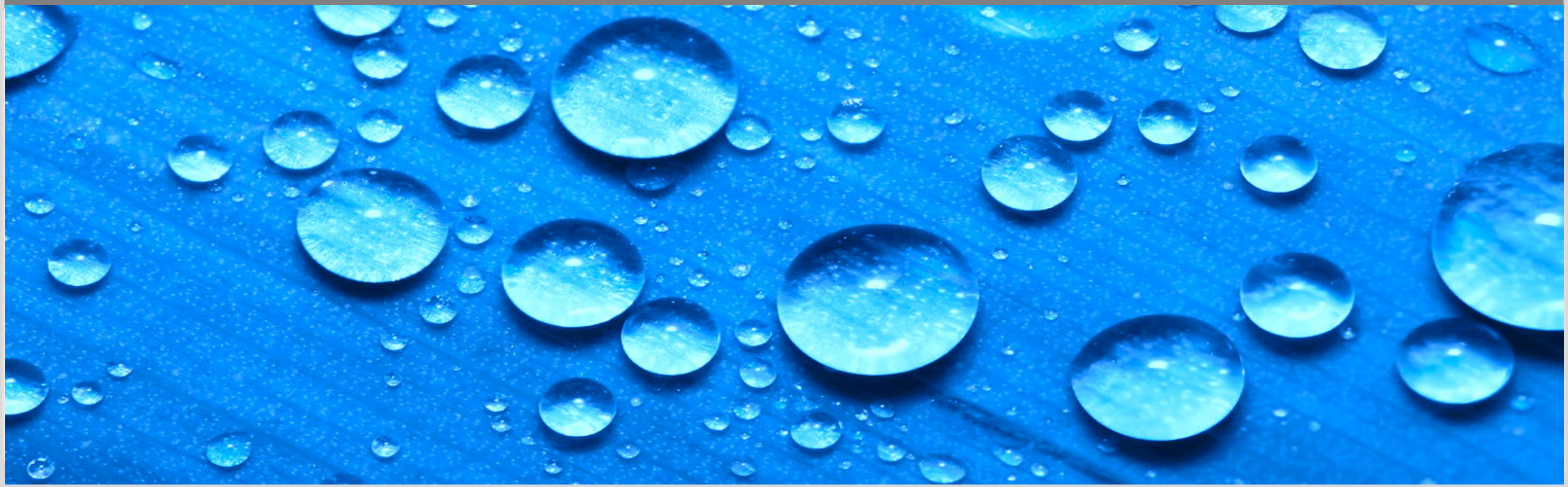
Karlsruhe Institute of Technology

# Numerical Study of Droplet Impact and Rebound on Hydrophobic Surface


**Xuan Cai, Yanchen Wu, Martin Wörner and Bettina Frohnapfel**

**Karlsruhe Institute of Technology (KIT), Germany**


70th Annual Meeting of the APS Division of Fluid Dynamics, November 19–21, 2017, Denver, Colorado

