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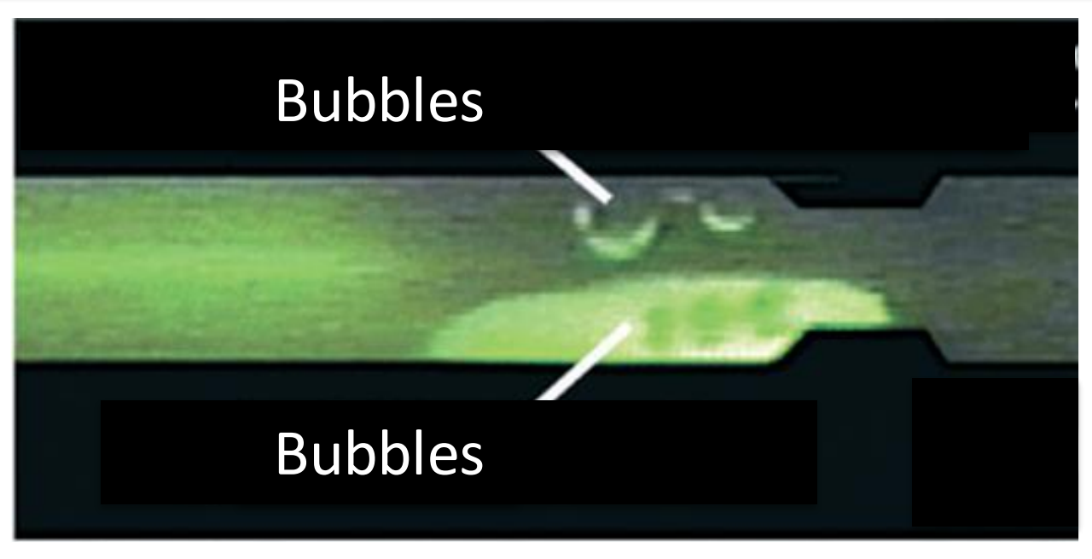
A Volume-of-Fluid-based approach for bubble growth in electrolytic solutions

PhD Student: Gabriele Gennari
Supervisors: Prof. Richard Jefferson-Loveday and Prof. Steve Pickering

Background

- The **Photo-Electro Project** is a multi-disciplinary research group focused on making chemical manufacturing more **sustainable**.
- From a sustainability point of view, **electrochemistry** is a very attractive methodology as physical reagents may be replaced by electrons generated from **green energy** sources.
- The **electric current** produced by the voltage difference between the electrodes may **generate gas molecules** dissolved in the liquid, leading to a **locally supersaturated** fluid. **Bubbles** are then generated on the electrodes surfaces.
- Bubbles reduce the **active electrocatalytic area** and induce a **non-uniform current** density distribution. They also **increase the resistance** of the electrolytic solution. All these effects are proven to be **detrimental for electrochemistry** [1].



Bubbles generation in an electrolytic solution [2].

Numerical Approach

- The Open Source Code **Basilisk** [3] is used to solve the incompressible **Navier-Stokes Equations**. We solve a single set of equations with variable density and viscosity (Single-Field Formulation).
- The **Continuity Equation** is modified to take into account the **Phase Change** effect:

$$\nabla\cdot\boldsymbol{u} = \dot{m}\left(\frac{1}{\rho_G}-\frac{1}{\rho_L}\right)\frac{A_\Sigma}{V}$$

- The **interface** is tracked with the **Volume of Fluid** Method:

$$\frac{\partial f}{\partial t}+\boldsymbol{u}\cdot\nabla f = \frac{\dot{m}}{\rho_f}\frac{A_\Sigma}{V}$$

