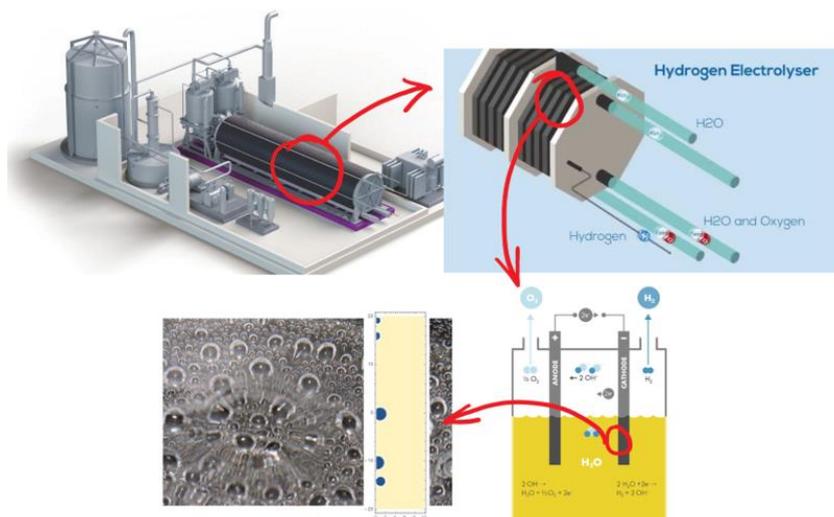


163 European Study Group with Industry



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PROCEEDINGS OF THE
163 EUROPEAN STUDY GROUP WITH
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Universidade de Vigo



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PROCEEDINGS OF THE 163 EUROPEAN STUDY GROUP WITH INDUSTRY (163 ESGI)

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Introduction

Initiated in Oxford in 1968, Study Groups with Industry provide a forum for industrial scientists to work alongside academic mathematicians on problems of direct industrial relevance. They are an internationally recognized method of technology and knowledge transfer between academic mathematicians and industry, usually lasting one week.

The success of the ESGI lies in its unique format which has been copied around the world, and which allows mathematicians to work on reduced groups to study problems presented by industry. These problems arise from any industrial and economic sector thanks to the versatility of Mathematics.

The objective is to present the capabilities of Mathematics and its applicability in a large part of the challenges and needs that industry presents. It aims to bring small, medium and large companies a technology with great potential, used by highly qualified researchers and which does not require large investments to use.

Therefore, collaboration between industry experts and researchers is a key point to address technological innovation issues by using successful mathematical techniques. ESGI contributes to the promotion of Mathematics and helps companies to use Mathematics to improve their processes.

The goals which want to be reached at the ESGI are:

- find solutions and bring new insights to existing industrial problems;
- establish lasting and productive working relations between industry and mathematicians;
- propose new lines of research based on business challenges;
- reinforce the importance of Mathematics in industry and mathematical profiles companies; and
- stimulate greater awareness of the power of Mathematics to provide solutions to solve real-world problems.

Finally, it should be pointed out that 70 researchers, students, professors and company technicians contributed to a successful 163 ESGI.

Santiago de Compostela on 20th January, 2022

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Nucleation, growth and detachment of bubbles formed by reaction over surfaces

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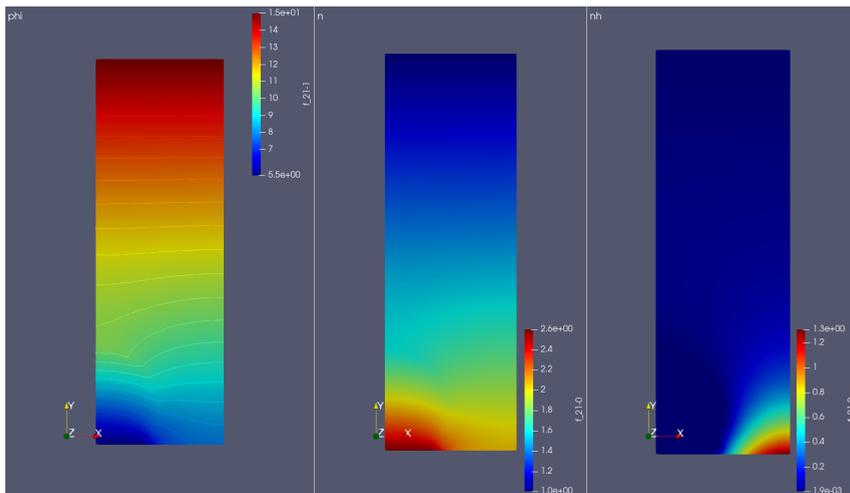
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Nucleation, growth and detachment of bubbles formed by reaction over surfaces

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Abstract

This article concerns a problem presented at the 163 European Study Group with Industry by Repsol company. After a description of the problem, a mathematical model is introduced which is formulated and solved, for a simple case, by using phase-field methods implemented in FEniCs software

