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BOY-127 TP 1

Numerische Simulation von Tropfenaufprallvorgängen im Hinblick auf die Bildung von Flüssigkeitsfilmen bei der SCR Abgasnachbehandlung

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Boysen Doktorandentage, 17.-18.05.2018, Altensteig

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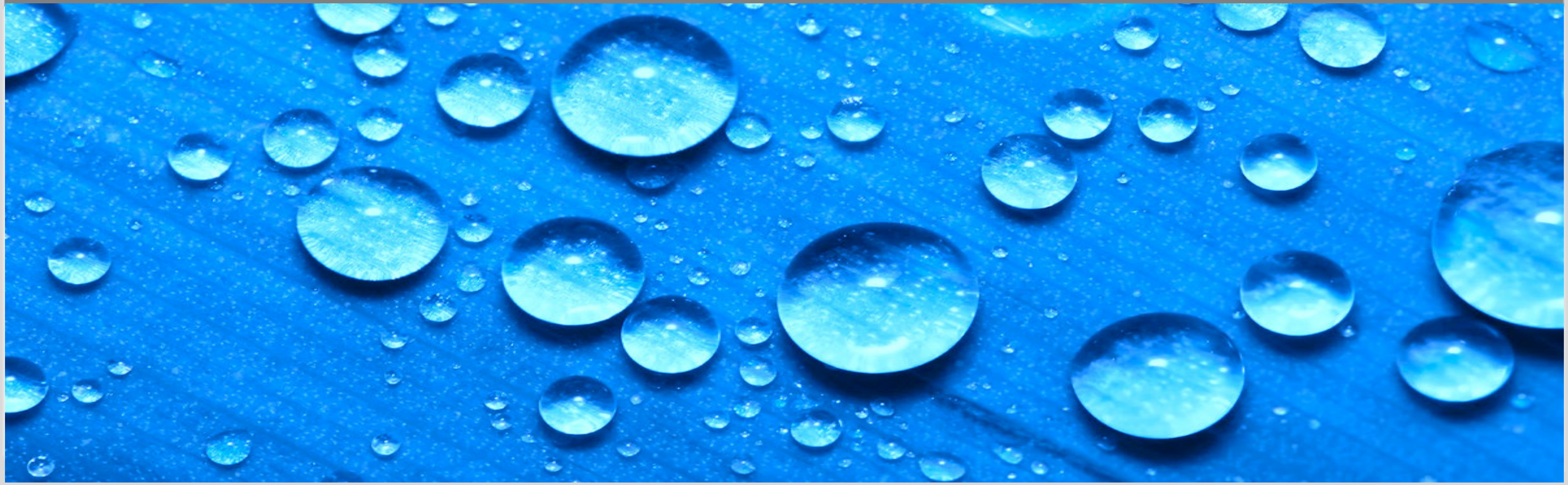
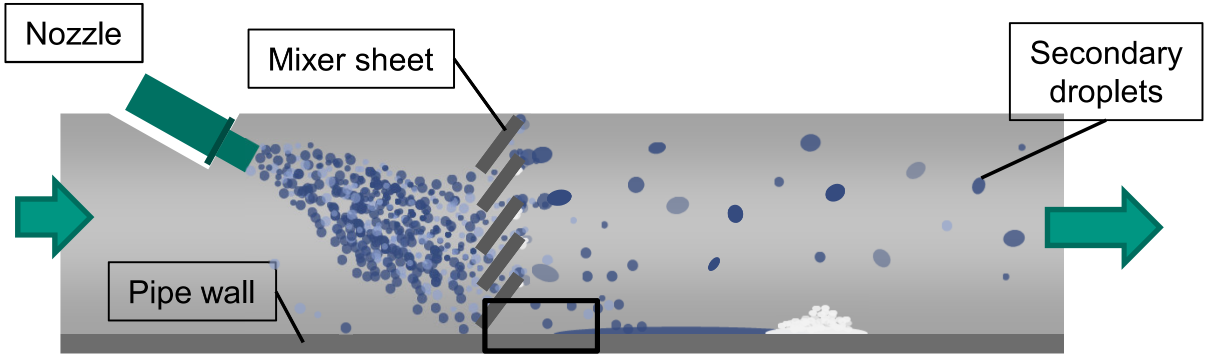


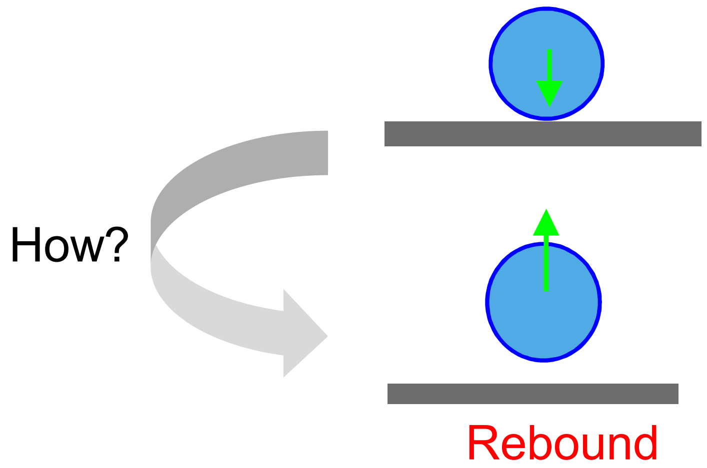
Outline

- Introduction and motivation
- Numerical simulations of
  - Single droplet impact and rebound
  - Coalescence of droplets
- Summary and outlook

