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HZB Helmholtz Zentrum Berlin

Bubble detachment from the surface of a (photo)electrode

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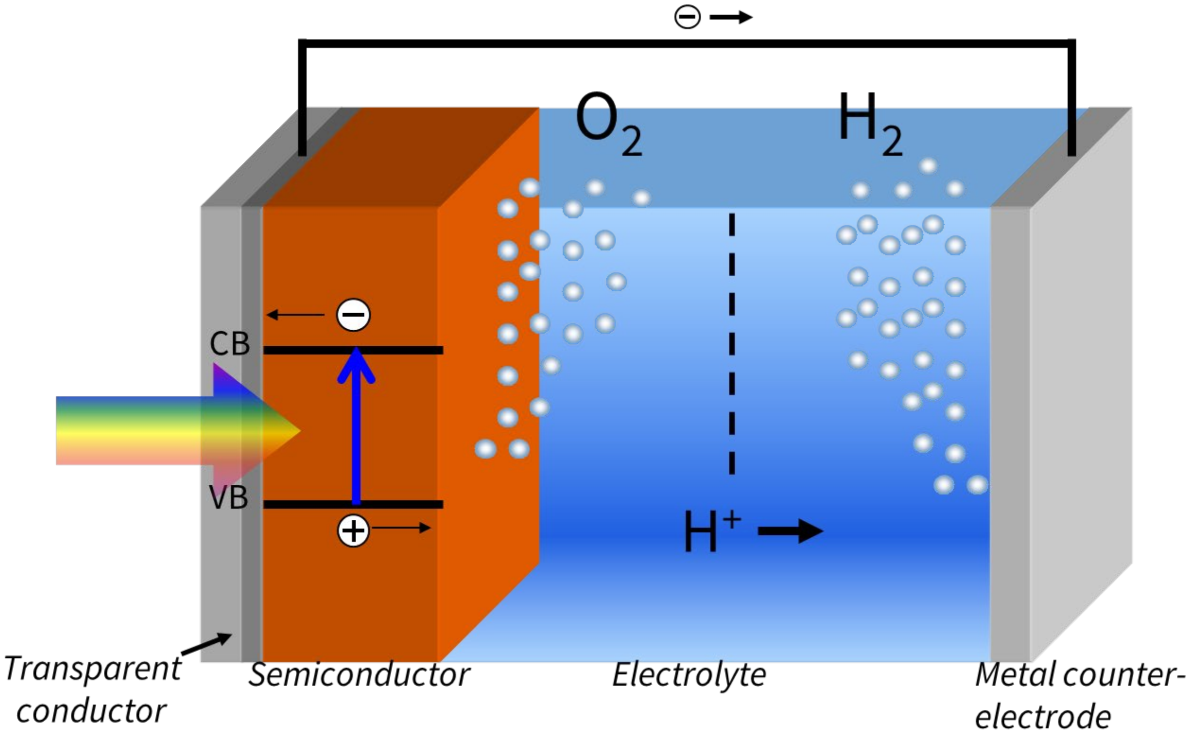
Computational Fluid Dynamics II

Photoelectrochemical water splitting



Schematic illustration of the (photo)electrochemical water splitting device

Bubble induced drawbacks:

blockage of the electro-catalyst surface,

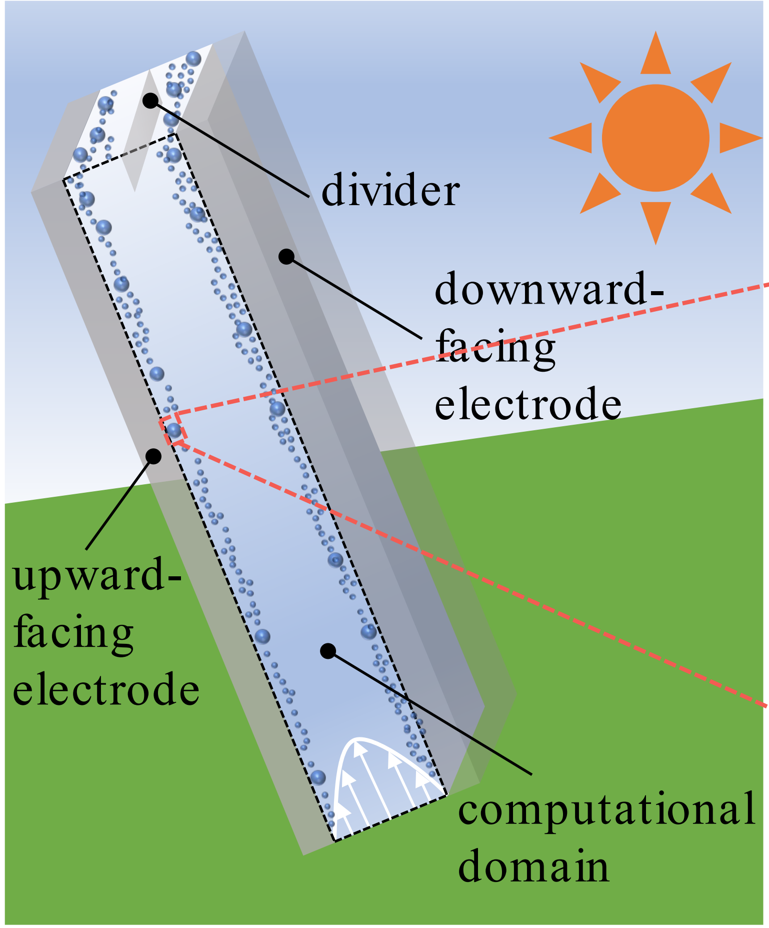
product crossover, i.e., mixture of H_2 and O_2

