

Evaporation of a thin sessile droplet in a shallow well

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Approach vs. Gradient Dynamics, 28th April to 3rd May 2019



- Motivation

Talk Outline

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- Assumptions and model

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- Comparison with experiments
- Extension to different well shapes
- Conclusions and further work

- Droplet evaporation occurs commonly in a vast range of circumstances in nature, industry and biology



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Motivation

- Droplet evaporation occurs every day, with applications in nature, industry and biology
- Crucial process in technological applications - inkjet printing, coating, spray cooling, etc.



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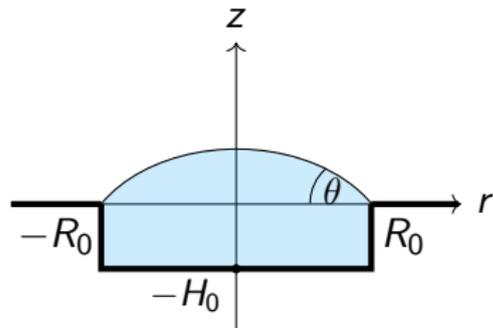
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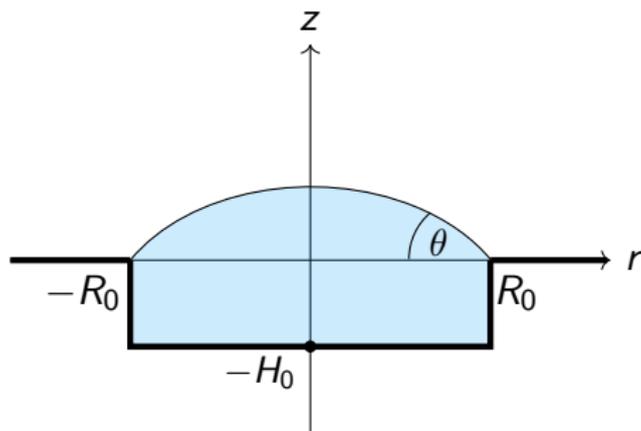
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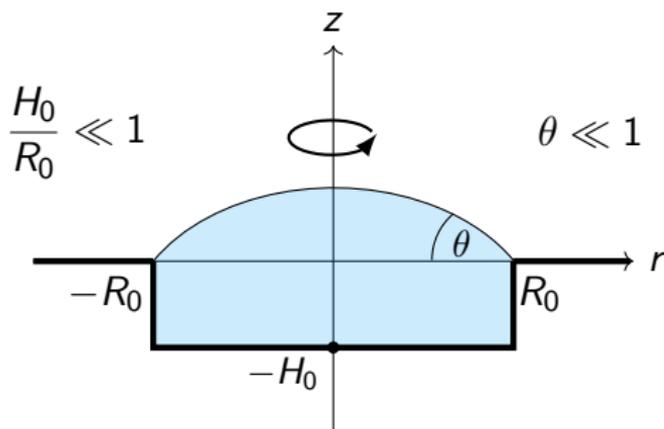
- Droplet evaporation occurs every day, with applications in nature, industry and biology
- Crucial process in technological applications - inkjet printing, coating, spray cooling, etc.
- The aim of the project is to understand droplet evaporation on textured substrates
- In this talk we look at the evolution and lifetime of a drying droplet in a shallow well



The Model - Assumptions

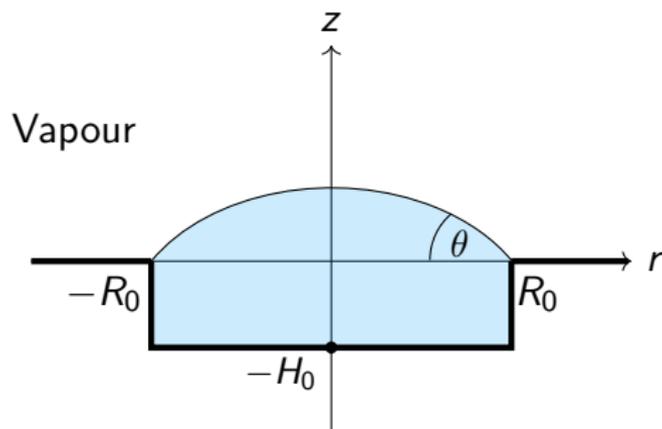


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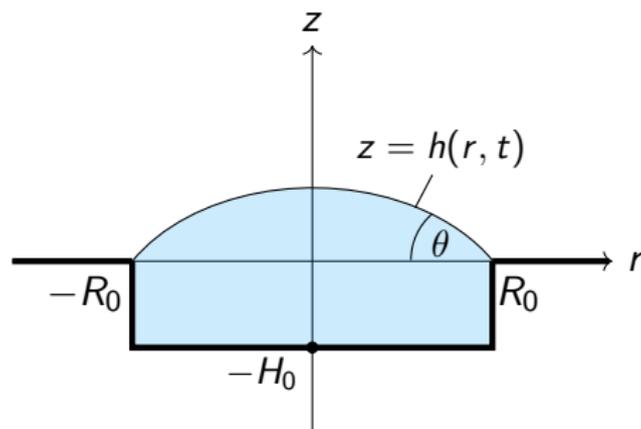
- We consider a **thin** axisymmetric sessile droplet in a **shallow** cylindrical axisymmetric well

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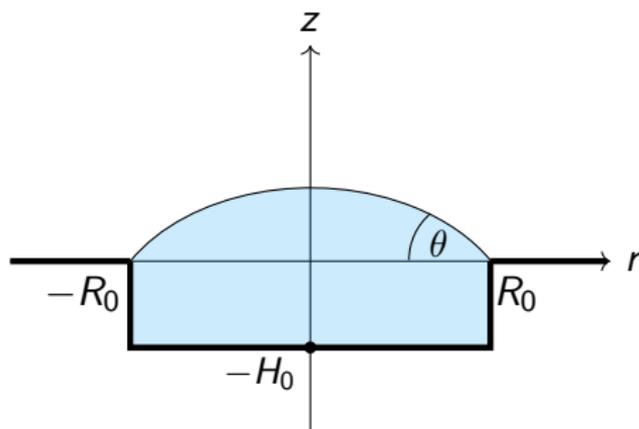
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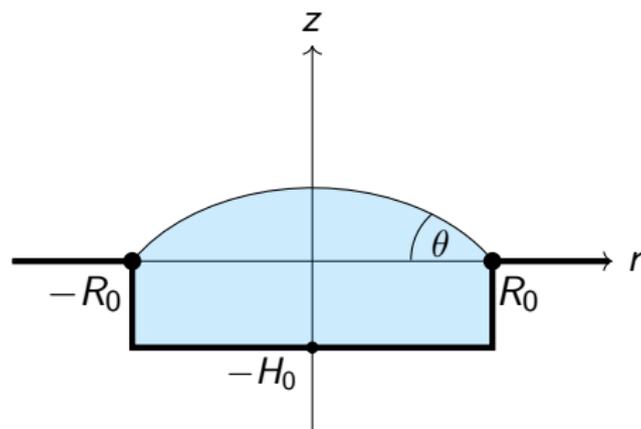
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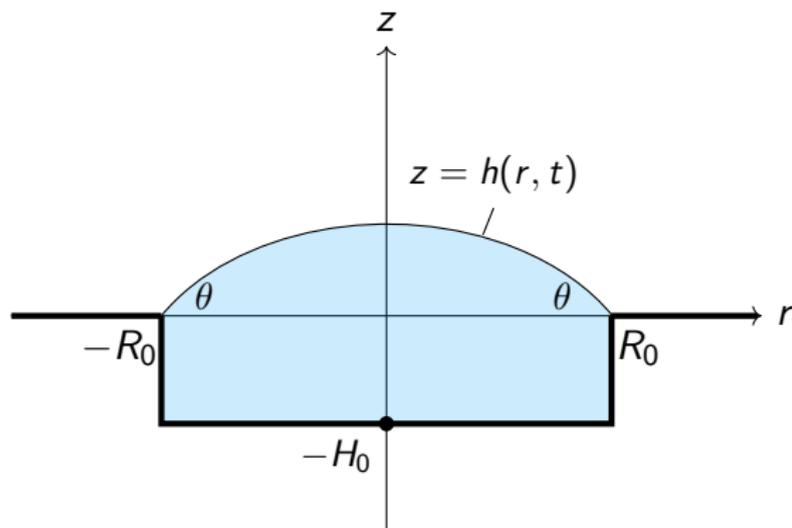
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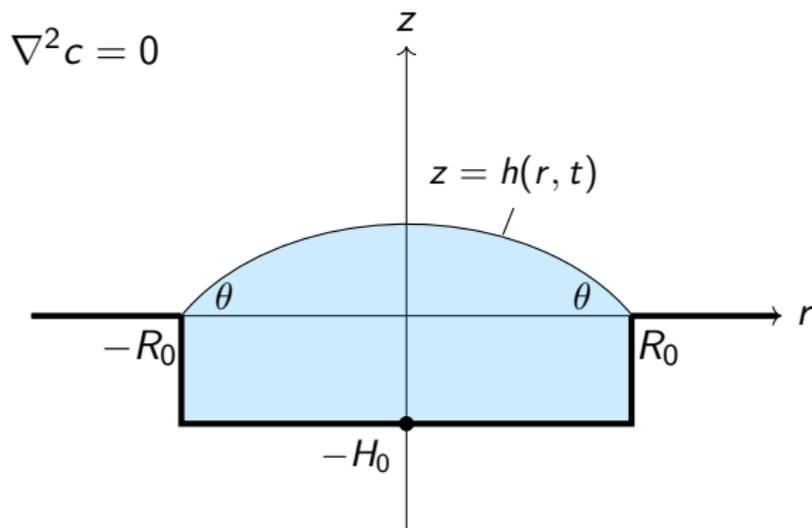


