Mathematical modelling and simulation of corrosion in an underground repository

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Thanks to many collaborators :
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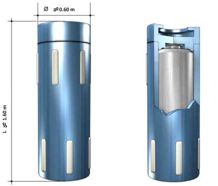
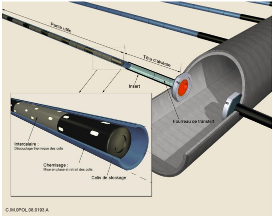
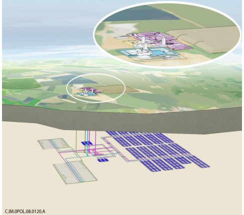
Nuclear waste repository



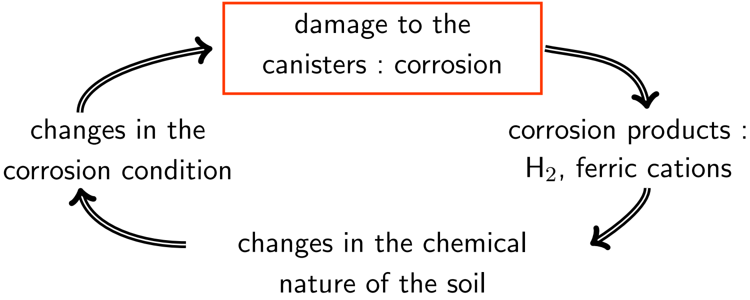




- Nuclear waste in a glass matrix, stored in steel candisters
- Canisters placed in a micro-tunnel done in a geological layer
- Several concerns, including the corrosion of the steel canisters

Nuclear waste repository

Storage under anaerobic conditions



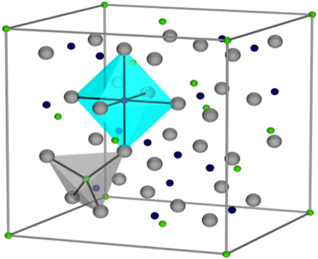
Main objectives

➤ Ensure safety, reliability and reversibility of storage..

- ➢ Assessment of container lifetime
- ➢ Evaluation of gas production (H_2)

The oxide layer

- Formation of an oxide layer,
- with a microscopic crystalline structure.

