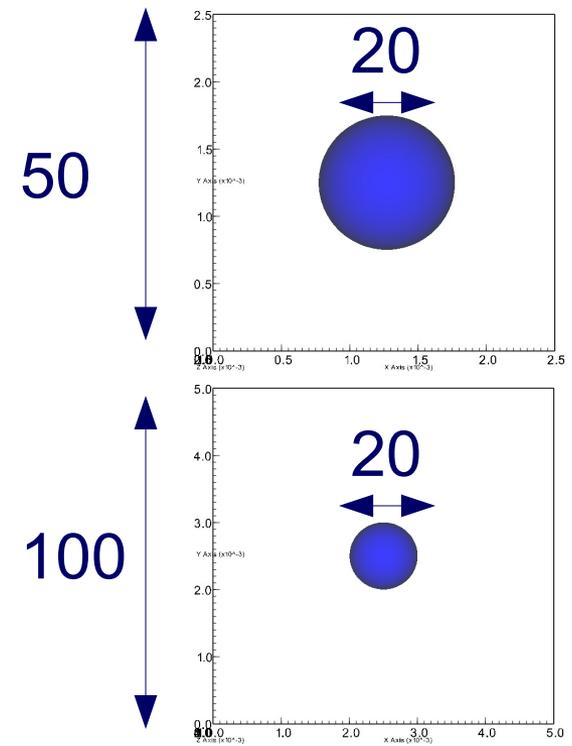
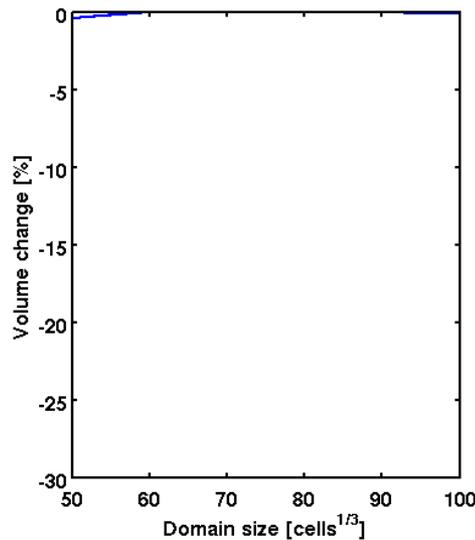
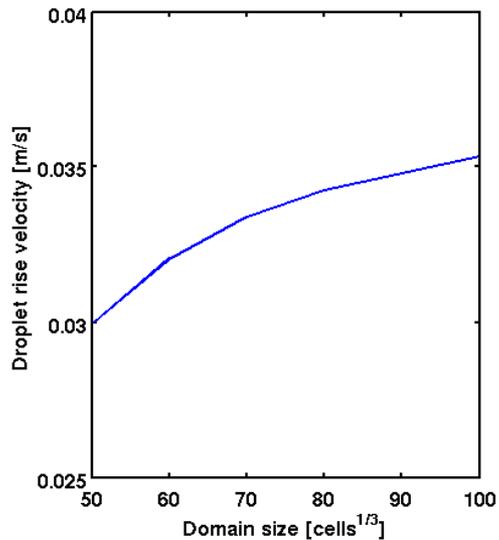
- Vary resolution in droplet, domain 5 times droplet size