optical loss, etc.

H. Vogt, *et al.*, *Electrochim. Acta*, 235 (2017), 495
K. Obata, *et al.*, *Cell Reports Physic. Sci.*, 2021, 100358
I. Holmes-Gentle, *et al.*, *J. phys. Chem. C*, 123 (2019), 17

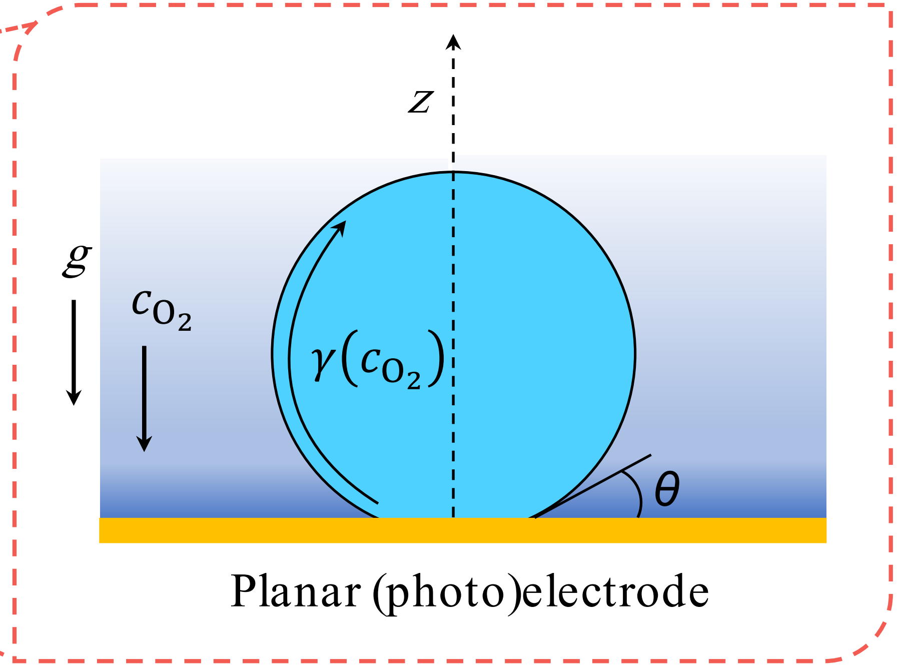
- Photoelectrochemical (PEC) water splitting can produce truly green hydrogen
- Bubbles in PEC devices play a crutial role in affecting energy conversion efficiency, lots of mechanisms, e.g., bubble detachment, however, remain unclear