Motivation

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





Numerical method and code

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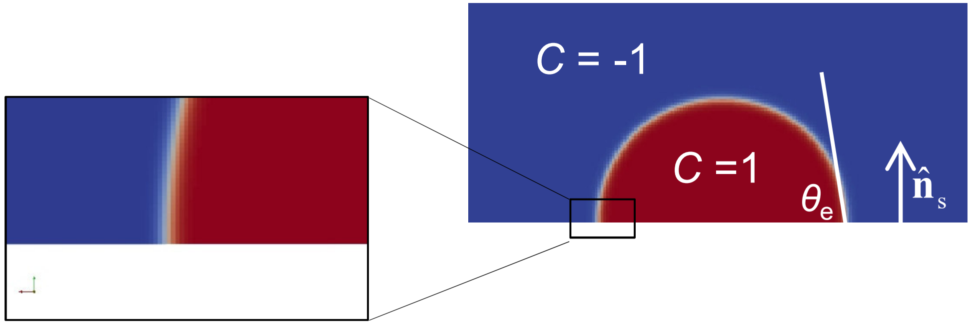
- **Phase-field method**
  - Gas-liquid-interface has a certain thickness (“diffuse-interface”)
  - Phase distribution is described by an order parameter *C*
  - Coupling of Cahn-Hilliard equation and Navier-Stokes equations
  - Particularly suitable for modelling of wetting process



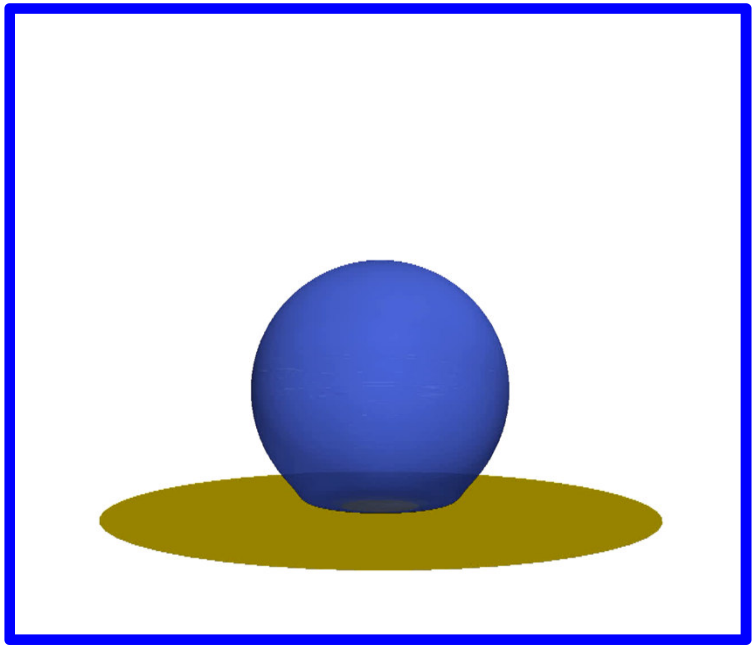
- **Code *phaseFieldFoam***
  - in the open-source CFD Software OpenFOAM implemented
  - Development in cooperation with Dr. H. Marschall (TU-Darmstadt)

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

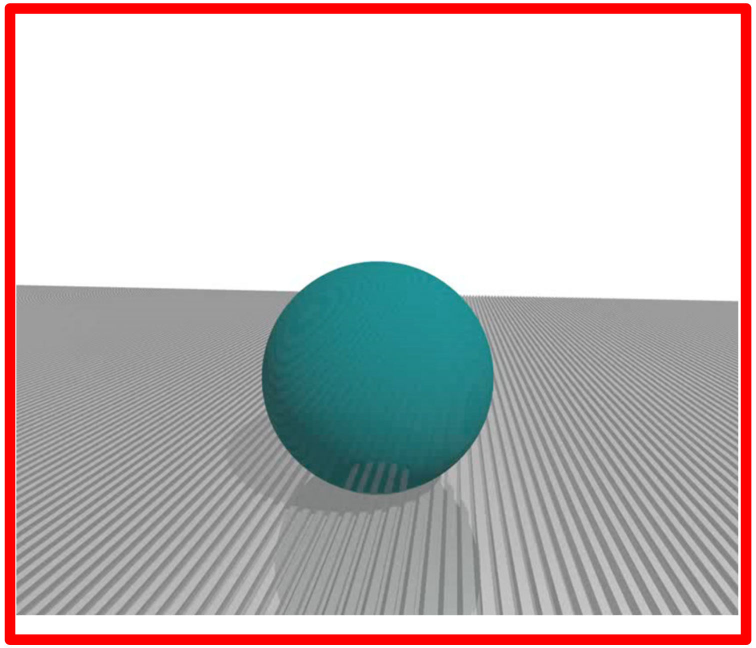
📖 Marschall, Cai, Wörner and Deutschmann, **2015,** 10th Int. OpenFOAM® Workshop, Ann Arbor, Michigan

Rebound on micro-structured surface

- Micro-structure → super-hydrophobicity → rebound



2D Axisymmetric Simulation for smooth surface



3D Simulation for micro-structured surface

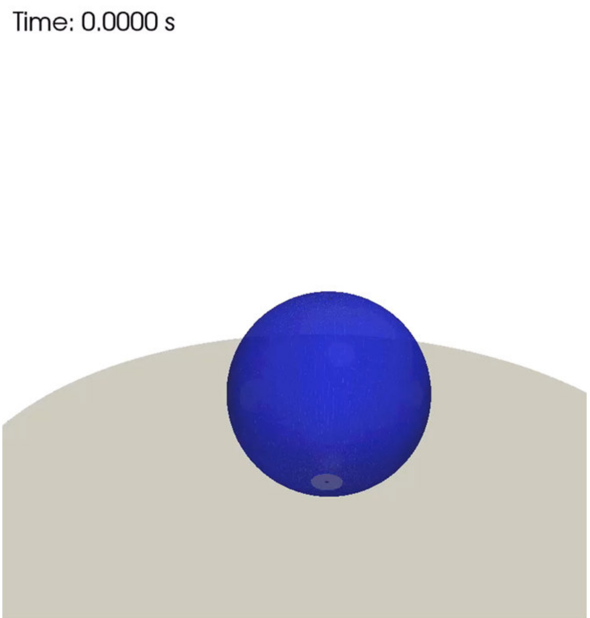
18 million cells and 800,000 CPU hours!