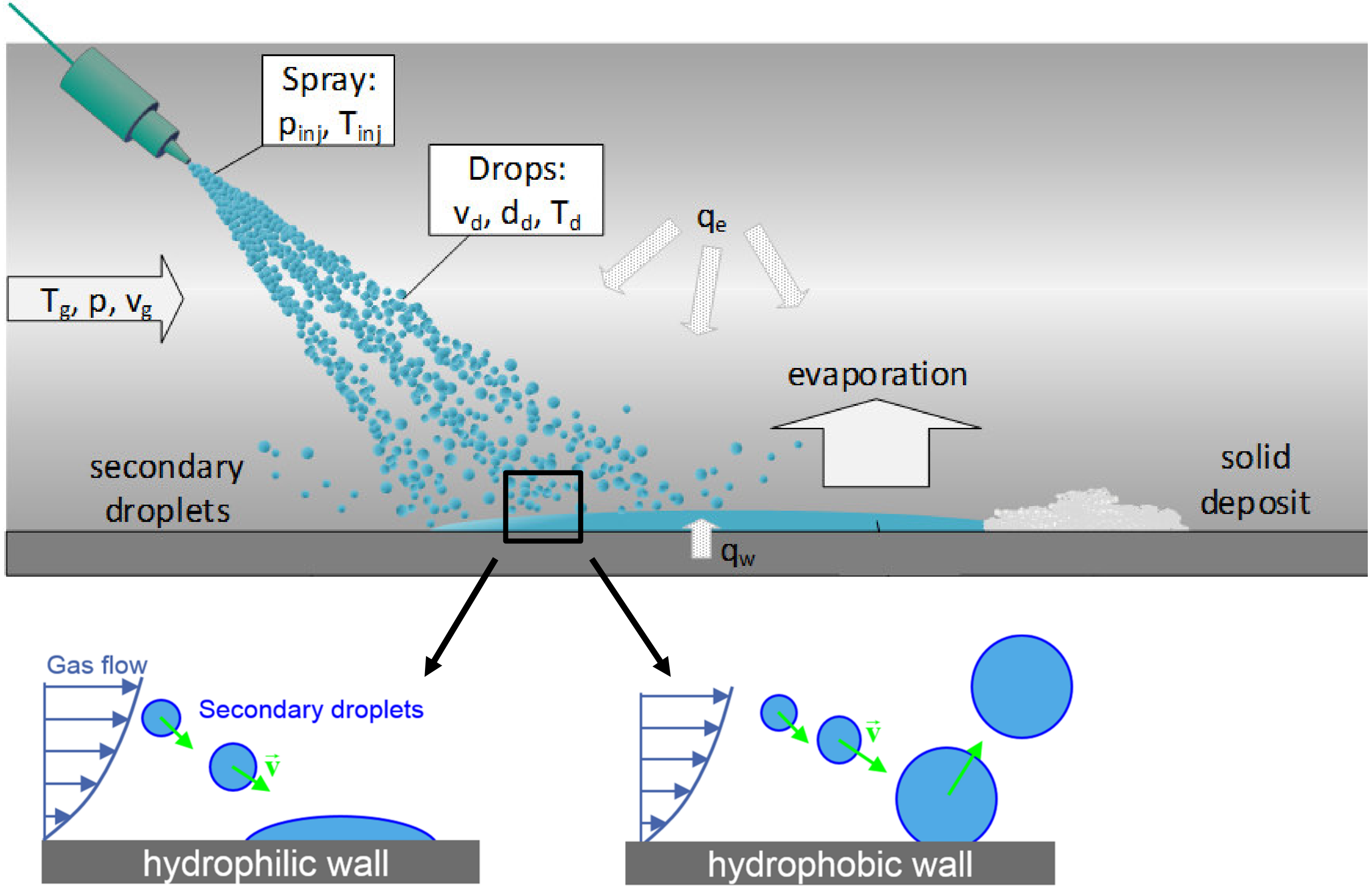


# Outline

- Motivation
- Phase-field method
- Validation for impact and rebound of water droplet on micro-structured and smooth surfaces
- Influence of impact parameters and surface wettability for Diesel-Exhaust-Fluid (DEF) droplets
- Summary and Outlook

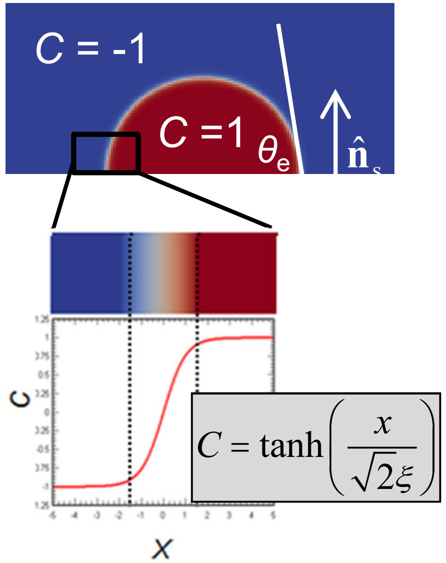
# Motivation

- Impact of Diesel-Exhaust-Fluid (DEF) droplets onto tailpipe wall, for exhaust gas after-treatment in diesel engine



# Phase Field Method

- Order Parameter ( $C$ ) as phase indictor
  - Smooth transition from -1 to 1 → **diffuse interface**




- $C$ evolution governed by Cahn-Hilliard equation

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

- Wetting boundary condition for equilibrium contact angle $\theta$

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

- Single-field Navier-Stokes equation:

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

- The method was implemented in the open-source CFD code OpenFOAM (H. Marschall and X. Cai)

$\Phi$ = chemical potential [J/m$^3$]
$\lambda$ = mixing energy [J/m]

**$\varepsilon$ = capillary thickness [m]**
**$\kappa$ = mobility [m$^3$s/kg]**
or dimensionless versions:
**Cahn number:**
***Cn = ε / L***
**Peclet number:**
**$Pe_C = (8/9)^{1/2} LU\varepsilon / (\kappa\,\sigma)$**

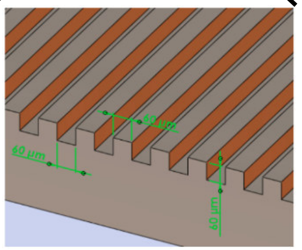
D. Jacqmin, *J. Comput. Phys.* **1999**, 155: 96-127.

# Outline

- Motivation
- Phase-field method
- Validation for impact and rebound of water droplet
- Influence of impact parameters and surface wettability for Diesel-Exhaust-Fluid (DEF) droplets
- Summary and Outlook

