Numerical Simulation Campaign on Droplet Rebound from Hydrophobic Surface

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Outline

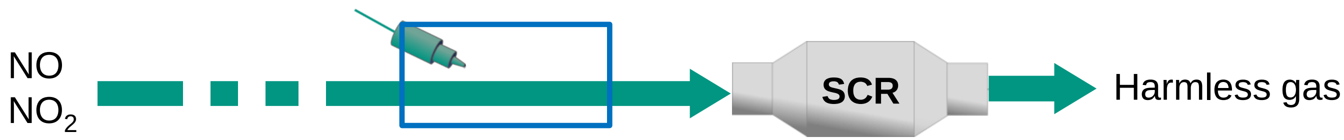
- Introduction and motivation
- Numerical method and validation for droplet rebound
- AdBlue® Droplet rebound regimes for operating parameters
- Summary and Outlooks

Introduction

- Project background: Selective Catalytic Reduction (SCR) system for exhaust gas after-treatment in diesel engine

Injection of urea $(NH_2)_2CO$ water solution (**AdBlue®**)

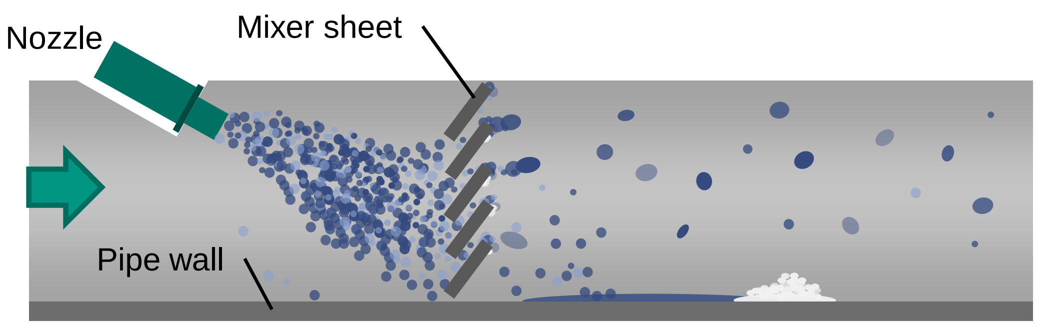
Diesel engine
Source: BMW

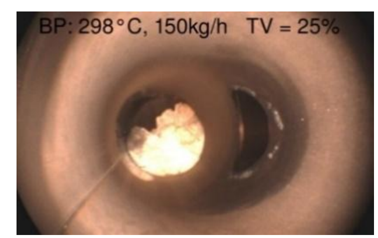


$(NH_2)_2CO$ (l) $\Rightarrow$ NH_3 (g) + HNCO (g)

HNCO (g) + H_2O (g) $\Rightarrow$ NH_3 (g) + CO_2 (g)

2 NH_3 + NO + NO_2 $\rightarrow$ 2 N_2 + 3 H_2O



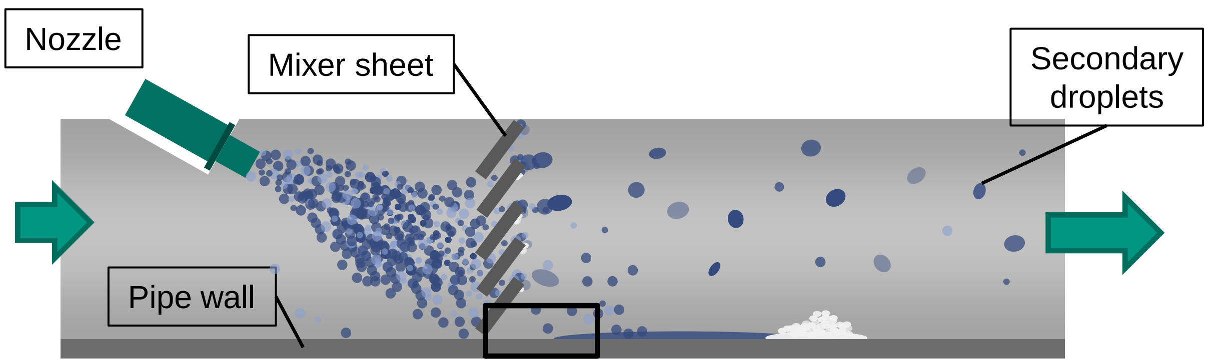


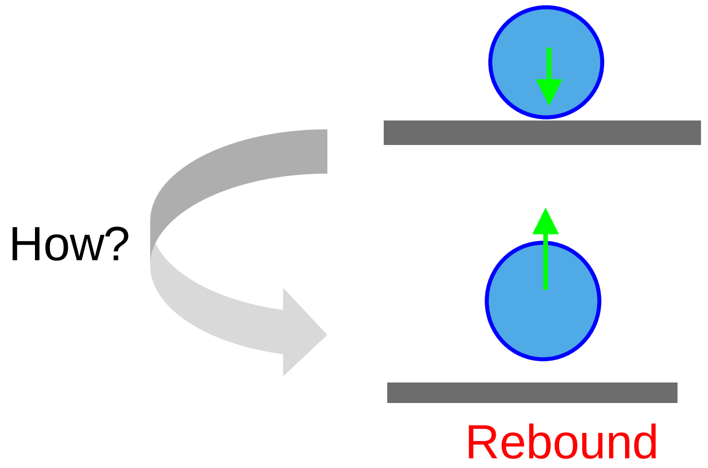
Pipe blockage by solid deposits in engine test bench (Brack 2014)

- Liquid film formation and solid deposit formation

Motivation

- **Numerical simulation of droplet impact and film formation on wall**





Phase-Field Method (PFM)

- Order parameter (C) as phase indictor
  - Smooth transition from -1 to 1 → **diffuse interface**
  - Its thickness characterized by capillary width ε
- C evolution governed by Cahn-Hilliard equation

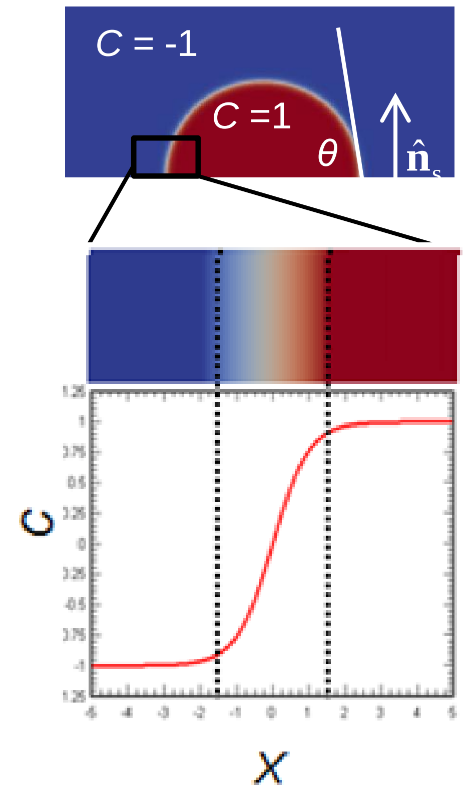
$$\frac{\partial C}{\partial t} + (\mathbf{u}\cdot\nabla)C = \kappa\nabla^2\phi(C) \qquad \phi = \frac{\lambda}{\varepsilon^2}C(C^2-1) - \lambda\nabla^2 C$$

describes motion of contact line!