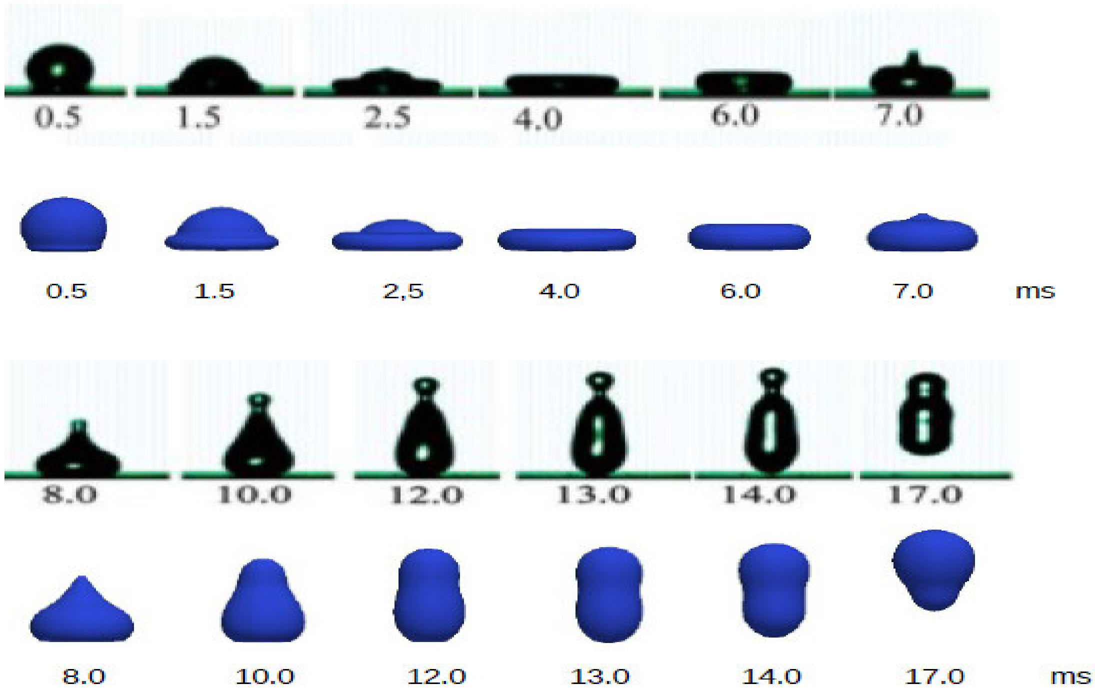
📖 Fink, Cai, Stroh, Bernard, Kriegseis, Frohnapfel, Marschall and Wörner, *Int. J. Heat & Fluid Flow,* **2018,** 70, 271-278

Rebound on smooth surface

- **Very large contact angle $\boldsymbol{\theta_{eq}}$** → super-hydrophobicity → rebound
- Validation against experiment Zang et al. (2013), θ_{eq} = 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





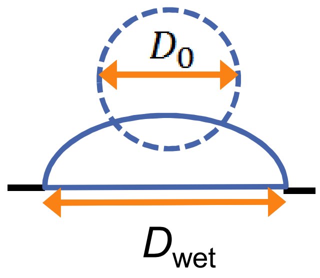
Zang et al. *Soft Matter* **2013**, 9(2): 394-400

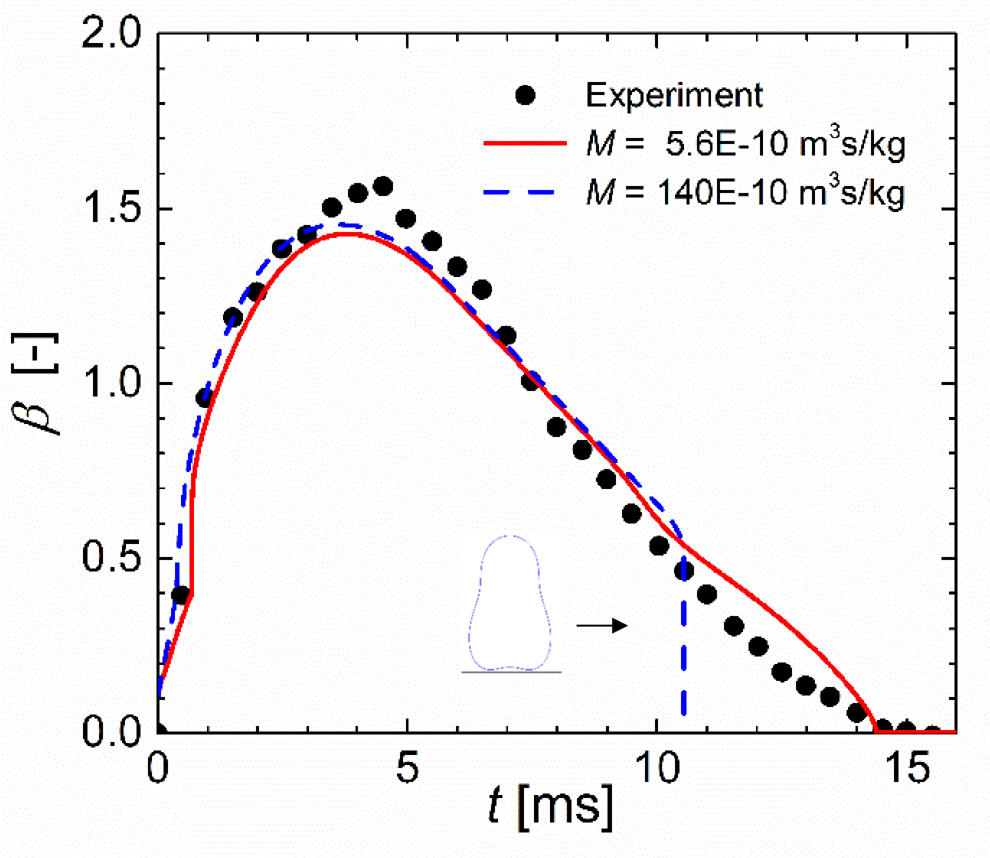
Rebound on smooth surface

- **Very large contact angle θ_{eq}** → super-hydrophobicity → rebound
- Validation against experiment Zang et al. (2013), θ_{eq} = 163°