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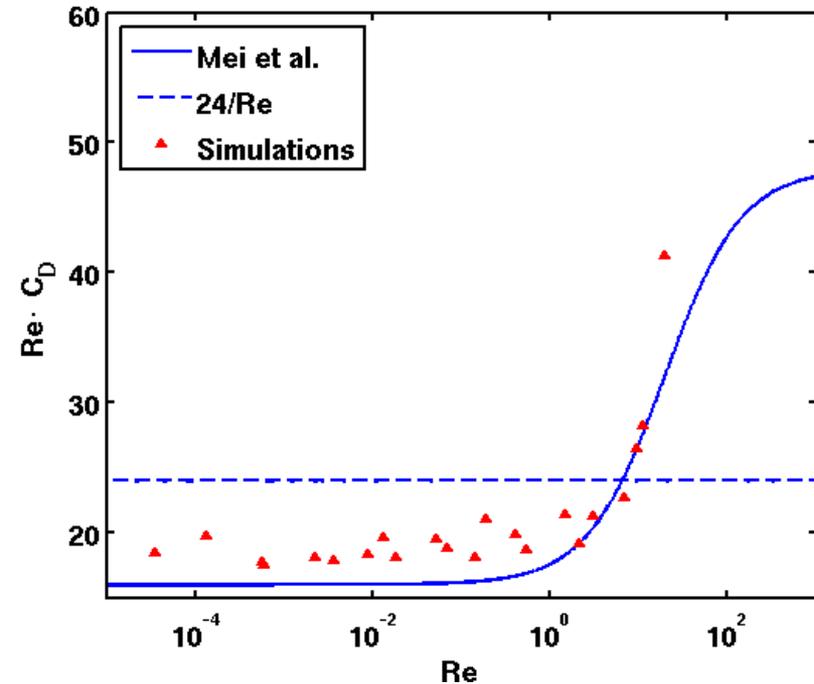
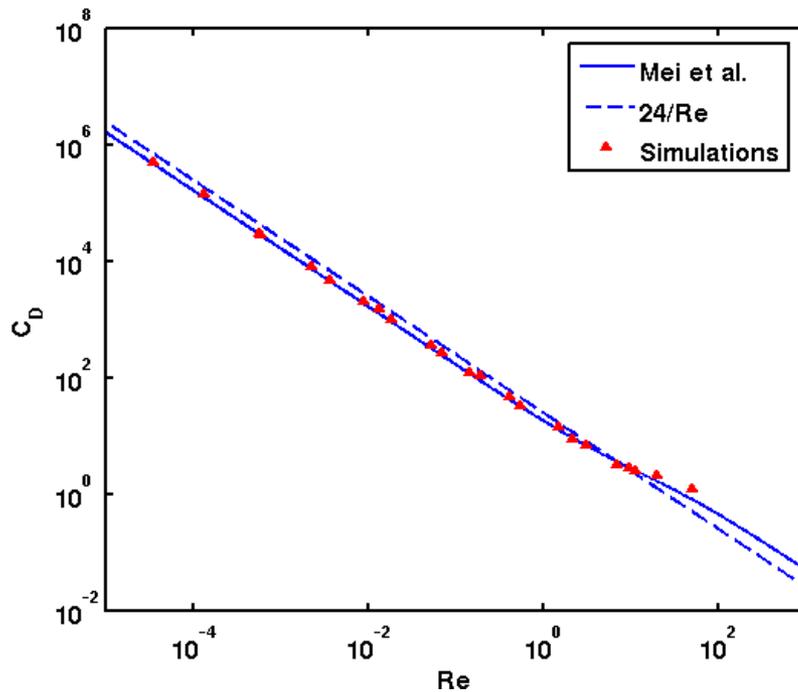