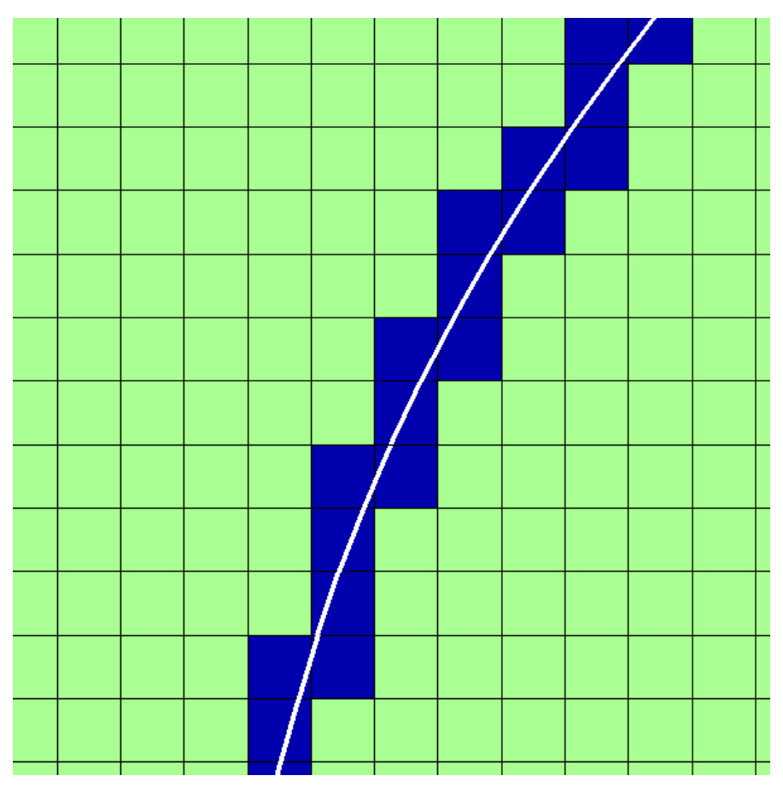
- **A two-scalar approach** [4] is used to compute the species concentration field. This requires the solution of an additional transport equation (**advection-diffusion-reaction**).

$$\frac{\partial c}{\partial t}+\boldsymbol{u}\cdot\nabla c = \nabla\cdot(D_c\nabla c)+\frac{\dot{m}}{M}\frac{A_\Sigma}{V}$$

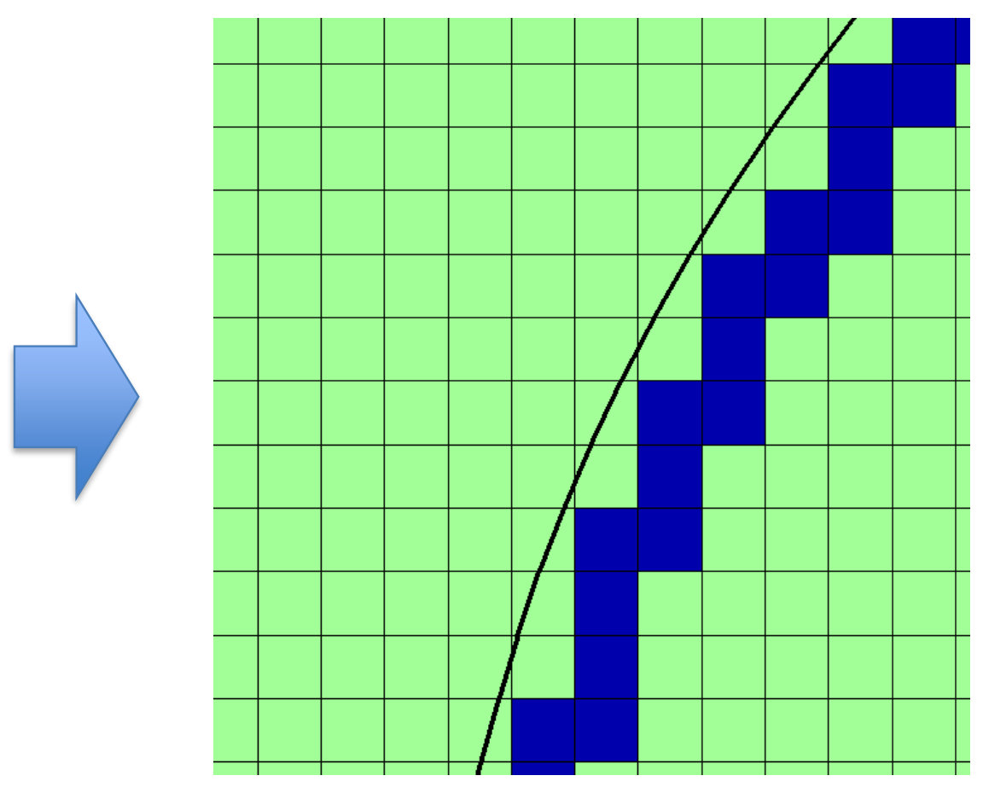
- **Mass Transfer** is computed in each interfacial cell. We evaluate the gradient on the liquid-side of the interface by using **quadratic** (2D) or **bi-quadratic** (3D) interpolation between the first two rows of neighbouring cells [4].