- We consider a **thin** axisymmetric sessile droplet in a **shallow** cylindrical axisymmetric well
- Diffusion-limited evaporation under ambient conditions
- Gravity is neglected - free surface determined by surface tension
- Free surface evolves quasi-statically
- Contact line remains pinned at the lip of the well throughout the entire evaporation

The Model - Prior to Touchdown

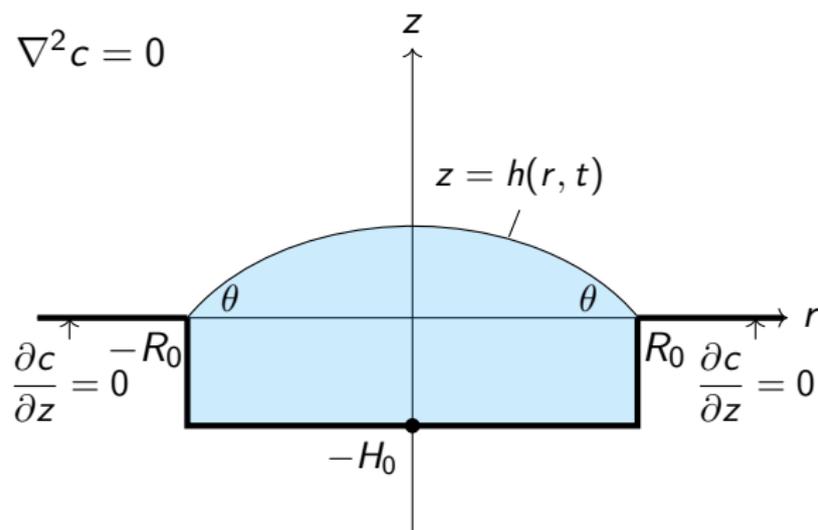


The Model - Prior to Touchdown



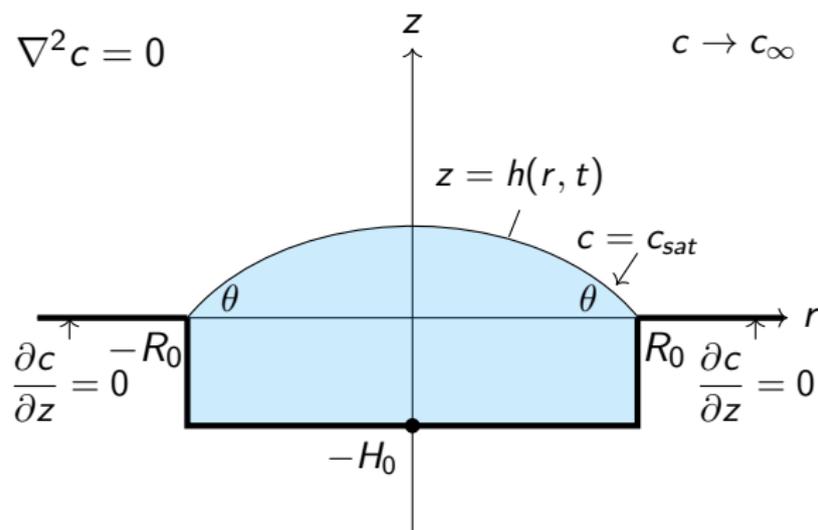
- c is the vapour concentration in the air

The Model - Prior to Touchdown



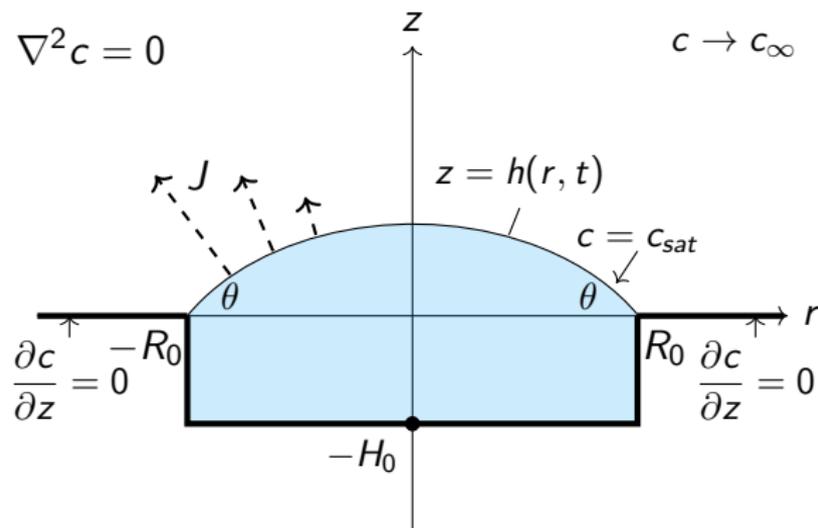
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The Model - Prior to Touchdown



- c is the vapour concentration in the air

The Model - Prior to Touchdown



- c is the vapour concentration in the air
- J is the local evaporative flux

The Model - Prior to Touchdown

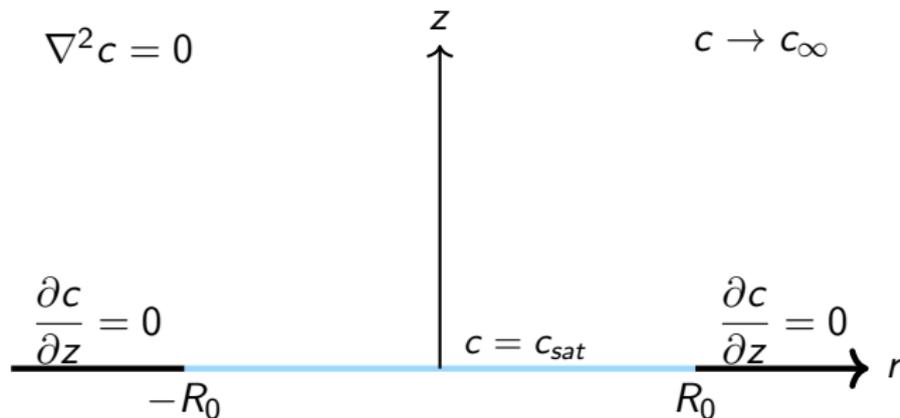


Figure: View of the droplet on the scale of the atmosphere

The Model - Prior to Touchdown

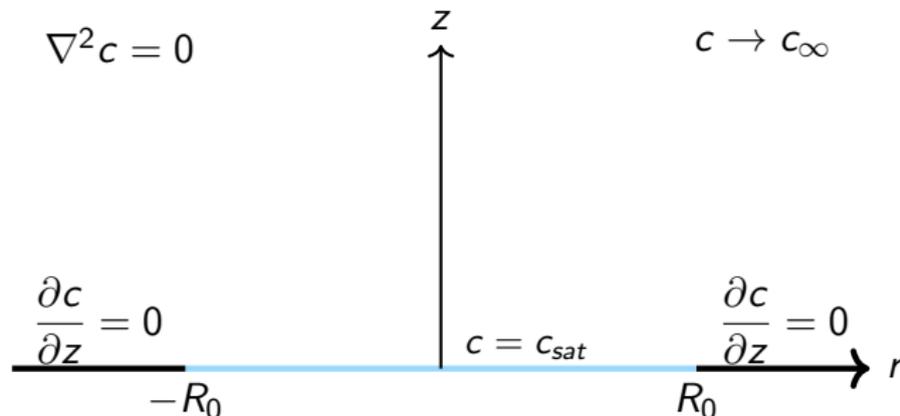


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Height Profile:
$$h(r, t) = h_m \left(1 - \frac{r^2}{R_0^2} \right), \quad h_m = h(0, t) = \frac{R_0 \theta}{2}$$