Closer look at the bubble on (photo)electrode

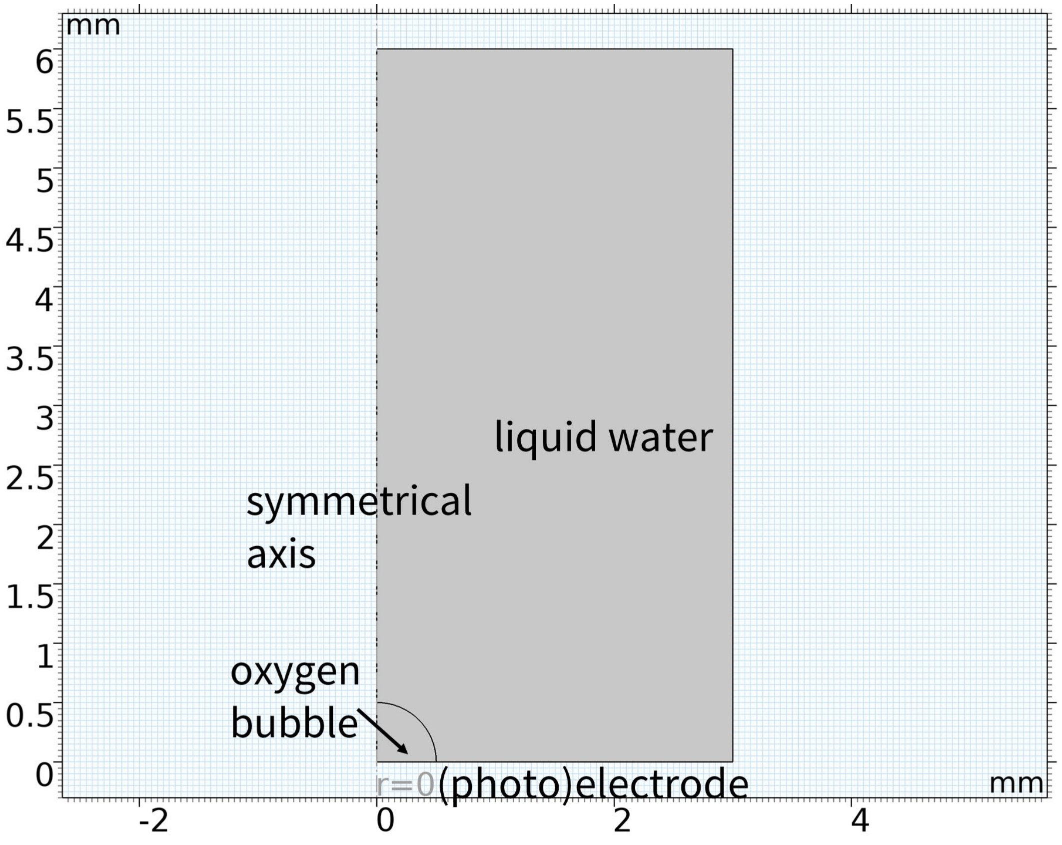


Schematic illustration of the (photo)electrochemical water splitting device

Problem concerned: **how does the supersaturated boundary layer of dissolved oxygen affect bubble detachment?**



Model description



Liquid flow:

Navier-Stokes equation

BCs: top (pressure outlet), bottom (wetted wall), right (no slip wall)

Bubble/electrolyte interface:

Level-set

BCs: top (no flow), bottom (wetted wall), right (no flow)

Convection of dissolved oxygen:

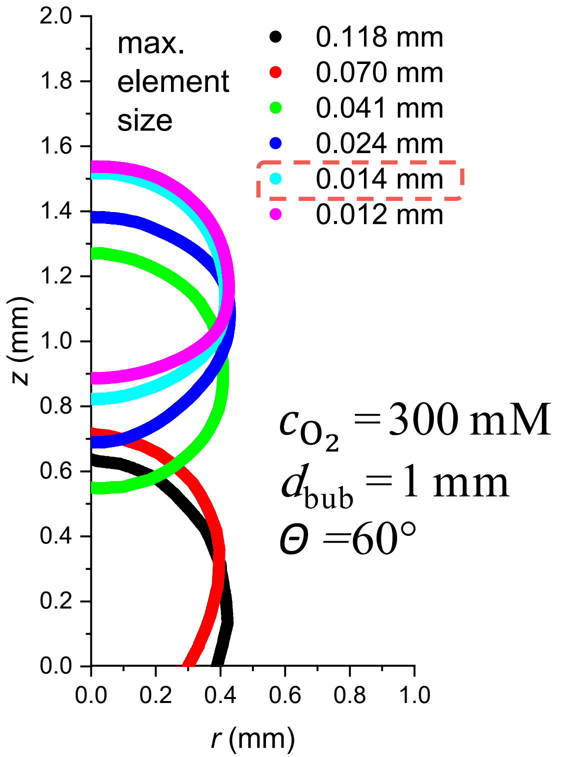
Transport equation

BCs: top (free outlet), bottom (no flux), right (no flux)