  - Φ = chemical potential [J/m^3]
  - λ = mixing energy [J/m]
  - κ = mobility [m^{3}s/kg]

- Wetting boundary condition for static contact angle θ

$$\hat{\mathbf{n}}_s \cdot \nabla C = \frac{\sqrt{2}}{2}\frac{\cos\theta}{\varepsilon}(1-C^2)$$



$$C = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right)$$

D. Jacqmin, *J. Comput. Phys.* **1999**, 155: 96-127.

PFM Coupled with Navier-Stokes Equations

Karlsruhe Institute of Technology

- Singe-field Navier-Stokes equation for incompressible Newtonian fluids

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial(\rho_C \mathbf{u})}{\partial t} + \nabla \cdot (\rho_C \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu_C \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathsf{T}} \right) \right] + \mathbf{f}_\sigma + \rho_C \mathbf{g}$$

therein $\rho_C = \frac{1+C}{2}\rho_{\mathsf{L}} + \frac{1-C}{2}\rho_{\mathsf{G}}, \quad \mu_C = \frac{1+C}{2}\mu_{\mathsf{L}} + \frac{1-C}{2}\mu_{\mathsf{G}}, \quad \mathbf{f}_\sigma = -C\nabla\phi$

- The method was implemented in the open-source CFD code OpenFOAM (H. Marschall and X. Cai)
  - A novel top-level solver *phaseFieldFoam*
  - Within foam-extend-1.6 and foam-extend-4.0
  - Validated for droplet wetting phenomena

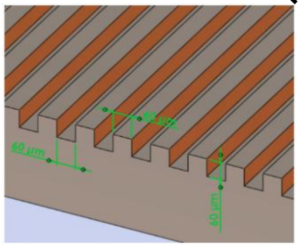
- Phase-field specific parameters:
  - Cahn number ***Cn*** = ***ε*** / *L* = 0.02 (*L* reference length scale, e.g. droplet diameter)
  - Number of cell for diffuse interface ***Nc*** = 6
  - Mobility ***M*** = O(ε^2)

D. Jacqmin, *J. Comput. Phys.* **1999**, 155: 96-127.

X. Cai, H. Marschall, M. Wörner and O. Deutschmann, *Chem. Eng. Technol.* **2015**, 38: 1985–1992

Rebound on micro-structured surface

- Micro-structure → super-hydrophobicity → rebound
- **Experiment** of water droplet impacting (D_0=2.1 mm, U_0=0.61 m/s) on smooth & micro-structured PDMS (for smooth surface, equilibrium contact angle ≈ 100°)



micro-grooved structures
characteristic dimension
s = 60 µm

📖 V. Fink, X. Cai, A. Stroh, R. Bernard, J. Kriegseis, B.Frohnapfel, H. Marschall, M. Wörner, Intl. Journal of Heat & Fluid Flow (Accepted)

Rebound on micro-structured surface

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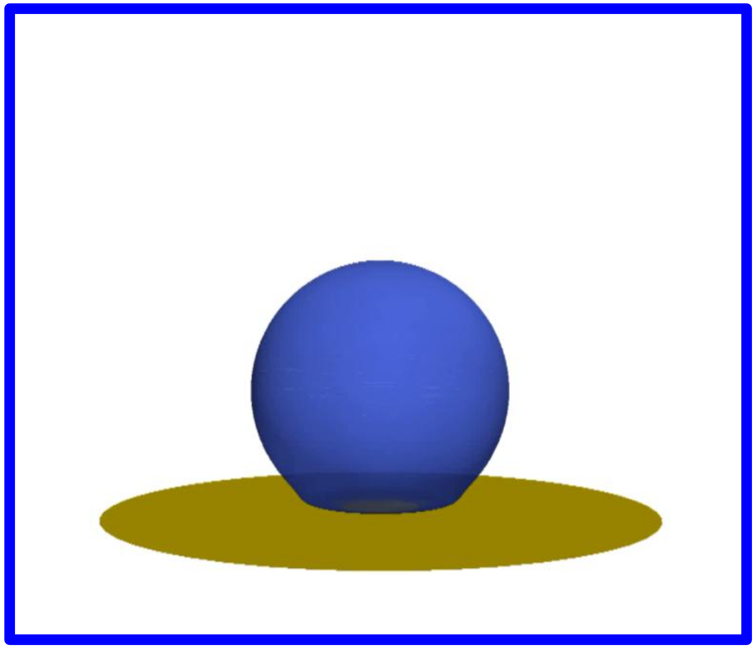
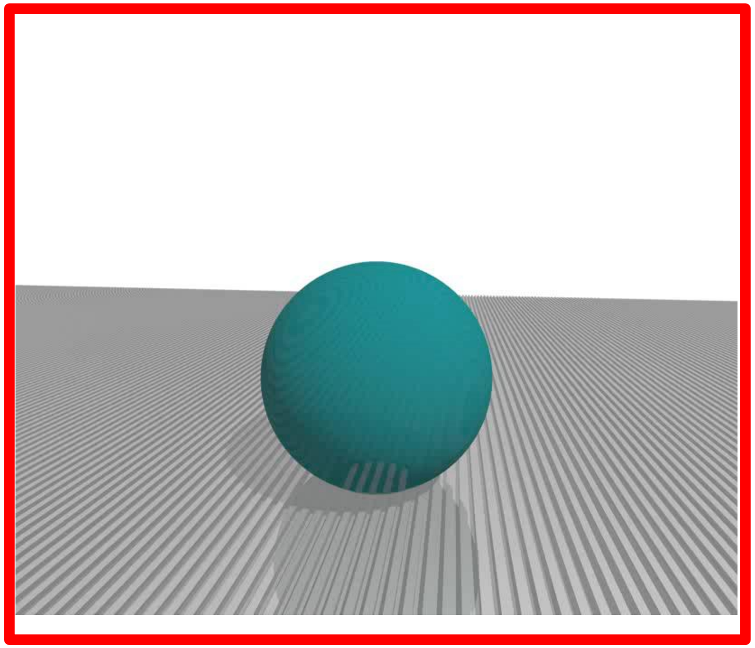