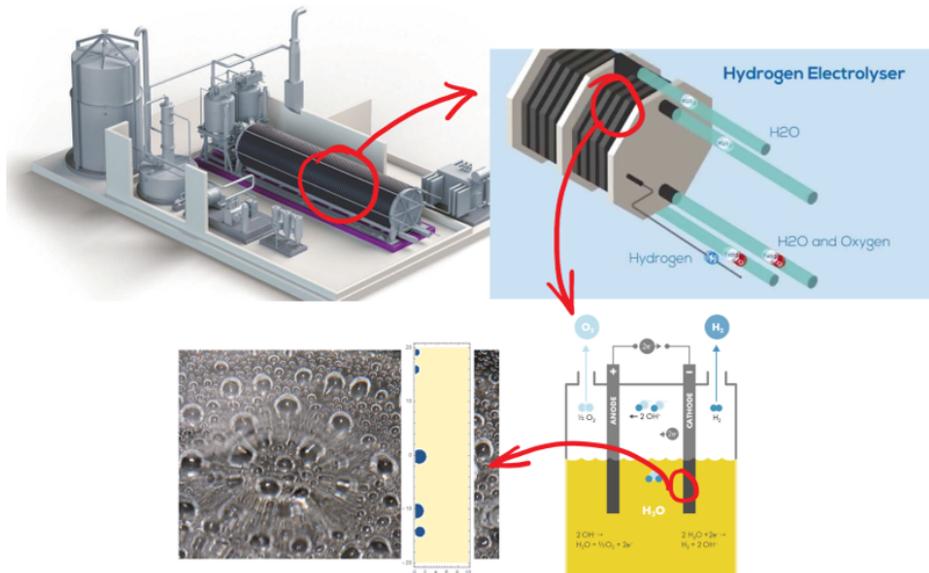


Figure 1: Example of electrochemical systems

1. Introduction

Repsol has been actively working in recent years on electrochemical systems. Batteries and electrolytic cells are two examples ... but also corrosion (which produce millionaire losses along the many kilometers of pipelines) or heterogeneous catalysts are closely related problems.

In electrolytic cells (i.e. to produce hydrogen at low pressure), either reduction or oxidation reaction at one electrode, requires that the ionic species travel towards the wall from the water. On the walls of the electrodes, small growing bubbles with gas, a product from the electrochemical reaction occurring in the interface electrode-electrolyte, are forming. Rapidly the surface of the electrodes are almost completely covered by the bubbles but only at those regions of the wall free of bubbles (insulate) are able to complete the reaction. Thus, only a small fraction of the wall is effective and the efficiency of the process is limited by the behavior of the attached bubbles.

When the bubbles become large they begin to feel the outer flow and the buoyancy. Detachment of the bubble occurs when finally those forces overcome the capillary force

If the bubbles are large we also may have troubles in the case of porous electrodes. It is very important to understand the process and mechanism by which a bubble born, grows and detaches and to determine the relevant parameters and their relation.

The outline of this article is as follows: first, a mathematical model using conservation laws is derived. Second, we do a “translation” of these sharp interface equations to a diffuse interface model using a phase field method. Third, we simulate a simplified scenario but at the same time, that includes all the important effects.

The main goals of the company are

- to understand the process and mechanisms by which a bubble (of H₂, for sake of concreteness) is born, grows and detach as product of an electrochemical reaction at the interface between an electrode and an electrolyte,
- to build a model that describes the process and allows us to simulate it.

From the company point of view, to get a phase field model would be desirable

2. Water electrolysis

Water electrolysis is the decomposition of water into hydrogen and oxygen using electric energy in an electrolytic cell. The electrochemical reactions involved are a reduction reaction at one of the electrodes (the cathode), where

hydrogen is produced, and an oxidation reaction at the other electrode (the anode), where oxygen is produced.

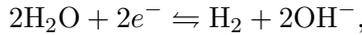
The rates of these reactions depend on the concentrations of the ionic species in the electrolyte surrounding the electrodes, and on the differences of electric potential between each electrode and the electrolyte around it.

The reactions are very slow in pure water, because the molar concentrations of H^+ and OH^- are very small; $n_H = n_{OH} = 10^{-7}$ mol/L at normal temperature and pressure, from the equilibrium of the dissociation reaction

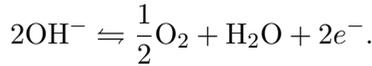


and the condition of electrical neutrality $n_H = n_{OH}$.

