

#### Jahrestreffen der DECHEMA-Fachgruppen Aerosoltechnik, Gasreinigung, Mehrphasenströmung und Partikelmesstechnik 28. – 30. März 2023, Paderborn

#### Entwicklung einer universellen analytischen Beziehung für die maximale Ausbreitung eines Tropfens beim Aufprall auf eine Wand

Development of a universal analytical relationship for the maximum spread of a drop when hitting a wall



Wörner et al., Applied Mathematical Modeling 95 (2021) 53-73

Drop impact on a <u>hydrophilic</u> surface Visser et al., *Soft Matter* **11** (2015)

#### www.kit.edu

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#### **Motivation**



Predicting the interaction of a single drop with a dry horizontal surface



#### Objective

- Maximum spread diameter depends on physical properties, on drop size/velocity and on wettability of the solid surface
  - Weber number  $We = \rho d_0 u_0^2 / \sigma$
  - Reynolds number  $Re = \rho d_0 u_0 / \mu$  (or  $Oh = \sqrt{We} / Re$ )
  - Contact angle  $\theta$  (static, equilibrium, advancing, receding, dynamic)
- Classification of theoretical models for maximum spreading
  - Models based on scaling relations valid in certain regimes
  - Mechanistic models based on momentum or energy balance
- A universal mechanistic model based on the energy balance is missing
  - Difficulty with low/high viscosity liquids and hydrophilic/hydrophobic surfaces
  - Here, significant progress in development of a <u>universal energy balance model</u> is reported



 $u_0$ 



 $d_0$ 

dror

g



### Outline

#### Introduction

Motivation and objective

#### Literature survey on models for maximum spreading

- Energy balance (EB) approach
- Scaling in different regimes
- New concepts for closure terms in the energy balance
  - Gas-liquid surface area
  - Dissipation upon maximum spread
- Closure of dissipation function and test of the novel model
  - Parameter determination by asymptotic analysis and experiments
  - Test against experimental data sets from literature
- Conclusions and outlook

### **Balance of mechanical energy**



- General energy balance between initial state (t = 0) and state at time t > 0
  - Consideration of liquid kinetic energy  $(E_k)$  and surface energy  $(E_s)$
  - Gravitational energy  $(E_a)$  can be neglected because  $E_a/E_s$  is typically small
  - Energy lost by (viscous) dissipation  $W \ge 0$
  - Normalization of EB by  $\sigma S_0$ , where  $S_0$  denotes the initial gas-liquid surface area

$$\frac{E_{k,0} - E_k(t)}{\sigma S_0} + \frac{E_{s,0} - E_s(t)}{\sigma S_0} = \frac{W(t)}{\sigma S_0} \qquad \frac{E_{k,0}}{\sigma S_0} = \frac{(\frac{1}{2}\rho u_0^2)(\frac{\pi}{6}d_0^3)}{\sigma \pi d_0^2} = \frac{\frac{\pi}{12}\rho u_0^2 d_0^3}{\sigma \pi d_0^2} = \frac{We}{12}$$

• Energy balance at time of maximum spreading  $(t = t_m)$  assuming  $E_k(t_m) = 0$ 



 $\rightarrow$  see slides 11 and 12

## Scaling in <u>capillary</u> regime $-\beta_m \sim We^{1/2}$



Young's equation

Initial kinetic energy is completely converted in surface energy at max. spread

$$\frac{E_{k,0}}{\sigma S_0} = \frac{We}{12} \sim \frac{E_{s,m}}{\sigma S_0}$$

- Estimation of surface energy
  - Change of Gibbs free interfacial energy (per unit area)  $\Delta G = \underbrace{\gamma_{gl}}_{=\sigma} + \underbrace{\gamma_{sl} \gamma_{sg}}_{-\sigma \cos \theta} = \sigma(1 \cos \theta)$  At maximum spread
  - At maximum spread

$$\frac{E_{s,m}}{\sigma S_0} \sim \frac{\Delta G \cdot A_{wet}}{\sigma S_0} = \frac{\sigma (1 - \cos \theta) \frac{\pi}{4} d_m^2}{\pi \sigma d_0^2} = \frac{1 - \cos \theta}{4} \beta_m^2 \quad \rightarrow \quad \beta_m \sim \sqrt{\frac{3We}{1 - \cos \theta}} \sim We^{1/2}$$