2D Axisymmetric Simulation for smooth surface



3D Simulation for micro-structured surface

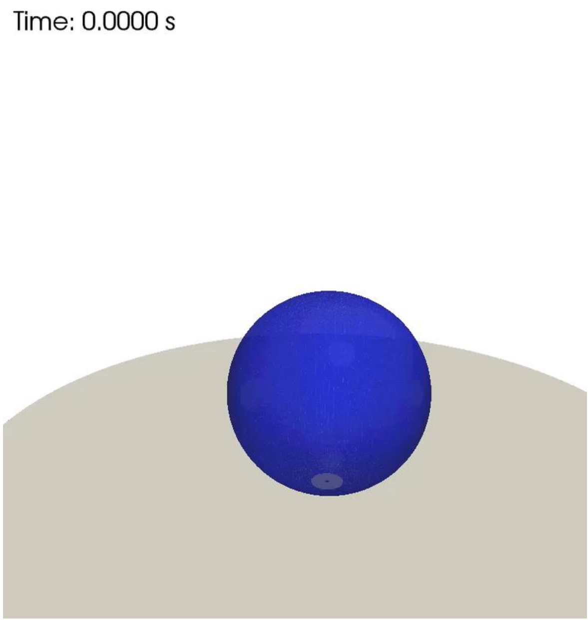
18 million cells and 800,000 CPU hours!

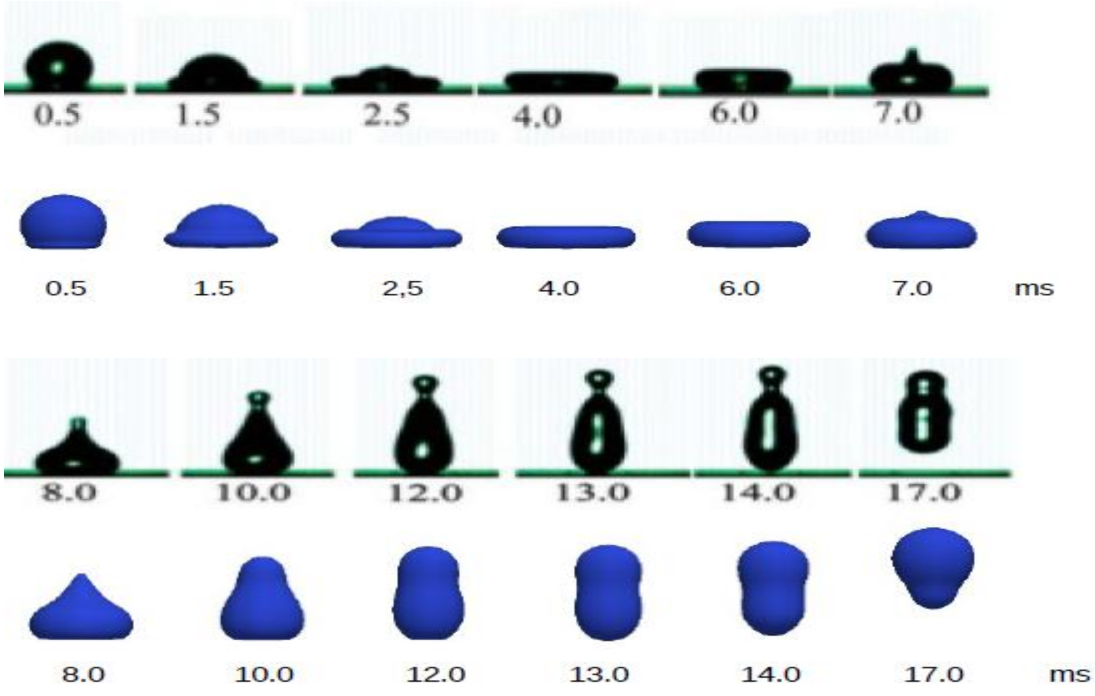
V. Fink, X. Cai, A. Stroh, R. Bernard, J. Kriegseis, B.Frohnapfel, H. Marschall, M. Wörner, Intl. Journal of Heat & Fluid Flow (Accepted)

Rebound on smooth surface

- **Very large contact angle θ** → super-hydrophobicity → rebound
- Validation against experiment Zang et al. (2013), θ = 163°
- Droplet impacts with D_0=2.1 mm, U_0=0.61 m/s

2D Axisymmetric Simulation
10,000 cells and 4 CPU hours





Zang et al. *Soft Matter* **2013**, 9(2): 394-400

Rebound on smooth surface

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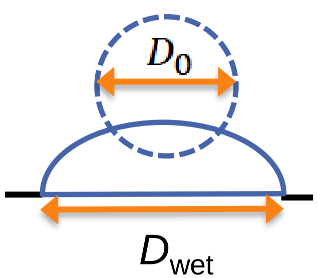
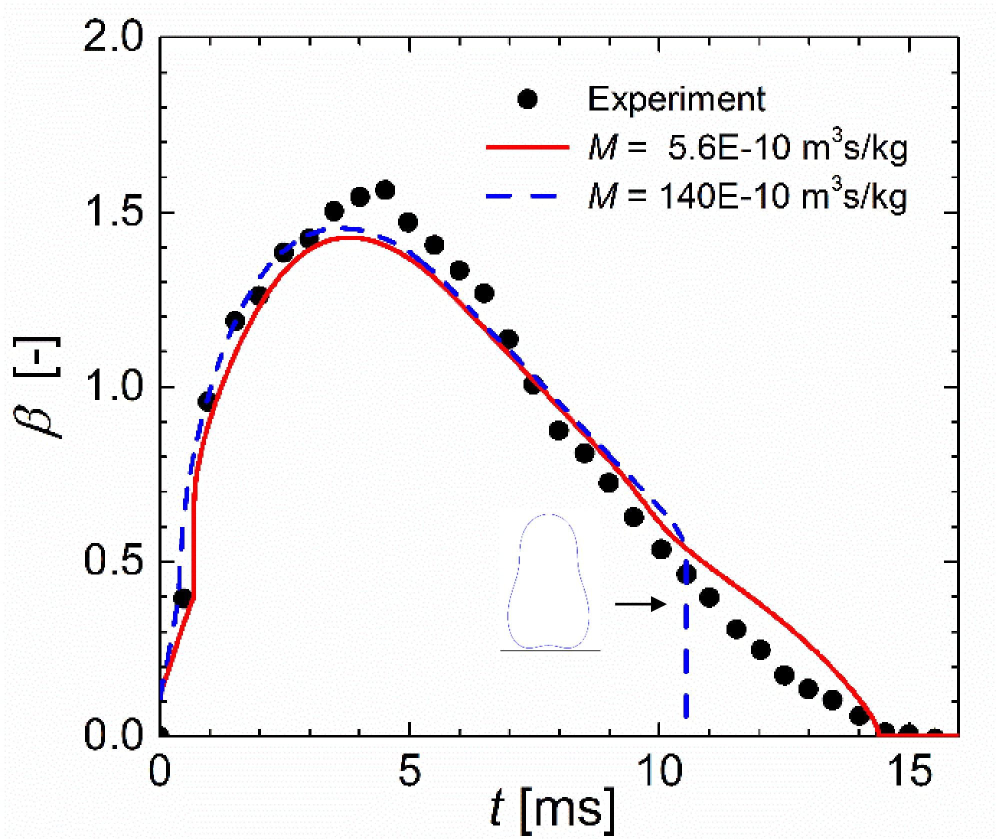
- Validation against experiment Zang et al. (2013), $\theta = 163°$