The Model - Prior to Touchdown

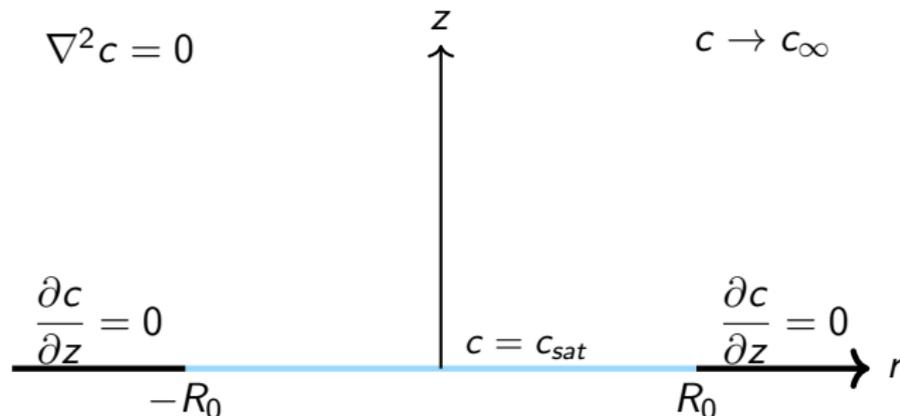


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Volume:
$$V(t) = V_{well} + V_{drop} = \pi H_0 R_0^2 + \frac{\pi R_0^3 \theta}{4}$$

The Model - Prior to Touchdown

- Mathematical model for a thin droplet evaporating in a shallow well prior to touchdown

$$\nabla^2 c = 0 \quad \text{for the half space } z > 0$$

$$c = c_{sat} \quad \text{on } z = 0 \text{ for } r \leq R_0$$

$$c \rightarrow c_\infty \quad \text{as } |\mathbf{r}| \rightarrow \infty$$

$$\frac{\partial c}{\partial z} = 0 \quad \text{on } z = 0 \text{ for } r > R_0$$

$$J = -D \frac{\partial c}{\partial z} \quad \text{on } z = 0 \text{ for } r \leq R_0$$

$$\rho \frac{dV}{dt} = -2\pi \int_0^{R_0} J r \, dr$$

The Vapour Problem - Prior to Touchdown

- We rescale so that the problem for the concentration c of vapour is

$$\nabla^2 c = 0 \quad \text{for the half space } z > 0$$

$$c = 1 \quad \text{on } z = 0 \text{ for } r \leq 1$$

$$c \rightarrow 0 \quad \text{as } |\mathbf{r}| \rightarrow \infty$$

$$\frac{\partial c}{\partial z} = 0 \quad \text{on } z = 0 \text{ for } r > 1$$

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- where

$$h = h_m(1 - r^2), \quad h_m = \frac{\theta}{2}$$

$$V = \pi H_0 + \frac{\pi\theta}{4}$$

Solution for Concentration - Prior to Touchdown

- The exact solution for c is well known and may be written as

$$c = \frac{2}{\pi} \sin^{-1} \left(\frac{2}{[(1+r)^2 + z^2]^{1/2} + [(1-r)^2 + z^2]^{1/2}} \right)$$

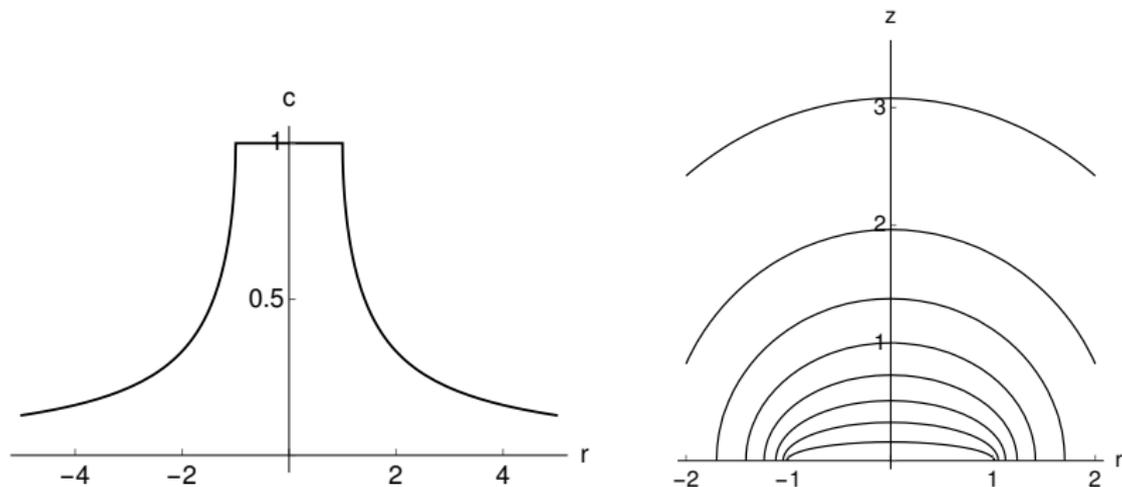


Figure: Plot of the concentration on $z = 0$ and a contour plot of c .

Solution for the Flux - Prior to Touchdown

- The evaporative flux from the free surface J is

$$J = -\left. \frac{\partial c}{\partial z} \right|_{z=0} = \frac{2}{\pi(1-r^2)^{1/2}} \quad \text{for } r < 1$$

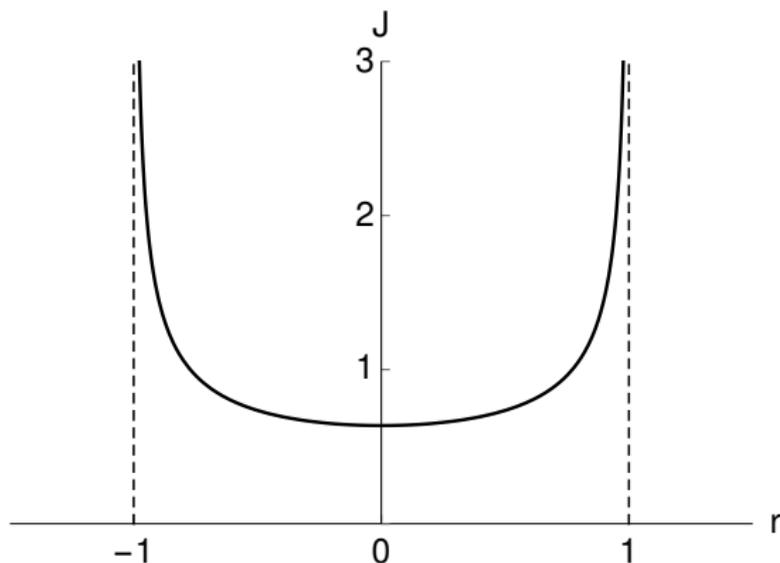


Figure: Solution for the evaporative flux J prior to touchdown

Evolution - Prior to Touchdown

- $\frac{dV}{dt}$ is given by

$$\frac{dV}{dt} = -2\pi \int_0^1 J r dr$$

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Evolution - Prior to Touchdown

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- The evolution of the droplet prior to touchdown is therefore given by

$$\begin{aligned}V &= V_0 - 4t, & V_0 = V(0) &= \pi H_0 + \frac{\pi}{4} \\ \theta &= \theta_0 - \frac{16}{\pi}t, & \theta_0 = \theta(0) &= 1\end{aligned}$$

Evolution - Prior to Touchdown

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- we now find t_{flat} and $t_{\text{touchdown}}$ to be

$$t_{\text{flat}} = \frac{\pi}{16} \approx 0.1963$$

$$t_{\text{touchdown}} = \frac{\pi(1 + 2H_0)}{16}$$

The Droplet - After Touchdown

- The free surface touches down at $r = 0$, $z = -H_0$ at $t = t_{\text{touchdown}}$

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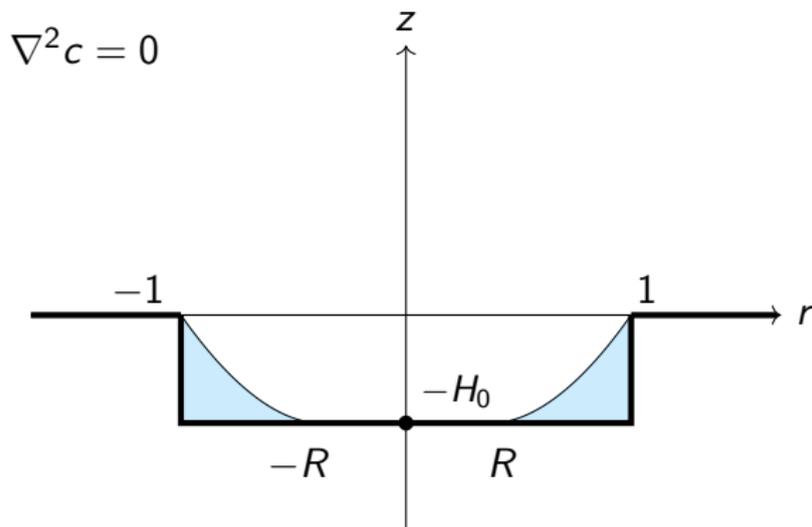


