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Bubble detachment from heterogeneous surfaces

27 Aug 2025, EFDC2, Dublin, Ireland.

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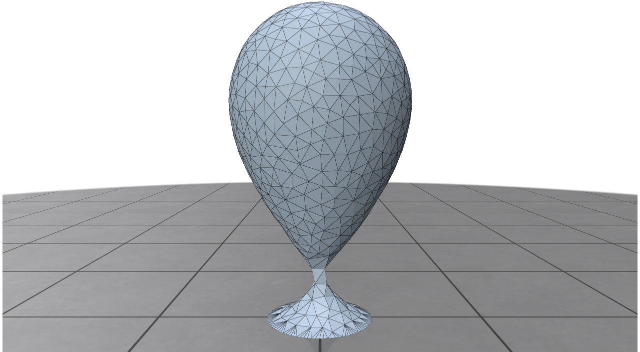
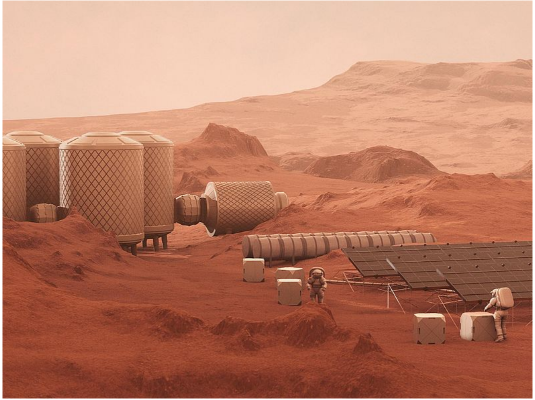


The need for hydrogen and oxygen

- Hydrogen and oxygen are needed as fuel for interplanetary travel.
- Less energy is needed to escape Earth's gravity if the rockets are refuelled on a lunar base
- Humans on the Moon and Mars will need supply of oxygen
- Ice is found at the poles and in craters on the Moon and Mars
- Solar photovoltaics can be used to generate electricity



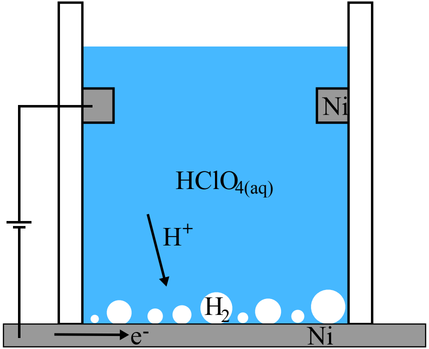
Joris Wegner, University of Bremen

ELECTROLYSIS OF ACIDIC WATER

- Hydrogen bubbles form at the anode

$$2H^+_{(aq)} + 2e^- \rightarrow H_{2(g)} \tag{1}$$

- Attached bubbles obstruct the motion of H^+ ions, reducing efficiency



Demirkr, a., Wood, J. A., Lohse, D., & Krug, D. (2024). *Langmuir*, (39)

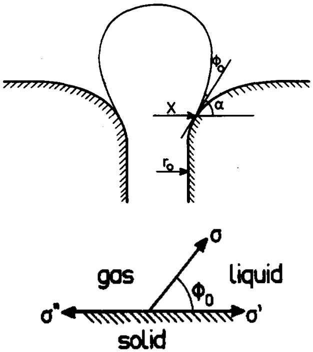
Aims

Question

What size are the bubbles when they detach from the electrode?

BUBBLE FORMATION

- Bubbles nucleate inside cavities on the electrode surface.
- The contact angle ϕ_0 between the three phases depends on their relative affinities.



Chesters, A. K. (1978). *International Journal of Multiphase Flow*, (3)

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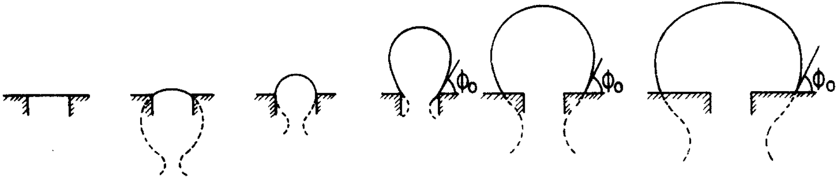
Pinned and spreading bubbles

- At first, the contact line lies on the curved edge of the cavity as the bubble grows.
- The contact line remains on the cavity as long as the angle of the bubble foot with the horizontal is more than ϕ_0
- This is known as the **pinned** state.
- If the angle of the interface decreases to ϕ_0, the bubble spread across the electrode.
- This is known as the **spreading** state.