Spread factor:

$\beta = D_{wet} / D_0$

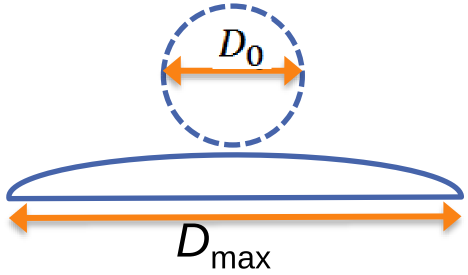




📖 Zang et al. *Soft Matter* **2013**, 9(2): 394-400

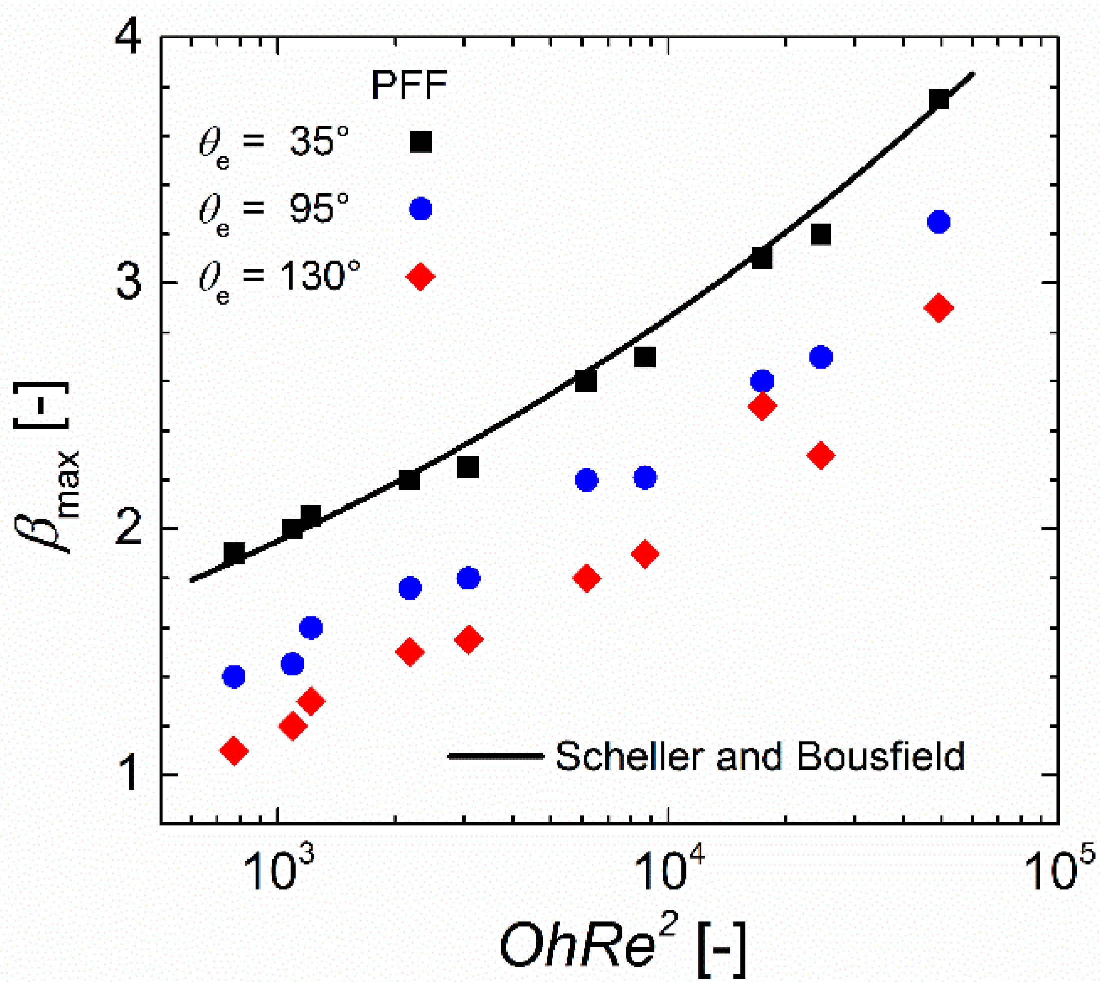
Maximal spread factor

$\beta_{max} = D_{max} / D_0$



$$Re = \frac{\rho U D}{\mu} \qquad Oh = \frac{\mu}{\sqrt{\rho \sigma D}}$$

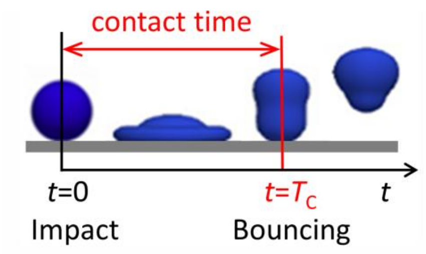
In Phase-Field Simulation (PFF):
0.05 mm < D_0 < 0.8 mm
5 m/s < U_0 < 10 m/s

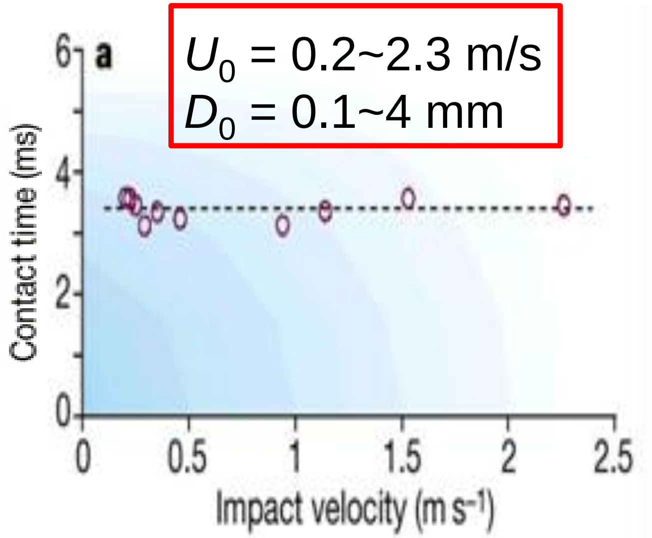


Scheller et al. *AIChE Journal* **1995** 41: 1357-1367.