# Rebound on micro-structured surface

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

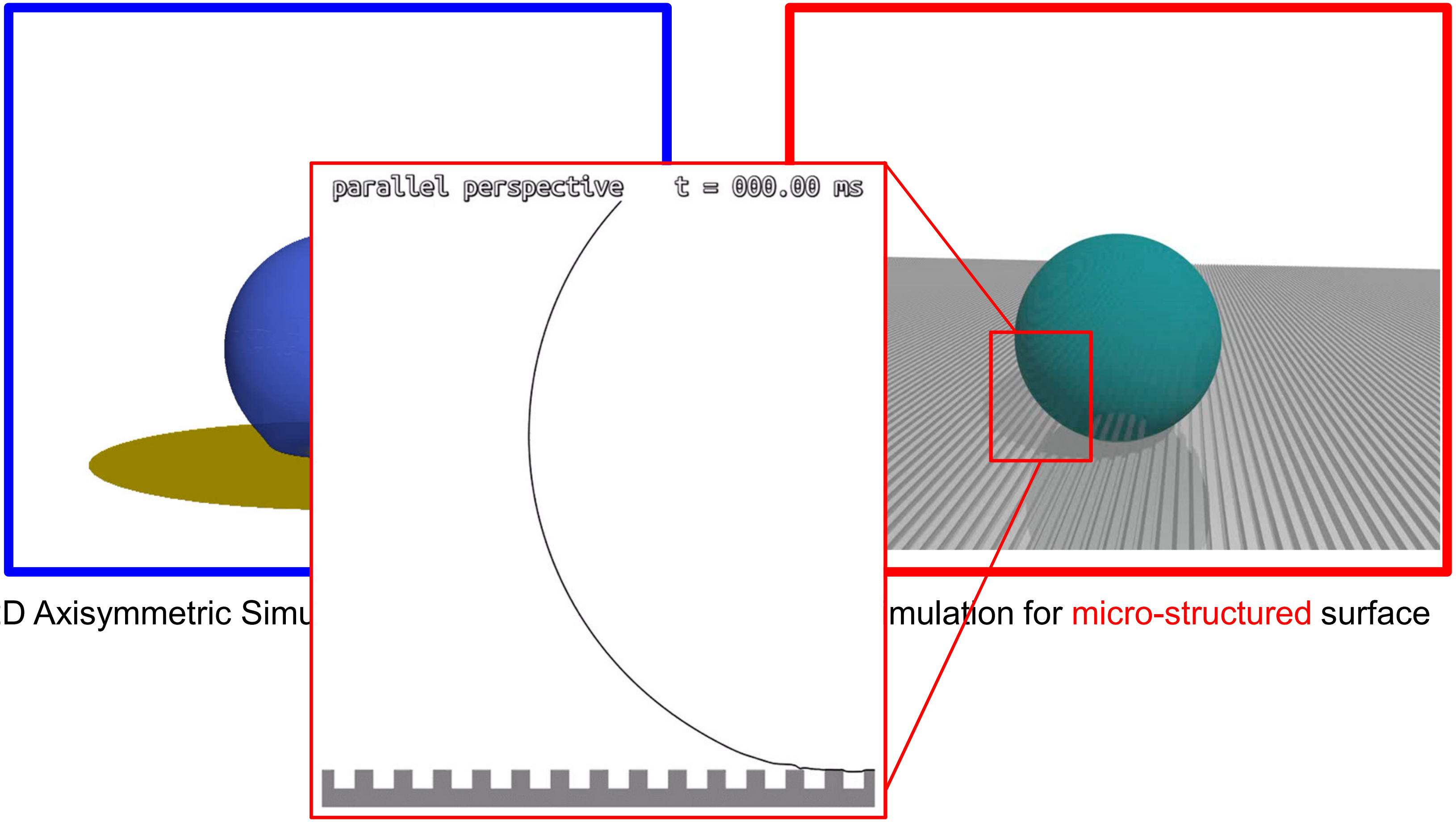


micro-grooved structures
characteristic dimension
*s* = 60 µm

📖 V. Fink, X. Cai, A. Stroh, R. Bernard, B. Frohnapfel, H. Marschall and M. Wörner (2017), under review

# Rebound on micro-structured surface

- Micro-structure → super-hydrophobicity → rebound




2D Axisymmetric Simu… …mulation for micro-structured surface

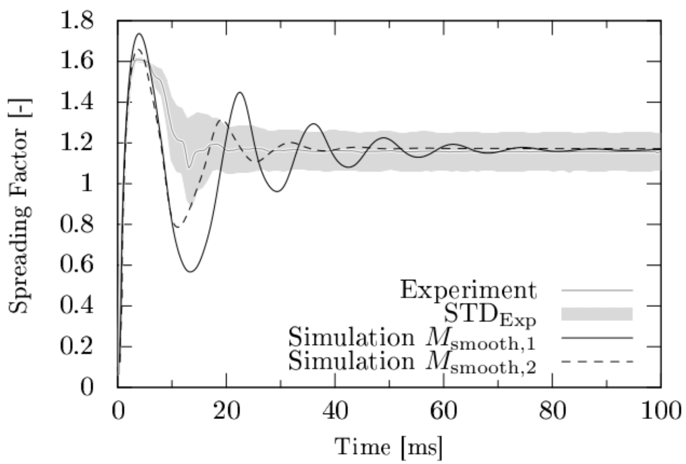
📖 V. Fink, X. Cai, A. Stroh, R. Bernard, B. Frohnapfel, H. Marschall and M. Wörner (2017), under review

# Rebound on micro-structured surface

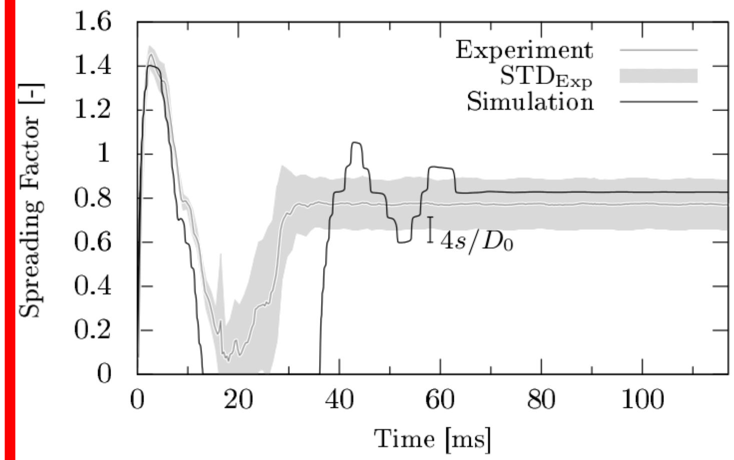
KIT Karlsruhe Institute of Technology

- Micro-structure → super-hydrophobicity → rebound

Droplet on smooth surface

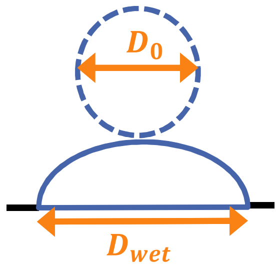



Droplet on micro-structured surface




Spread factor:

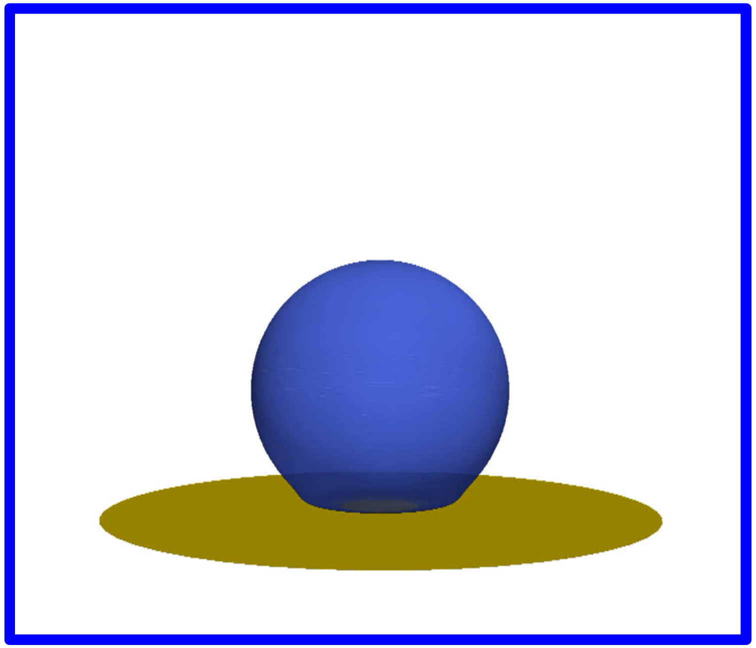
$\beta = D_{wet} / D_0$



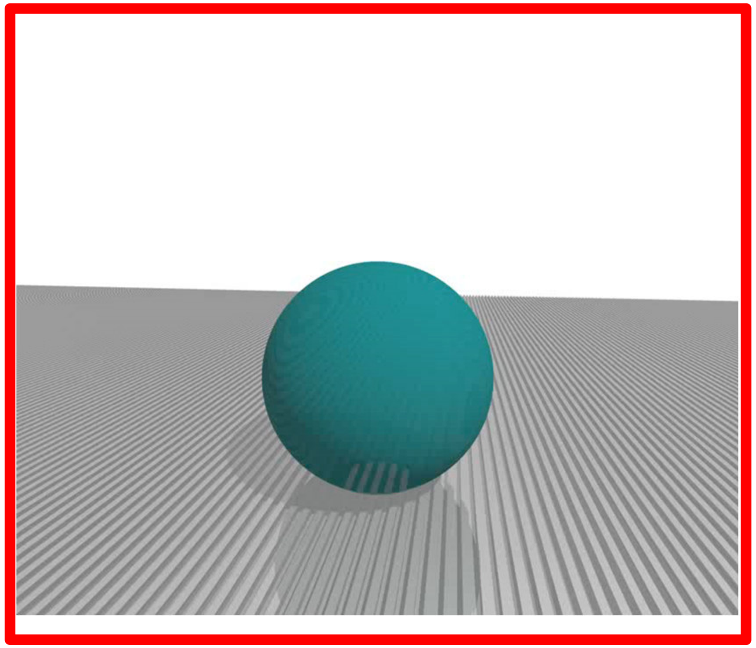

📖 V. Fink, X. Cai, A. Stroh, R. Bernard, B. Frohnapfel, H. Marschall and M. Wörner (2017), under review

# Rebound on micro-structured surface

- Micro-structure → super-hydrophobicity → rebound



2D Axisymmetric Simulation for smooth surface



3D Simulation for micro-structured surface

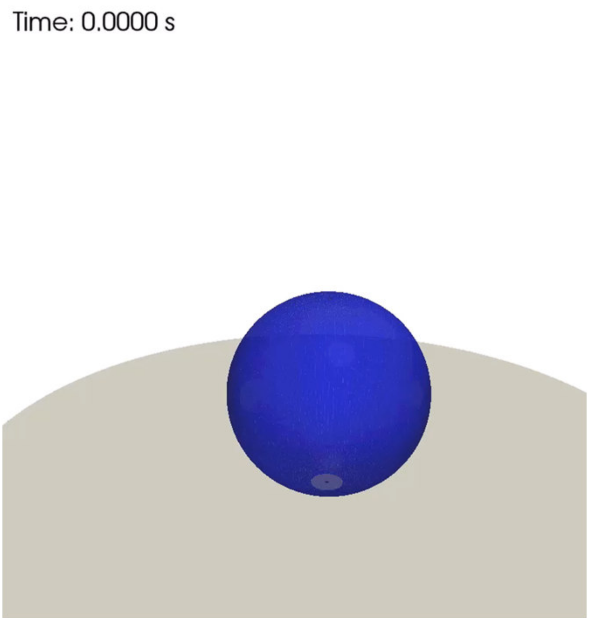
**18 million cells and 800,000 CPU hours!**

