A Cross-Validation Study of Computational Methods for Droplet Impact

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Introduction

- In this talk, we look droplet impact on a smooth surface.
- **Impact, Spread, Retraction**

  In the land of splashes, what the scientist knows as Inertia and Surface Tension are the sculptors in liquids, and fashion from them delicate shapes none the less beautiful because they are too ephemeral for any eye but that of the high-speed camera [Yarin, Annu. Rev. Fluid Mech. (2006)]

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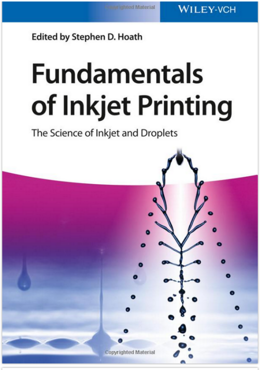
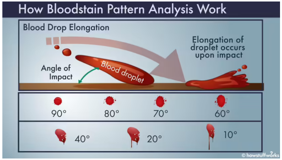
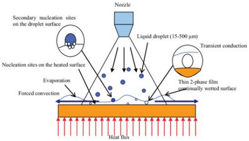
- Highlights the importance of **parameters** in such studies; key parameters are the **Weber number**, $\mathrm{We} =$ Inertia/Surface Tension, and the **Reynolds number** – *sculptor has two tools*.
- Droplet spreading below **splash threshold**, $K \lesssim 3,000$, where $K = \mathrm{We}\sqrt{\mathrm{Re}}$

Motivation

- Industry (inket printing, cooling, bloodstain pattern analysis)







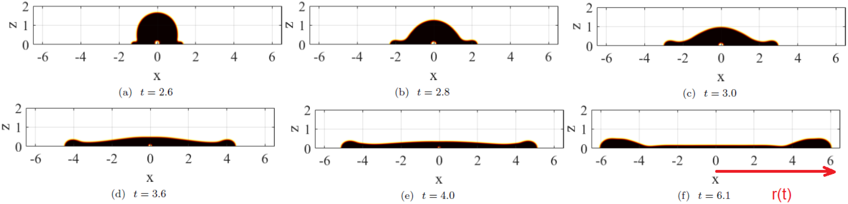
- **Scientific curiosity**...

Motivation, continued

Model systems in Fluid Mechanics, metaphors for more complicated realistic systems, help with understanding.

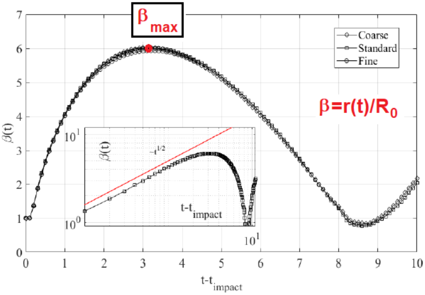
- Exactly solvable:
  1. Couette Flow, Poiseuille Flow
  2. Stokes Flow past a sphere
  3. Point vortices
- Significant analytical progress possible:
  1. Navier-Stokes Flow past a cylinder
  2. Blasius Boundary Layer
  3. Parallel flow (Orr–Sommerfeld)
  4. Free-Surface Flow, Long-wave limit (Shallow water, lubrication theory, Benney equation...)
- Other simple systems enabling significant numerical or experimental investigation:
  1. Turbulence in a periodic box;
  2. **Droplet Impact**

Aim of Present Work



Want to find $r_{max}(\mathrm{We}, \mathrm{Re})$, or

$$\beta_{max} = r_{max}/R_0.$$

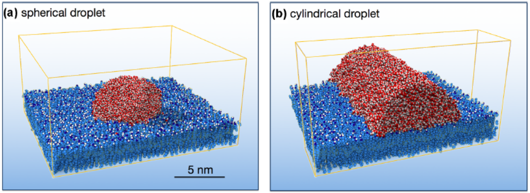


Point of departure

- Mechanistic models for β_{max} exist – based on energy budget.
- All terms in energy budget well modelled... except **dissipation**.
- At least two known loss channels in dissipation:
  - Boundary layer dissipation in lamella;
  - Head loss

This work uses 2D cylindrical droplet simulations to build up database of simulations, to better quantify dissipation loss.