Contact time

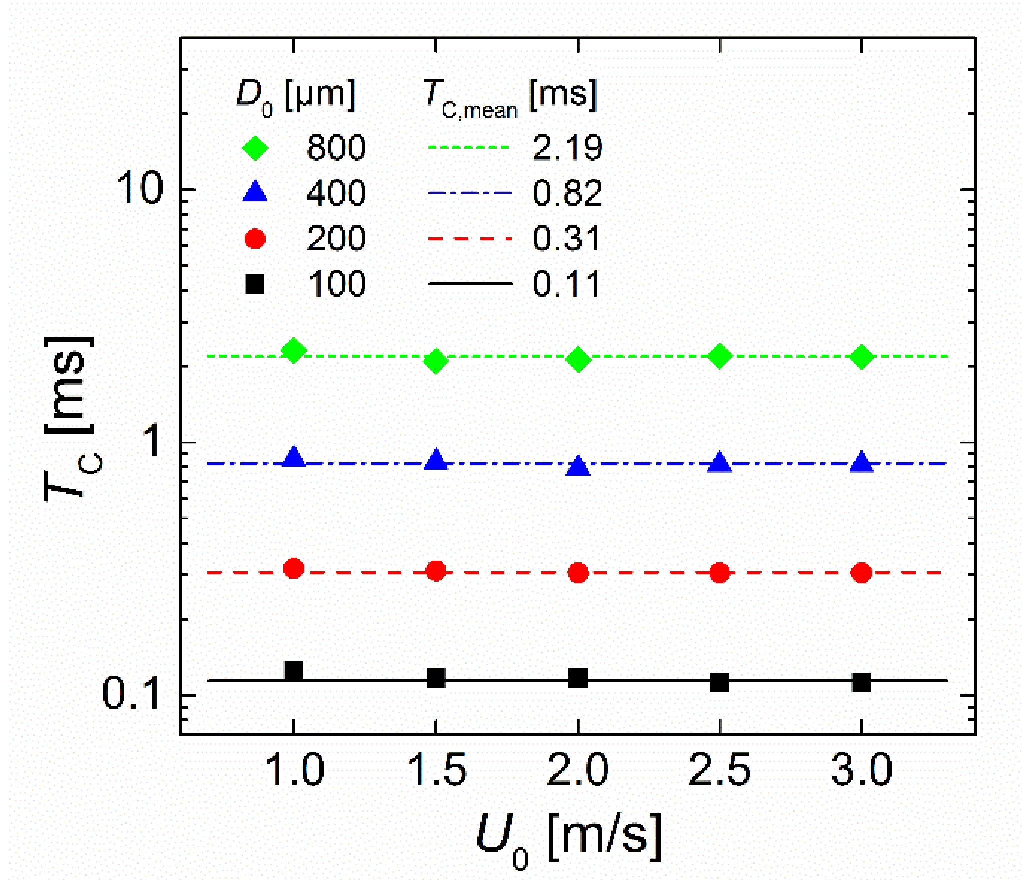
- Richard et al. (2002) found contact time does not depend on impact velocity





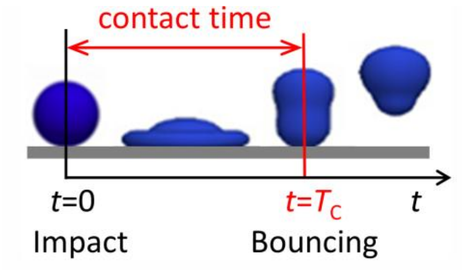
(source: Richard et al.)

θ=170º



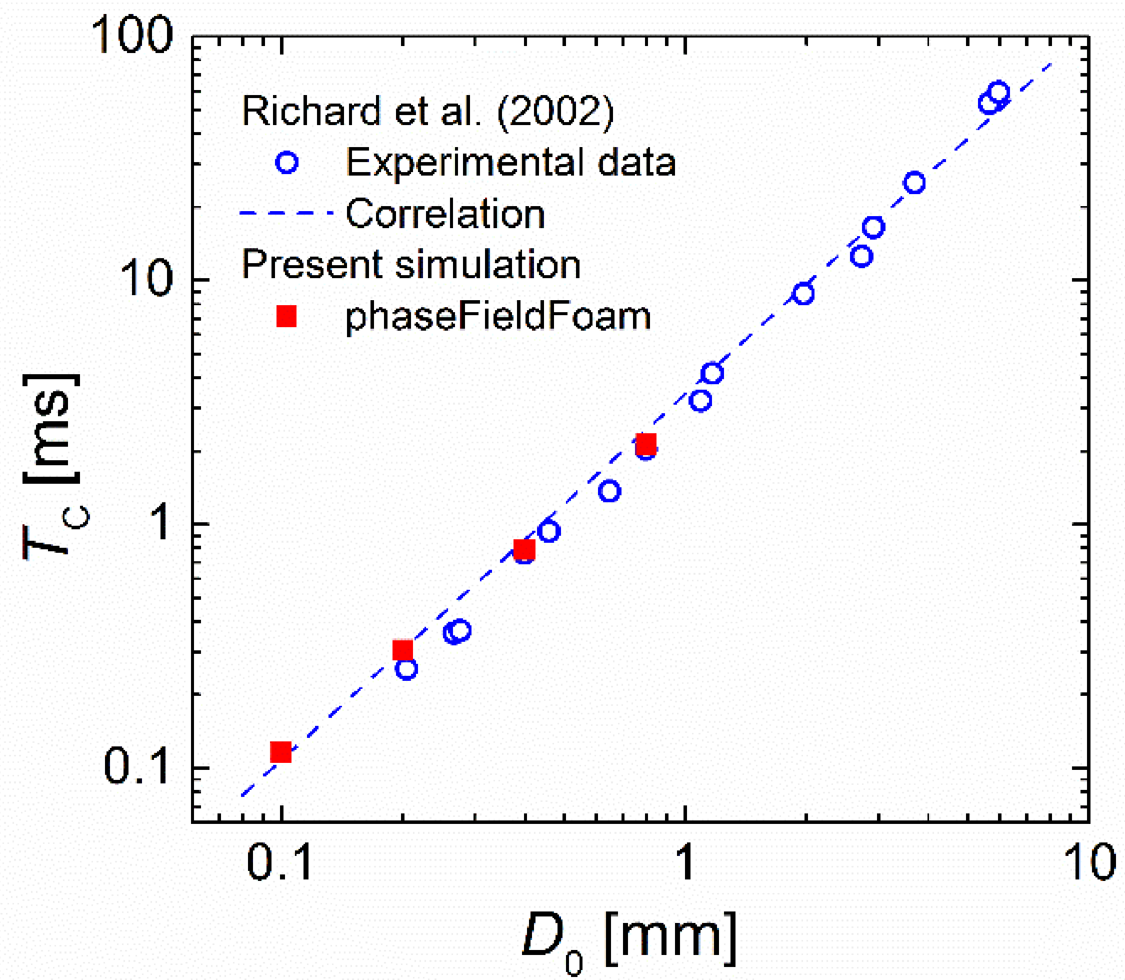
Richard et al. *Nature* **2002** 417: 811-811.