Chesters, A. K. (1978). *International Journal of Multiphase Flow, (3)*

Bubble shape

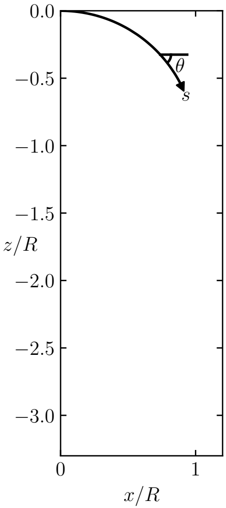
- The curvature of the interface is given by the Young-Laplace equation,

$$\sigma\left(\frac{1}{R_1}+\frac{1}{R_2}\right)=p_{out}-p_{in} \tag{2}$$

- Assume axial symmetry,

$$\sigma\left(\frac{d\theta}{ds}+\frac{\sin\theta}{x}\right)=(\rho_{in}-\rho_{out})zg-\frac{2\sigma}{R} \tag{3}$$

Bashforth, F., & Adams, J. C. (1883). Cambridge University Press



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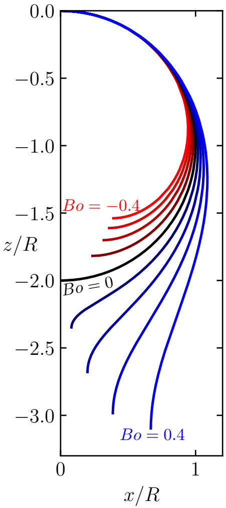
BUBBLE SHAPE

- Group dimensional variables in the Bond number $\mathrm{Bo} = \frac{(\rho_{in} - \rho_{out}) g R^2}{\sigma}$;

$$\frac{d\theta}{d(s/R)} + \frac{R}{x}\sin\theta = \mathrm{Bo}\frac{z}{R} - 2. \tag{4}$$

Bashforth, F., & Adams, J. C. (1883). Cambridge University Press



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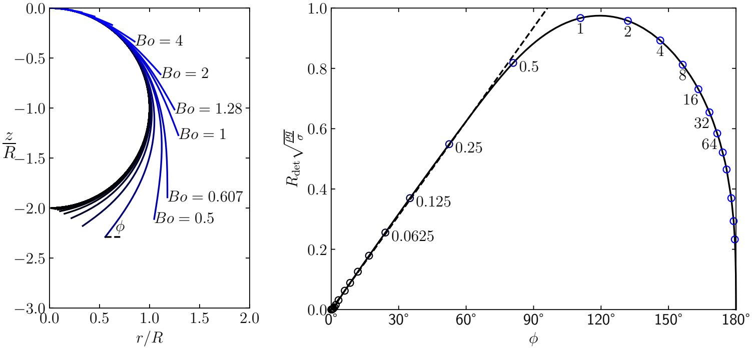
DETACHMENT SIZE OF SPREADING BUBBLES



- For each Bond number Bo, we find the largest bubble with a given contact angle ϕ.
- The largest spreading bubble has a contact angle of 121° and radius of 0.97 capillary lengths.
- The dashed line $R_{\mathrm{det}}\sqrt{\frac{\rho g}{\sigma}} = 0.104\phi$, is the result of Fritz, 1935.

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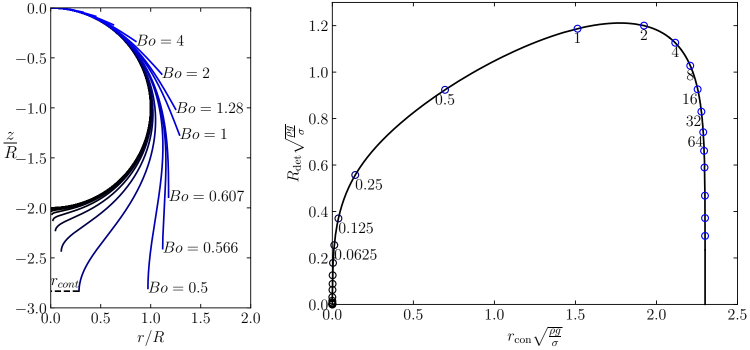
Detachment size of pinned bubbles



- For each Bond number Bo, we find the largest bubble with a given cavity radius r.
- The largest possible bubble has $R_{\mathrm{det}}\sqrt{\frac{\rho g}{\sigma}} \approx 1.2$.