Spread factor:

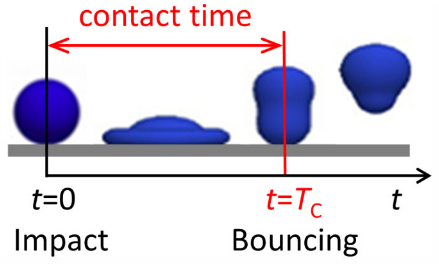
$$\beta = D_{wet} / D_0$$





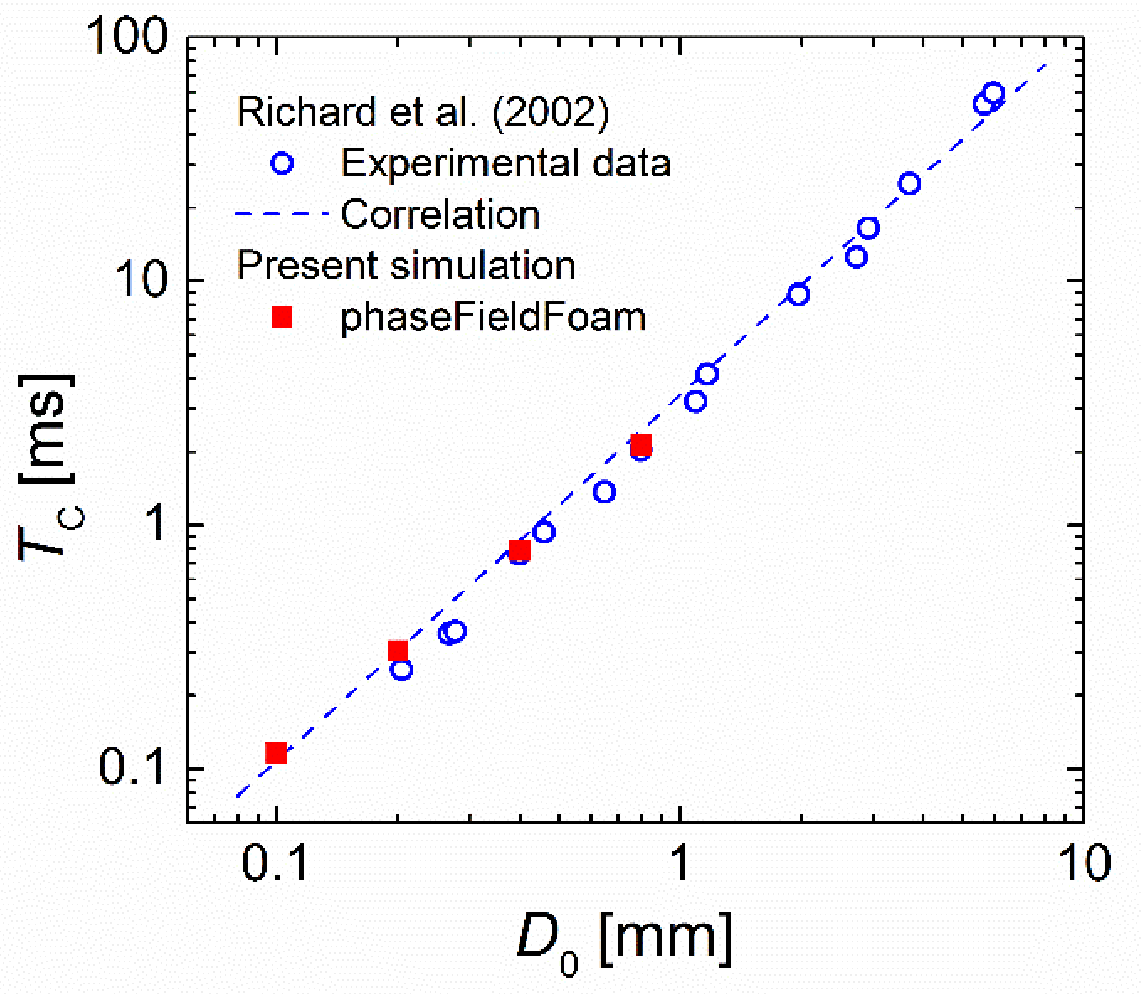
📖 Zang et al. *Soft Matter* **2013**, 9(2): 394-400

Contact time



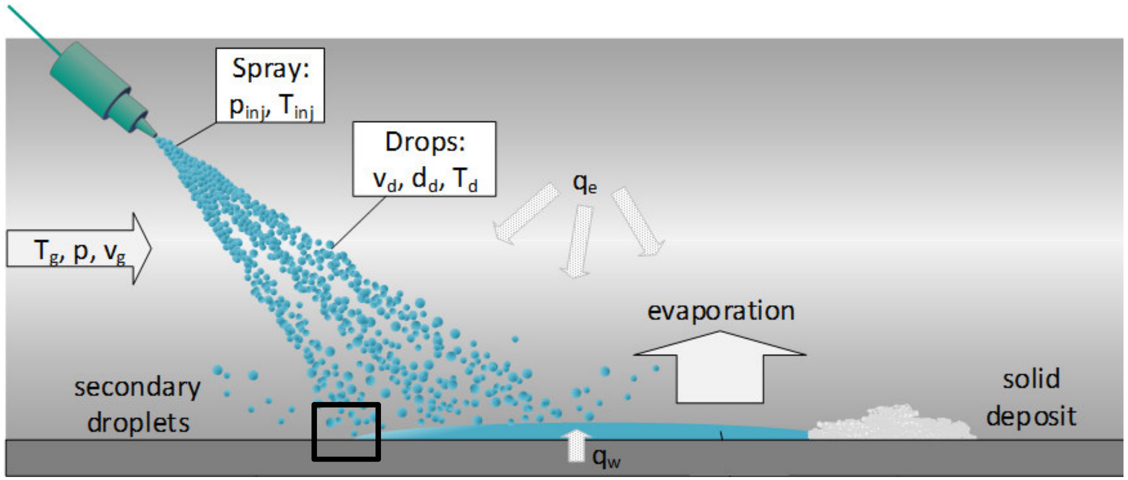
- Richard et al. (2002) correlated *Tc* with droplet radius D_0