Contact time



- Richard et al. (2002) correlated *Tc* with droplet radius D_0

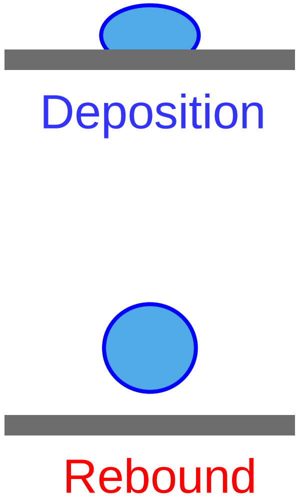
$$T_C = 2.6\left(\frac{\rho}{\sigma}\right)^{1/2}\left(\frac{D_0}{2}\right)^{3/2}$$

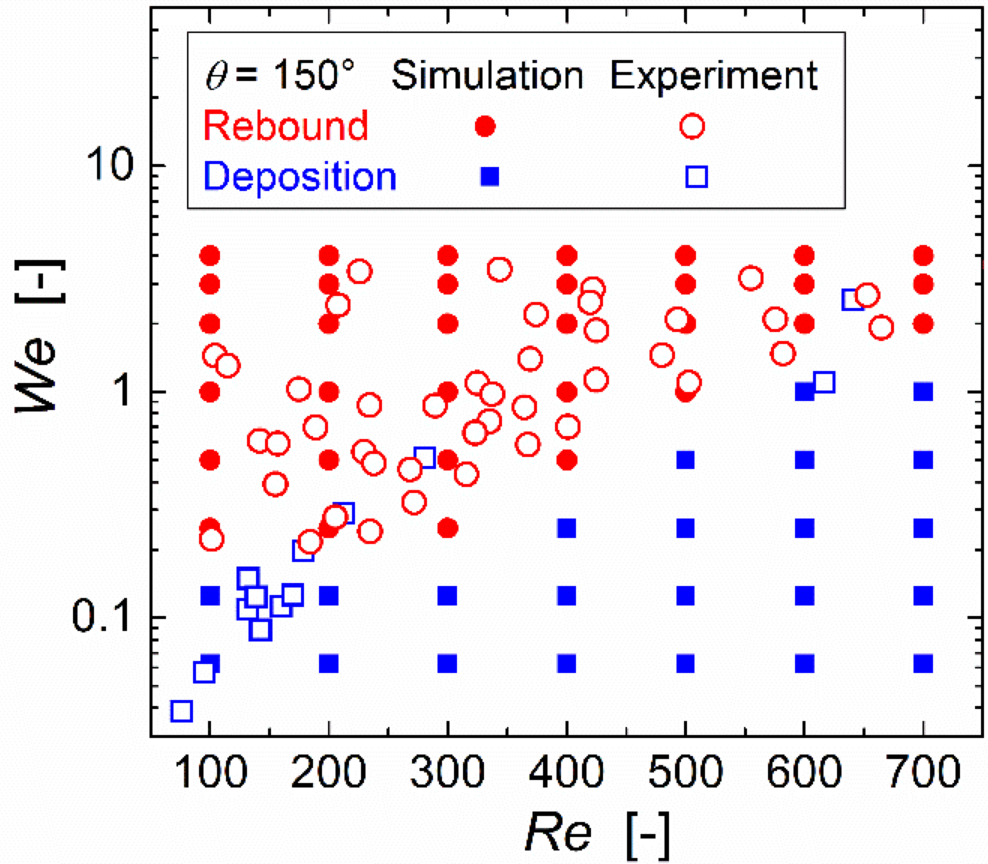


📖 Richard et al. *Nature* **2002** 417: 811-811.

Regime map for rebound and deposition

- For Weber number *We* and Reynolds number *Re*
  - Simulations in comparison with experimental data from Rioboo et al. 2008
    (Each symbol ■ or ● represents one simulation)





📖 Rioboo et al. *Langmuir* **2008** (24), 14074-14077

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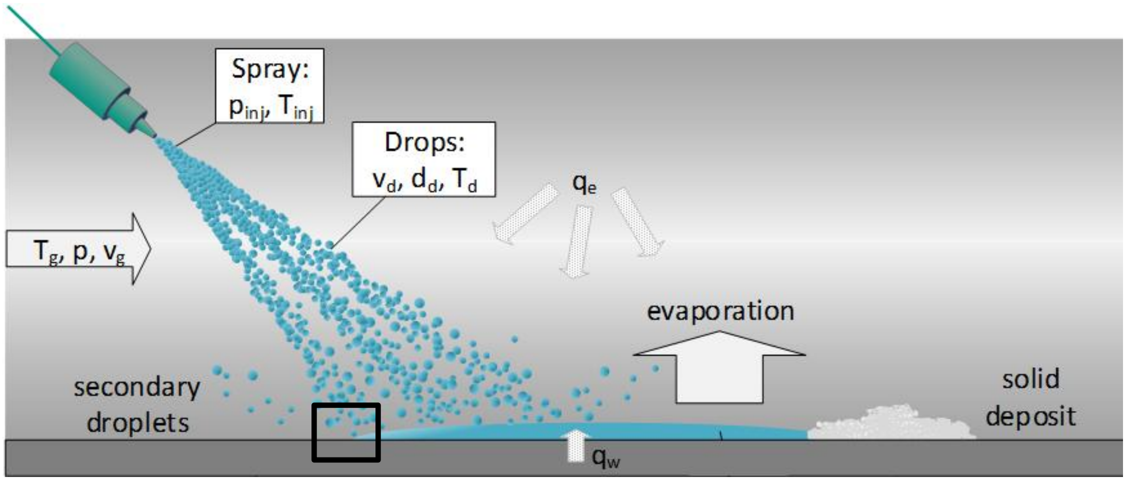
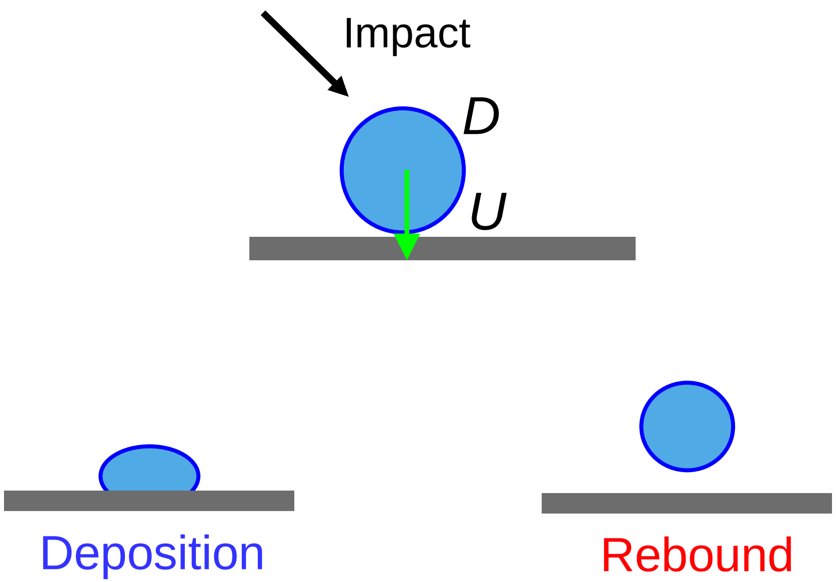
AdBlue® droplet onto wall