$$\dot{m} = D_c\cdot M\cdot\left.\frac{\partial c}{\partial n}\right|_\Sigma$$

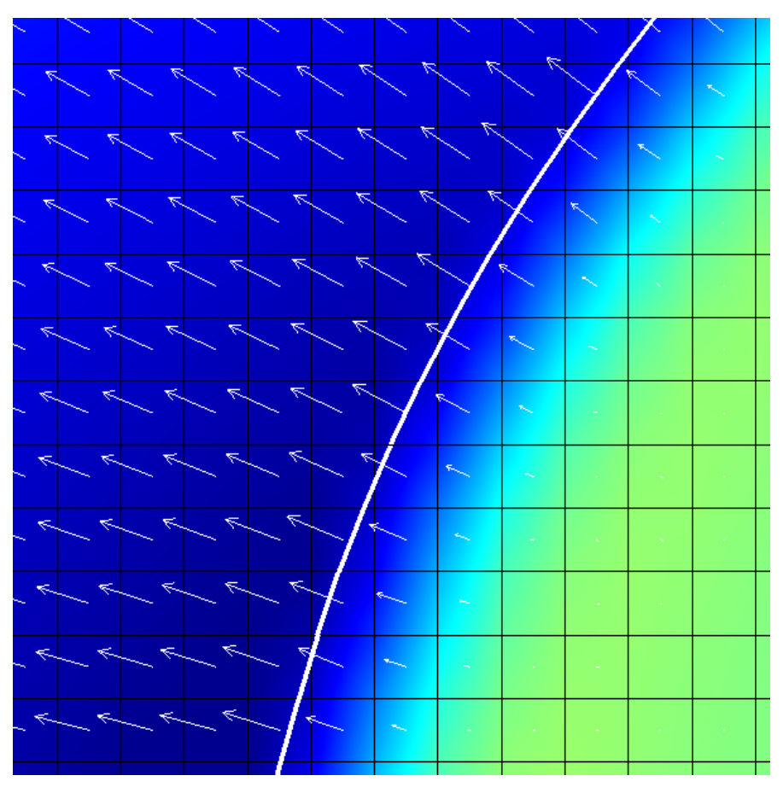
- The concentration value at the interface is given by **Henry's Law** for saturated interfaces.
- To make the incompressible VOF scheme compatible with the **non-solenoidal velocity field**, we propose an approach inspired by the Ghost Fluid Method [5]. We smoothly extend the liquid velocity film across the interface by **shifting the mass source term** to the first row of pure gas cells.



Mass transfer computation in interfacial cells.