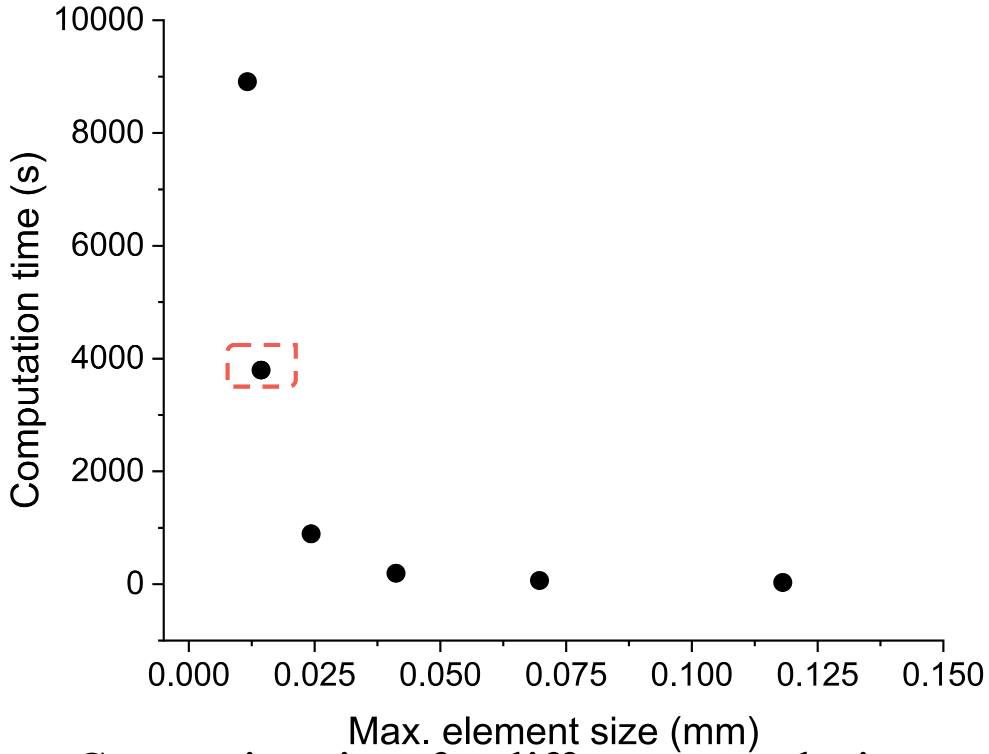
Note: diffusive mass transfer is ignored due to the Péclet number (Pe) is in the order of magnitude of 10^4;

mass transfer through the interface is not included due to short simulation time (5 ms)

Mesh independence check



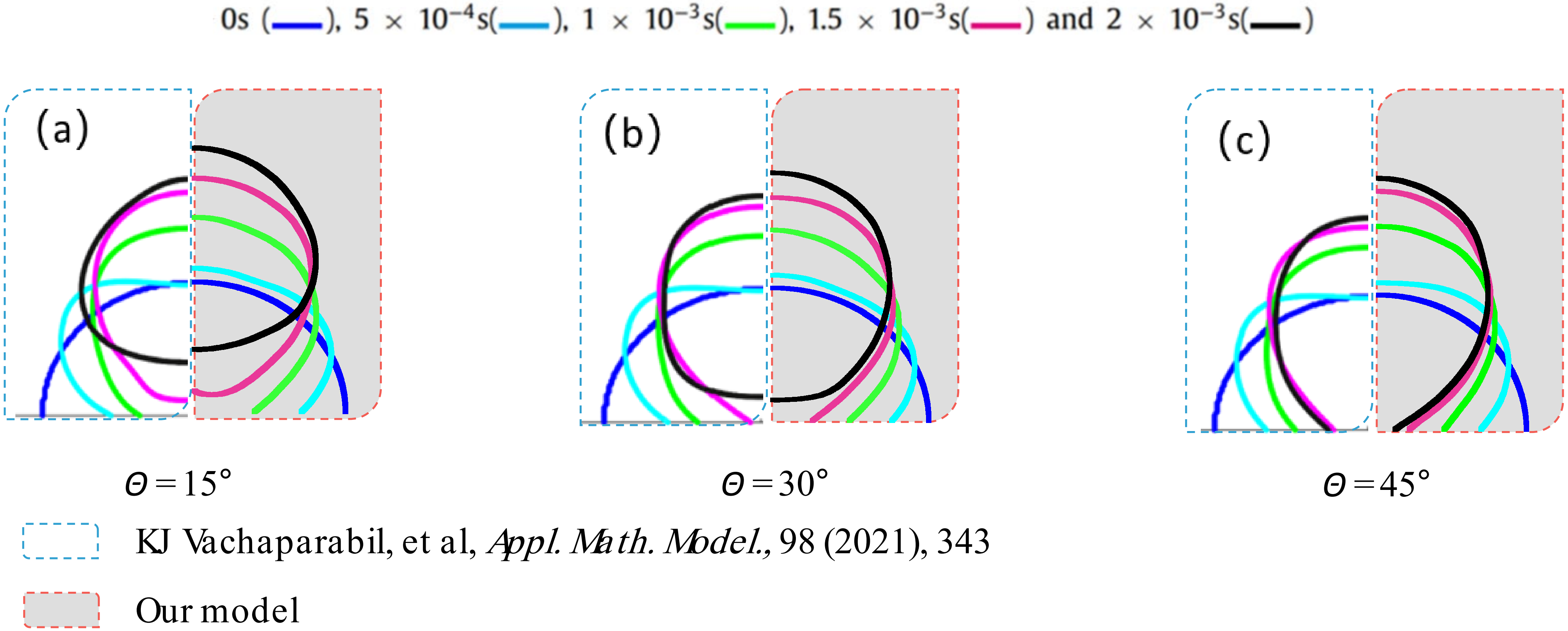
Bubble/electrolyte interface at 5 ms for diff. max. mesh size