Figure: Sketch of the annular droplet at some instant after touchdown

The Droplet - After Touchdown

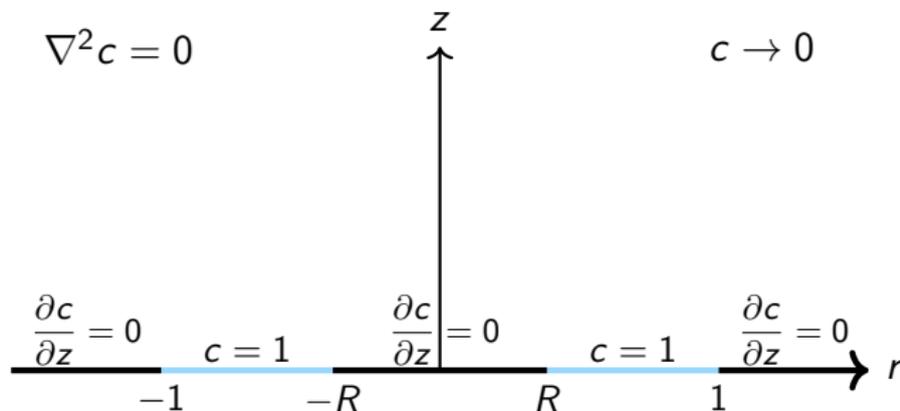


Figure: View of the droplet on the scale of the atmosphere after touchdown

The Droplet - After Touchdown

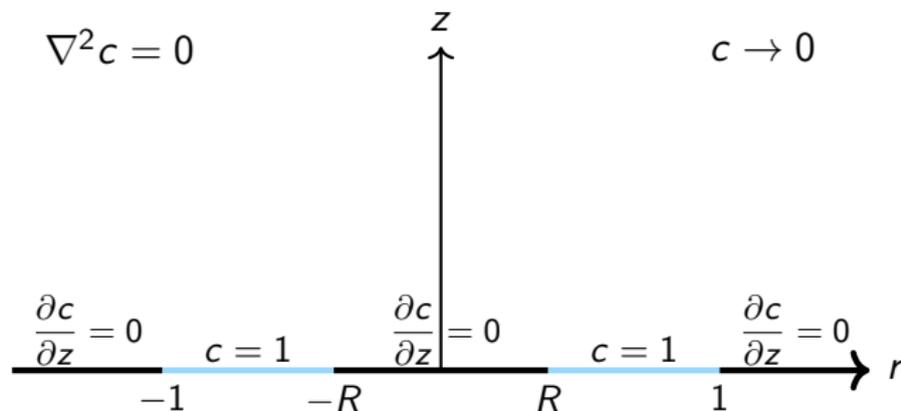


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$$\text{Height Profile: } h(r, t) = \frac{H_0(r^2 - 1 - 2R^2 \log r)}{1 - R^2 + 2R^2 \log r}, \quad R = R(t)$$

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$$c \rightarrow 0 \quad \text{as } |\mathbf{r}| \rightarrow \infty$$

$$\frac{\partial c}{\partial z} = 0 \quad \text{on } z = 0 \text{ for } 0 \leq r < R \text{ and for } r > 1$$

$$J = -\frac{\partial c}{\partial z} \quad \text{on } z = 0 \text{ for } R \leq r \leq 1$$

$$\frac{dV}{dt} = -F(R), \quad F(R) = 2\pi \int_R^1 J r \, dr$$

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- No simple closed form solution is available for c
- Our main concern is finding the total flux F

- How to find the evaporative flux J and total flux F ?

Solution - After Touchdown

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 - We also used the finite-element package COMSOL to find the solution for c and hence J and F
 - The two approaches were found to be in very good agreement for F

Solution - After Touchdown

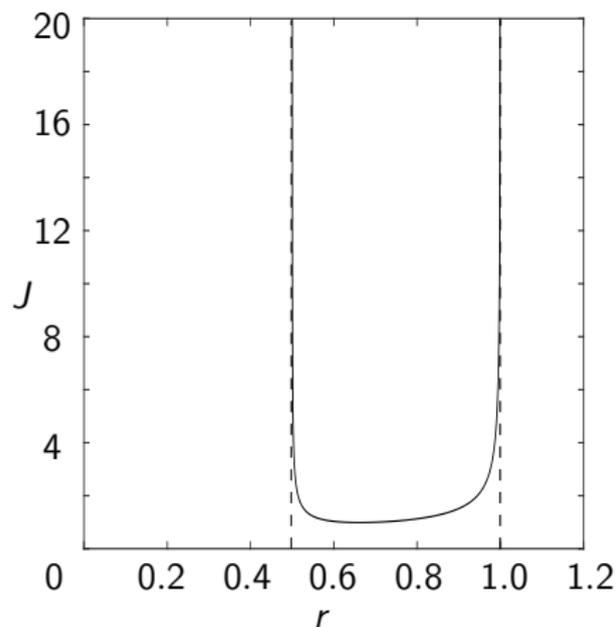
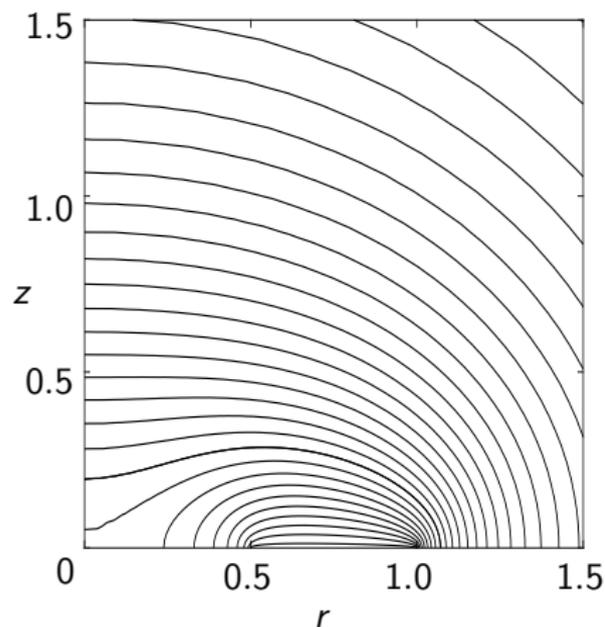


Figure: Contour plot of the concentration c and a plot of the evaporative flux J for an annular droplet in $R \leq r \leq 1$ in the case $R = 1/2$

Solution - After Touchdown

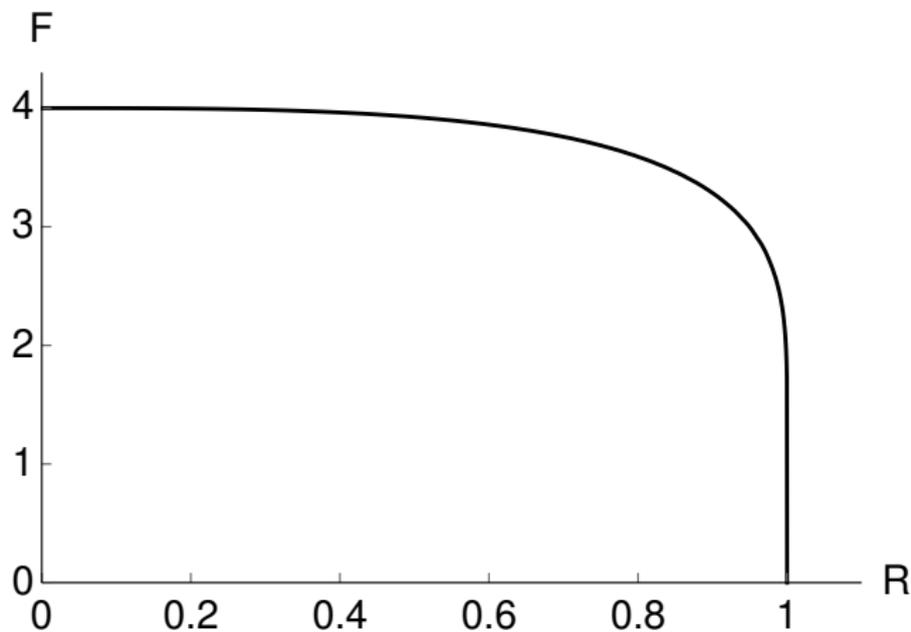


Figure: The numerical solution for the total evaporative flux F , obtained via COMSOL

$$V = \frac{\pi H_0(1 - R^4 + 4R^2 \log R)}{2(1 - R^2 + 2R^2 \log R)} = \pi H_0 f(R), \quad \frac{dV}{dt} = -F(R)$$