Why 2D?



- 2D cylindrical droplets are not often encountered in nature.
- Easy to simulate numerically... but not a good enough reason to study them.

Energy-budget arguments in 2D lead to development of novel expressions for β_{max}, yet another test / validation of corresponding expressions for β_{max} in 3D.

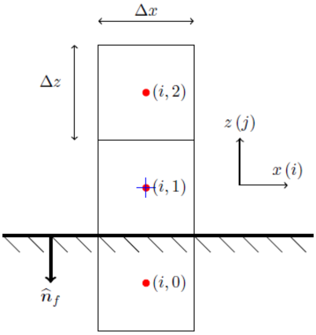
Methodology

- Incompressible Navier–Stokes equations (one-fluid formulation, Korteweg stress term for the modelling of the surface tension).
- Diffuse-Interface Method for Interface Capturing and contact-line dynamics, discretization on a MAC grid.
- Geometric boundary condition, θ_0 is the equilibrium contact angle:

$$\widehat{\boldsymbol{n}_f} \cdot \nabla C = -\tan\left(\tfrac{1}{2}\pi - \theta_0\right) \left|\nabla C - \left(\widehat{\boldsymbol{n}_f} \cdot \nabla C\right) \widehat{\boldsymbol{n}_f}\right|,$$

- Implementation of BC on MAC grid:

$$C_{i,0} = C_{i,2} + \tan\left(\tfrac{1}{2}\pi - \theta_0\right) \left|C_{i+1,1} - C_{i-1,1}\right|$$



Setup

Realistic parameter values for mm scale droplet:

	Water (L)	Air (G)
Dynamic Viscosity (μ)	$8.9 \times 10^{-4}\,\mathrm{Pa\,s}$	$1.837 \times 10^{-5}\,\mathrm{Pa\,s}$
Density (ρ)	$1000\,\mathrm{kg\,m^{-3}}$	$1.225\,\mathrm{kg\,m^{-3}}$

Droplet Radius (R_0)	$3\,\mathrm{mm}$
Surface Tension (σ)	$0.072\,\mathrm{N\,m^{-1}}$

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Bond Number scaling: timescale $T_0 = R_0/U_0$, $U_0 = \sqrt{gR_0}$, hence strength of surface tension is $1/\mathrm{Bo}$:

$$\mathrm{Bo} = \frac{\rho_L g R_0^2}{\sigma} = 1.226.$$

Also,

$$\mathrm{Re} = \frac{\rho_L R_0 U_0}{\mu_L} = 578.0.$$

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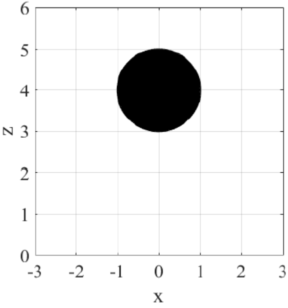
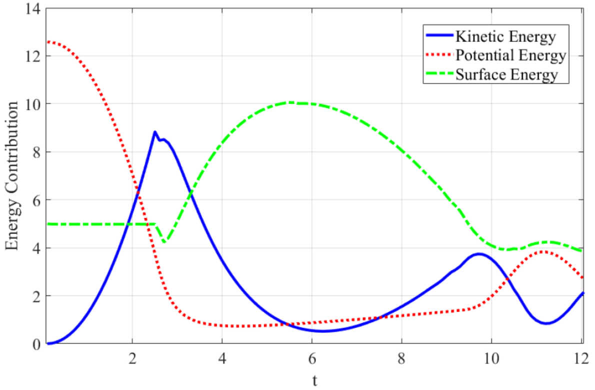
Droplet released from a height:



Energy Budget

Energy of Droplet:

$$E_D = \underbrace{\int_\Omega \frac{1}{2}\boldsymbol{u}^2 \left[\frac{1}{2}(1+C)\right] \mathrm{d}^3x}_{\text{Kinetic}} + \underbrace{\int_\Omega z \left[\frac{1}{2}(1+C)\right] \mathrm{d}^3x}_{\text{Gravitational}} + \underbrace{F[C]}_{\text{Surface (Cahn–Hilliard)}}$$



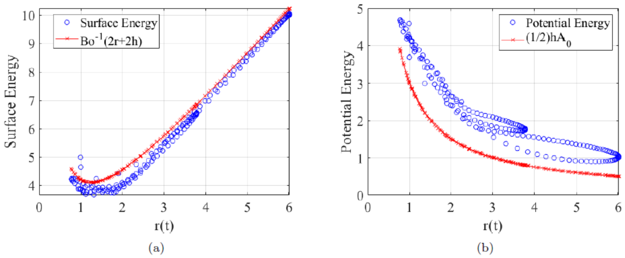
Energy budget for the case $\theta_0 = 90°$.