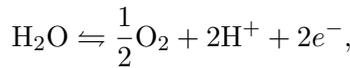
An alkaline solution is obtained by dissolving in water a species that dissociates into OH^- and a cation (KOH is used in most commercial electrolyzers), so that the $\text{H}^+ - \text{OH}^-$ equilibrium is displaced toward increasing the concentration of OH^- , and the cations supplied by the dissociated species enforce quasineutrality. The overall reduction reaction at the cathode is then



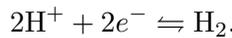
and the OH^- travels to the anode to undergo the oxidation reaction



An acidic solution is obtained by dissolving a species (e.g. H_2SO_4) that displaces the $\text{H}^+ - \text{OH}^-$ equilibrium toward increasing the concentration of H^+ , with the anions of the dissociated species enforcing quasi-neutrality. The oxidation reaction at the anode is then



and the H^+ ions travel to the cathode to be reduced in the reaction



2.1. Cathode reaction

We focus on the reduction reaction going on at the cathode and use the Butler-Volmer model to write its rate in the form

$$\omega = \frac{i_o^s}{2F} \left[e^{2\alpha F(\phi_0 - \phi_0^{eqs})/RT} \left(\frac{n_{\text{H}_2\text{O}}}{n_w} \right)^2 - e^{-2(1-\alpha)F(\phi_0 - \phi_0^{eqs})/RT} \left(\frac{n_{\text{OH}}}{n^s} \right)^2 \frac{n_{\text{H}_2}}{n^s} \right],$$

in the alkaline case, and

$$\omega = \frac{i_o^s}{2F} \left[e^{2\alpha F(\phi_0 - \phi_0^{eqs})/RT} \left(\frac{n_H}{n^s} \right)^2 - e^{-2(1-\alpha)F(\phi_0 - \phi_0^{eqs})/RT} \frac{n_{\text{H}_2}}{n^s} \right],$$

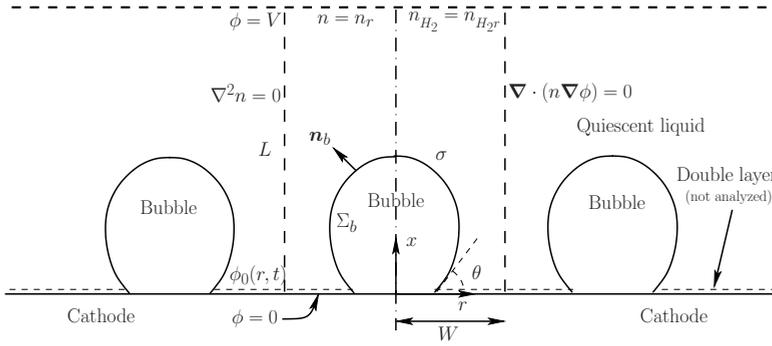


Figure 2: Definition sketch.

in the acidic case.

Here ω is the number of moles of hydrogen produced per unit time and unit electrode area; n_j with $j = \text{H}_2\text{O}, \text{OH}, \text{H}, \text{H}_2$, are the molar concentrations of the species taking part in the reaction, with $n^s = 1 \text{ mol/L}$ the molar concentration of all the electroactive species in the so-called standard reference state, in which $n_{\text{H}_2\text{O}} = n_w = 55.55 \text{ mol/L}$ (pure water); ϕ_0 is the electric potential at the edge of the double layer relative to the electrode (where $\phi = 0$) and ϕ_0^{eqs} is the equilibrium value of ϕ_0 at which $\omega = 0$ in the standard reference state; i_0^s is the exchange current in the standard reference state, which is a function of the material and structure of the electrode; R , F and T are the universal gas constant, the Faraday constant and the temperature; and α , the transfer coefficient, is a model constant.

Since the solubility of hydrogen in water is very small, the solution rapidly becomes supersaturated and hydrogen bubbles nucleate on the cathode.

2.2. Model formulation

A quiescent, dilute solution is considered, in which hydrogen bubbles grow quasi-statically at the electrode due to the diffusion flux of dissolved hydrogen reaching their surfaces from the supersaturated liquid around the electrode. The bubbles detach when surface tension ceases to be able to balance buoyancy. In the model, the bubbles are equispaced and grow synchronously, so that only the conditions around one bubble need be computed. In addition, the bubbles are assumed to be axisymmetric. In these conditions, the concentrations of ions (n) and dissolved hydrogen (n_{H_2}), and the electric potential (ϕ) satisfy

$$\nabla^2 n = \nabla^2 n_{\text{H}_2} = 0, \quad \nabla \cdot (n \nabla \phi) = 0$$

outside the double layer on the electrode. These equations are obtained by linearly combining the conservation equations for the two ionic species and the dissolved hydrogen, and imposing quasi-neutrality.

In the region of the electrode surface ($x = 0$) not covered by bubbles, the boundary conditions

$$\frac{\partial n}{\partial x} = \mp \frac{2Z}{(1+Z)D_{\mp}}\omega, \quad \frac{\partial n}{\partial x} \pm \frac{ZF}{RT} \frac{\partial \phi}{\partial x} = 0, \quad -D_{H_2} \frac{\partial n_{H_2}}{\partial x} = \omega$$

must be satisfied. These conditions express the balance of the flux of each electroactive species entering or leaving the double layer (by diffusion and migration from the bulk), and the rate at which that species is consumed or produced by the electrode reaction. Upper signs are for the an alkaline solution and lower signs are for an acidic solution. Z is the modulus of the charge number of the cations in the first case and of the anions in the second; and D_{\pm} and D_{H_2} are the diffusivities of H^+ , OH^- and dissolved hydrogen.