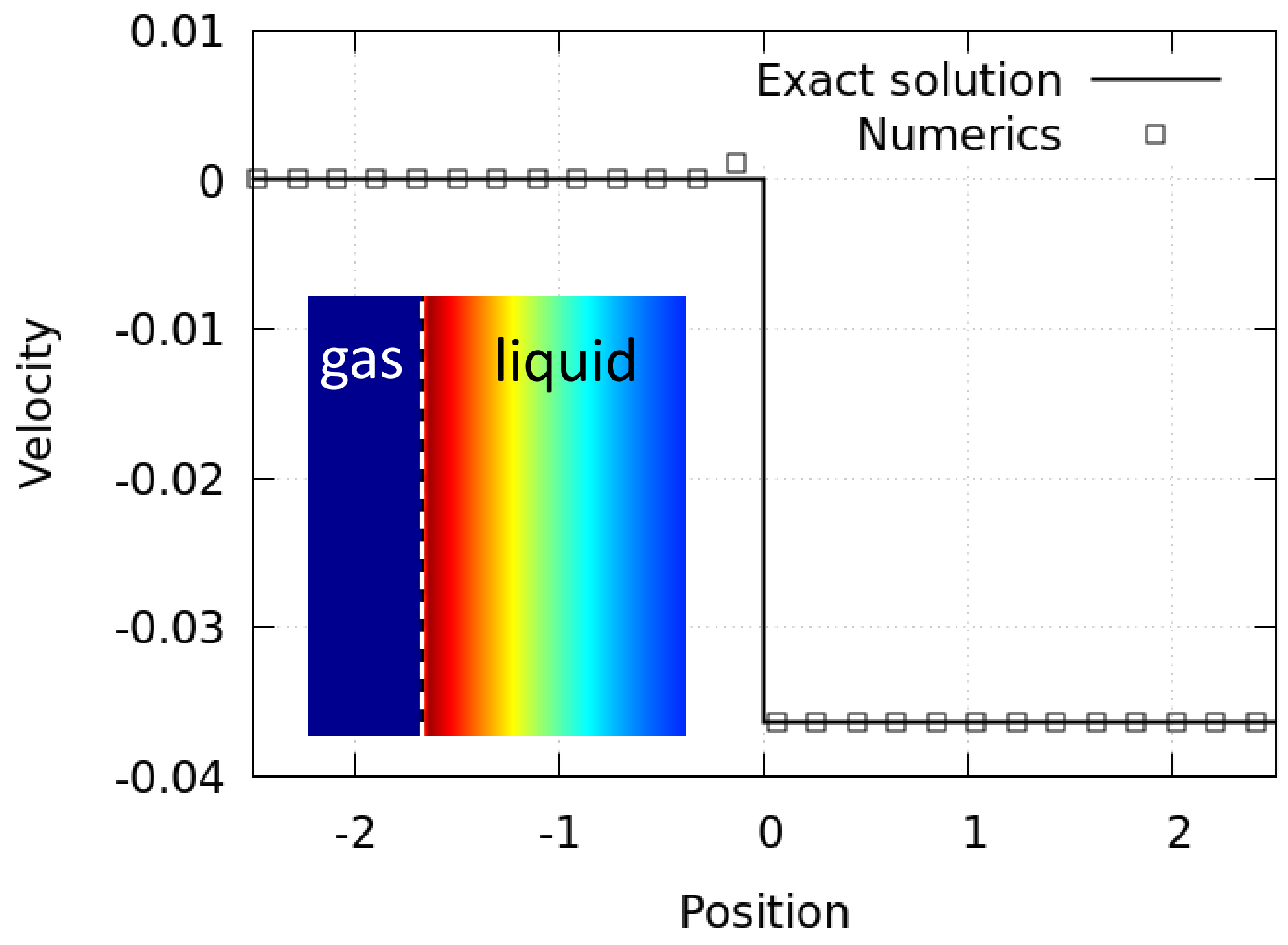
Mass transfer distribution after the shifting step.