- Physical properties
  - ρ_L = 1090 kg/m^3
  - μ_L = 1.3 mPa s
  - σ_L = 0.073 N/m

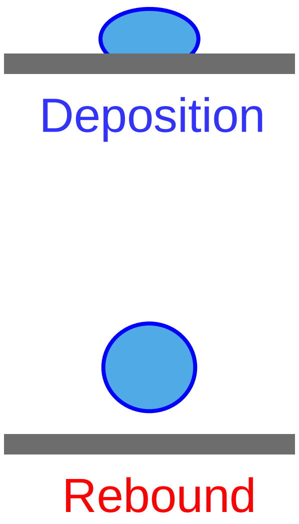
- Typical operating conditions:
  - **10 µm < D_0 < 800 µm**
  - **0 < U_0 < 10 m/s**

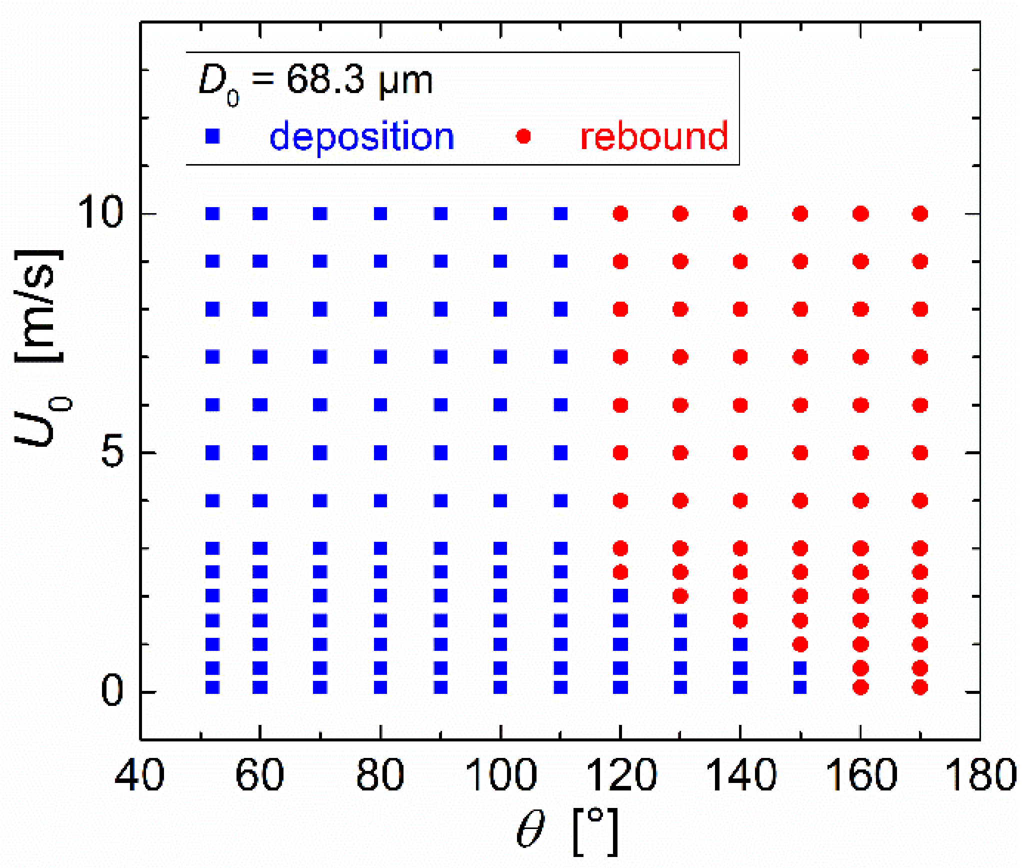
- Contact angle
  90° < θ < 170°

Regime map for physical parameters

- Regime map for impact velocity U_0 and equilibrium contact angle θ

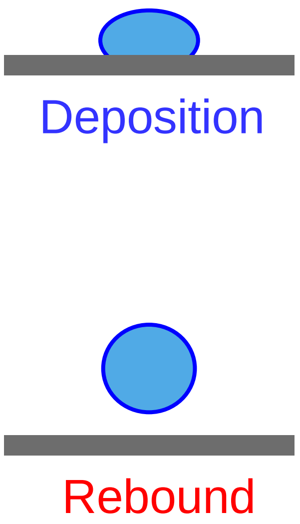
  (Each symbol ■ or ● represents one simulation)