R.E. Ford, C.G.L. Furmidge, Impact and spreading of spray drops on foliar surfaces, Society of Chemical Industry, London, 1967, 417-432 B.W. Collings, A.J. Markworth, J.K. McCoy, J.H. Saunders, J. Mater. Sci. 25 (1990) 3677-3682 I. Bennett, D. Poulikakos, J. Mater. Sci. 28 (1993) 963-970



### Scaling in <u>capillary</u> regime $-\beta_m \sim We^{1/4}$

- Experiments of Clanet et al. (2004)
  - Impact of water droplets on smooth superhydrophobic surface ( $\theta_{eq} = 170^\circ$ )
  - Observed experimental scaling  $\beta_m \sim We^{1/4}$
  - Explanation by "effective gravity" force due to drop deceleration after impact
- Exp. by Attane et al. (2007), Laan et al. (2014)
  - Scaling  $\beta_m \sim We^{1/4}$  is consistent for water but does not hold for other liquids (e.g. blood)
  - The exact conditions under which this scaling occurs are still unclear



C. Clanet, C. Beguin, D. Richard, D. Quere, Maximal deformation of an impacting drop, *J. Fluid Mech.* 517 (2004) 199-208
 P. Attane, F. Girard, V. Morin, An energy balance approach of the dynamics of drop impact on a solid surface, *Phys. Fluids* 19 (2007) 012101
 N. Laan, K.G. de Bruin, D. Bartolo, C. Josserand, D. Bonn, *Physical Review Applied* 2 (2014) 044018

### Scaling in viscous regime



Initial kinetic energy is mainly dissipated at maximum spread

$$\frac{E_{k,0}}{\sigma S_0} = \frac{We}{12} \sim \frac{W_m}{\sigma S_0} \qquad \qquad W_m = \int_{0}^{t_m} \int_{V_{drop}} \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) : \nabla \mathbf{u} \, \mathrm{d}V \mathrm{d}t$$

Chandra & Avedisian (1991)

$$W_m \sim \mu \frac{u_0^2}{h_m^2} \cdot \frac{d_0^3}{u_0} \cdot \frac{d_0}{u_0} \sim \frac{\mu u_0 d_0^4}{h_m^2}$$

$$h_m d_m^2 \sim d_0^3 \longrightarrow \beta_m \sim Re^{1/4}$$

volume conservation ( $h_m$  = drop height at maximum spread)

Clanet et al. (2004)

$$W_m \sim \mu \frac{u_0^2}{h_m^2} \cdot \frac{d_m d_0^2}{u_0} \cdot \frac{d_0}{u_0} \sim \frac{\mu u_0 d_m d_0^3}{h_m^2} \longrightarrow \beta_m \sim Re^{1/5} \quad (\text{Scaling observed in experiment of Madejski})$$

S. Chandra, C.T. Avedisian, *Proc. Royal Society London. Series A: Mathematical and Physical Sciences* 432 (1991) 13-41
 C. Clanet, C. Beguin, D. Richard, D. Quere, Maximal deformation of an impacting drop, *J. Fluid Mech.* 517 (2004) 199-208
 J. Madejski, Solidification of droplets on a cold surface, *Int. J. Heat Mass Transf.* 19 (1976) 1009-1013

#### **Transition between both regimes**

- Capillary regime P < 1
  - All initial energy is transferred in surface energy at maximum spreading
- Viscous regime P > 1
  - Clanet et al. (2004), Fedorchenko et al. (2005), Roisman (2009)
- Impact parameter P serves to distinguish both regimes
  - b = 4/5 (Clanet), b = 1/2 (Fedorchenko), b = 2/5 (Eggers)
- Rescaling methods (e.g. Laan et al., 2014)
  - Regime discrimination parameter A = 1.24 is of order 1
- C. Clanet, C. Beguin, D. Richard, D. Quere, Maximal deformation of an impacting drop, J. Fluid Mech. 517 (2004) 199-208
- A.I. Fedorchenko, A.-B. Wang, Y.-H. Wang, *Phys. Fluids* **17** (2005) 093104
- I.V. Roisman, Inertia dominated drop collisions, Part II., *Phys. Fluids* **21** (2009)
- J. Eggers, M.A. Fontelos, C. Josserand, S. Zaleski, *Phys. Fluids* 22 (2010) 062101
- III N. Laan, K.G. de Bruin, D. Bartolo, C. Josserand, D. Bonn, *Physical Review Applied* 2 (2014) 044018