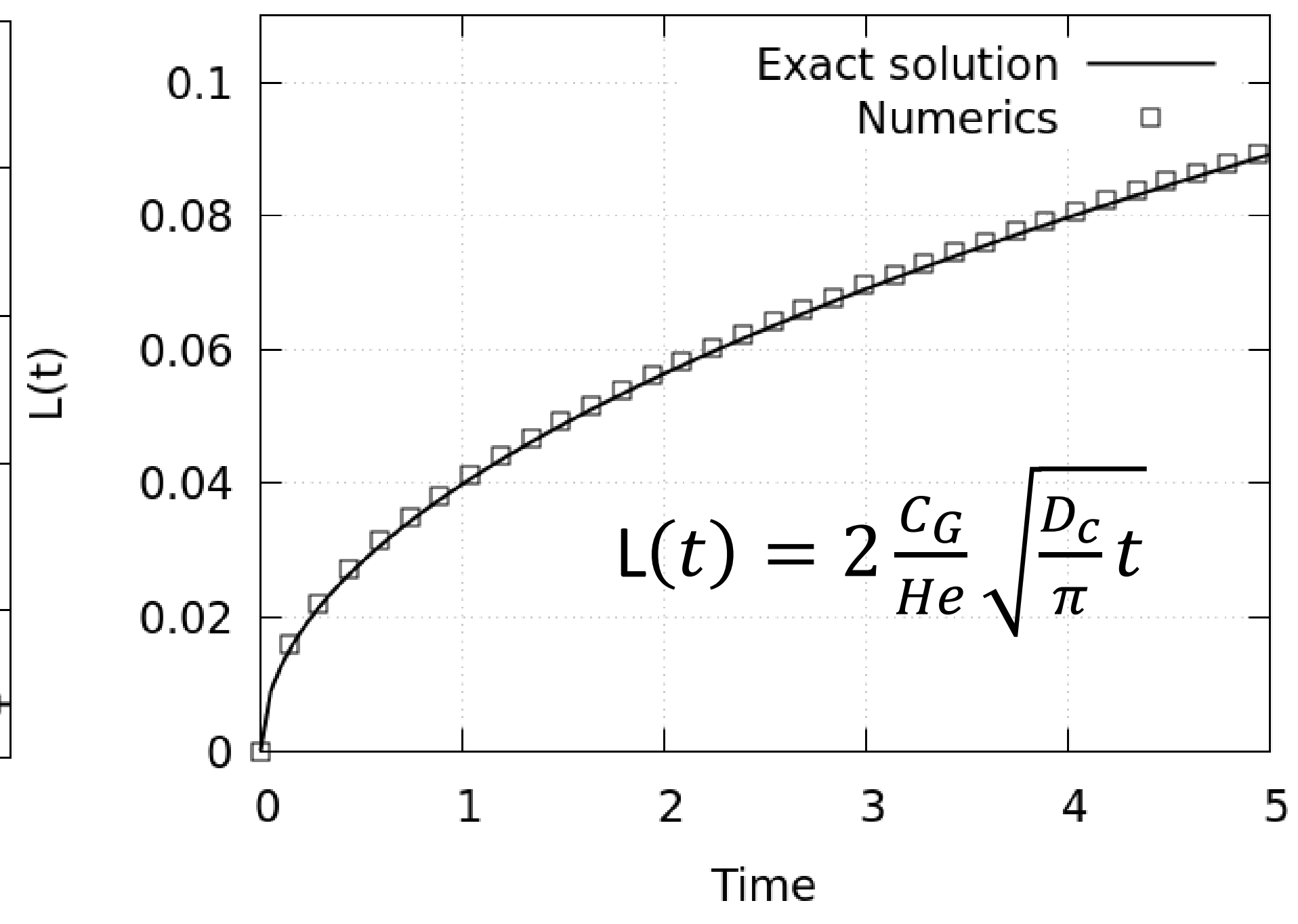
Velocity Field and contour of the horizontal velocity component.