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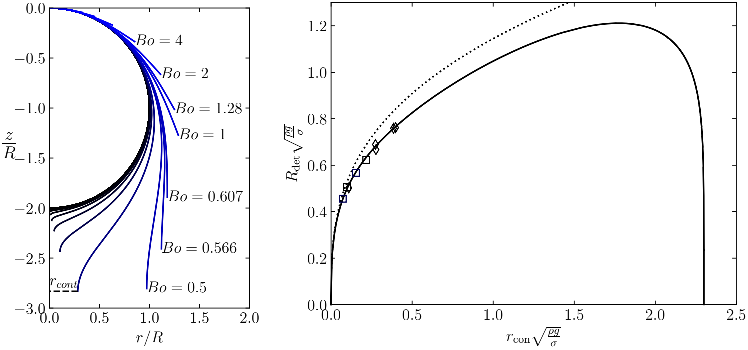
DETACHMENT SIZE OF PINNED BUBBLES

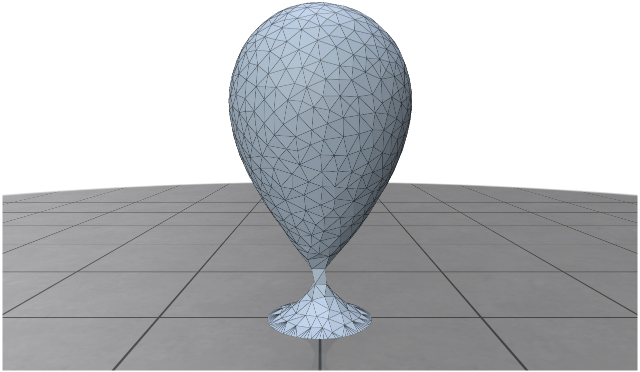


- Our results agree with the carbonated water experiments of Mori and Baines, 2001 and the boiling experiments of Lesage and Marois, 2013.
- We measure a maximum possible cavity radius of 2.40, agreeing with the stability analysis of Pitts, 1974.

AIMS

QUESTION

Can we predict the shape of generic 3D bubbles?

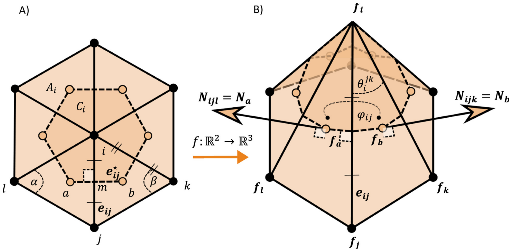


Surface tension force

- Triangulate the interface so that vertices lie on the surface.
- Compute the total curvature at each vertex using discrete differential geometry.

$$\widehat{H\mathbf{N}A}_i = \frac{1}{2} \sum_{j \in st(\mathbf{f_i})} (\cot \alpha_{ij} + \cot \beta_{ij}) \left(\boldsymbol{f}_i - \boldsymbol{f}_j \right). \quad (5)$$

- Apply a surface tension force $\boldsymbol{S_i} = \sigma \widehat{H\mathbf{N}A}_i$.
- Endres, S. C., Avila, M., & Lutz, M. (2022). *Chemical Engineering Science*



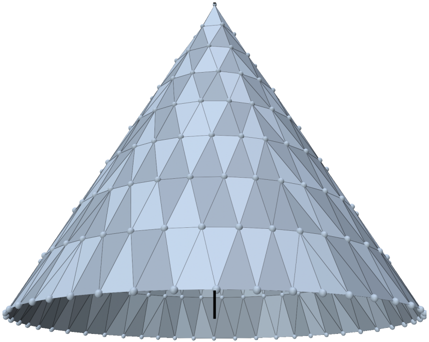
Pressure forces

- Initialise the bubble as a cone with volume V_0 and base radius R_{foot}
- Outer pressure assumed to be hydrostatic.

$$p_{\mathrm{out}} = \Delta\rho g z \tag{6}$$

- Inner pressure enforces volume conservation.