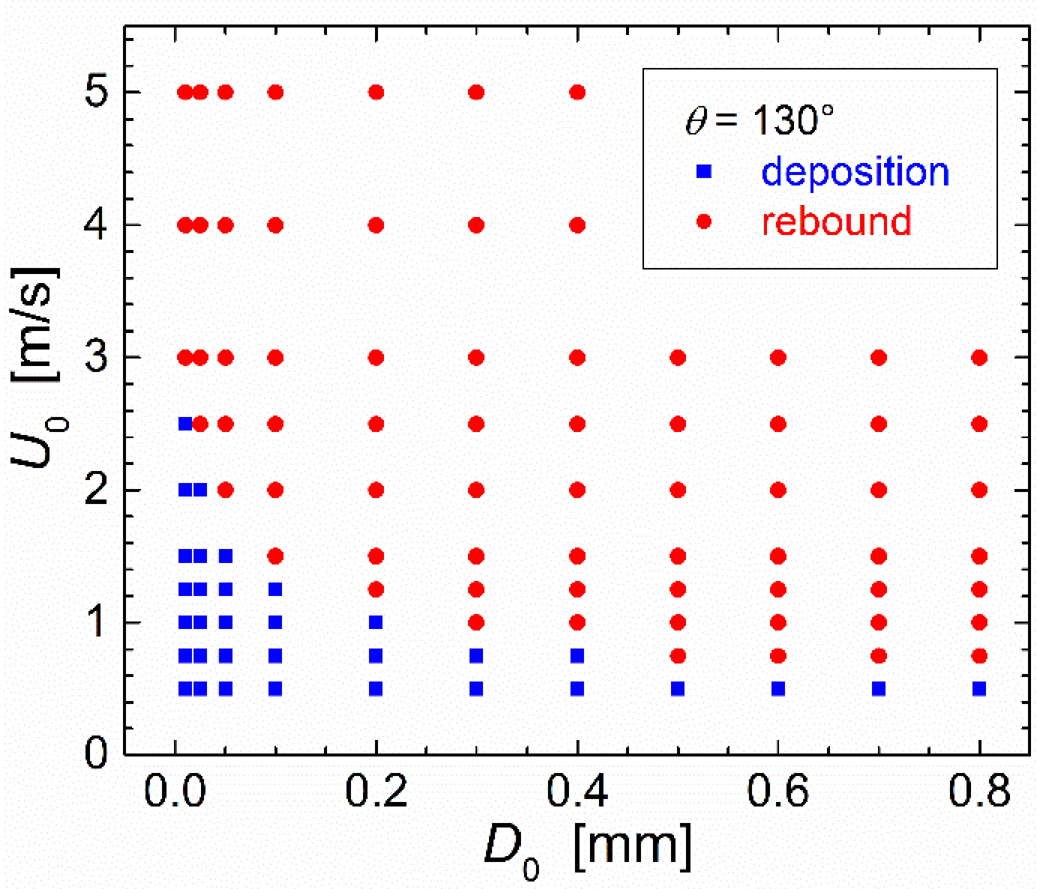




Regime map for physical parameters

- Regime map for impact velocity U_0 and initial droplet diameter D_0
  (Each symbol ■ or ● represents one simulation)

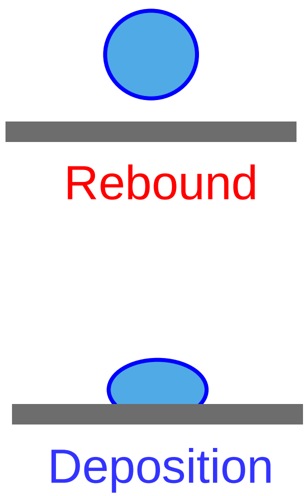


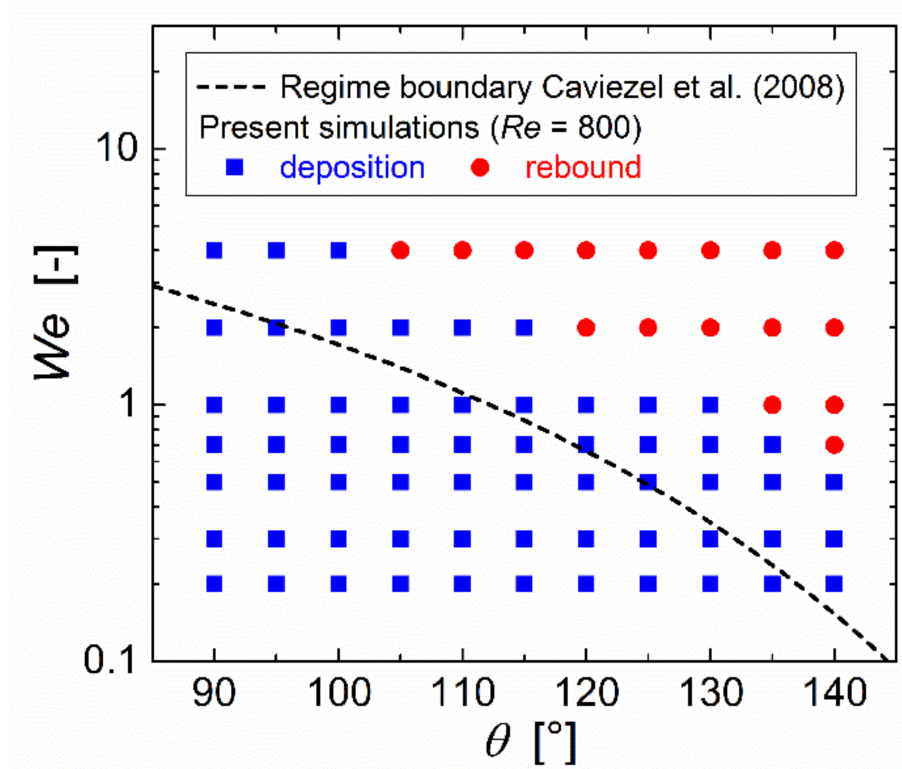


Regime map for dimensionless quantities

- For Weber number *We* and equilibrium contact angle θ
  - Simulations in comparison with Caviezel's analytical limit between the two regime:

$$We_{\text{critical}} = 12\{1-(2-3\cos\theta + \cos^3\theta)[2(1-\cos\theta)(2-\cos\theta-\cos^2\theta)]^{-2/3}\}$$

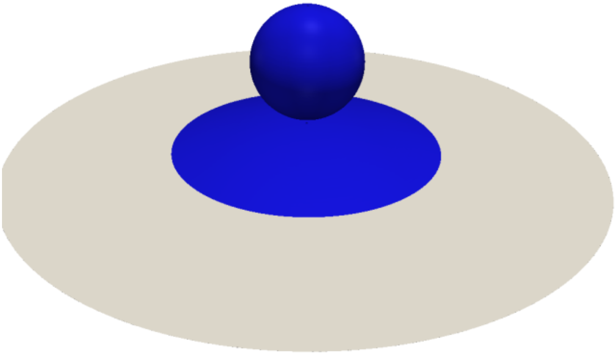




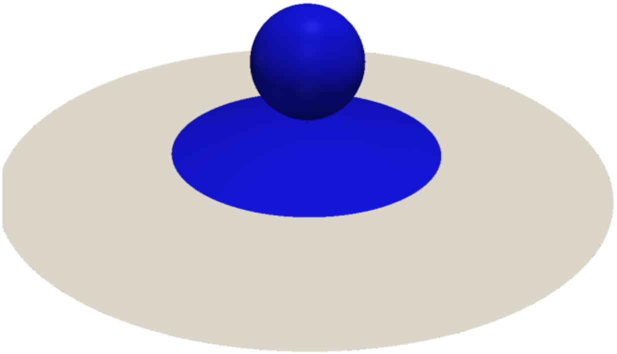
Caviezel et al. *Microfluidics and Nanofluidics* **2008**, 5(4): 469-478

Summary and outlooks

- The numerical code is validated for single droplet rebound process
- Rebound regime maps obtained by our simulation campaign show:
  - contact angle↑, impact velocity↑ , diameter↑ or Weber↑
    → rebound occurrence↑
- Outlooks
  - Contact angle hysteresis model with specification of θ_a and θ_r
  - Droplet coalescence



U_0 = 0.8 m/s



U_0 = 2.1 m/s

Friedrich und Elisabeth Boysen-Stiftung (BOY-127)

Thank you for your attention!