Computing time for diff. max. mesh size

Compromise between model accuracy and computation time

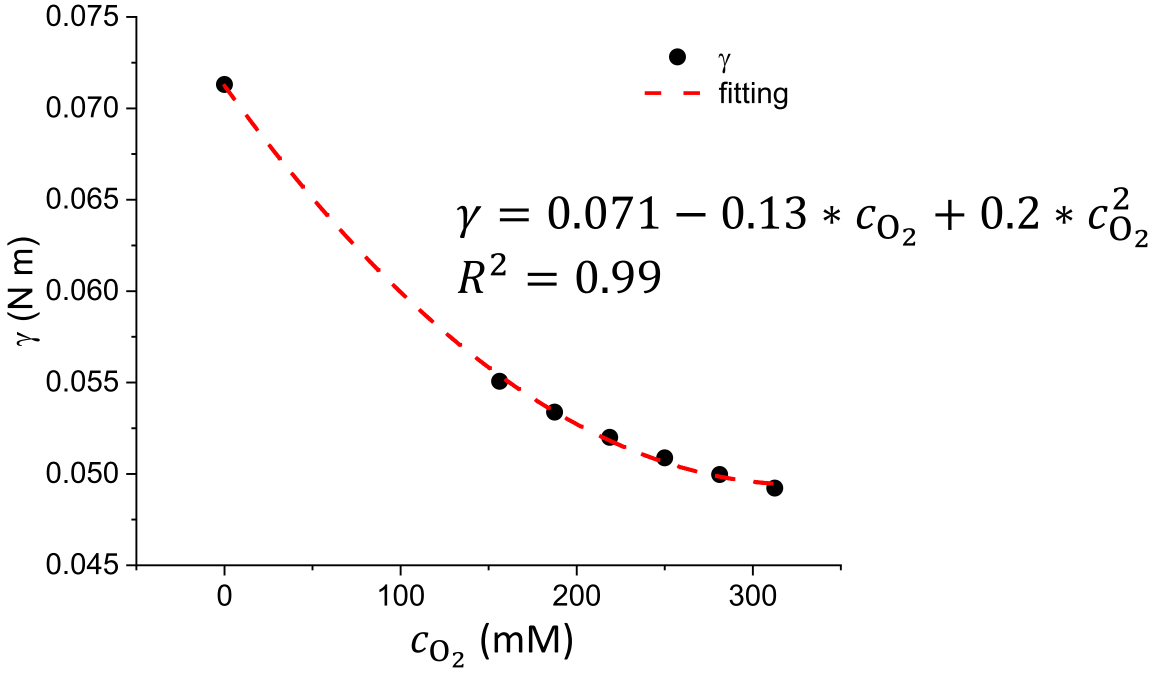
Model validation



Small differences attributed to slight variation of the material properties; however, the simulated bubble interface from our model agrees well with the literature results