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- Solving with the condition $R(t_{\text{touchdown}}) = 0$ gives

$$t = t_{\text{touchdown}} - \pi H_0 \int_0^R \frac{f'(\hat{R})}{F(\hat{R})} d\hat{R}$$

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- Then using the fact that $R(t_{\text{lifetime}}) = 1$ we obtain

$$t_{\text{lifetime}} = t_{\text{touchdown}} + \pi \alpha H_0 = \frac{\pi}{16} [1 + 2(1 + 8\alpha)H_0],$$

$$\text{where } \alpha = - \int_0^1 \frac{f'(R)}{F(R)} dR \approx 0.1369$$

Evolution - R and V

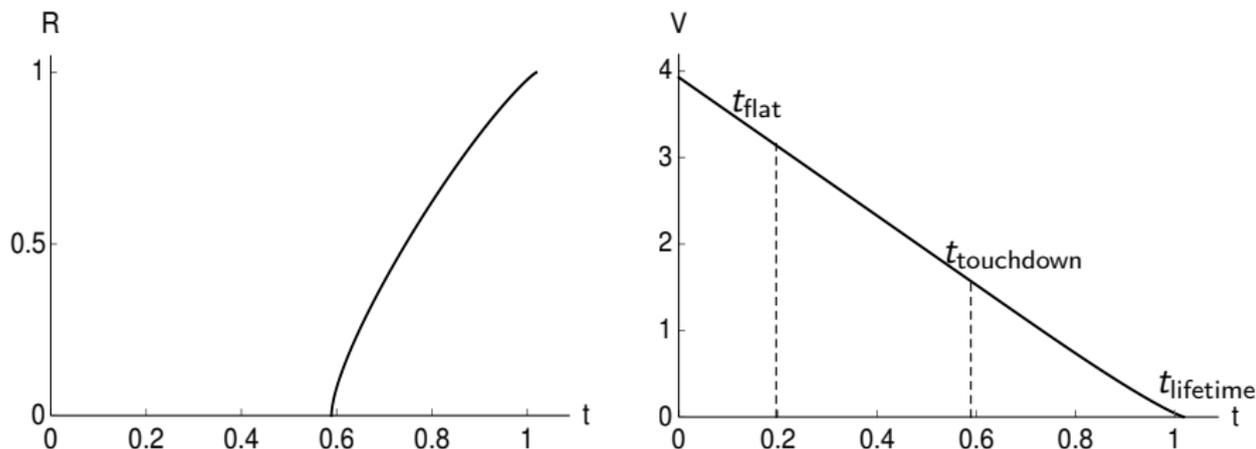


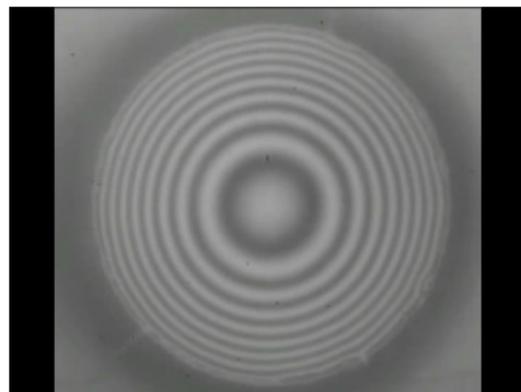
Figure: Evolution of the moving inner contact radius R and the volume V for $t = 0 \dots t_{\text{lifetime}}$ in the case $H_0 = 1$

Comparison with experiments

- We compare the theory to experiments conducted in Durham on droplets of methyl benzoate evaporating (into ambient air) from the wells in polished glass substrates coated with ITO

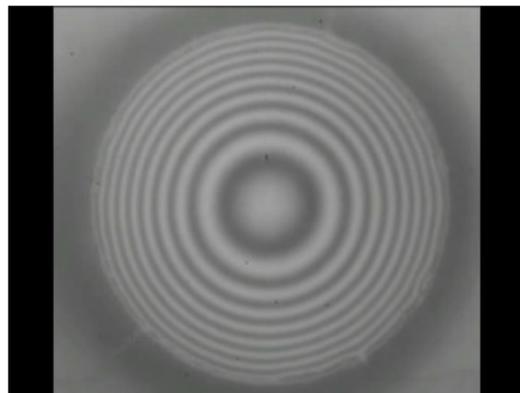
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- Droplets were deposited into wells of radius 30, 50 and 75 μm



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- We compare the theory to experiments conducted in Durham on droplets of methyl benzoate evaporating (into ambient air) from the wells in polished glass substrates coated with ITO
- Droplets were deposited into wells of radius 30, 50 and 75 μm
- Behaviour of the height profile, R , and V were measured



Comparison with experiments

- The following parameter values were used in the comparison of the theory with experiments

$$D = 6.899 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}, \quad \rho = 1.085 \times 10^3 \text{ kg m}^{-3},$$

$$c_{\text{sat}} = \begin{cases} 2.330 \times 10^{-3} \text{ kg m}^{-3} & \text{Book Value 1} \\ 2.252 \times 10^{-3} \text{ kg m}^{-3} & \text{Book Value 2} \end{cases}$$

$$c_{\infty} = 0$$

Comparison with Experiments - Height Profile

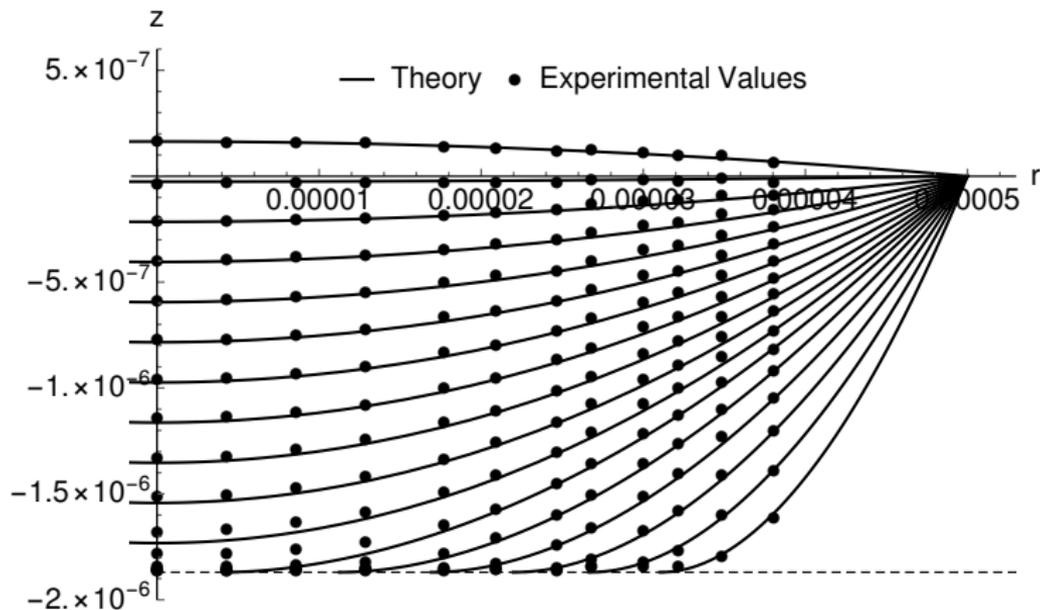


Figure: Comparison of the height profile predicted by the theory with the measured experimental values of a methyl benzoate droplet in a well of radius $50 \mu\text{m}$ at times $t = 0, 0.26 \dots 4.16 \text{ s}$

Comparison with Experiments - R

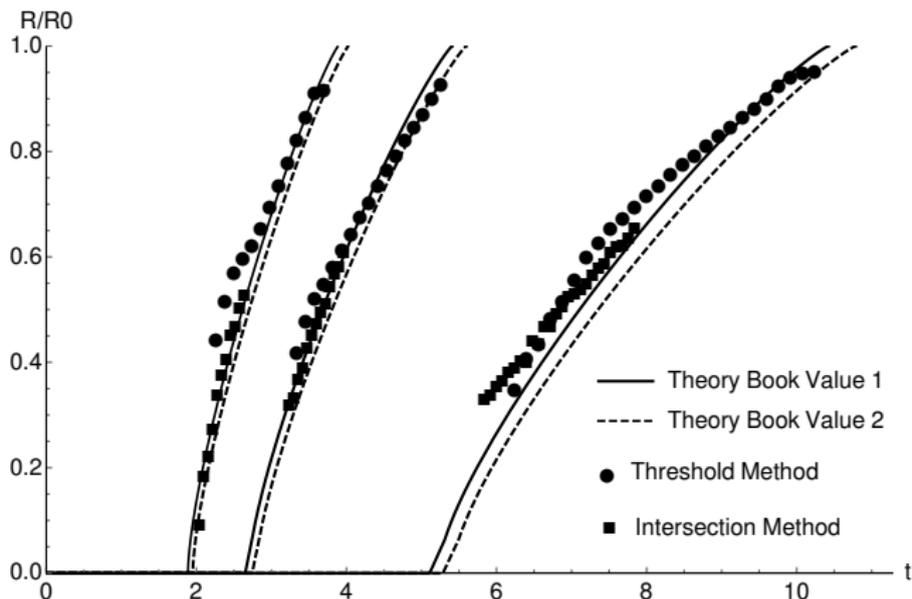


Figure: Comparison of the evolution of the moving inner contact radius R predicted by the theory with the measured experimental values for droplets of methyl benzoate in wells of radii 30, 50 and 75 μm