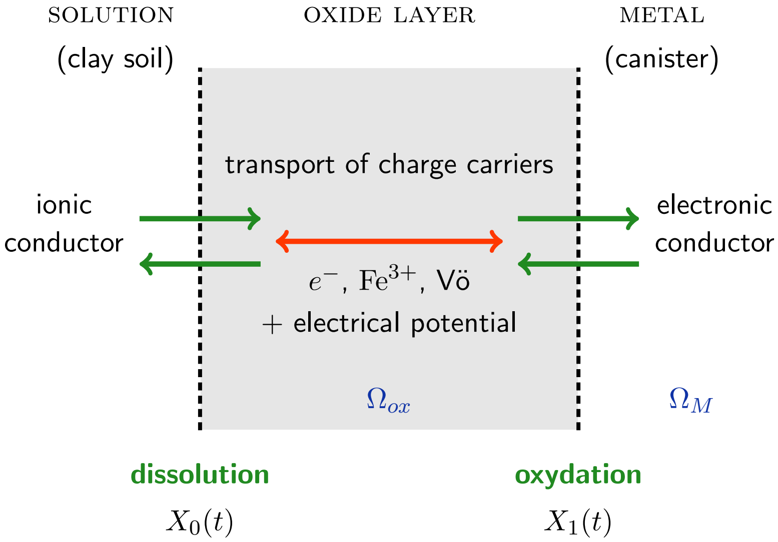


O^{2-}, Fe^{2+}, Fe^{3+}

tetrahedral/octahedral sites

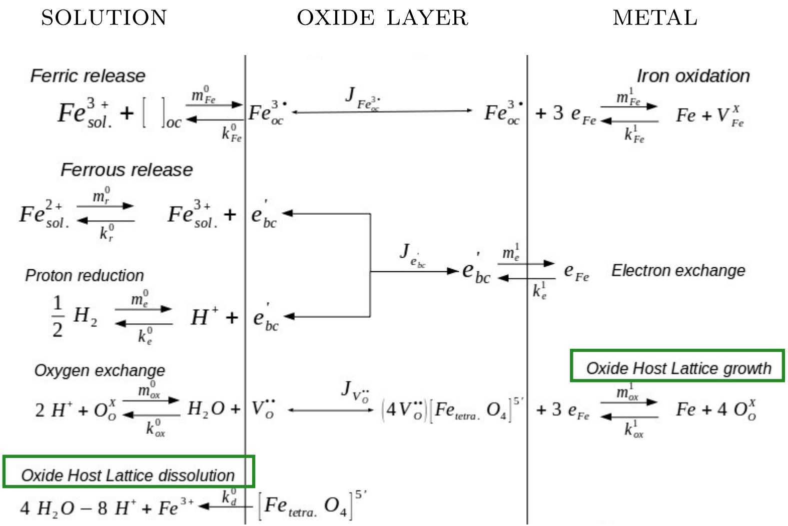
- Charge transport induced by an electrical field/a difference of electrical potentials

The oxide layer



Chemical reaction summary

- Bataillon *et al.*, EA 2010



Organization of the lecture

PART I :

The Diffusion Poisson Coupled Model :
overview, mathematical and numerical results

PART II :

First results on a new model,

the variational Diffusion Poisson Coupled Model

PART I :

The Diffusion Poisson Coupled Model : overview, mathematical and numerical results

- BATAILLON *et al.*, Electrochimica Acta 2010

Outline of Part I

Overview of the Diffusion Poisson Coupled Model

Unknowns

- Densities of species : C_e, C_{Fe}, C_{V} (e^-, Fe^{3+} and Vö)

  $z_e = -1$, $z_{\mathrm{Fe}} = 3$, $z_V = 2$, the charges

  J_e, J_{Fe}, J_{V}, the associated current densities.
- Electrical potential Φ.
- Interfaces : X_0, X_1.

Equations

- Convection-diffusion equations for the charge carriers

  $+$ kinetics of the electrochemical reactions at the interfaces

- Poisson equation for the electrical potential

  $+$ boundary conditions given by Gauss-Helmholtz laws

- Moving boundaries equations

DPCM in physical units : the equations

Poisson equation for the electric potential

$$-\chi\chi_0\partial^2_{xx}\Phi = F \sum_{s\in\{e,\mathrm{Fe},\mathrm{V}\}} z_s C_s + \rho_{hl}$$

- χ, χ_0 dielectric constants, F : Faraday constant,
- ρ_{hl} charge density of the host lattice ($\rho_{hl} = -5\dfrac{F}{\Omega_{ox}}$).

Charge transport in the oxide

For each species $s \in \{e, \mathrm{Fe}, \mathrm{V}\}$,

$$\partial_t C_s + \partial_x J_s = 0$$
$$J_s = -D_s(\partial_x C_s - z_s\gamma C_s\nabla\Phi)$$

- D_s diffusion constant of the species,
- $\gamma = \dfrac{F}{RT}$ in V^{-1}

DPCM in physical units : the equations

Poisson equation for the electric potential

$$-\chi\chi_0\partial_{xx}^2\Phi = F\sum_{s\in\{e,\mathrm{Fe},\mathrm{V}\}} z_s C_s + \rho_{hl}$$

Charge transport in the oxide

$$\partial_t C_s + \partial_x J_s = 0$$
$$J_s = -D_s(\partial_x C_s - z_s\gamma C_s\nabla\Phi)$$

Moving boundary equations

$$X_1'(t) = -4\Omega_M\Big(J_{\mathrm{V}}(X_1(t)) - X_1'(t)C_{\mathrm{V}}(X_1(t))\Big)$$
$$X_0'(t) = v_d(t) + X_1'(t)(1 - R_{\mathrm{PB}})$$

- v_d dissolution speed of the oxide in the solution
- R_{PB} Pilling-Bedworth ratio, $R_{\mathrm{PB}} = \dfrac{\Omega_{ox}}{3\Omega_M}$.