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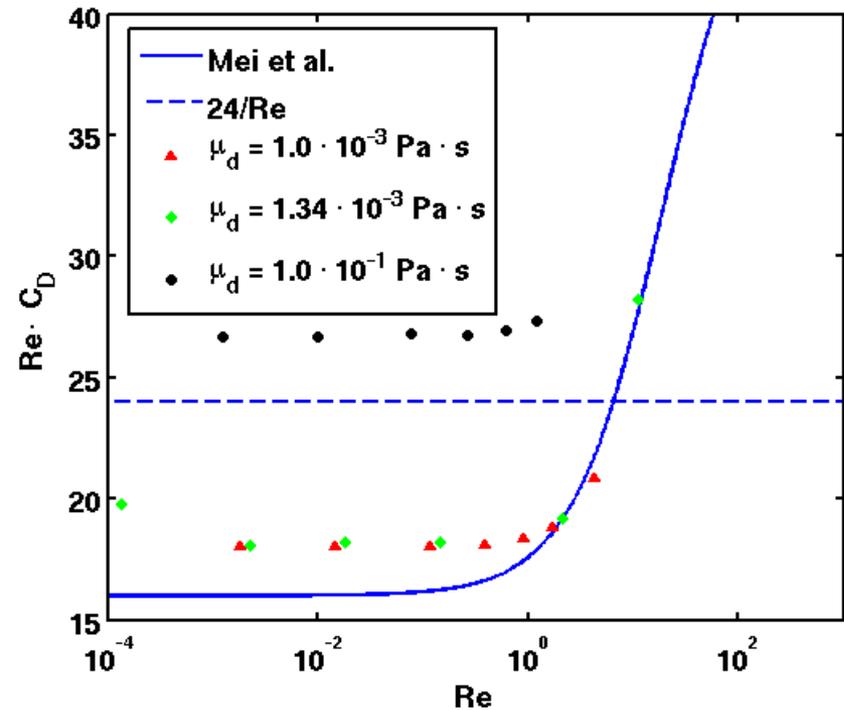
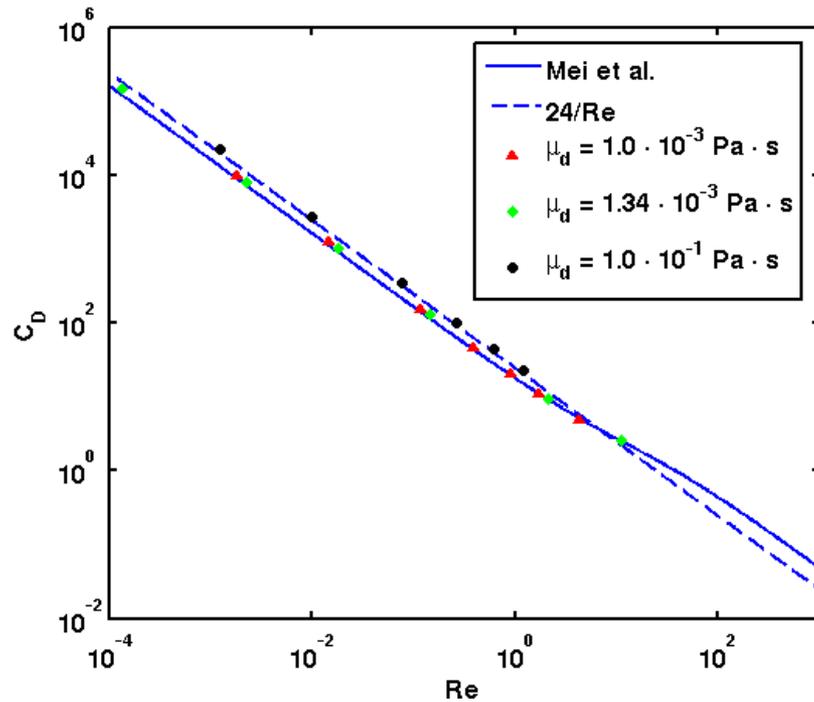
- Used settings:
  - 20 grid cells in droplet diameter
  - $100^3$  grid cells in domain
- Variation of continuous phase viscosity between 0.001 - 0.2 Pa·s
- Variation of equivalent droplet diameter between 0.2 – 5 mm
- “Dodecane droplet in water” system:
  - $\rho_c = 1000 \text{ kg/m}^3$ ;
  - $\rho_d = 746 \text{ kg/m}^3$ ;      $\mu_d = 1.34 \cdot 10^{-3} \text{ Pa}\cdot\text{s}$
  - $\sigma = 0.0529 \text{ N/m}$ ;