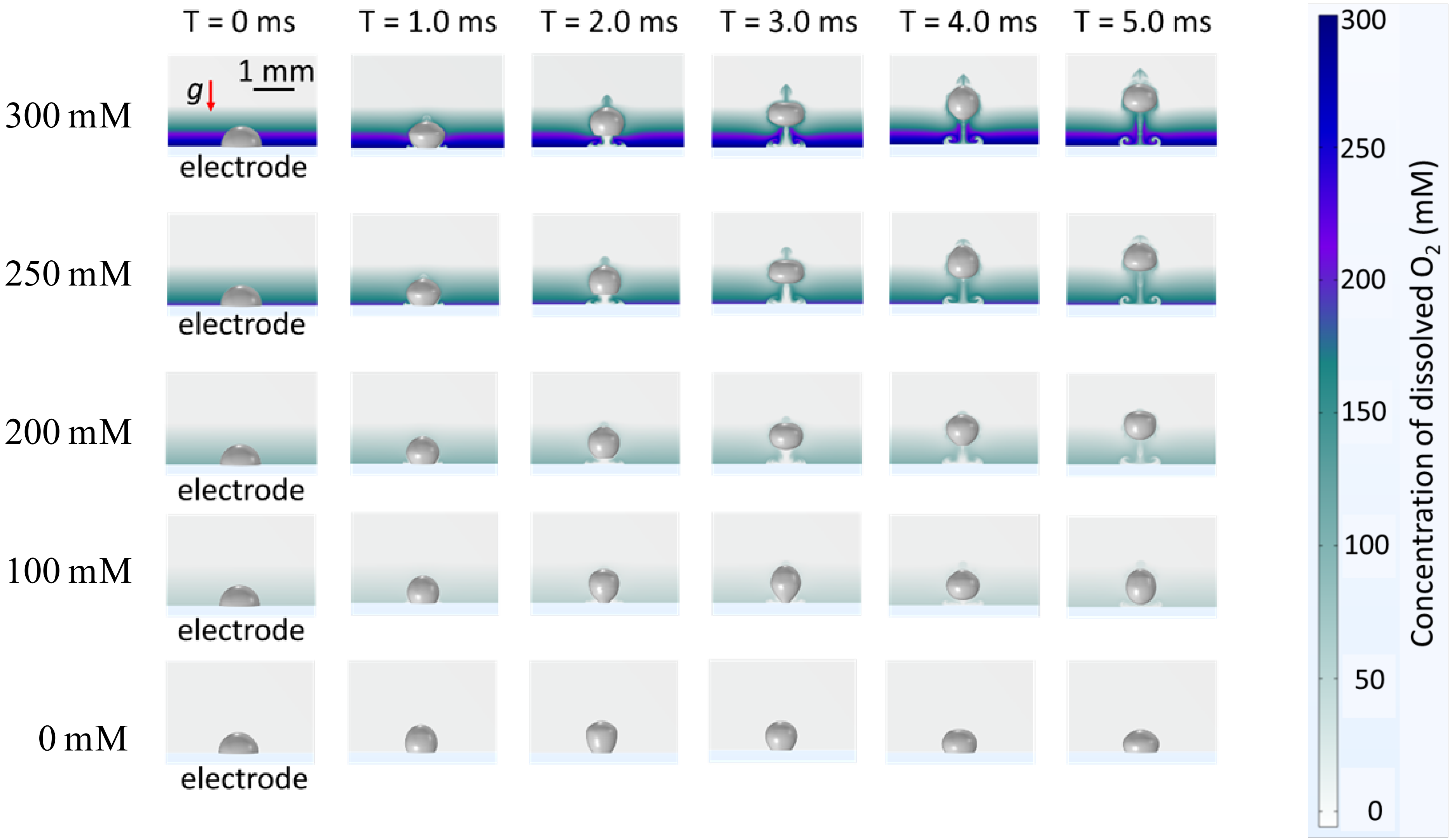
Dependence of γ on dissolved O_2 concentration

S Jain, et al, *AIP Adv.*, 7 (2017), 045001



Surface tension coeff. is significantly affected by the concentration of dissolved oxygen