Comparison with Experiments - V

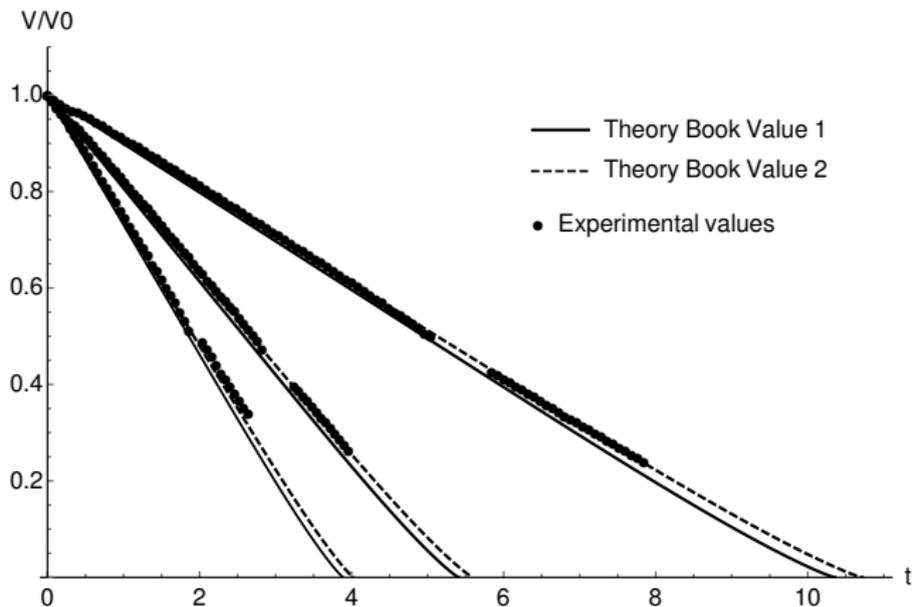


Figure: Comparison of the evolution of the volume V predicted by the theory with the measured experimental values for droplets of methyl benzoate in wells of radii 30, 50 and 75 μm

Comparison with Experiments - Critical Times

Well Dimensions (μm)	Critical Times	Experiments	Theory BV 2	% diff.
$R_0 = 30, H_0 = 2.38$	t_{flat}	0.07 s	0.06 s	-14%
	$t_{\text{touchdown}}$	1.90 s	1.95 s	+3%
	t_{lifetime}	3.98 s	4.03 s	+1%
$R_0 = 50, H_0 = 1.87$	t_{flat}	0.23 s	0.23 s	$\pm 0\%$
	$t_{\text{touchdown}}$	2.88 s	2.79 s	-3%
	t_{lifetime}	5.44 s	5.60 s	+3%
$R_0 = 75, H_0 = 2.39$	t_{flat}	0.46 s	0.49 s	+6%
	$t_{\text{touchdown}}$	5.05 s	5.40 s	+7%
	t_{lifetime}	10.40 s	10.79 s	+4%

Table: Comparison of experimental results for the critical times with theory

Different Shapes of Well

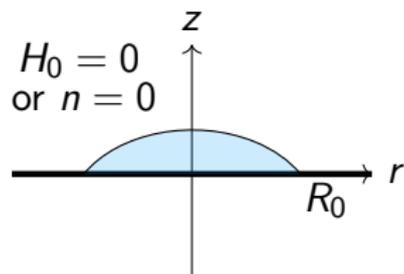
- We have extended this approach to wells with height profile

$$z = H(r) = -H_0 \left[1 - \left(\frac{r}{R_0} \right)^n \right]$$

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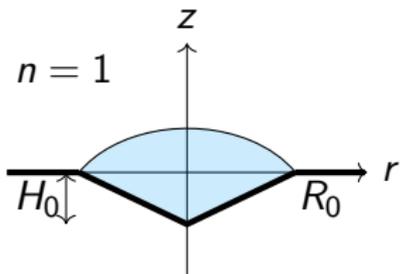
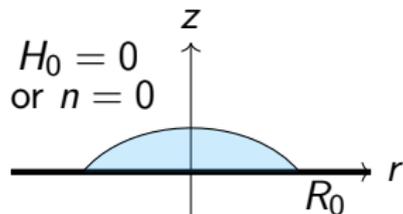
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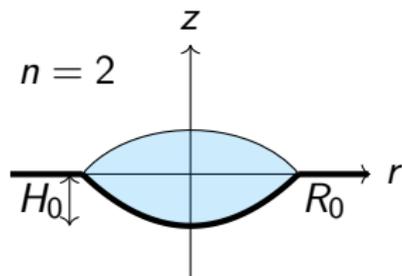
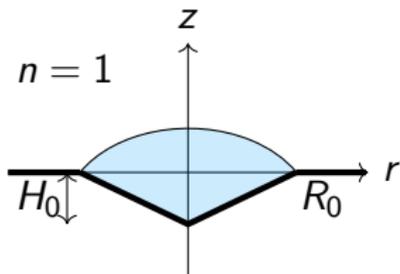
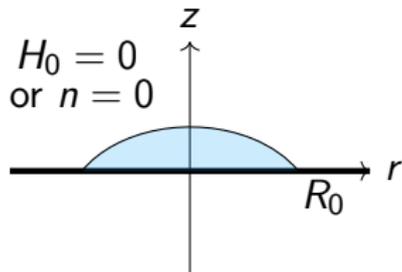
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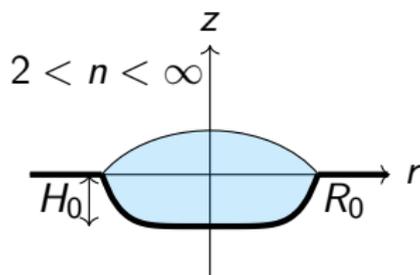
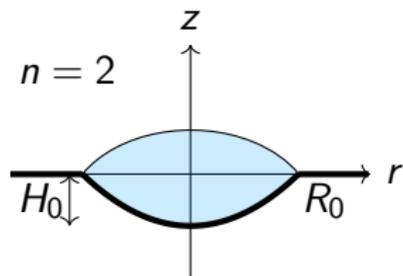
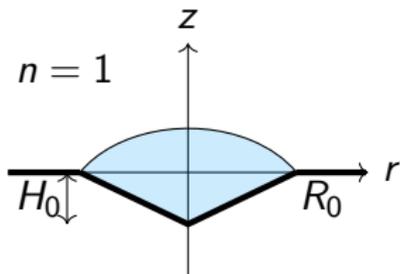
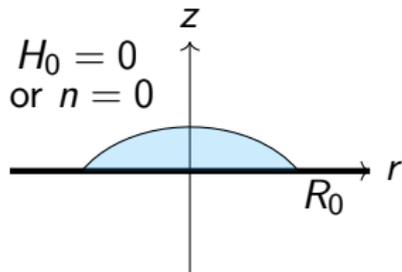
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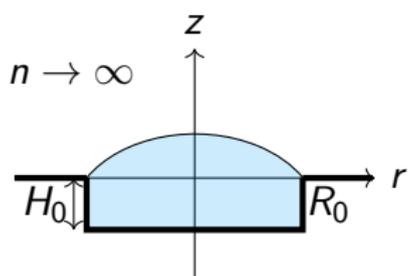
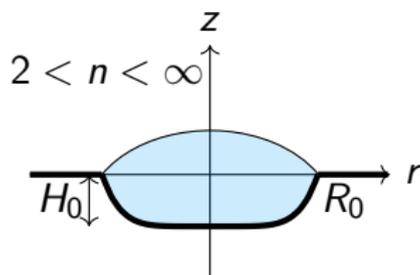
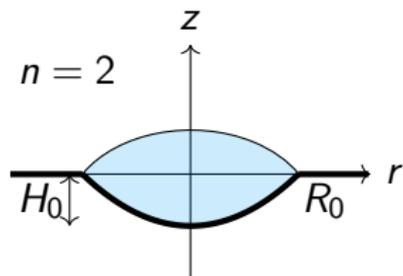
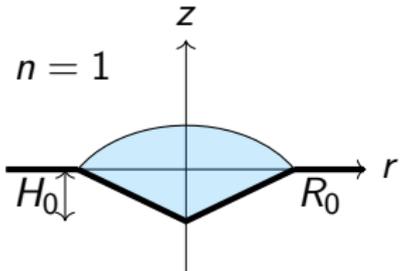
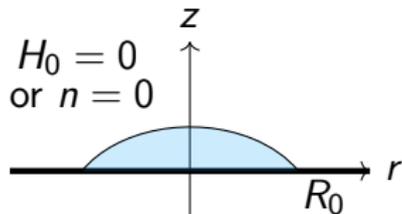
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Conclusions and Future Work

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- We used the COMSOL Multiphysics package and Chebyshev-Gauss quadrature to obtain the evaporative flux J and the total flux F after touchdown
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- We found good agreement with experimental data for the height profile, R , V and the critical times

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- Extend analysis to other modes of evaporation

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- Extend analysis to other modes of evaporation
- Multicomponent droplets

Thank You for Listening!