At the surface $\Sigma_b(t)$ of a growing bubble, the conditions that the fluxes of both types of ions be zero and the concentration of dissolved hydrogen be the saturation concentration n_s read

$$\mathbf{n}_b \cdot \nabla n = \mathbf{n}_b \cdot \nabla \phi = 0, \quad n_{H_2} = n_s \quad \text{at} \quad \Sigma_b,$$

where \mathbf{n}_b is the unit normal to the bubble surface.

In addition to these, conditions of zero flux mimicking a periodic array of bubbles are imposed at a distance W from the symmetry axis:

$$\frac{\partial n}{\partial r} = \frac{\partial n_{H_2}}{\partial r} = \frac{\partial \phi}{\partial r} = 0 \quad \text{at} \quad r = W.$$

Finally, the conditions

$$n = n_r, \quad n_{H_2} = n_{H_{2r}}, \quad \phi = V \quad \text{at} \quad x = L$$

are imposed at a distance L above the electrode.

With n_r , $n_{H_{2r}}$ and V constant, these conditions can be approximately realized if the cathode is at the bottom of a recess of depth L and a stream flows horizontally above the recess that uniformizes the concentrations of all the species without inducing a significant flow in the recess. The anode (not analyzed) would be a horizontal electrode much larger than the cathode and located far above the recess, so that it acts as a nonpolarizable electrode.

2.3. Bubble growth and average current density

Once the solution of this problem is found for a given equilibrium shape of the bubble, the mass flux of hydrogen reaching the bubble can be evaluated as

$$\dot{m} = W_{H_2} D_{H_2} \int_{\Sigma_b} \mathbf{n}_b \cdot \nabla n_{H_2} \, dA,$$

where W_{H_2} is the molecular mass of hydrogen, and the rate of growth of the bubble volume, V_b , whose shape is an equilibrium shape at any time, is

$$\frac{dV_b}{dt} = \frac{RT}{W_{H_2} p_g(t)} \dot{m}(t) - \frac{RT}{W_{H_2} p_g(t)^2} \int_0^t \dot{m}(t') dt' \frac{dp_g}{dt},$$

where $p_g(t)$ is the pressure of the gas (hydrogen) in the bubble, which is a known function of the bubble volume.

The electric current density averaged over the surface of the electrode is

$$\bar{i}(t) = \frac{2\pi \int_{r_c}^W 2\omega r dr}{\pi W^2}.$$

where $r_c(t)$ is the radius of the contact line of the bubble with the electrode.

This current density is further averaged over the time of growth of a bubble and scaled with $FD_{OH}n_r/\ell_c$ in the alkaline case and with $FD_H n_r/\ell_c$ in the acidic case, where $\ell_c = (\gamma/\rho g)^{1/2}$ is the capillary length, with ρ , γ , g the density and surface tension of the liquid, and the acceleration of gravity.

2.4. Results: Average current density as a function of voltage

Figure 3 shows the space and time averaged current density as a function of the modified dimensionless voltage $\tilde{V} = F(V - \phi_0^{eqs})/RT$ for various values of other parameters in alkaline (left) and acidic (right) cases.

Solid curves give the current density in the absence of bubbles. In the alkaline case (in which water consumption has been neglected) the current increases exponentially with the voltage. In the acidic case, the concentration of H^+ at the electrode tends to zero when the voltage increases, and the current density saturates at a finite value.

The current density increases in all cases with the exchange current i_0^s , which is a measure of the catalytic activity of the electrode.

Hydroxide ions are a reaction product in the alkaline case. The current density decreases when the concentration of this species is increased at the upper boundary by increasing n_r .

In the acidic case, H^+ is a reactant. The current density increases when its concentration is increased at the upper boundary.

Symbols are numerical results with bubbles. As can be seen, the current density increases when bubbles are present. This beneficial effect of the bubbles can be traced to their role as sinks of dissolved hydrogen. Since hydrogen is the product of the cathode reaction, decreasing its concentration increases the forward rate of the reaction, and thus the electric current.

In the framework of this model, this effect overcomes the negative effect of attached bubbles, which cover a fraction of the electrode area, rendering it inactive for the electrochemical reaction.