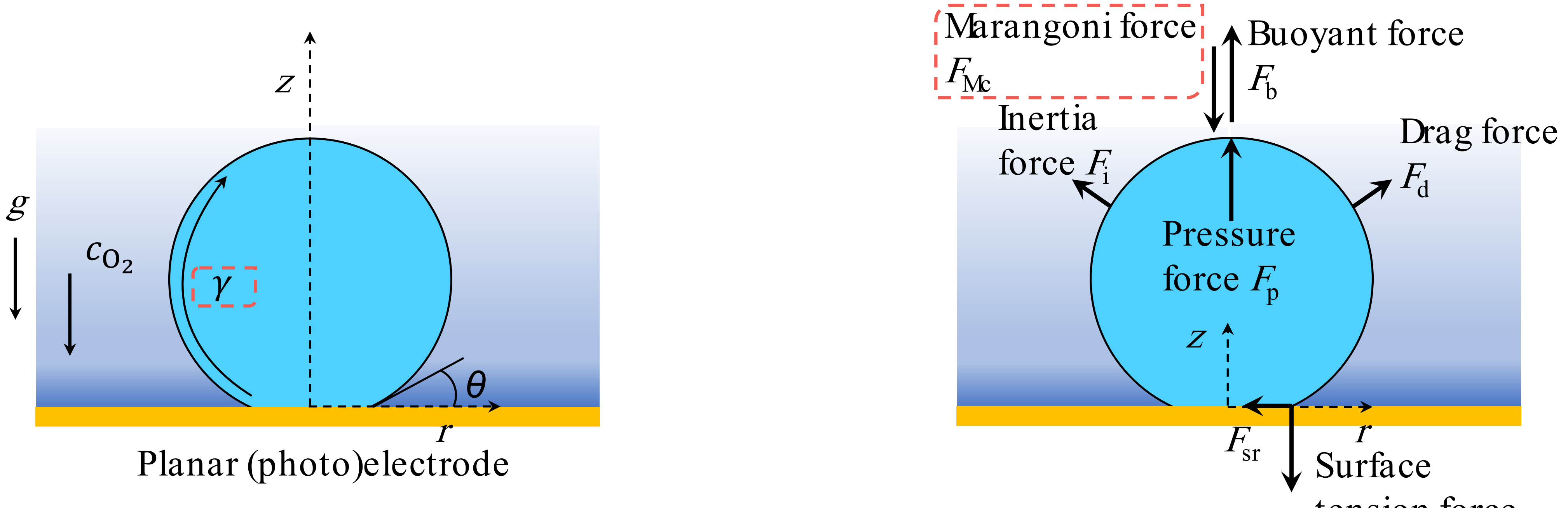
Snapshots of the bubble/electrolyte interface

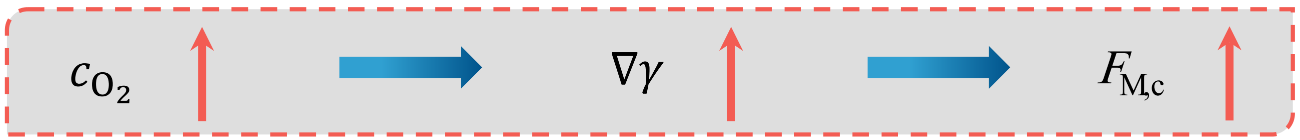


Super-saturated boundary layer of the dissolved oxygen facilitates bubble detachment

Does the Marangoni force dominate in bubble departure?