$$P = \frac{We}{Re^b}$$

 $\beta_m \sim W e^{1/2}$ 

 $\beta_m \sim Re^{1/5}$ 



### **EB** – Modeling of gas-liquid surface area $s_m$





R.E. Ford, C.G.L. Furmidge, Impact and spreading of spray drops on foliar surfaces, Society of Chemical Industry, London, 1967, 417-432
 T. Mao, D.C.S. Kuhn, H. Tran, Spread and rebound of liquid droplets upon impact on flat surfaces, *AIChE J.* 43 (1997) 2169-2179
 H. Park, W.W. Carr, J. Zhu, J.F. Morris, Single drop impaction on a solid surface, *AIChE J.* 49 (2003) 2461-2471

# **EB** – Modeling of dissipation $w_m$

- Mechanistic dissipation models  $W_m = \int_{0}^{t_m} \int_{V_{\text{disc}}} \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^{\text{T}} \right) : \nabla \mathbf{u} \, \mathrm{d}V \mathrm{d}t$ 
  - $\approx \mu \cdot u_c^2 \cdot L_c^{-2} \cdot t_m \cdot V_{\rm diss}$
  - Various proposals for  $u_c, L_c, t_m$ all yield  $w_m = W_m/(\sigma S_0) \sim \beta_m^n$ with exponent n = 2 - 6.5
- Combinations of models for s<sub>m</sub> and w<sub>m</sub> give energy balance models of very different form
- Is dissipation model appropriate? Different dissipation contributions: viscous b.l., c.l. friction, ...



Wildeman et al. (2016)<sup>9</sup>

Literature

 $+\left(\frac{1}{D} + \frac{1}{D}\sin\theta_{a}\right)\left(\frac{3}{\sqrt{Re}} - \cos\theta_{a}\right)$  $\frac{12}{We} + \frac{1}{2} = \beta_{max}^{2}\frac{3(1 - \cos\theta)}{We} + \frac{\alpha}{\sqrt{Re}}\beta_{max}^{2}\sqrt{\beta_{max} - 1}$ no-slip, We > 30

Energy models

Table from Aksoy et al., Phys. Fluids 34 (2022) 042106





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#### New concepts for closure terms in the energy balance

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#### New model for gas-liquid surface area



#### New concept for modeling of dissipation



Existing models do not respect the upper physical bound for dissipation
 Energy balance between initial state and terminal deposition state ( $t = t_{eq}$ )

$$\frac{We}{12} + 1 - \frac{S(t_{eq})}{\underbrace{S_0}_{=s_{eq}}}{\underbrace{S_0}_{=s_{eq}}} + \frac{\cos\theta}{4} \beta_{eq}^2 = \underbrace{\frac{W(t_{eq})}{\sigma S_0}}_{=w_{eq}} \longrightarrow w_{eq} = \frac{We}{12} + \underbrace{1 - \sqrt[3]{(2 + \cos\theta)(1 - \cos\theta)^2 / 4}}_{0 \le w_{eq,s} \le 1}$$

$$s_{eq} = s_{sc}(\theta) = \sqrt[3]{\frac{2}{(2 + \cos\theta)^2(1 - \cos\theta)}} \qquad \beta_{eq} = \beta_{sc}(\theta) = \sqrt[3]{\frac{4\sin^3\theta}{(2 + \cos\theta)(1 - \cos\theta)^2}}$$

<u>New model</u> for dissipation upon maximum spread
 Dissipation function *f<sub>w</sub>* needs to be determined

$$w_m = f_w w_{eq}, \quad 0 \le f_w \le 1$$



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#### Energy balance with the two new concepts