Scaling of the DPCM

Poisson equation for the electric potential

$$-\chi\chi_0\partial^2_{xx}\Phi = F\sum_{s\in\{e,\mathrm{Fe},\mathrm{V}\}} z_s C_s + \rho_{hl}$$

$$x \to Lx,\ \ \Phi \to \frac{\Phi}{\gamma} = \frac{RT}{F}\Phi,\ \ C_s \to \frac{C_s}{\Omega_{ox}}, \rho_{hl} \to \frac{F}{\Omega_{ox}}\rho_{hl}$$

Scaling of the DPCM

Poisson equation for the electric potential

$$-\lambda^2 \partial^2_{xx} \Phi = \sum_{s \in \{e, \mathrm{Fe}, \mathrm{V}\}} z_s C_s + \rho_{hl}, \quad \lambda^2 = \frac{\chi \chi_0 RT}{F^2 L^2}$$

$$x \to Lx, \ \Phi \to \frac{\Phi}{\gamma} = \frac{RT}{F} \Phi, \ C_s \to \frac{C_s}{\Omega_{ox}}, \rho_{hl} \to \frac{F}{\Omega_{ox}} \rho_{hl}$$

Scaling of the DPCM

Poisson equation for the electric potential

$$-\lambda^2 \partial_{xx}^2 \Phi = \sum_{s \in \{e, \mathrm{Fe}, \mathrm{V}\}} z_s C_s + \rho_{hl}, \quad \lambda^2 = \frac{\chi \chi_0 RT}{F^2 L^2}$$

$$x \to Lx, \;\; \Phi \to \frac{\Phi}{\gamma} = \frac{RT}{F}\Phi, \;\; C_s \to \frac{C_s}{\Omega_{ox}}, \rho_{hl} \to \frac{F}{\Omega_{ox}}\rho_{hl}$$

Charge transport in the oxide

$$\partial_t C_s + \partial_x J_s = 0, \quad J_s = -D_s(\partial_x C_s - z_s \gamma C_s \nabla \Phi)$$

$$t \to \frac{L^2}{D_{\mathrm{Fe}}} t, \;\; J_s \to \frac{D_s}{\Omega_{ox} L} J_s$$

Scaling of the DPCM

Poisson equation for the electric potential

$$-\lambda^2 \partial_{xx}^2 \Phi = \sum_{s \in \{e, \mathrm{Fe}, \mathrm{V}\}} z_s C_s + \rho_{hl}, \quad \lambda^2 = \frac{\chi \chi_0 RT}{F^2 L^2}$$

$$x \to Lx, \;\; \Phi \to \frac{\Phi}{\gamma} = \frac{RT}{F}\Phi, \;\; C_s \to \frac{C_s}{\Omega_{ox}}, \rho_{hl} \to \frac{F}{\Omega_{ox}}\rho_{hl}$$

Charge transport in the oxide

$$\frac{D_{\mathrm{Fe}}}{D_s}\partial_t C_s + \partial_x J_s = 0, \quad J_s = -(\partial_x C_s - z_s C_s \nabla \Phi)$$

$$t \to \frac{L^2}{D_{\mathrm{Fe}}} t, \;\; J_s \to \frac{D_s}{\Omega_{ox} L} J_s$$

Scaling of the DPCM

$$-\lambda^2 \partial_{xx}^2 \Phi = \sum_{s \in \{e, \mathrm{Fe}, \mathrm{V}\}} z_s C_s + \rho_{hl}, \qquad \lambda^2 = \frac{\chi \chi_0 RT}{F^2 L^2}$$

$$\frac{D_{\mathrm{Fe}}}{D_s} \partial_t C_s + \partial_x J_s = 0, \quad J_s = -(\partial_x C_s - z_s C_s \nabla \Phi)$$

Moving boundary equations

$$X_1'(t) = -4\Omega_M \Big(J_{\mathrm{V}}(X_1(t)) - C_{\mathrm{V}}(X_1(t)) X_1'(t) \Big)$$

$$X_0'(t) = v_d(t) + X_1'(t)(1 - R_{\mathrm{PB}})$$

$$X_0 \to L X_0, \; X_1 \to L X_1, \; t \to \frac{L^2}{D_{\mathrm{Fe}}} t,$$

$$J_{\mathrm{V}} \to \frac{D_{\mathrm{V}}}{\Omega_{ox} L} J_{\mathrm{V}}, \; v_d \to \frac{D_{\mathrm{Fe}}}{L} v_d$$