Hannah-May D'Ambrosio

Brian Duffy

Teresa Colosimo

Colin Bain

Dan Walker

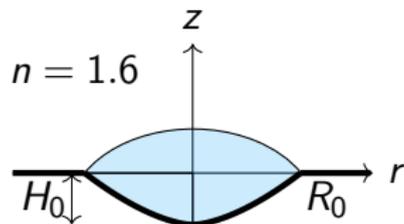
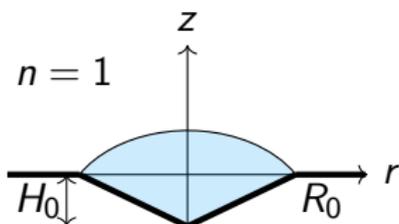
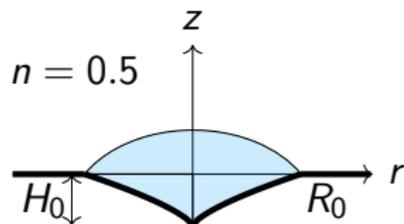
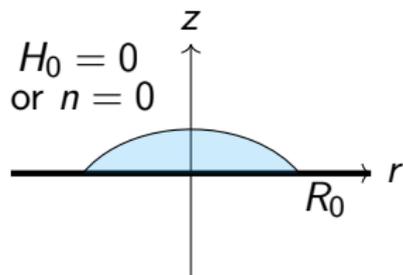


Different Shapes of Wells

- For $0 < n < 2$

$$t_{\text{touchdown}} = \frac{\pi(1 + nH_0)}{16}$$

$$t_{\text{lifetime}} = \frac{\pi(1 + n + 3nH_0)}{16(1 + n)}$$



Different Shapes of Wells

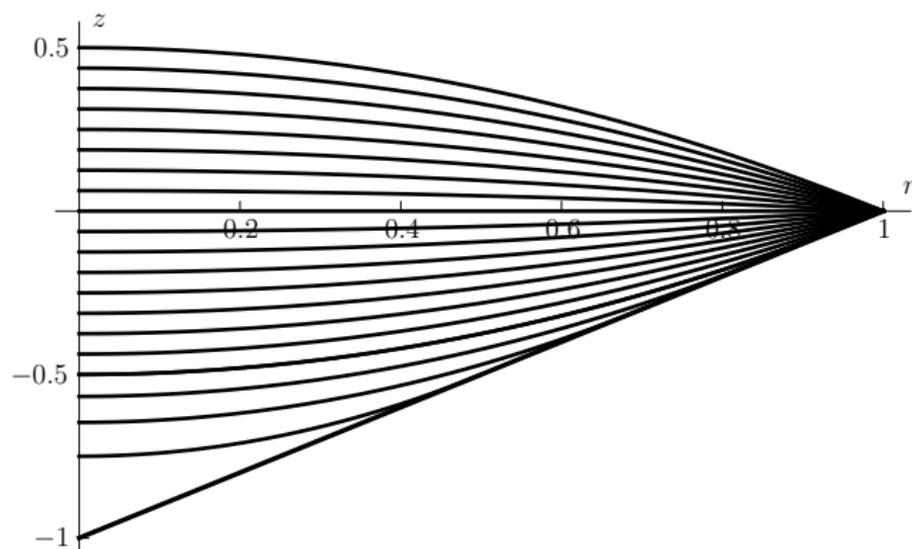
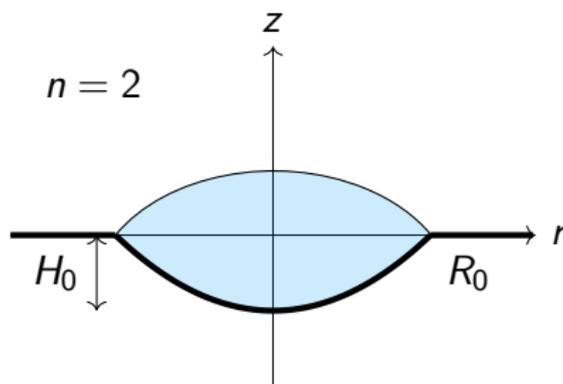


Figure: Evolution of the height profile of a droplet in a conical well from the theory where $n=1$.

Different Shapes of Wells

- For $n = 2$

$$t_{\text{touchdown}} = t_{\text{lifetime}} = \frac{\pi(1 + 2H_0)}{16}$$



Different Shapes of Wells

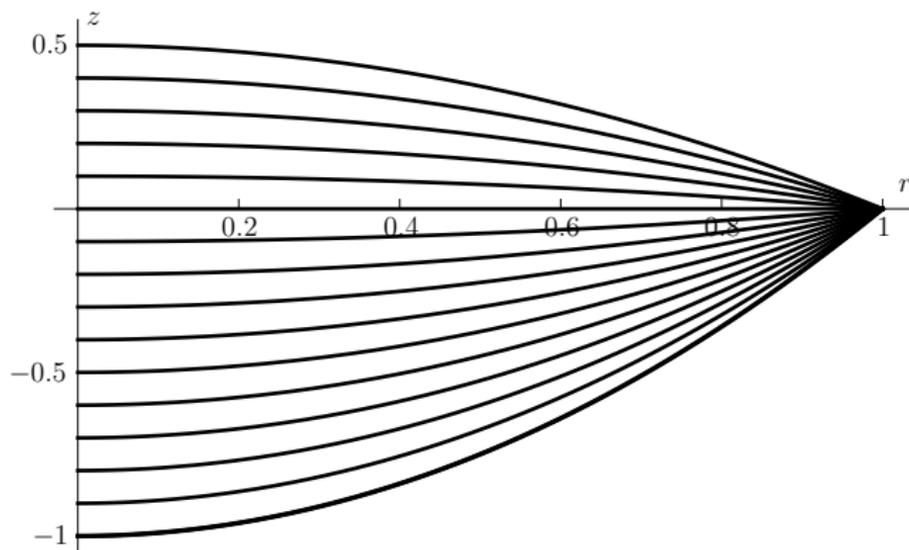


Figure: Evolution of the height profile of a droplet in a parabolic well from the theory where $n=2$.

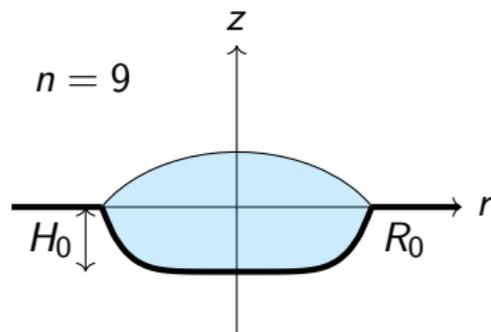
Different Shapes of Wells

- For $2 < n < \infty$

$$t_{\text{touchdown}} = \frac{\pi(1 + 2H_0)}{16}$$

$$t_{\text{lifetime}} = \frac{\pi}{16} [1 + 2(1 + 8\alpha)H_0]$$

$$\alpha = - \int_0^1 \frac{f'(R)}{F(R)} dR (> 0)$$



Different Shapes of Wells

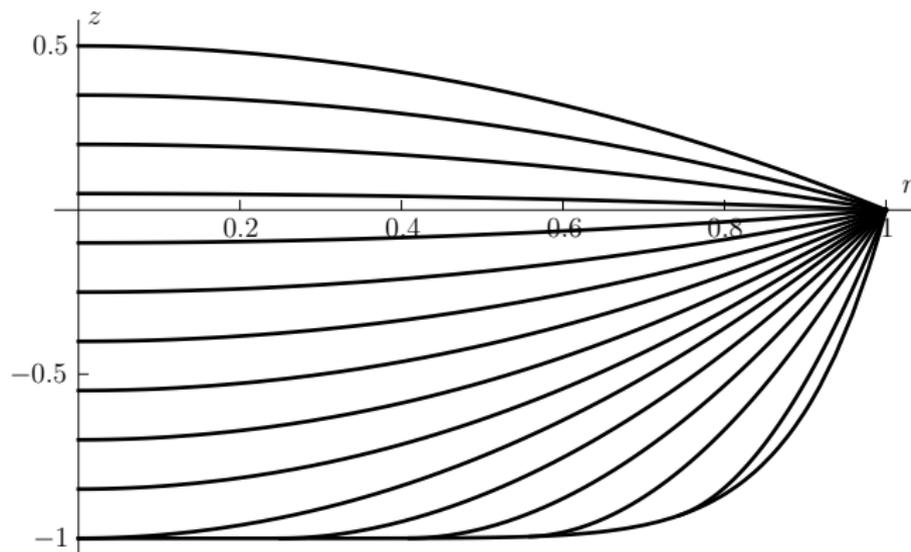


Figure: Evolution of the height profile in an axisymmetric well from the theory where $n=9$.