J W Chen, et al, *Electrochim. Acta, 274* (2018), 57

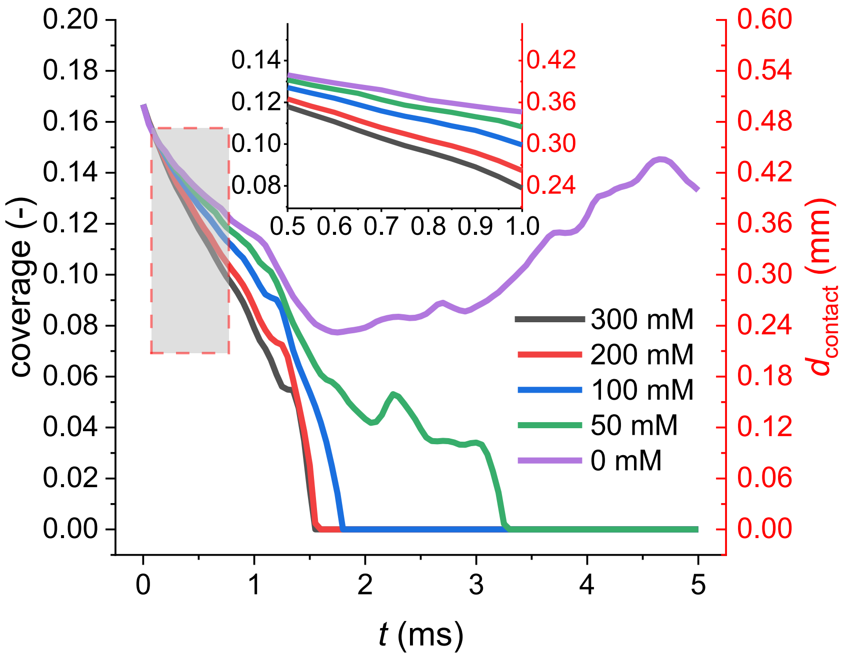


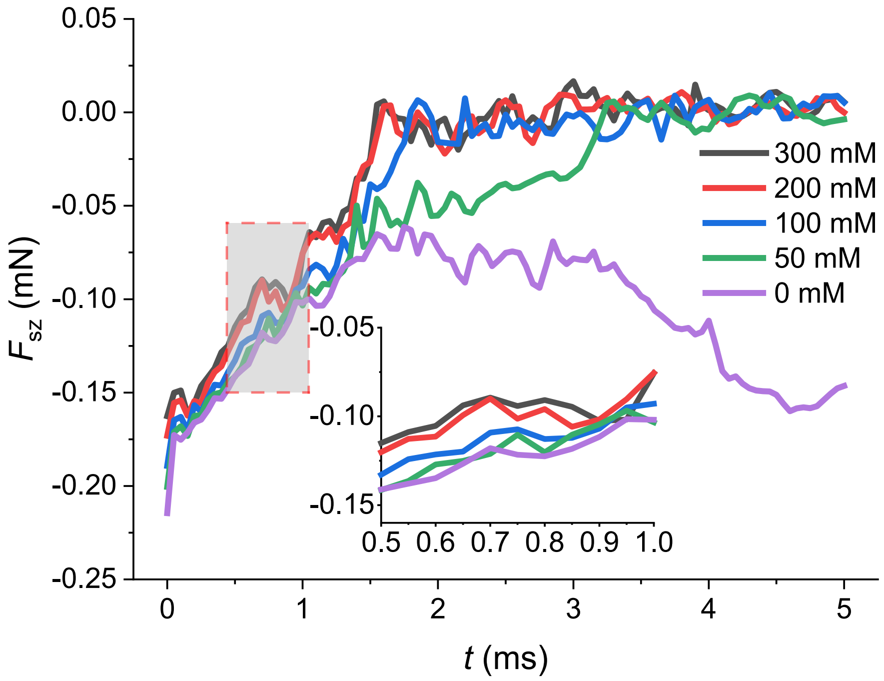


- Surface tension gradient induces the Marangoni convection, which leads to a downward (against the bubble departure trajectory) Marangoni force on bubble, F_{Mc}

- F_{Mc} is not the determining force during bubble departure

Surface tension force in *z* direction, F_{sz}





- Bubble coverage on the (photo)electrode follows the same trend as F_{sz}
- Surface tension gradient due to the concentration difference of dissolved oxygen causes dramatic morphological changes at the bubble/electrolyte interface, thus decreases the bubble coverage on (photo)electrode, which is the determining factor in bubble detachment

Summary

We developed a simple model to describe how the super-saturated boundary layer of dissolved oxygen affects bubble detachment

- Surface tension coefficient is significantly affected by the concentration of dissolved oxygen
- Super-saturated boundary layer of dissolved gas facilitates bubble detachment
- Surface tension gradient induces the Marangoni convection, thus leads to a downward (against the bubble departure trajectory) Marangoni force, F_{Mc}, which is, however, not the determining factor
- Surface tension force in z direction, F_{SZ}, is the dominant force which prevents bubble departure

c_{O_2} ↑ → $\nabla\gamma$ ↑ → Marangoni convection ↑ → morphological change of interface ↑ → bubble coverage ↓ → F_{SZ} ↓ → bubble departure ↑

Acknowledgements

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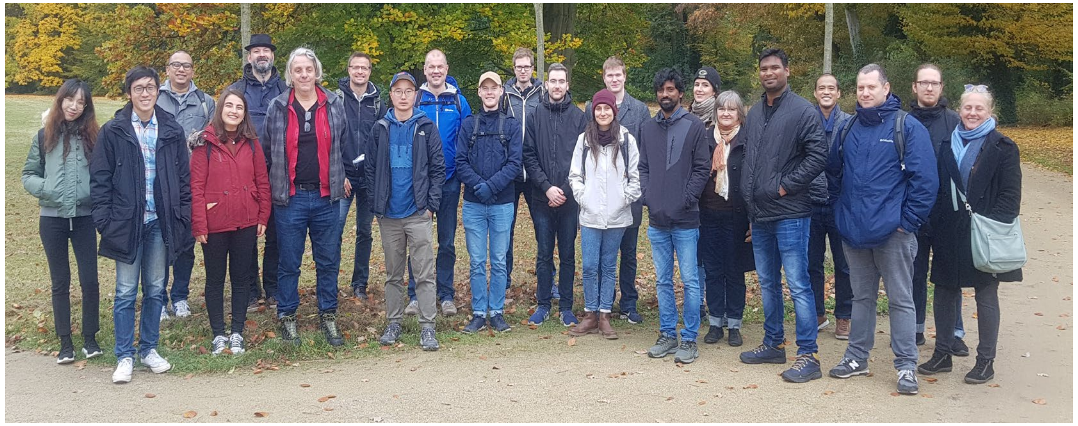

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