Scaling of the DPCM

$$-\lambda^2 \partial_{xx}^2 \Phi = \sum_{s \in \{e, \mathrm{Fe}, \mathrm{V}\}} z_s C_s + \rho_{hl}, \qquad \lambda^2 = \frac{\chi \chi_0 RT}{F^2 L^2}$$

$$\frac{D_{\mathrm{Fe}}}{D_s} \partial_t C_s + \partial_x J_s = 0, \quad J_s = -(\partial_x C_s - z_s C_s \nabla \Phi)$$

Moving boundary equations

$$X_1'(t) = -\frac{4}{3R_{\mathrm{PB}}} \frac{D_{\mathrm{V}}}{D_{\mathrm{Fe}}} \Big(J_{\mathrm{V}}(X_1(t)) - \frac{D_{\mathrm{Fe}}}{D_{\mathrm{V}}} X_1'(t) C_{\mathrm{V}}(X_1(t)) \Big)$$
$$X_0'(t) = v_d(t) + X_1'(t)(1 - R_{\mathrm{PB}})$$

$$X_0 \to L X_0, \; X_1 \to L X_1, \; t \to \frac{L^2}{D_{\mathrm{Fe}}} t,$$

$$J_{\mathrm{V}} \to \frac{D_{\mathrm{V}}}{\Omega_{ox} L} J_{\mathrm{V}}, \; v_d \to \frac{D_{\mathrm{Fe}}}{L} v_d$$

The scaled DPCM : the equations

New notations

- P, N, C, scaled densities of Fe^{3+}, e^- and Vö
- $z_P = 3$, $z_N = -1$, $z_C = 2$
- Dimensionless numbers :

$$\lambda^2, \text{ Debye length, } R_{\mathrm{PB}} \text{ Pilling-Bedworth ratio,}$$

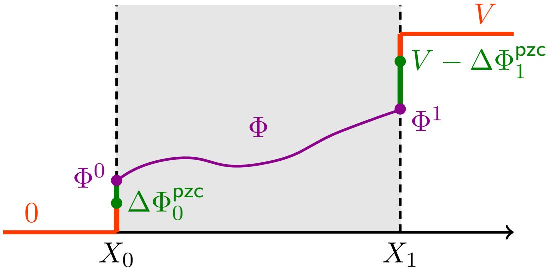
$$\varepsilon_P = 1, \quad \varepsilon_N = \frac{D_{\mathrm{Fe}}}{D_e} \ll 1, \quad \varepsilon_C = \frac{D_{\mathrm{Fe}}}{D_{\mathrm{V}}} \approx 10^2.$$

The equations

$$\begin{cases} -\lambda^2 \partial^2_{xx}\Phi = z_P P + z_N N + z_C C + \rho_{hl} & \text{in } (X_0(t), X_1(t)) \\ \varepsilon_U \partial_t U + \partial_x J_U = 0,\ J_U = -\partial_x U - z_U \partial_x \Phi & \text{in } (X_0(t), X_1(t)) \\ \qquad \text{for } U = P, N, C & \\ X_0'(t) = v_d(t) + X_1'(t)(1 - R_{\mathrm{PB}}) & \\ X_1'(t) = -\dfrac{4}{3R_{\mathrm{PB}}\varepsilon_C}\left(J_C - \varepsilon_C X_1'(t) C\right) & \end{cases}$$

The scaled DPCM : the boundary conditions

On the electrical potential : Gauss-Helmholtz laws

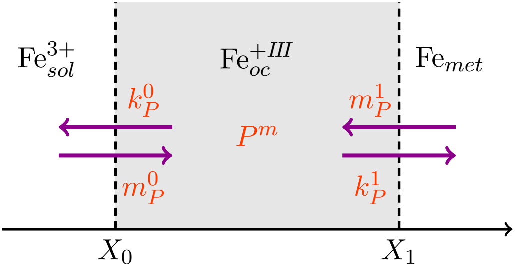


$$\Phi - \alpha_0 \partial_x \Phi = \Delta\Phi_0^{\text{pzc}}$$

$$\Phi + \alpha_1 \partial_x \Phi = V - \Delta\Phi_1^{\text{pzc}}$$

The scaled DPCM : the boundary conditions

On the densities of species : Butler-Volmer laws



- Interface oxide/solution, X_0 :

$$-(J_P - \varepsilon_P X_0' P) = -m_P^0 e^{-3b_P^0 \Phi}(P^m - P) + k_P^0 e^{3a_P^0 \Phi} P$$