- Variation of continuous phase viscosity



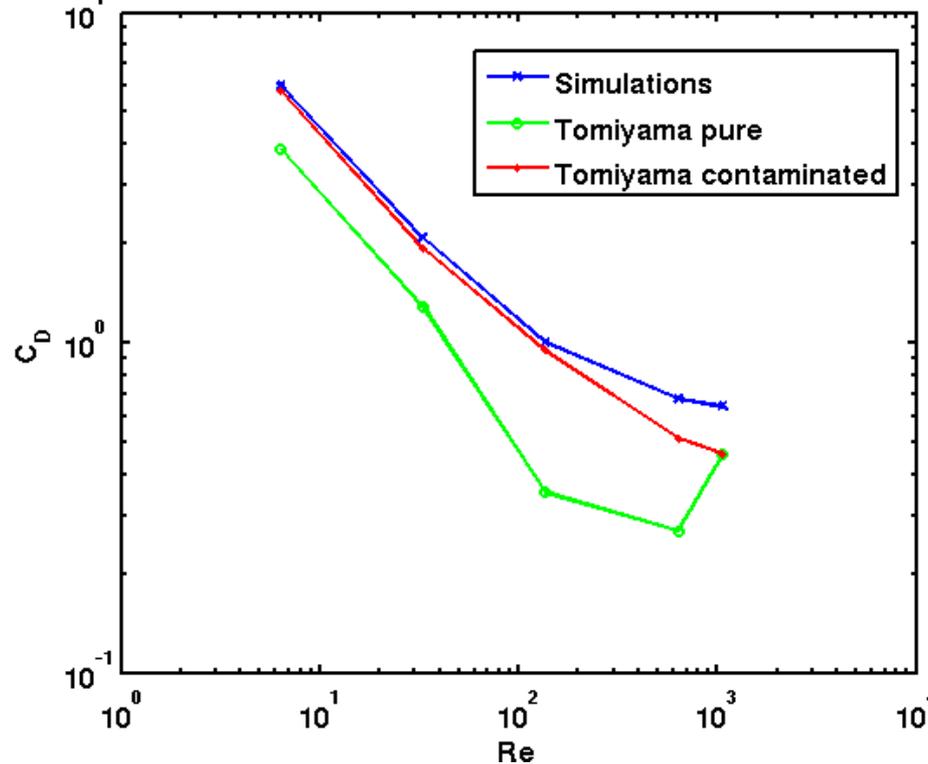
- Variation of dispersed phase viscosity between  $10^{-3}$  –  $10^{-1}$  Pa·s
- Variation of equivalent droplet diameter between 0.2 – 7 mm
- Physical properties
  - $\rho_c = 1000$  kg/m<sup>3</sup>;  $\mu_c = 10^{-1}$  Pa·s
  - $\rho_d = 800$  kg/m<sup>3</sup>;
  - $\sigma = 0.0529$  N/m;

- Variation of dispersed phase viscosity



- Due to volume losses more detailed simulations:
  - Computational grid  $150^3$  cells
  - 30 cells within droplet diameter
  - Higher surface tension

Drag force coefficient compared to Tomiyama correlations (high Re)



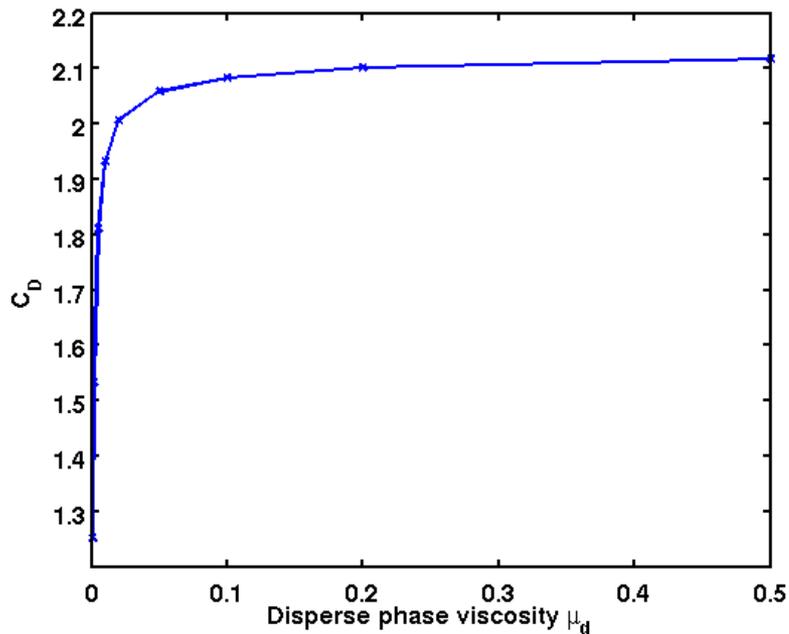
Simulation parameters:

$$\rho_c = 1000 \text{ kg/m}^3; \quad \mu_c = 10^{-3} \text{ Pa}\cdot\text{s}$$

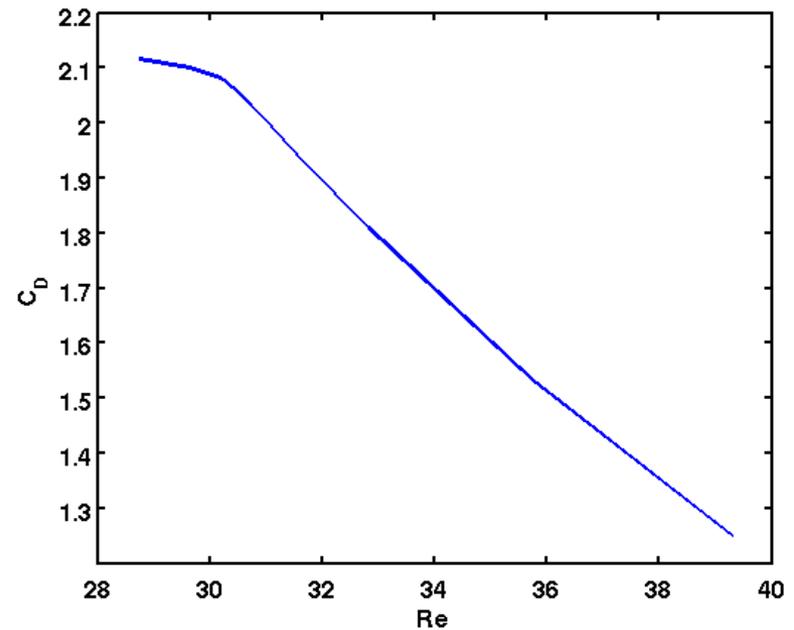
$$\rho_d = 800 \text{ kg/m}^3; \quad \mu_d = 10^{-1} \text{ Pa}\cdot\text{s}$$

$$\sigma = 0.1 \text{ N/m}; \quad d_{eq} = 0.5 - 7 \text{ mm}$$

Drag force for different  $\mu_d$  of a 1 mm droplet in water



Variation of  $C_D$  at different  $\mu_d$



Simulation parameters:

$$\rho_c = 1000 \text{ kg/m}^3; \quad \mu_c = 10^{-3} \text{ Pa}\cdot\text{s}$$

$$\rho_d = 800 \text{ kg/m}^3; \quad \mu_d = 10^{-3} - 0.5 \text{ Pa}\cdot\text{s}$$

$$\sigma = 0.1 \text{ N/m}; \quad d_{eq} = 1 \text{ mm}$$

- Front tracking model can simulate dispersed liquid phases but a high resolution is required
- Volume loss strongly depending on droplet resolution
- Correlations of Mei et al. and Tomiyama for bubbly flow are well predicted
  - Some overshoot due to wall effects
- Transition of free-slip to no-slip condition as a function of  $\mu_d$  shown
- Outlook:
  - Eo dependence of drag force coefficient
  - Droplet and bubble swarms

Thank you for your attention

Surface tension is mapped from the interface mesh to the Eulerian grid.

$$\vec{F}_a = \sigma (\vec{t}_{m,a} \times \vec{n}_a)$$

$$\vec{F}_b = \sigma (\vec{t}_{m,b} \times \vec{n}_b)$$

$$\vec{F}_c = \sigma (\vec{t}_{m,c} \times \vec{n}_c)$$