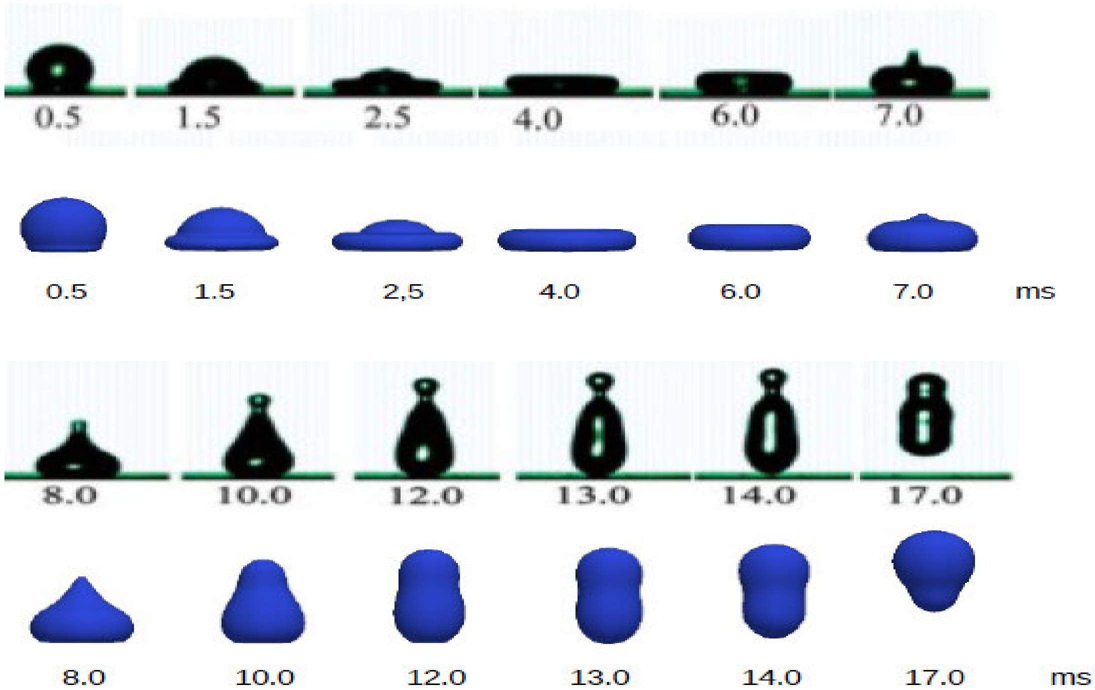
📖 V. Fink, X. Cai, A. Stroh, R. Bernard, B. Frohnapfel, H. Marschall and M. Wörner (2017), under review

# Rebound on smooth surface

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

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



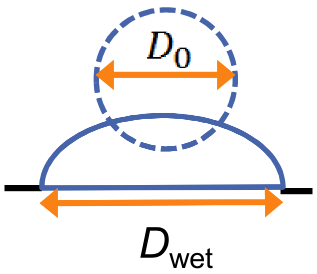

📖 Zang et al. *Soft Matter* **2013**, 9(2): 394-400

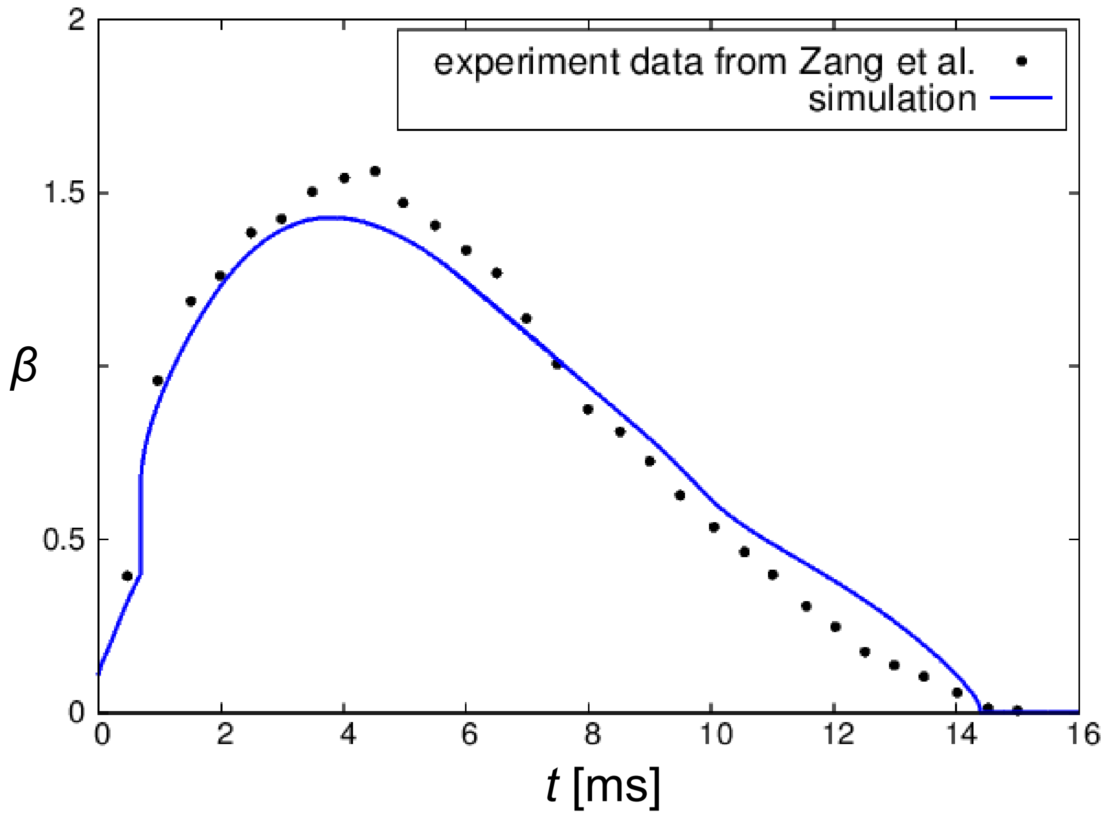
# Rebound on smooth surface

- **Very large contact angle *θ*** → super-hydrophobicity → rebound
- Validation against experiment Zang et al. (2013), $\theta$ = 163°