- Interface oxide/metal X_1 :

$$J_P - \varepsilon_P X_1' P = k_P^1 e^{3a_P^1 (V-\Phi)}(P^m - P) - m_P^1 e^{-3b_P^1 (V-\Phi)} P$$

The scaled DPCM : the boundary conditions

On the electrical potential

$$\Phi - \alpha_0 \partial_x \Phi = \Delta\Phi_0^{\mathrm{pzc}}$$
$$\Phi + \alpha_1 \partial_x \Phi = V - \Delta\Phi_1^{\mathrm{pzc}}$$

On the densities of species

$$\begin{aligned} -(J_U - \varepsilon_U X_0'(t) U) &= r_U^0(U(X_0(t)), \Phi(X_0(t))) && \text{on } X_0(t) \\ J_U - \varepsilon_U X_1'(t) U(t) &= r_U^1(U(X_1(t)), \Phi(X_1(t)), V) && \text{on } X_1(t) \end{aligned}$$

with

$$r_U^0(s, x) = \beta_U^0(x) s - \gamma_U^0(x)$$
$$r_U^1(s, x, V) = \beta_U^1(V - x) s - \gamma_U^1(V - x)$$

$\beta_U^\Gamma, \gamma_U^\Gamma$ positive functions for $\Gamma \in \{0, 1\},\ U = P, N, C.$

The scaled DPCM : the boundary conditions

On the electrical potential

$$\Phi - \alpha_0 \partial_x \Phi = \Delta\Phi_0^{\mathrm{pzc}}$$
$$\Phi + \alpha_1 \partial_x \Phi = V - \Delta\Phi_1^{\mathrm{pzc}}$$

On the densities of species

$$-(J_U - \varepsilon_U X_0'(t) U) = r_U^0(U(X_0(t)), \Phi(X_0(t))) \quad \text{on } X_0(t)$$
$$J_U - \varepsilon_U X_1'(t) U(t) = r_U^1(U(X_1(t)), \Phi(X_1(t)), V) \quad \text{on } X_1(t)$$

with
$$r_U^0(s,x) = \beta_U^0(x)s - \gamma_U^0(x)$$
$$r_U^1(s,x,V) = \beta_U^1(V-x)s - \gamma_U^1(V-x)$$

$\beta_U^\Gamma, \gamma_U^\Gamma$ positive functions for $\Gamma \in \{0,1\},\ U = P, N, C.$

Potentiostatic/galvanostatic case

V given / V prescribed by an additional equation

Outline of Part I

Numerical scheme for DPCM (CALIPSO)

Main requirements

- Stability in long time
- Stability with respect to the parameters

Overview

1. A change of variables toward a fixed domain
2. A finite volume scheme in space

   with Scharfetter-Gummel numerical fluxes
3. An implicit in time Euler scheme
4. Potentiostatic and galvanostatic case

❑ Bataillon , Bouchon, C.-H., Fuhrmann, Hoarau, Touzani, JCP'12

The change of variables

Definition with $L(t) = X_1(t) - X_0(t)$

$$\bigcup_{0\le t\le T} [X_0(t), X_1(t)] \times \{t\} \to [0,1] \times [0,T]$$
$$(x,t) \mapsto \left(\xi(x,t) = \frac{x - X_0(t)}{L(t)}, t\right)$$

Application to $f(x,t) = \bar{f}(\xi, t)$

$$\partial_t f = \frac{1}{L(t)}\left(\partial_t (L(t)\bar{f}) - \partial_\xi \left(X_0'(t) + L'(t)\xi \bar{f}\right)\right)$$
$$\partial_x f = \frac{1}{L(t)} \partial_\xi \bar{f}.$$

DPCM in the fixed domain $[0,1]$ (with x instead of ξ)

Equation and boundary conditions for Φ

$$-\frac{\lambda^2}{L(t)^2}\partial^2_{xx}\Phi = 3P - N + 2C - 5 \quad \text{in } [0,1]$$

$$\Phi - \frac{\alpha_0}{L(t)}\partial_x\Phi = \Delta\Phi_0^{\text{pzc}} \quad \text{on } x = 0$$

$$\Phi + \frac{\alpha_1}{L(t)}\partial_x\Phi = V - \Delta\Phi_1^{\text{pzc}} \quad \text{on } x = 1$$