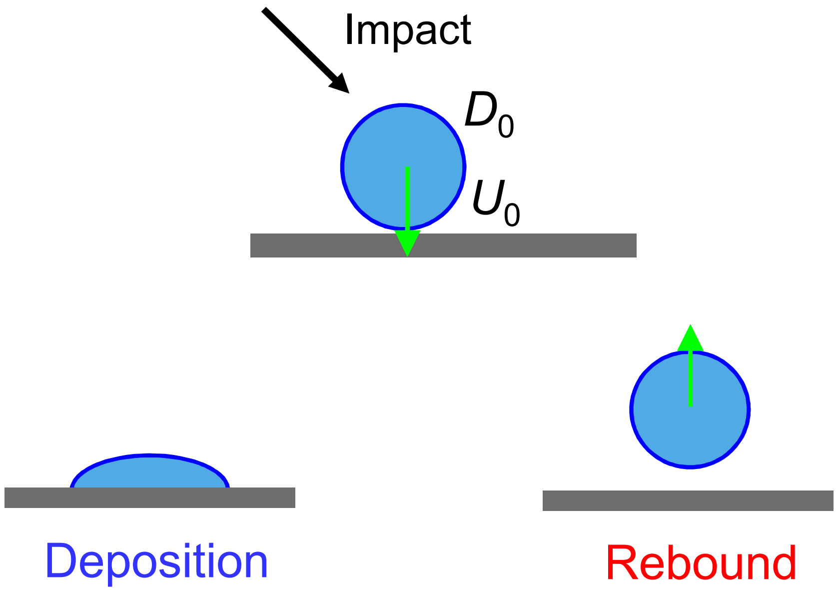
$$T_C = 2.6\left(\frac{\rho}{\sigma}\right)^{1/2}\left(\frac{D_0}{2}\right)^{3/2}$$



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

AdBlue® droplet onto wall



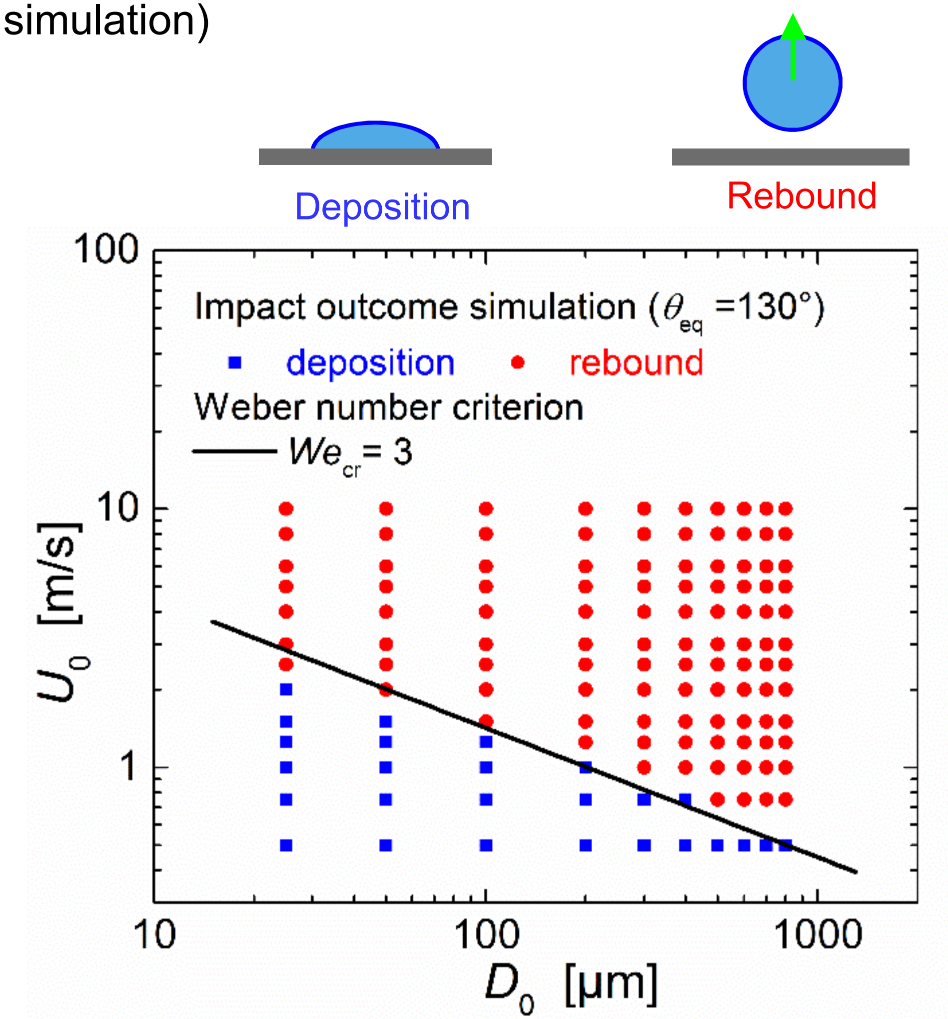


- Physical properties
  - ρ_L = 1090 kg/m^3
  - μ_L = 1.3 mPa s
  - σ_L = 0.073 N/m
- Typical operating conditions:
  - **25 µm ≤ D_0 ≤ 800 µm**
  - **0 < U_0 ≤ 10 m/s**
- Contact angle
  90° ≤ θ_{eq} ≤ 170°