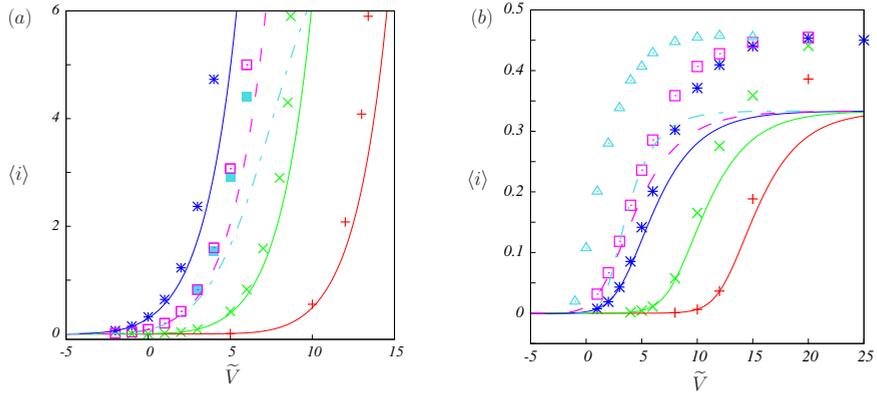


Figure 3: Space and time averaged current density as a function of the voltage \tilde{V} , for alkaline solutions (a) and acidic solutions (b). Shown are results for $W = 1$, $\theta = 45^\circ$ and $n_r = 0.1$ mol/L, $i_0^s = 10^{-3}$ A/m² (pluses), $n_r = 0.1$ mol/L, $i_0^s = 0.1$ A/m² (crosses), $n_r = 0.1$ mol/L, $i_0^s = 10$ A/m² (stars), and $n_r = 0.5$ mol/L, $i_0^s = 10$ A/m² (open squares). The thin curves show the current density in the absence of bubbles. Solid curves are for $n_r = 0.1$ mol/L, with i_0^s increasing from right to left, and the dashed curve is for $n_r = 0.5$ mol/L, $i_0^s = 10$ A/m². In addition, the filled squares and the chain curve in (a) are results for $n_r = 0.5$ mol/L, $i_0^s = 10$ A/m² taking water consumption into account, and the triangles and the chain curve in (b) are results for $n_r = 0.1$ mol/L, i_0^s infinite.

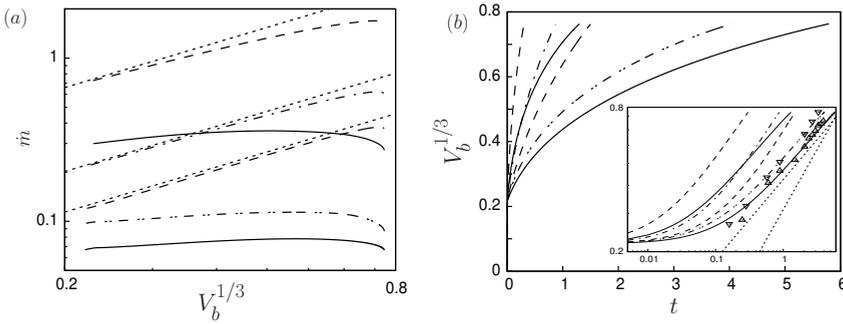


Figure 4: (a) Mass of hydrogen vaporizing per unit time as a function of the cubic root of the bubble volume, and (b) cubic root of the bubble volume as a function of time, in linear and logarithmic scales (inset), for some sample cases. Solid: acidic, $\tilde{V} = 2$ and 5 , $W = 1$; dashed: acidic, $\tilde{V} = 2$ and 5 , $W = 3$; dash-double-dot: alkaline, $\tilde{V} = -2$, $W = 1$; dash-dot: alkaline, $\tilde{V} = -2$, $W = 3$. The dotted lines in (a) have slope $1/2$, and the dotted lines at the lower part of (b) are $V_b^{1/3} = 0.3t^{1/2}$ and $V_b^{1/3} = 0.4t^{1/3}$.

2.5. Results: Growth of a bubble

Figure 4 shows the mass of hydrogen vaporizing per unit time as a function of the size of the bubble, defined as the cubic root of its volume, and the right-hand side figure shows this size as a function of time.

The rate of intake of hydrogen is nearly proportional to the size of the bubble when the bubble spacing (W) is large compared with the capillary length. This leads to a size that grows nearly as the square root of time.

When the spacing of the bubbles is decreased, most of the hydrogen produced at the electrode reaches the bubbles, because the channels left between bubbles are too narrow for the hydrogen to escape through them. The vaporization flux is nearly independent of the size of the bubble, and their volume increases nearly linearly with time.

3. Phase field formulation

A useful approach to simulation of problems involving moving interfaces separating two different phases is by means of a so-called phase field. This approach amounts to introducing a phase field scalar function $\Psi(\mathbf{x}, t)$ so that $\Psi = 1$ in one phase and $\Psi = -1$ in the other phase. The function Ψ will have a very sharp transition between the two limiting values -1 and 1 across the interface. In this way, sharp interfaces are replaced by "diffuse interfaces" which are not exactly surfaces but space regions where the level lines of Ψ with values between -1 and 1 concentrate. The easiest way to introduce the phase field into a model comes from the observation that a free energy involving the area