Equations and boundary conditions for $U = P, N, C$

$$\varepsilon_U L(t)\partial_t(L(t)U) + \partial_x\hat{J}_U = 0 \quad \text{in } [0,1]$$

$$\hat{J}_U = -\partial_x U - \Big(z_U\partial_x\Phi + \varepsilon_U L(t)(X_0'(t) + xL'(t))\Big)U$$

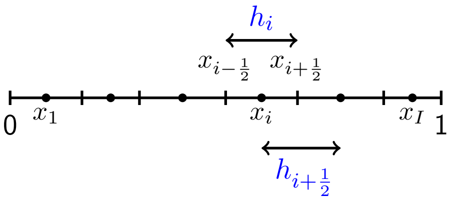
$$-\hat{J}_U = L(t)r_U^0(U,\Phi) \quad \text{on } x = 0$$

$$\hat{J}_U = L(t)r_U^1(U,\Phi,V) \quad \text{on } x = 1$$

FV scheme in space : the Poisson equation

$$-\frac{\lambda^2}{L^2}\partial^2_{xx}\Phi = 3P - N + 2C - 5$$

Notations for the mesh



$$h = \max h_i,$$

Scheme for Φ

$$d\Phi_{i+\frac{1}{2}} = \frac{\Phi_{i+1} - \Phi_i}{h_{i+\frac{1}{2}}} \quad (\approx \partial_x \Phi(x_{i+\frac{1}{2}}))$$

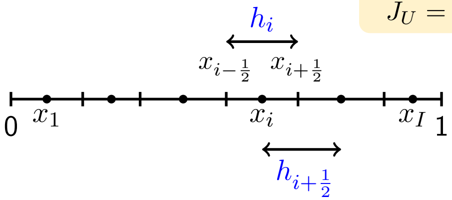
$$-\frac{\lambda^2}{L^2}(d\Phi_{i+\frac{1}{2}} - d\Phi_{i-\frac{1}{2}}) = h_i(3P_i - N_i + 2C_i - 5), \quad 1 \leq i \leq I,$$

$$\Phi_0 - \frac{\alpha_0}{L} d\Phi_{\frac{1}{2}} = \Delta\Phi_0^{\text{pzc}},$$

$$\Phi_{I+1} + \frac{\alpha_1}{L} d\Phi_{I+\frac{1}{2}} = V - \Delta\Phi_1^{\text{pzc}}.$$

Approximation of linear convection-diffusion fluxes

$$J_U = -\partial_x U + \mathbf{w} U$$



Scharfetter-Gummel numerical fluxes

$$\begin{aligned} \mathcal{F}_{U,i+\frac{1}{2}} &\approx J_U(x_{i+\frac{1}{2}}) \\ \mathbf{w}_{i+\frac{1}{2}} &\approx \mathbf{w}(x_{i+\frac{1}{2}}) \end{aligned}$$

$$\mathcal{F}_{U,i+\frac{1}{2}} = \frac{1}{h_{i+\frac{1}{2}}} \Big(B\big(-h_{i+\frac{1}{2}} \mathbf{w}_{i+\frac{1}{2}}\big) U_i - B\big(h_{i+\frac{1}{2}} \mathbf{w}_{i+\frac{1}{2}}\big) U_{i+1} \Big),$$

and $B(x) = \dfrac{x}{e^x - 1}$ (Bernoulli function).

Special case $\mathbf{w} = -z_U \partial_x \Phi$

$$\mathcal{F}_{U,i+\frac{1}{2}} = \frac{1}{h_{i+\frac{1}{2}}} \Big(B\big(z_U(\Phi_{i+1} - \Phi_i)\big) U_i - B\big(-z_U(\Phi_{i+1} - \Phi_i)\big) U_{i+1} \Big)$$

FV scheme for a linear convection-diffusion equation

$$\partial_t U + \partial_x J_U = 0$$

Balance law

$$h_i \frac{U_i^n - U_i^{n-1}}{\delta t} + \mathcal{F}^n_{U,i+\frac{1}{2}} - \mathcal{F}^n_{U,i-\frac{1}{2}} = 0.$$