Validation Benchmarks

1. Stefan Problem – 1D planar interface

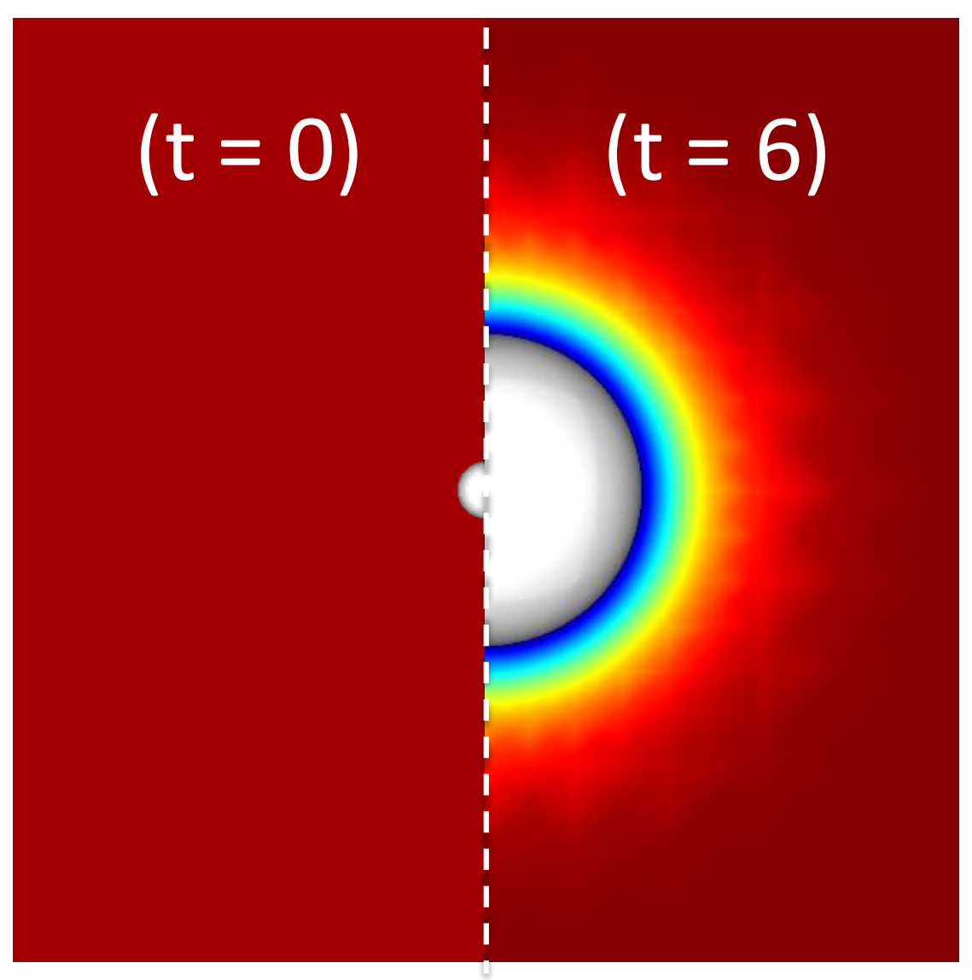


Discontinuous Velocity profile across the interface and contour of species concentration.