Introducing the proposed models for  $s_m$  and  $w_m$  in the energy balance yields

$$\frac{1}{4}\frac{\beta_m^4}{\beta_m^2 + 4a} - \frac{\cos\theta}{4}\beta_m^2 - \left[\frac{We}{12} + 1 - a - f_w\left(\frac{We}{12} + 1 - \sqrt[3]{(2 + \cos\theta)(1 - \cos\theta)^2/4}\right)\right] = 0$$

Solution of this fourth order equation in  $\beta_m$ 

$$\beta_m = \sqrt{\frac{2(Q + a\cos\theta) + 2\sqrt{(Q + a\cos\theta)^2 + 4aQ(1 - \cos\theta)}}{1 - \cos\theta}}$$

$$Q > 0 \rightarrow \beta_m > 0$$

Assumed relationship for the dissipation function

The exponents b of the Reynolds number and c of the impact parameter are determined by asymptotic analysis

$$f_w = \frac{P^c}{A + P^c}$$

 $P = WeRe^{-b}$ 

### Asymptotic analysis (a = 1) - Case 1



• Assumption  $(Q + \cos \theta)^2 \gg 4Q(1 - \cos \theta)$  i.e.  $Q \gg 4 - 6\cos \theta$ 

$$\beta_m = \sqrt{\frac{2(Q + \cos\theta) + 2\sqrt{(Q + \cos\theta)^2 + 4Q(1 - \cos\theta)^2}}{1 - \cos\theta}} \approx \sqrt{\frac{4Q}{1 - \cos\theta}} \approx \sqrt{\frac{4}{1 - \cos\theta}} \frac{A}{A + P^c} \frac{We}{12}$$

$$P^c = We^c Re^{-bc}$$

• Assumption  $We \gg 12$ 

$$Q = \frac{We}{12} - f_w \left( \frac{We}{12} + 1 - \sqrt[3]{(2 + \cos\theta)(1 - \cos\theta)^2 / 4}} \right) \rightarrow Q \approx (1 - f_w) \frac{We}{12} = \frac{A}{A + P^c} \frac{We}{12}$$

Capillary regime  $P^{c} < A$  $\beta_{m} \approx \sqrt{\frac{We}{3(1-\cos\theta)}} \sim We^{1/2} \checkmark$ Viscous regime  $P^{c} > A$   $P = WeRe^{-2/5}$   $P = WeRe^{-2/5}$   $\beta_{m} \approx \sqrt{\frac{AP^{-c}We}{3(1-\cos\theta)}} \sim We^{(1-c)/2}Re^{bc/2} \stackrel{!}{=} Re^{1/5} \rightarrow c = 1, b = 2/5$ 

### Asymptotic analysis (a = 1) - Case 2



• Assumption  $(Q + \cos \theta)^2 \ll 4Q(1 - \cos \theta)$  i.e.  $Q \ll 4 - 6\cos \theta \le 10$ 

$$\beta_m = \sqrt{\frac{2(Q + \cos\theta) + 2\sqrt{(Q + \cos\theta)^2 + 4Q(1 - \cos\theta)}}{1 - \cos\theta}} \approx \sqrt[4]{\frac{16Q}{1 - \cos\theta}} \approx \sqrt[4]{\frac{16}{1 - \cos\theta}} \frac{A}{A + P^c} \frac{We}{12}$$

$$P^c = We^c Re^{-bc}$$

• Assumption  $We \gg 12$ 

$$Q = \frac{We}{12} - f_w \left( \frac{We}{12} + 1 - \sqrt[3]{(2 + \cos\theta)(1 - \cos\theta)^2 / 4}} \right) \rightarrow Q \approx (1 - f_w) \frac{We}{12} = \frac{A}{A + P^c} \frac{We}{12}$$

Capillary regime 
$$P^c < A$$
  
 $\beta_m \approx \sqrt[4]{\frac{4}{3} \frac{We}{1-\cos\theta}} \sim We^{1/4} \checkmark$ 
Viscous regime  $P^c > A$ 
Clanet (2004)  
 $P = WeRe^{-4/5}$   
 $\beta_m \approx \sqrt[4]{\frac{4}{3} \frac{AP^{-c}We}{1-\cos\theta}} \sim We^{(1-c)/4}Re^{bc/4} \stackrel{!}{=} Re^{1/5} \rightarrow c = 1, b = 4/5$ 