δt : the time step

choice of a Backward Euler scheme in time

Application to $\varepsilon_U L(t)\partial_t(L(t)U) + \partial_x \hat{J}_U = 0$

$$\varepsilon_U L^n h_i \frac{L^n U_i^n - L^{n-1} U_i^{n-1}}{\delta t} + \hat{\mathcal{F}}^n_{U,i+\frac{1}{2}} - \hat{\mathcal{F}}^n_{U,i-\frac{1}{2}} = 0$$

$$\hat{J}_U = -\partial_x U + \mathbf{w} U$$

with $\mathbf{w} = -\Big(z_U \partial_x \Phi + \varepsilon_U L(t)(X_0'(t) + x L'(t))\Big)$,

$+$ natural definition for $\mathbf{w}^n_{i+\frac{1}{2}}$.

Comment on the choice of the Bernoulli function

Thermal equilibria at the continuous level

$$J_U = -\partial_x U - z_U \partial_x \Phi \; U$$

Therefore,

$$U = \lambda \exp(-z_U \Phi) \Longrightarrow J_U = 0.$$

Thermal equilibria at the discrete level

$$\mathcal{F}_{U,i+\frac{1}{2}} = \frac{1}{h_{i+\frac{1}{2}}} \Big(B\big(z_U(\Phi_{i+1} - \Phi_i)\big) U_i - B\big(-z_U(\Phi_{i+1} - \Phi_i)\big) U_{i+1} \Big)$$

Therefore, with the Bernoulli function,

$$U_i = \lambda \exp(-z_U \Phi_i) \Longrightarrow \mathcal{F}_{U,i+\frac{1}{2}} = 0.$$

About the time discretization for the DPCM

Guideline

- The scheme in time is a backward Euler scheme.
- At each time step, we solve a nonlinear system of equations on

$$((P_i^n, N_i^n, C_i^n, \Phi_i^n)_{0\leq i\leq I+1}, X_0^n, X_1^n, L^n).$$

- The nonlinear system is solved with the Newton's method.

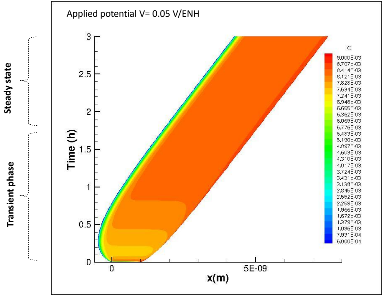
Why ?

- We could try to decouple the scheme for the Poisson equation from the scheme for the convection-diffusion equations.
- Main advantage : we only solve linear systems of equations at each time step.
- Main drawback : the stability condition

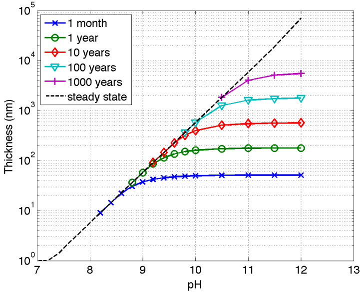
$$\Delta t \leq \varepsilon_N \lambda^2 = 10^{-20} \text{ !!!}$$

Numerical results

Evolution of the density of oxygen vacancies



Oxide layer thickness *vs* pH and time



Observation :

Convergence in time towards a traveling wave solution

Outline of Part I

The 2-species DPCM on a fixed domain

A drift-diffusion system of equations

$$\partial_t P + \partial_x J_P = 0, \quad J_P = -\partial_x P - 3P\partial_x \Phi$$
$$\varepsilon_N \partial_t N + \partial_x J_N = 0, \quad J_N = -\partial_x N + N\partial_x \Phi$$
$$-\lambda^2 \partial_{xx}^2 \Phi = -N + 3P - 5$$

- Gajewski, Gröger 1986, 1989
- Markowich, 1986
- Markowich, Ringhofer, Schmeiser, 1990

Originality : the Robin boundary conditions

$$J_U(x=1) = m_U^1 U e^{-3b_U^1(V-\Phi)} - k_U^1(U^m - U)e^{3a_U^1(V-\Phi)}$$
$$J_U(x=0) = m_U^0(U^m - U)e^{-3b_U^0\Phi} - k_U^0 U e^{3a_U^0\Phi}$$

$$\Phi - \alpha_0\partial_x\Phi = \Delta\Phi_0^{\text{pzc}} \qquad \text{on } x=0,$$
$$\Phi + \alpha_1\partial_x\Phi = V - \Delta\Phi_1^{\text{pzc}} \quad \text{on } x=1.$$