Spread factor:

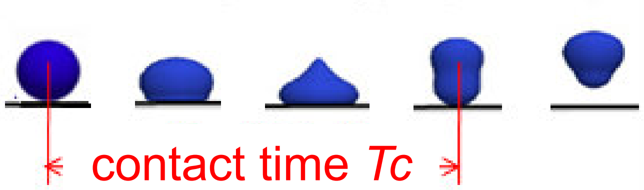
$\beta = D_{wet} / D_0$



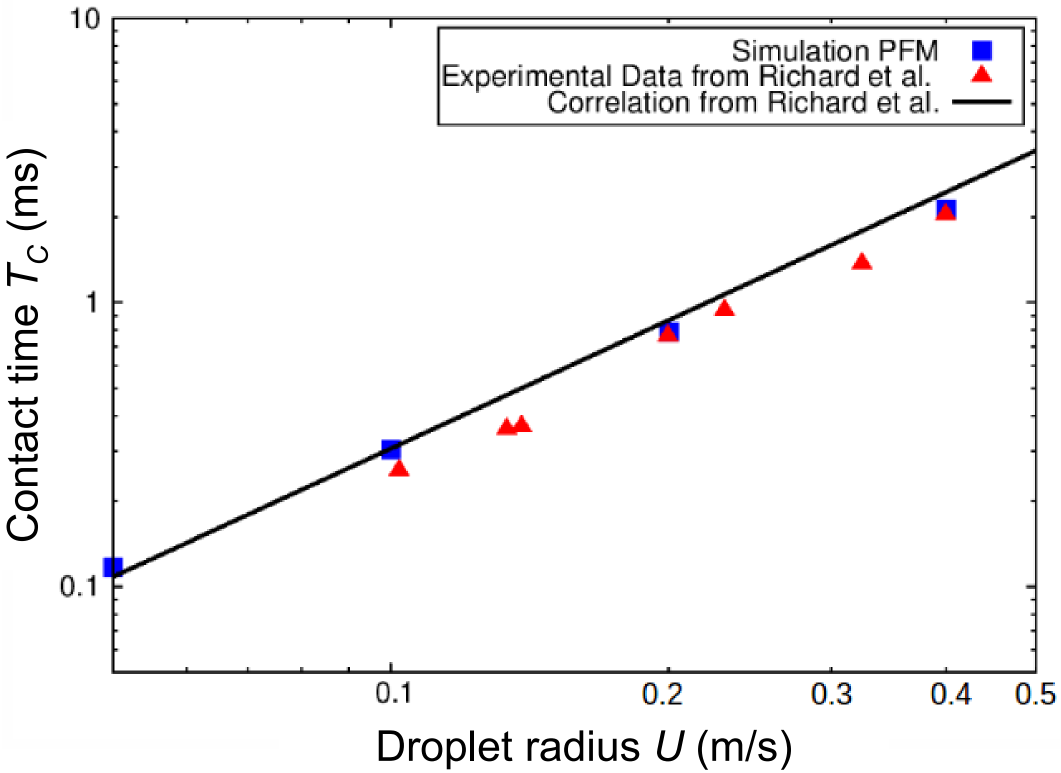

📖 Zang et al. *Soft Matter* **2013**, 9(2): 394-400

# Contact time




- Richard et al. (2002) correlated *Tc* with droplet ($U$ = 0.2 ~ 2.3 m/s) radius $R$

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

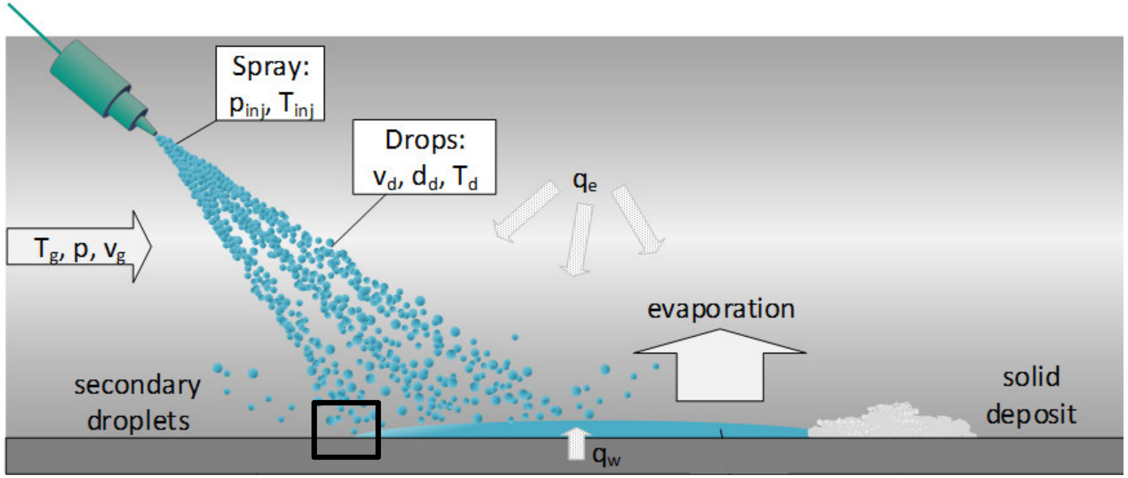


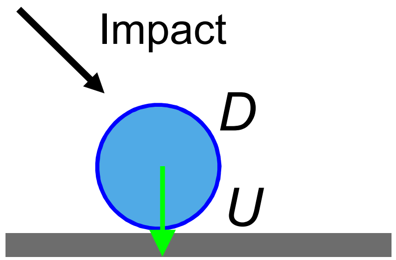

Richard et al. *Nature* **2002** 417: 811-811.