A of an interface

$$F = \gamma A$$

is well approximated by the following phase-field energy

$$F_\delta = \gamma_0 \int \left(\delta \frac{|\nabla \Psi|^2}{2} + \frac{1}{\delta} W(\Psi) \right)$$

where

$$W(\Psi) = (1 - \Psi^2)^2.$$

Classical works (see, for instance [1], [3] and references therein for more information) show that minimizers of F_δ , that is interfacial shapes that minimize F_δ , converge (in a suitable sense) to minimizers of F as $\delta \rightarrow 0$ provided $\gamma = \frac{4\sqrt{2}}{3}\gamma_0$. The level lines of Ψ concentrate in a $O(\delta)$ region along the normal direction to the interface and the function Ψ in that direction approaches the explicit form $\Psi = \tanh \frac{x}{\delta}$ with x the coordinate in the normal direction. This stationary version of the phase field methodology extends more or less automatically to evolutionary problems where interfacial energies come into play like, for instance, a gradient flow involving F that is replaced by a gradient flow of F_δ . This yields, depending on the kind of gradient flow considered, to the well-known Allen-Cahn equation (first introduced in [2])

$$\Psi_t = -\frac{\delta F_\delta}{\delta \Psi}$$

and the Cahn-Hilliard equation (cf. [4])

$$\Psi_t = -\nabla \cdot \left(M(\Psi) \nabla \frac{\delta F_\delta}{\delta \Psi} \right)$$

which are typically the evolution equations for Ψ when coupled with other physical field equations. An important difference between Allen-Cahn and Cahn-Hilliard is that the later preserves the volume enclosed by a level surface of Ψ . This is important, for instance, when modelling incompressible fluids. Phase field formulation, with Ψ solving Cahn-Hilliard equations, for two-phase fluids satisfying Navier-Stokes equations under the effects of surface tension has been introduced to successfully model drops and bubbles (see [1] and the references on classical works presented there). The great advantages of a diffuse interface models with respect to classical sharp interface models is that it allows to continue solutions after topological changes such as bubble detachment, coalescence or collapse and allows solving for multiple bubbles at the same time (see [5] for instance or [6] for the specific problem of the detachment of a bubble). In addition, since no sharp moving interfaces are present, one does not have to deal with boundary conditions there and this represents an enormous advantage for numerical implementation.

In our problem, we have to couple the phase field Ψ with the other fields in the model so that equations and boundary conditions are satisfied as $\delta \rightarrow 0$. In this spirit, we replace the ion concentration equation

$$\nabla^2 n = 0$$

to be satisfied in the liquid medium with the equation

$$\nabla \cdot (a(\Psi)\nabla n) = 0$$

where

$$a(\Psi) = \frac{1 + \Psi}{2}$$

so that both equations coincide when $\Psi = 1$ but ions do not diffuse inside the bubble where $a(\Psi) \simeq 0$. Analogously, for the electric field equation

$$\nabla \cdot (n\nabla\phi) = 0$$

we write in terms of the phase field Ψ

$$\nabla \cdot (a(\Psi)n\nabla\phi) = 0$$

At the surface of the bubble, continuity of $a(\Psi)\nabla n \cdot \mathbf{n}$ and $a(\Psi)n\nabla\phi \cdot \mathbf{n}$ in the normal direction implies that necessarily $\nabla n \cdot \mathbf{n} \simeq 0$ and $n\nabla\phi \cdot \mathbf{n} \simeq 0$ when approaching the bubble from the liquid interface. In this way, boundary conditions at the bubble are satisfied. Finally, for the H_2 concentration n_{H_2} we replace the equation

$$-\nabla^2 n_{H_2} = 0$$

with the equation

$$-\nabla \cdot (a(\Psi)\nabla n_{H_2}) + b(\Psi)(n_{H_2} - n_s) = 0$$

where the term $b(\Psi)(n_{H_2} - n_s)$ represents a penalization that cancel at the liquid region but imposes $n_{H_2} = n_s$ inside the bubble and at its boundary. This is achieved by taking

$$b(\Psi) = C \frac{1 - \Psi}{2}$$

with $C > 1$ and sufficiently large.

At the electrode, we impose the same conditions but replacing the Damköhler number Da with a Ψ dependent one:

$$Da(\Psi) = \frac{1 + \Psi}{3}$$

Concerning the phase field Ψ , we must guarantee that the bubble grows when H_2 enters inside it. The volume of the drops V_b satisfies

$$\frac{dV_b}{dt} = - \int_{int} \nabla n_{H_2} \cdot \mathbf{n} dS = 0 \quad (1)$$

which is fulfilled in the equation

$$\Psi_t + \nabla n_{H_2} \cdot \nabla \Psi = 0 \quad (2)$$

where the volume enclosed by a level surface of Ψ satisfies (1). Nevertheless, equation (2) is not sufficiently suitable for two reasons: first it is first order and hence prone to numerical instabilities, and secondly it does not guarantee an equilibrium bubble surface. A solution to these two problems is to modify (2) in the form of the following Cahn-Hilliard version:

$$\Psi_t + \nabla n_{H_2} \cdot \nabla \Psi = -\nabla \cdot \left(M(\Psi) \nabla \frac{\delta F_\delta}{\delta \Psi} \right)$$

to be solved together with boundary conditions imposing that mass flow across the solid substrate is negligible and motion of contact lines of the interface touching the solid substrate. The first condition is fulfilled by imposing