Regime map for physical parameters

- Regime map for impact velocity U_0 and initial droplet diameter D_0

  (Each symbol ■ or ● represents one simulation)



- Critical Impact velocity

$$U_{0,\,cr} \sim \sqrt{\frac{\sigma}{\rho_L D_0}}$$

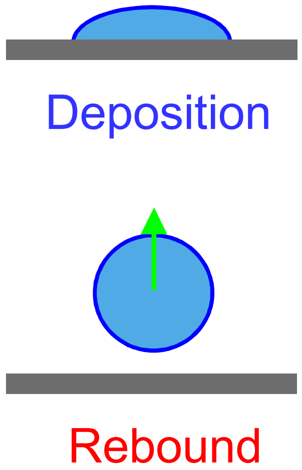
- Critical Weber number

$$We_{cr} = \frac{\rho_L D_0 U_{0,cr}^2}{\sigma}$$

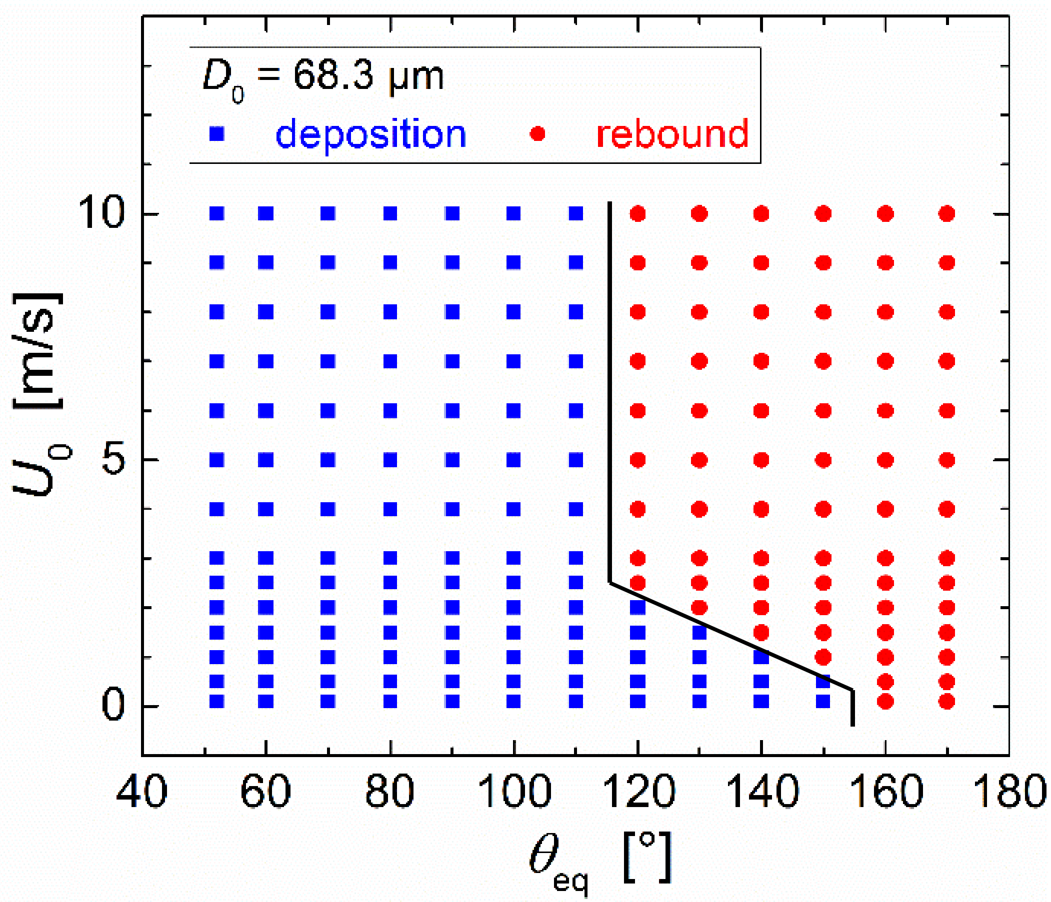
Reyssat et al. *Europhysics Letters* **2006**, 74, 306-312

Regime map for physical parameters

- Regime map for impact velocity U_0 and equilibrium contact angle θ_{eq}
  (Each symbol ■ or ● represents one simulation)