Different Shapes of Wells - Evolution of α

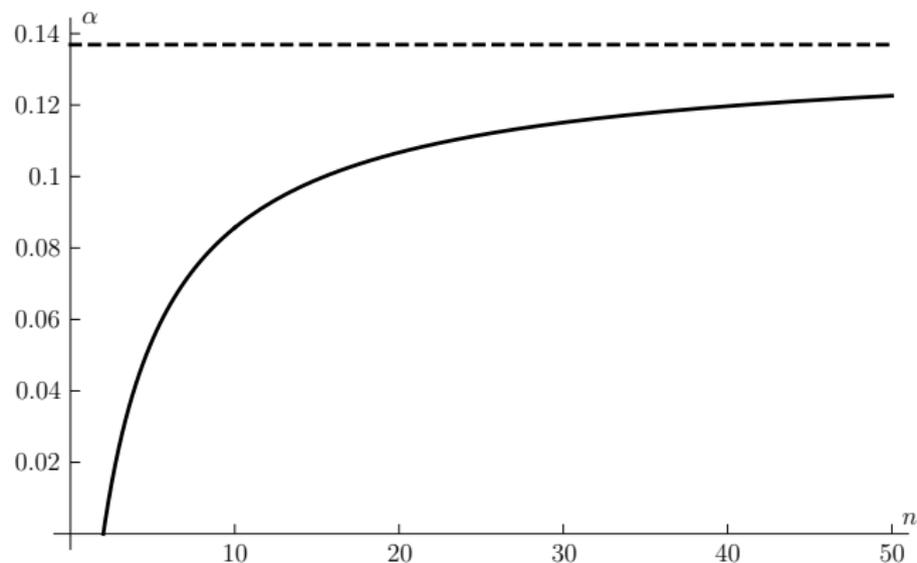


Figure: Evolution of parameter α for varying n .

Experimental Analysis

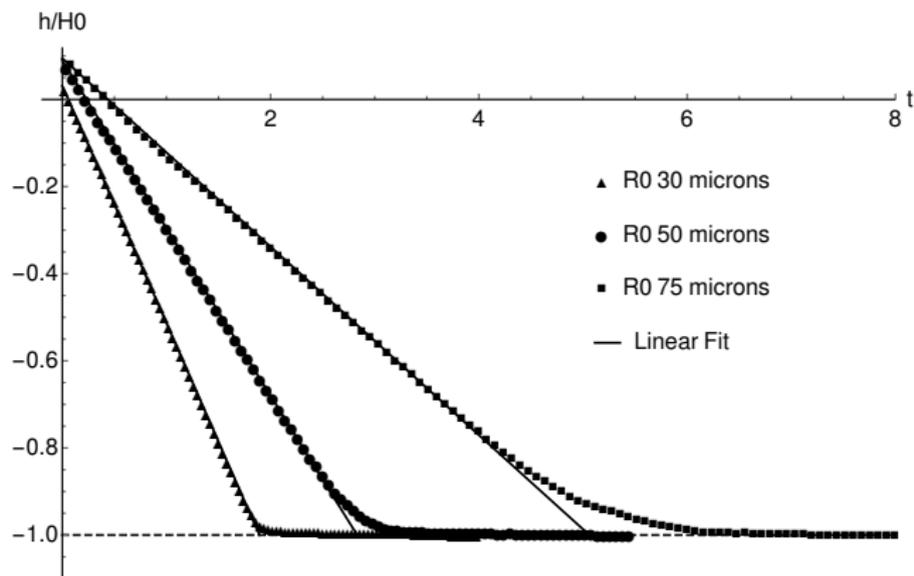
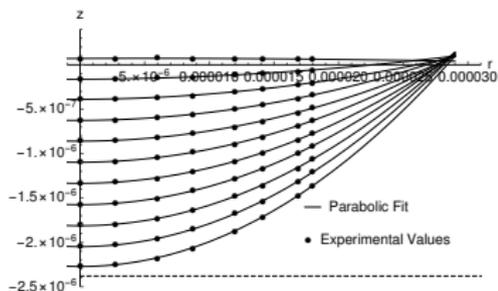
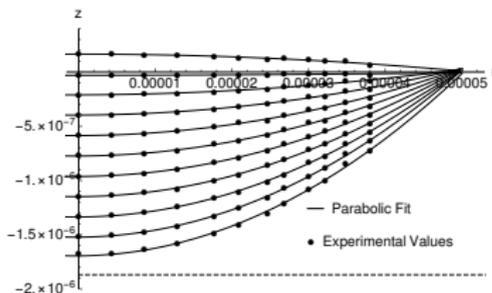


Figure: Experimental values for the height in the middle of the droplet h_m for three wells of radius 30, 50 and 75 μm .

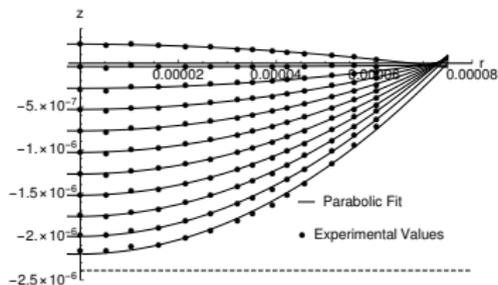
Experimental Analysis



(a) $R_0 = 30 \mu\text{m}$



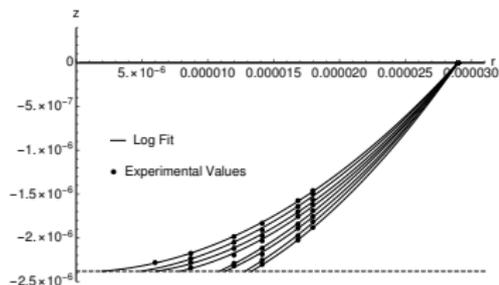
(b) $R_0 = 50 \mu\text{m}$



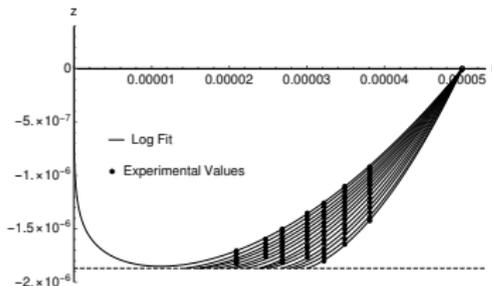
(c) $R_0 = 75 \mu\text{m}$

Figure: Parabolic fits of the experimental values for the height profile of a droplet in wells of radius 30, 50 and 75 μm before touchdown at time intervals of (a) $t = 0, 0.18 \dots 1.80$ s, (b) $t = 0, 0.26 \dots 2.60$ s and (c) $t = 0, 0.48 \dots 4.80$ s.

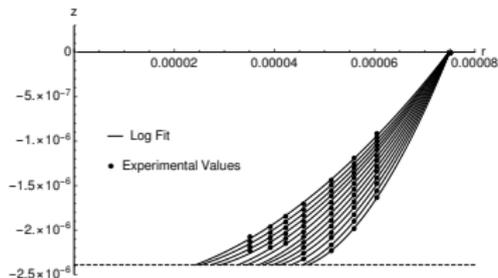
Experimental Analysis



(a) $R_0 = 30 \mu\text{m}$



(b) $R_0 = 50 \mu\text{m}$



(c) $R_0 = 75 \mu\text{m}$

Figure: Modified fits of the experimental values for the height profile of a droplet in wells of radius 30, 50 and 75 μm after touchdown at time intervals of (a) $t = 1.92, 1.98 \dots 2.52$ s, (b) $t = 3.12, 3.18 \dots 3.78$ s and (c) $t = 5.68, 5.84$