$$M(\Psi) \nabla \frac{\delta F_\delta}{\delta \Psi} \cdot \mathbf{n} = 0$$

while the second can be implemented with

$$\gamma_0 \delta \frac{\partial \Psi}{\partial n} + \gamma'_{fs}(\Psi) = 0$$

with

$$\gamma_{fs}(\Psi) = \frac{\gamma_{fs}^{(1)} - \gamma_{fs}^{(2)}}{2} \sin \frac{\pi \Psi}{2}$$

where $\gamma_{fs}^{(1)} - \gamma_{fs}^{(2)}$ is the jump of interfacial tensions between the liquid-solid and the gas-solid interface. It can be shown (see [1]) that, in rest, the level lines of Ψ touch the substrate with an approximate angle θ so that

$$\cos \theta = \frac{\gamma_{fs}^{(1)} - \gamma_{fs}^{(2)}}{\gamma}$$

3.1. Results: A simplified model

A simplified model is employed to test the phase field formulation. In this case the phase field Ψ is define as a static field:

$$\Psi(\mathbf{x}) = \begin{cases} -1 & \text{if } \mathbf{x} \in B(R, \mathbf{x}_c), \\ 1 & \text{if } \mathbf{x} \notin B(R, \mathbf{x}_c), \end{cases} \quad (3)$$

where $R \in \mathbb{R}$ is a fixed scalar that represents the radius of the bubble and $\mathbf{x}_c \in \mathbb{R}^2$ is its center.

A 2D problem with only one bubble, defined by $\Psi(\mathbf{x})$, is solved avoiding the resolution of the evolution of the phase field equation (Allen-Cahn or

Cahn-Hilliard). The weak formulation of the equations is obtained multiplying each equation by a test function, integrating over the domain and applying a Green's formula:

$$\int_{\Gamma^E} a(\Psi) \nabla n \cdot \mathbf{m} \tilde{n} ds - \int_{\Omega} a(\Psi) \nabla n \cdot \nabla \tilde{n} dx = 0 \quad \forall \tilde{n} \in H_{\Gamma^D}^1(\Omega) \quad (4)$$

$$\int_{\Gamma^E} a(\psi) n \nabla \phi \cdot \mathbf{m} \tilde{\phi} ds - \int_{\Omega} a(\Psi) n \nabla \phi \cdot \nabla \tilde{\phi} dx = 0 \quad \forall \tilde{\phi} \in H_{\Gamma^D}^1(\Omega) \quad (5)$$

$$\begin{aligned} & - \int_{\Gamma^E} a(\Psi) \nabla n_{H_2} \cdot \mathbf{m} \tilde{n}_{H_2} ds + \int_{\Omega} a(\Psi) \nabla n_H \cdot \nabla \tilde{n}_{H_2} dx \\ & + \int_{\Omega} b(\Psi) (n_{H_2} - n_s) \tilde{n}_{H_2} dx = 0 \quad \forall \tilde{n}_{H_2} \in H_{\Gamma^D}^1(\Omega) \end{aligned} \quad (6)$$

where

$$a(\Psi) = \frac{1 + \Psi}{2}$$

is a function that is 0 inside the bubble,

$$b(\Psi) = 10^6 \frac{1 - \Psi}{2}$$

is a penalty term to force $n_{H_2} = n_s$ inside the bubble and Γ^E is the electrode boundary, the bottom side of the rectangle that defines the computational domain. On the top side, Γ^D , the Dirichlet boundary conditions are applied. A solution of this problem can be seen in Figure 5. The solution is obtained by using the FEniCS package [7], a set of libraries for the solution of Partial Differential Equations (PDE) by the Finite Element Method (FEM).

4. Conclusion

A model has been set up to extend the so-called sharp interface model (a model for which the interphase is a surface). The computational domain of the new model includes both the bubbles and the liquid around. The free boundary between them is handled by using a phase field method. Preliminary numerical results obtained by using FEniCS package are very promising as they exhibit good agreement between the two models. Pending developments are,

- Including gravity and other body forces
- Handling several bubbles. Allowing coalescence and bubble formation (nucleation)
- Including motion of the electrolyte