The 2-species DPCM on a fixed domain

A drift-diffusion system of equations

$$\partial_x J_P = 0, \quad J_P = -\partial_x P - 3P\partial_x \Phi$$
$$\partial_x J_N = 0, \quad J_N = -\partial_x N + N\partial_x \Phi$$
$$-\lambda^2 \partial_{xx}^2 \Phi = -N + 3P - 5$$

- Gajewski, Gröger 1986, 1989
- Markowich, 1986
- Markowich, Ringhofer, Schmeiser, 1990

Originality : the Robin boundary conditions

$$J_U(x=1) = m_U^1 U e^{-3b_U^1(V-\Phi)} - k_U^1(U^m - U)e^{3a_U^1(V-\Phi)}$$
$$J_U(x=0) = m_U^0 (U^m - U)e^{-3b_U^0\Phi} - k_U^0 U e^{3a_U^0\Phi}$$

$$\Phi - \alpha_0 \partial_x \Phi = \Delta\Phi_0^{\mathrm{pzc}} \quad \text{on } x = 0,$$
$$\Phi + \alpha_1 \partial_x \Phi = V - \Delta\Phi_1^{\mathrm{pzc}} \quad \text{on } x = 1.$$

Mathematical results for the 2-species model

Existence results for the 2-species model

- C.-H., Lacroix-Violet, '12 : the stationary case
  by a fixed-point theorem applied to $(N, P) \to \Phi \to (\widetilde{N}, \widetilde{P})$
- C.-H., Lacroix-Violet, '15 : the evolutive case
  by convergence of a semi-discretization in time,
  under some special assumptions on the parameters.

Numerical analysis of the 2-species model

- Bataillon, C.-H., '08 : the stationary case
- C.-H, Colin, Lacroix-Violet, '15 : the evolutive case
  with the same strategy than in the continuous case.

Existence of traveling waves for the DPCM

- C.-H, Gallouët, '16 : study of a simplified model

Definition of the traveling waves

- $L(t) = X_1(t) - X_0(t) = \ell$, $X_1'(t) = X_0'(t) = \delta$
- the profiles de not depend on time in the oxide layer

Main assumption leading to a simplified model

- we assume the electroneutrality inside the oxide layer,
- so that Φ is an affine function.

Outline of the proof of existence

- We can compute $(\Phi_\ell, C_\ell, \delta_\ell)$, for any ℓ.
- Then, we can define F such that $F(\ell) = -K\hat{J}_{C_\ell}/(\ell\delta_\ell)$.
- Existence is obtained as $\exists \ell_s > 0$ such that $F(\ell_s) = 1$.

Existence of traveling waves for the DPCM

- Breden, C.-H, Zurek, '21 : a computer-assisted proof

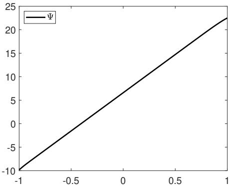
For a given set of parameters, there exist

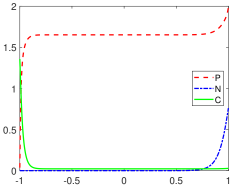
- analytic functions $\Phi, C, N, P : [-1,1] \to \mathbb{R}$ and $\delta, \ell > 0$ defining a traveling wave,
- $\bar{\Phi}$, $\bar{C}$, $\bar{N}$ and $\bar{P}$ explicitly known functions satisfying

$$\sup_{[-1,1]} |\Phi - \bar{\Phi}| \lesssim 10^{-9}, \qquad \sup_{[-1,1]} |U - \bar{U}| \lesssim 10^{-10}$$

$$\delta \in [33.4947256\mathbf{0}, 33.4947256\mathbf{4}]$$

$$\ell \in [1.703352535\mathbf{2}, 1.703352535\mathbf{6}]$$





Main issues from now on

- How to tackle the whole model ?
- A gradient flow structure would ensure existence, uniqueness and long time behaviour.
- Compatibility of the model with thermodynamics ?