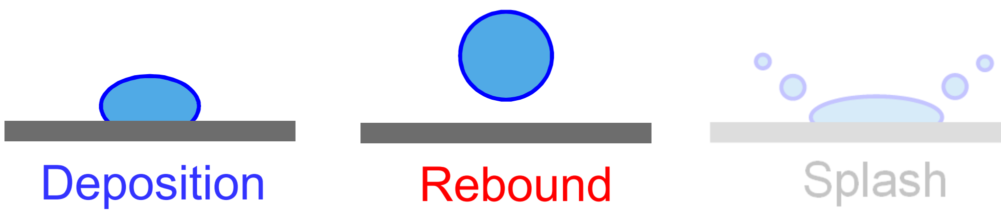
# Outline

- Motivation
- Phase-field method
- Validation for impact and rebound of water droplet
- Influence of impact parameters and surface wettability for Diesel-Exhaust-Fluid (DEF) droplets
- Summary and Outlook

# Diesel Exhaust Fluid (DEF) droplet onto wall



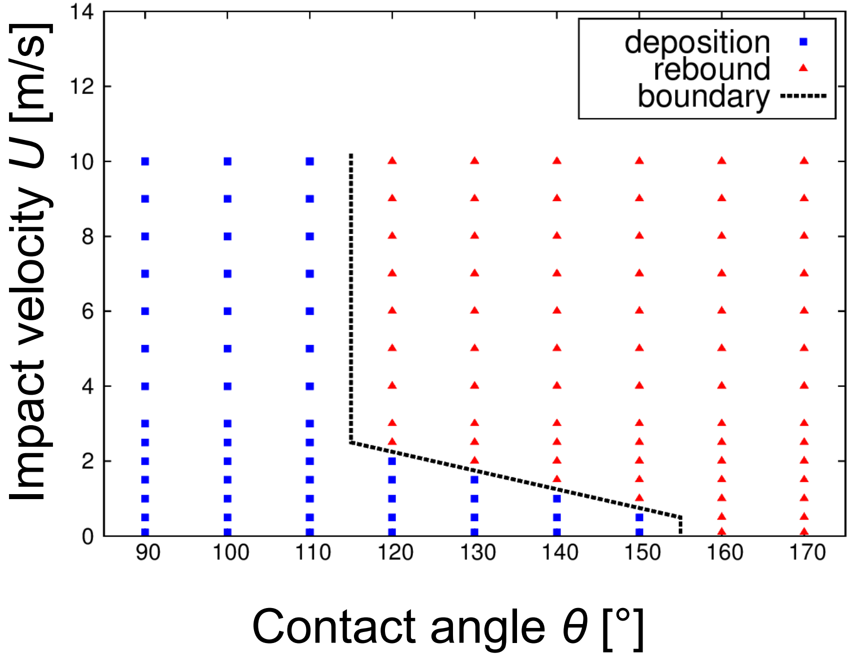




- Physical properties of DEF
  - $\rho$ = 1090 kg/m$^3$
  - $\mu$ = 1.3 mPa s
  - $\sigma$ = 0.073 N/m
- Representative of a typical operating conditions:
  - ***D* = 0.07 mm**
  - ***U* = 7 m/s**
- Contact angle
  **90° < $\theta$ < 170°**
- 0<*We*<90
  0<*Re*<500
  **splash doesn't occur**

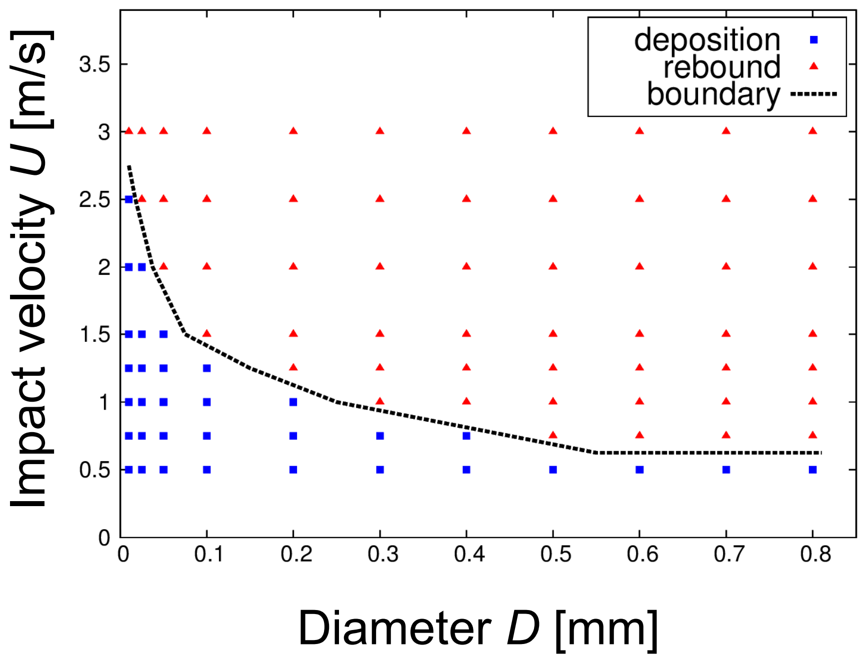
# Regime maps for DEF-droplet impacting on wall