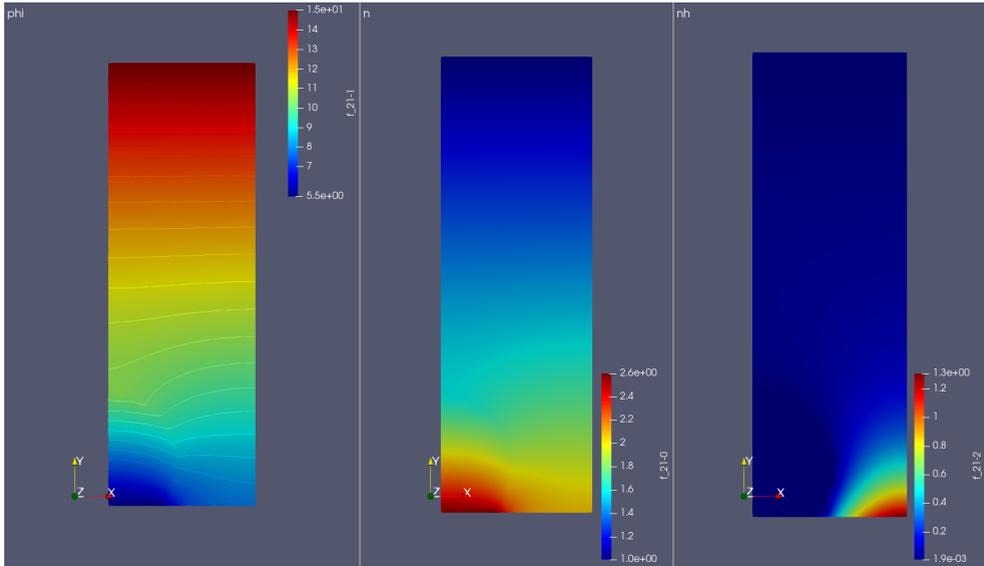


Figure 5: ϕ , n , n_{H_2} fields obtained by the phase field strategy.

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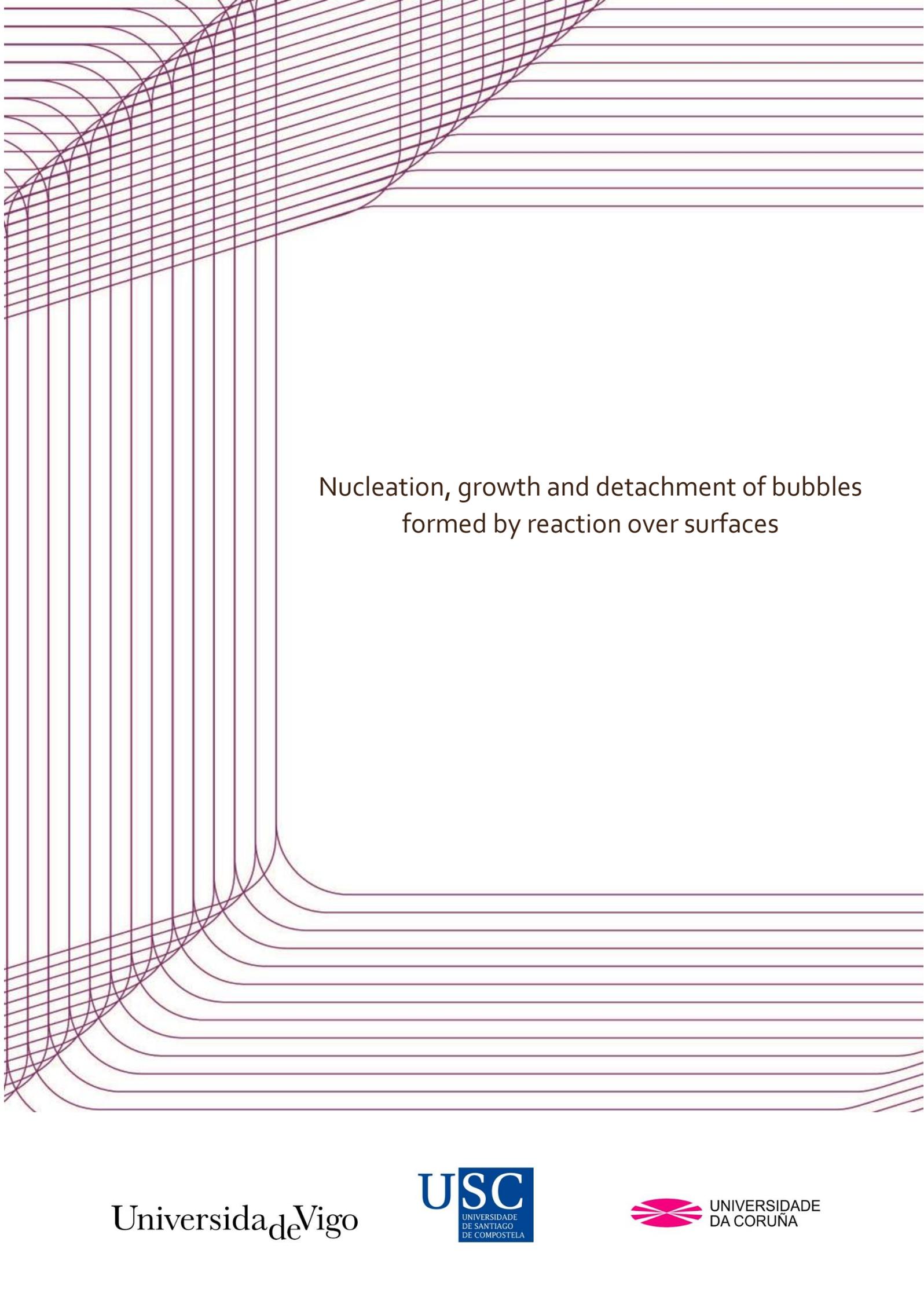
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Nucleation, growth and detachment of bubbles
formed by reaction over surfaces