#### **Determination of parameter** *A* in $f_w = P/(A + P)$

Evaluation of relative dissipation from literature data on maximum spread



#### **Determination of parameter** A in $f_w = P/(A + P)$

Evaluation of relative dissipation from literature data on maximum spread



Seven different liquids, 57 < We < 460, 4 < Re < 9200,  $\theta_a = 100^\circ$  (294 data points)

III Y.T. Aksoy, P. Eneren, E. Koos, M.R. Vetrano, Spreading of a droplet impacting on a smooth flat surface, *Phys. Fluids* 34 (2022) 042106 C. Clanet, C. Beguin, D. Richard, D. Quere, Maximal deformation of an impacting drop, J. Fluid Mech. 517 (2004) 199-208

#### Determination of parameter A (continued)



Regime discrimination parameter *A* depends on the advancing contact angle  $\theta_a$ Experimental data of Lee et al. (2016); reported  $\theta_d$  and  $\theta_{eq}$ , assumption  $\theta_a = \theta_d$ 

Three different liquids and surfaces, 1 < We < 1200, 40 < Re < 17800,  $44^{\circ} < \theta_a < 123^{\circ}$ 



Model for the dissipation function
$$f_{w} = \frac{WeRe^{-2/5}}{\underbrace{1.2 - \cos \theta_{a}}_{=A(\theta_{a})} + WeRe^{-2/5}}$$
For fixed impact parameter P = WeRe^{-2/5}

■ For fixed impact parameter P = WeRe<sup>-2/5</sup> hydrophobic surfaces dissipate less energy upon maximum spreading as compared to hydrophilic surfaces → enables drop rebound

I.B. Lee et al., Universal rescaling of drop impact on smooth and rough surfaces, J. Fluid Mech. 786 (2016) R4

#### Test of the proposed new model



- Parity plot against experimental data
  - Agreement is within  $\pm 20\%$
  - For all experimental data it is Q > 0

Y.T. Aksoy, P. Eneren, E. Koos, M.R. Vetrano, Spreading of a droplet impacting on a smooth flat surface, *Phys. Fluids* 34 (2022) 042106
 J.B. Lee et al., Universal rescaling of drop impact on smooth and rough surfaces, *J. Fluid Mech.* 786 (2016) R4

C. Clanet, C. Beguin, D. Richard, D. Quere, Maximal deformation of an impacting drop, J. Fluid Mech. 517 (2004) 199-208





#### Conclusions



- Existing energy balance models for max. spread have two shortcomings
  - Gas-liquid area is not properly modelled for superhydrophobic surfaces (low  $\beta_m$ )
  - Models for dissipation to do not account for proper upper physical limit
- Proposal of new concepts for the two closure terms in the energy balance
  - <u>Approximate spherical cap (asc) model for gas-liquid surface area</u>
  - Model for dissipation that respects the upper physical limit
- Proposal of a new 'universal' energy balance model for maximum spread
  - Model comprises power law scaling for viscous regime and <u>both</u> capillary regimes
  - Model is explicit and thus no iteration is required
  - **Dissipation function is determined from exp. data with wide ranges of** We, Re,  $\theta_a$
  - Model is in good agreement with exp. with a maximum deviation of about 20%

#### Outlook



#### Directions for model refinement

- The current model assumes zero kinetic energy at maximum spread
- The current model for total dissipation  $w_{eq}$  assumes zero c.a. hysteresis
- Test model against further experimental and numerical data from literature
- **Goal**: regime discrimination parameter  $A = A(\theta_a, \Delta \theta)$ 
  - $\rightarrow$  measurement of the advancing and the receding contact angle is required

#### Extend model to surfaces with regular roughness

Wenzel and Cassie-Baxter wetting states



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Deutsche DFG Peutsche Forschungsgemeinschaft

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I Y.T. Aksov, P. Eneren, E. Koos, M.R. Vetrano, Spreading of a droplet impacting on a smooth flat surface, *Phys. Fluids* **34** (2022) 042106 III J.B. Lee et al., Universal rescaling of drop impact on smooth and rough surfaces, J. Fluid Mech. 786 (2016) R4