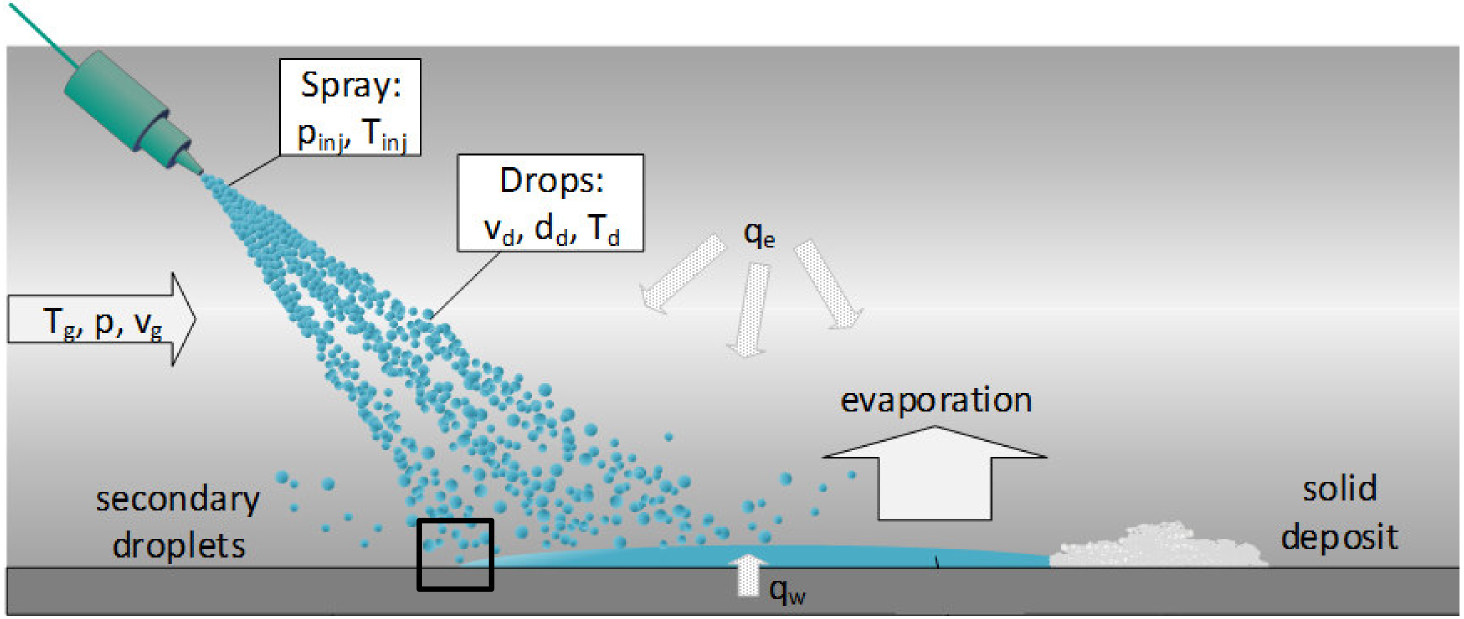


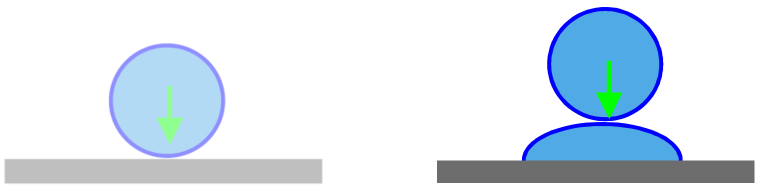
$$We_{cr} = f(\theta_{eq})$$



Coalescence of droplets

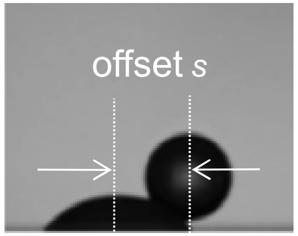
- Droplet impacts onto another droplet that has already deposited on surface





Coalescence of water droplets

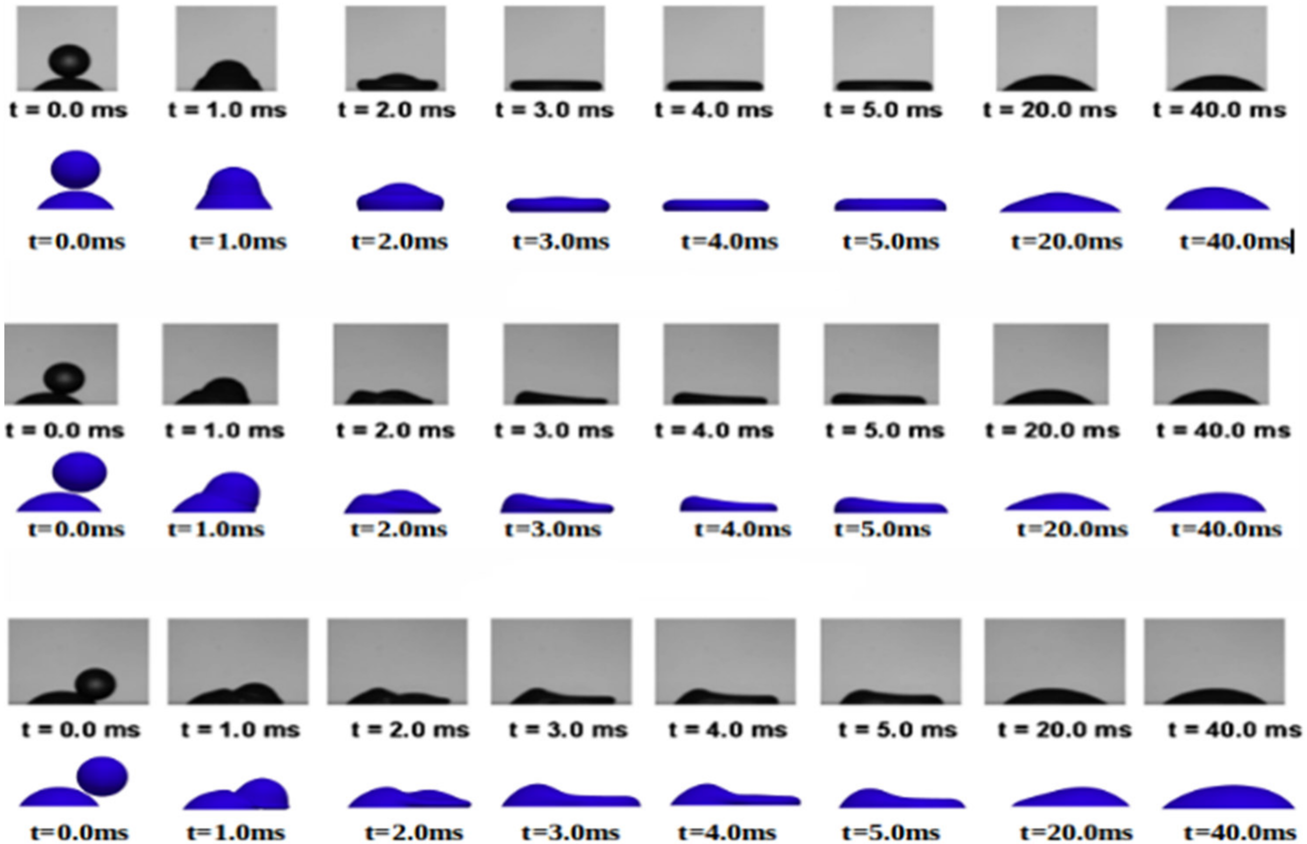
- Head-on coalescence versus coalescence with a given offset *s*