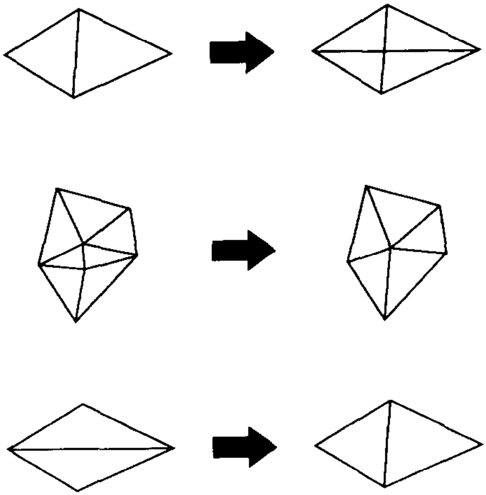
$$p_{\mathrm{in}} = \frac{2\sigma}{R}\left(\frac{V_0}{V}\right)^5 \tag{7}$$



REMESHING

Use the method described in Unverdi, S. O., & Tryggvason, G. (1992). *Journal of Computational Physics, (1)*;

- Split edges longer than $0.2R$
- Merge edges shorter than $0.1R$
- Reconnect diagonals if it shortens them by more than a factor of 1.5.



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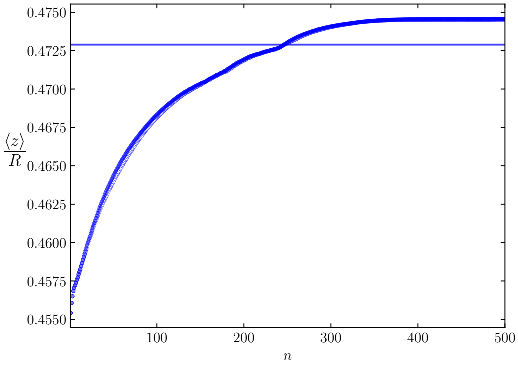
Minimising free energy

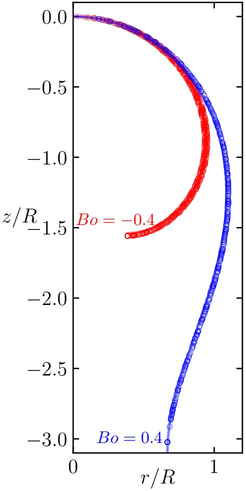
Use the Adams Bashforth method to find the locations $\mathbf{x_i}$ where resultant forces $\mathbf{F_i}$ on the vertices are zero;

$$\mathbf{x_i^{n+1}} = \mathbf{x_i^n} + \alpha \frac{3}{2}\mathbf{F_i^n} - \alpha \frac{1}{2}\mathbf{F_i^{n-1}} \tag{8}$$



Validation: bubble shape

For a fixed contact line, we can replicate the bubble shape for a range of Bond numbers, $\mathrm{Bo} = \dfrac{\Delta\rho g R^2}{\sigma}$.



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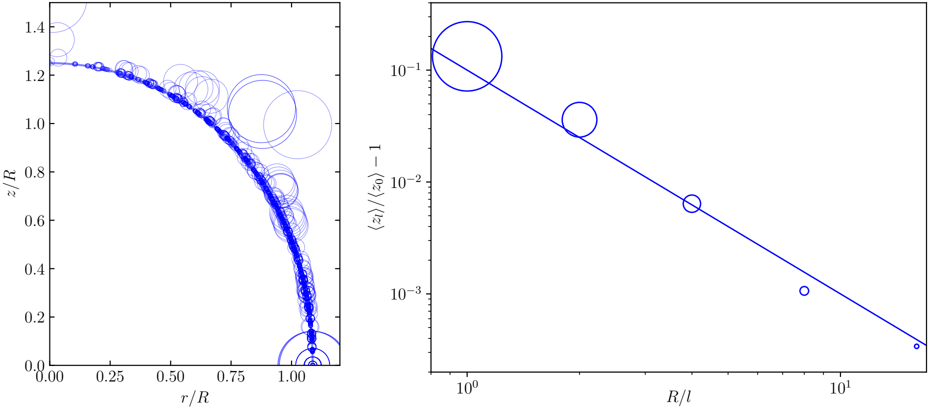
Validation: grid dependence



The error in the height of the centre of mass has a quadratic dependence on the grid size,

$$\frac{\langle z_l \rangle}{\langle z_0 \rangle} - 1 = 0.1 \left(\frac{R}{l} \right)^{-2}. \tag{9}$$

Conclusions

- The largest detaching bubble has a radius of 1.2 capillary lengths.
- The largest cavity that can support a bubble has a radius of 2.4 capillary lengths.
- We developed a discrete differential geometric formulation with second-order convergence.

Thank you!

https://ianto-cannon.github.io/

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