Energy Budget (continued)

Gravitational and surface energy terms are well approximated by treating cylindrical droplet as a sheet (3D equivalent would be disc):

$$\text{Surface Energy} \approx \frac{1}{\mathrm{Bo}}\left(2r+2h\right), \qquad \text{Gravitational Energy} \approx \tfrac{1}{2}hA_0,$$

here $A_0 = \pi R_0^2$ is the initial droplet area (volume), and by conservation of mass, $h = A_0/(2r)$ (**nondimensionless**).



Dependency of the different energy terms on the instantaneous droplet extent $r(t)$

Droplet Spread Correlation

2D droplet spread correlation for β_{max} via energy argument. Initial energy:

$$E_{init} = \rho_L g H_0(\pi R_0^2 \lambda) + 2\pi R_0 \sigma \lambda, \qquad \lambda = \text{length of cylinder (irrelevant)}$$

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At maximum extent, energy is all potential (no kinetic):

$$E_{final} = \sigma \left(\Pi - 2 r_{max} \cos\theta_0 \right) \lambda + \rho_L g (\pi R_0^2 \lambda) d_c$$

where

- Π is the droplet perimeter;
- $\sigma(-2 r_{max} \cos\theta_0)\lambda$ is the energy term coming from the liquid-substrate interaction (Laplace–Young condition);
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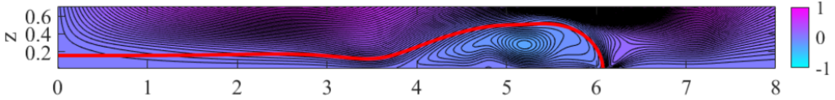
Energy budget:

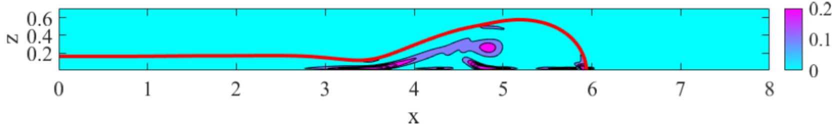
$$E_{init} = E_{final} + \Delta E, \qquad \Delta E = \text{Energy loss due to dissipation}$$

Dissipation

ΔE is the total energy loss up to the time of maximum spreading. Knowledge of internal structure of droplet required:



Instantaneous streamfunction at $t = 6.1$, near the point of maximum droplet spreading.



Instantaneous dissipation function $\text{Diss} = (\widehat{\mu}/\text{Re})\left(u_x^2 + u_z^2 + w_x^2 + w_z^2\right)$ at $t = 6.1$.

Evidence of **boundary layer** in lamella and **recirculation zone** in rim – boundary-layer dissipation modelled in standard fashion:

$$\Delta E_{bl} \approx \text{Const.} \times \frac{1}{\sqrt{\text{Re}}}\rho_L U_0^2 \beta_{max}\sqrt{\beta_{max} - 1}(R_0^2\lambda).$$

Head Loss

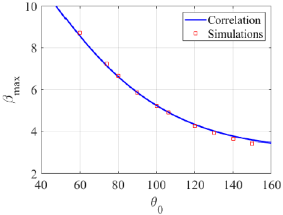
Dissipation in recirculation zone modelled as 'head loss':

> *According to Wilderman et al. and Villermaux and Bossa, the head loss can be estimated as a simple fraction of the initial kinetic energy of the droplet prior to impact.*[1]