Head-on
***s* = 0**

***s* = 0.9 mm**

***s* = 2.0 mm**

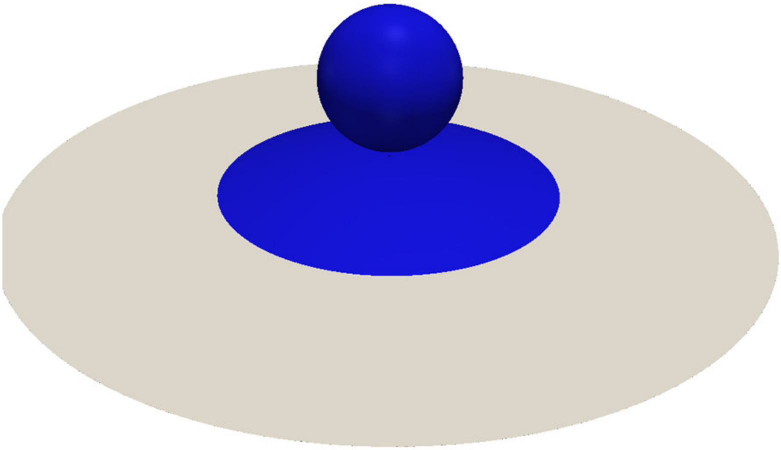


📖 Castrejon-Pita et al. *Biomicrofluidics* **2011**, 0141212

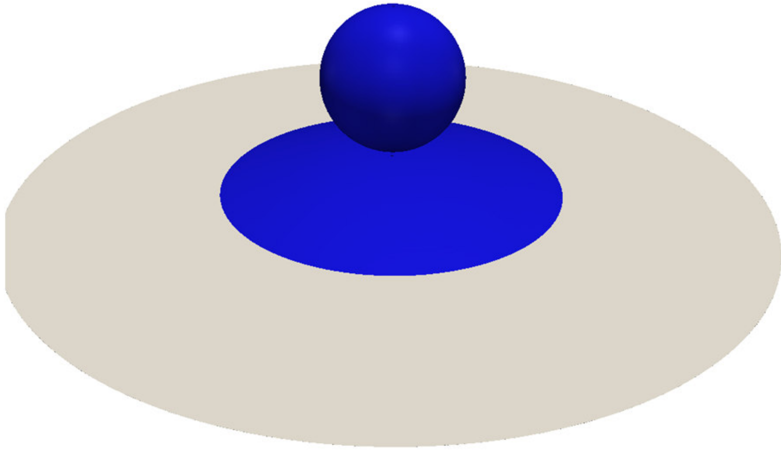
Coalescence of water droplets - crown formation

- 2D axisymmetric phase-field simulations

Impact velocity U = 0.8 m/s



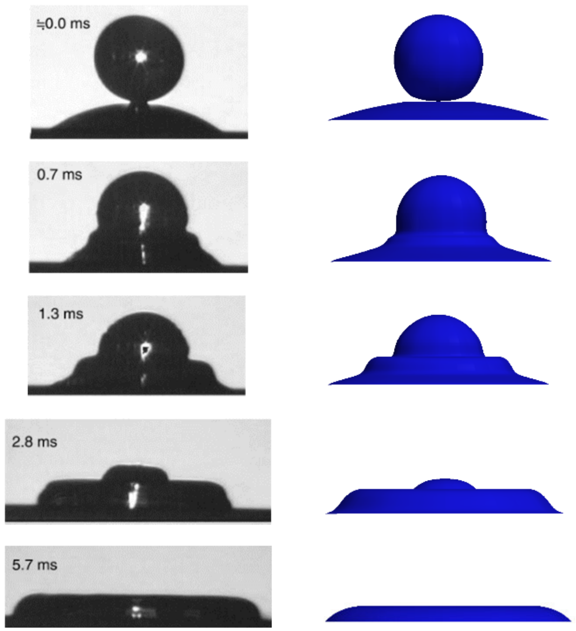
Impact velocity U = 2.1 m/s



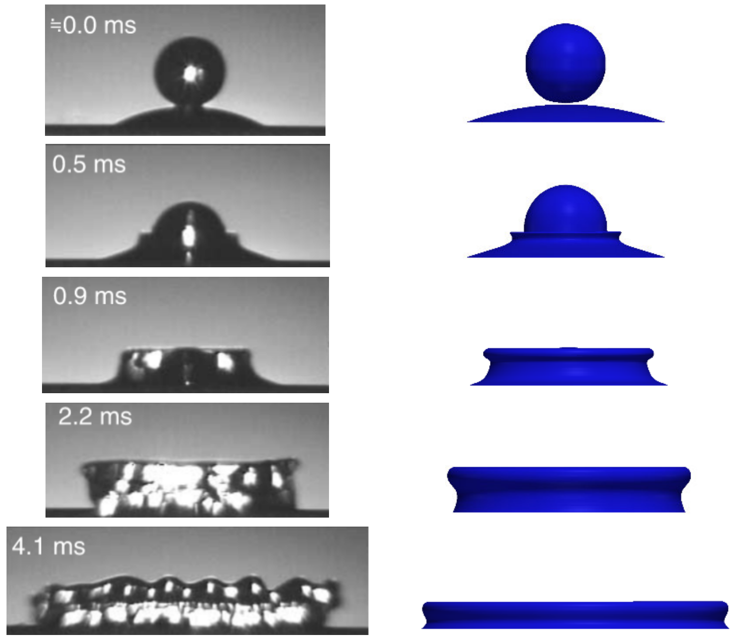
Coalescence of water droplets - crown formation

- The comparison of the experiment and present 2D axisymmetric phase-field simulation

Impact velocity U = 0.8 m/s



Impact velocity U = 2.1 m/s



📖 Fujimoto et al. *Intl. J. Multiphase Flow* **2001** 27: 1227-1245

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
  - Film formation