Deposition　　Rebound

*U* - *θ* map, *D* fixed as 0.07 mm

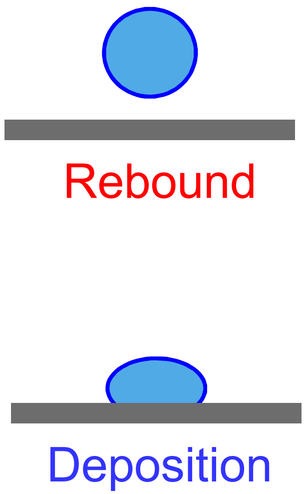


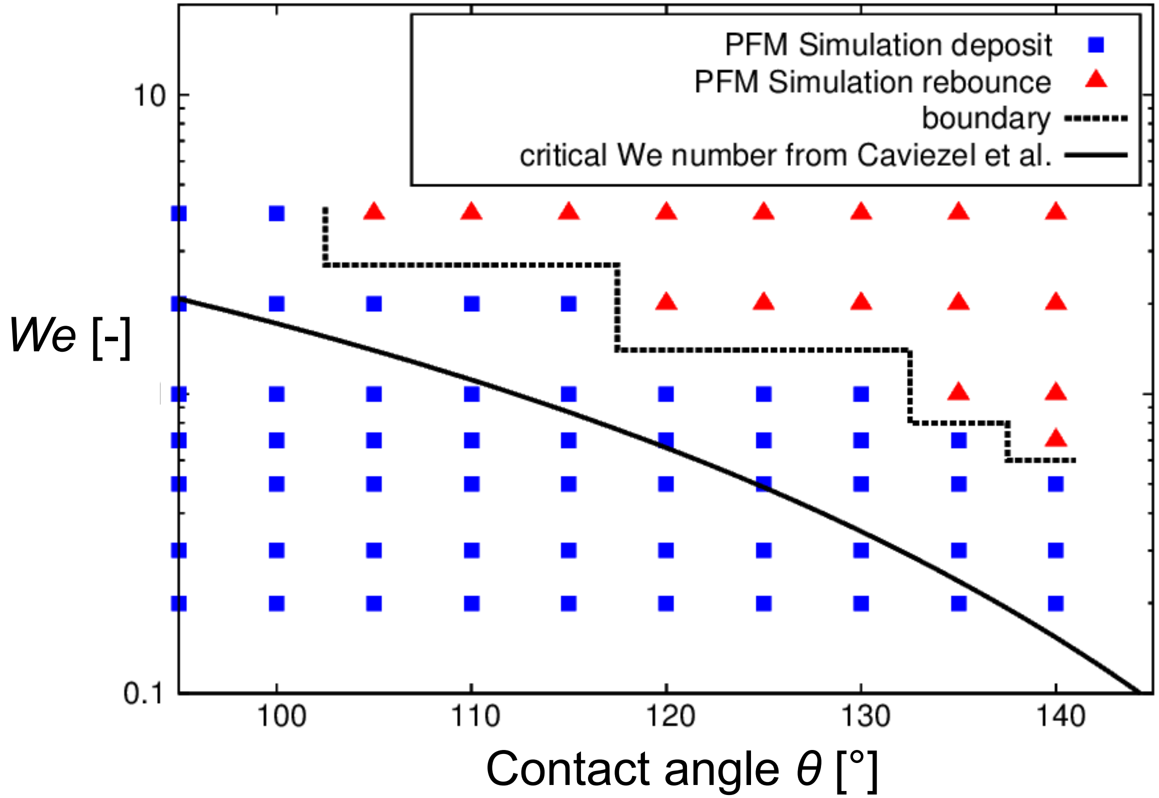

*U* - *D* map, *θ* fixed as 130°



# Comparison with Caviezel theory

- Caviezel et al. (2008) proposed an analytical limit between deposition and rebound regime based on Weber number and contact angle
  - valid for negligible viscous dissipation

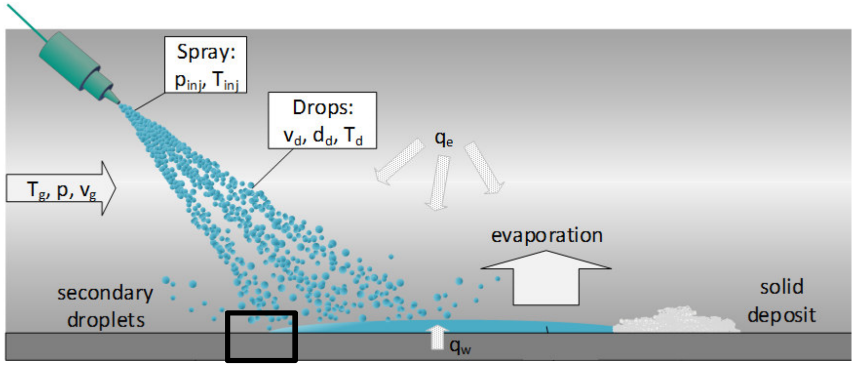



📖 Caviezel et al. *Microfluidics and Nanofluidics* **2008**, 5(4): 469-478

# Conclusions and outlook

- The numerical code can reproduce droplet rebound on micro-structured surface and on smooth surface using very large contact angle
- The numerical code is validated for instantaneous droplet shape, spread factor and contact time
- Rebound occurrence is determined by contact angle together with impact velocity and diameter (or Weber number)
- Outlook: multiple droplet coalescence on solid surface



# Acknowledgement for Financial Support

- Friedrich und Elisabeth Boysen-Stiftung
- DFG foundation, SFB/Transregio 150 “Turbulent, chemical reacting multi-phase flows near walls”