Final result – correlation for β_{max}, valid for cylindrical droplets:

$$\pi(H_0/R_0) + \frac{2\pi}{\mathrm{Bo}} = \frac{1}{\mathrm{Bo}}\left[2\beta_{max}\left(1-\cos\theta_0\right) + \frac{\pi}{\beta_{max}}\right] + \pi\left(\frac{\pi}{4\beta_{max}}\right) + \frac{2a}{\sqrt{\mathrm{Re}}}\beta_{max}\sqrt{\beta_{max}-1} + \pi(H_0/R_0)b.$$

Parameters a and b fixed once and then correlation is used predictively:



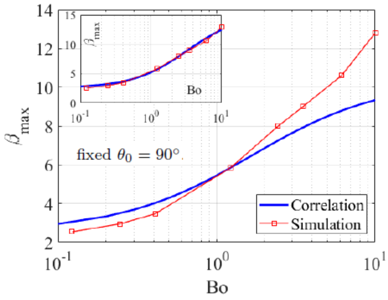
Dependence of β_{max} on the static contact angle for fixed Bo and Re. Squares: Simulations. Solid line: correlation

[1] Wildeman, Visser, Sun, and Lohse. On the Spreading of Impacting Drops. JFM (2016); Villermaux and Bossa. Drop Fragmentation on Impact. JFM (2011).

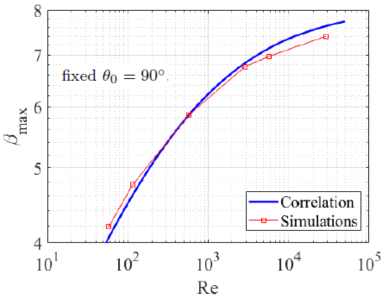
Wider Parameter Study

For wider parameter study, three parameters are required for fitting. Physical intuition: low surface tension, smaller rim, less head loss.

$$\Delta E_h \approx \left(\frac{b}{1 + c\mathrm{Bo}} \right) \rho_L g H_0 (\pi R_0^2 \lambda)$$



Fixed Re = 578 and varying Bo



Fixed Bo = 1.225 and varying Re

Results in Context of Existing Literature

Refer more easily to existing literature, no gravity, surface tension parametrized by $\mathrm{We} = \rho_L u_0^2 R_0 \sigma$. Two-parameter model becomes:

$$\frac{\pi}{2} + \frac{2\pi}{\mathrm{We}} = \frac{1}{\mathrm{We}}\left[2\beta_{max}(1-\cos\theta_0) + \frac{\pi}{\beta_{max}}\right] + \frac{2a}{\sqrt{\mathrm{Re}}}\beta_{max}\sqrt{\beta_{max}-1} + \frac{b\pi}{2}.$$

Limiting cases:

- $\mathrm{Re} \to \infty$ with We large but finite: For We large but finite, this further reduces to:

  $$\beta_{max} \approx \frac{\mathrm{We}\,\pi(1-b)}{4(1-\cos\theta_0)}.$$

  The equivalent scaling behavior for axisymmetric droplets is:

  $$\beta_{max} \approx \sqrt{\frac{4}{1-\cos\theta_0}\left[\tfrac{1}{12}(1-b)\mathrm{We}+1\right]},$$

  hence, $\beta_{max} \sim \mathrm{We}$ for cylindrical droplets and $\beta_{max} \sim \mathrm{We}^{1/2}$ for axisymmetric droplets.

Results in Context of Existing Literature (Continued)

- For $\mathrm{We} \to \infty$ energy balance reduces to:

$$\frac{\pi}{2}(1-b) \approx \frac{2a}{\sqrt{\mathrm{We}}}\beta_{max}\sqrt{\beta_{max}-1},$$

For Re large but finite, this gives $\beta_{max} \sim \mathrm{Re}^{1/3}$. The corresponding result for axisymmetric droplets is $\beta_{max} \sim \mathrm{Re}^{1/5}$.

Conclusions

- Looked at simulations of droplet impact and droplet spread in 2D cylindrical droplets.
- **Cross-validation** of simulation results using several approaches including independent OpenFOAM methodology (no time!).
- Formulated new theory for β_{max} as a function of Re and We.
- Indirectly validates the same approach for 3D droplets.
- Three-parameter model is a simple ‘fit’ accounting for head loss, a more detailed description of dissipation in rim is required in future.