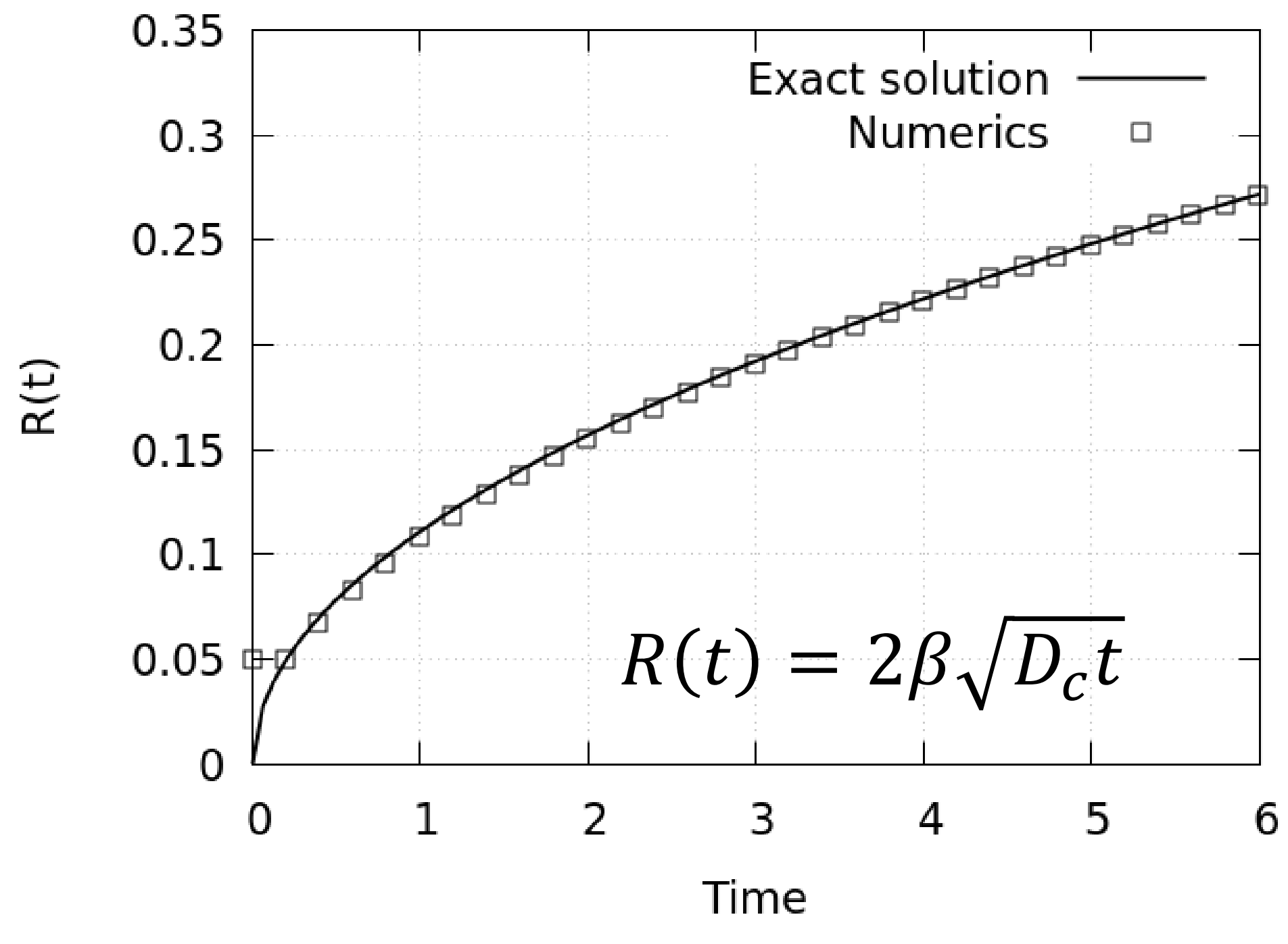


Displacement of the interface vs time.

2. Bubble growth in a supersaturated solution



Bubble shape and species concentration in the liquid at t=0 (left) and t=6 (right).



Bubble Radius vs time.

Future Work

- Model validation for moving bubbles (rising bubbles, bubbles in shear flows)
- Modelling of bubble growth on an electrode surface
- Modelling of a full electrochemical reactor
- Investigation on the influence of bubbles on the performance of electrochemical reactors

References

[1] Angulo, A.; van der Linde, P.; Gardeniers, H.; Modestino, M.; Fernández Rivas, D., Influence of Bubbles on the Energy Conversion Efficiency of Electrochemical Reactors. *Joule* **2020,** *4* (3), 555-579.

[2] S. Z. Hua, F. Sachs, D. X. Yang and H. D. Chopra, Anal. Chem., 2002, 74, 6392–6396.

[3] http://basilisk.fr/

[4] S. Fleckenstein, D. Bothe, A volume-of-fluid-based numerical method for multi-component mass transfer with local volume changes, J. Comput. Phys. 301 (2015) 35–58.

[5] D. Nguyen, R. Fedkiw, M. Kang, A boundary condition capturing method for incompressible flame discontinuities, J. Comput. Phys. 172 (2001) 71–98.

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