Finite Volume Scheme for a Corrosion Model

Claire CHAINAIS

Laboratoire de Mathématiques
Clermont-Ferrand, France

Collaboration with Christian Bataillon, CEA
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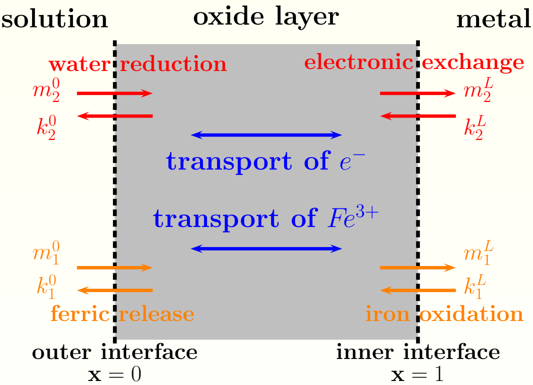
Outline of the talk

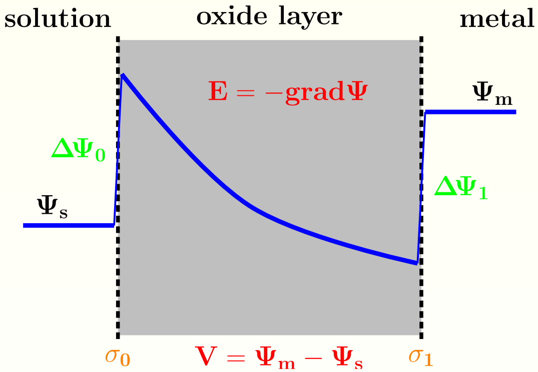
1. Introduction to corrosion modelling
2. Presentation of the scheme
3. Numerical analysis of the scheme
4. Numerical experiments

Introduction to corrosion modelling



Convection-diffusion equations on $\begin{cases} N : & \text{density of electrons} \\ P : & \text{density of cations} \end{cases}$

Introduction to corrosion modelling



Poisson equation on Ψ (electrostatic potential)

Introduction to corrosion modelling : the system

Equation and boundary conditions for P

$$\partial_t P + \partial_x J_P = 0, \quad J_P = -\partial_x P - 3P\partial_x \Psi$$

$$J_P(x=1) = m_1^L P e^{-3b_1^L(V-\Psi)} - (P_m - P)k_1^L e^{3a_1^L(V-\Psi)}$$

$$J_P(x=0) = -P k_1^0 e^{3a_1^0 \Psi}.$$

Equation and boundary conditions for N

$$\mathbf{D_1/D_2}\ \partial_t N + \partial_x J_N = 0, \quad J_N = -\partial_x N + N\partial_x \Psi$$

$$J_N(x=1) = m_2^L N e^{b_2^L(V-\Psi)} - (N_m - N)k_2^L e^{-a_2^L(V-\Psi)}$$

$$J_N(x=0) = -N k_2^0 e^{-a_2^0 \Psi}.$$

Equation and boundary conditions for Ψ

$$-\lambda^2 \partial_{xx}^2 \Psi = -N + 3P - 5$$

$$\Psi - \alpha_0 \partial_x \Psi = \Delta\Psi_0^{pzc} \qquad \text{on } x = 0,$$

$$\Psi + \alpha_1 \partial_x \Psi = V - \Delta\Psi_1^{pzc} \qquad \text{on } x = 1.$$

Introduction to corrosion modelling : the system

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Presentation of the scheme

Scheme for P : $\mathcal{F}_{i+\frac{1}{2}} - \mathcal{F}_{i-\frac{1}{2}} = 0,\ 1 \le i \le I$

$$\mathcal{F}_{\frac{1}{2}} = m_1^0 e^{-3b_1^0\Psi_0} P_m - \left(k_1^0 e^{3a_1^0\Psi_0} + m_1^0 e^{-3b_1^0\Psi_0}\right) P_0,$$

$$\mathcal{F}_{I+\frac{1}{2}} = \left(k_1^L e^{3a_1^L(V-\Psi_{I+1})} + m_1^L e^{-3b_1^L(V-\Psi_{I+1})}\right) P_{I+1} - k_1^L e^{3a_1^L(V-\Psi_{I+1})} P_m.$$

Scheme for N : $\mathcal{G}_{i+\frac{1}{2}} - \mathcal{G}_{i-\frac{1}{2}} = 0,\ 1 \le i \le I$

$$\mathcal{G}_{\frac{1}{2}} = m_2^0 e^{b_2^0\Psi_0} N_m - \left(m_2^0 e^{b_2^0\Psi_0} + k_2^0 e^{-a_2^0\Psi_0}\right) N_0,$$

$$\mathcal{G}_{I+\frac{1}{2}} = \left(m_2^L e^{b_2^L(V-\Psi_{I+1})} + k_2^L e^{-a_2^L(V-\Psi_{I+1})}\right) N_{I+1} - k_2^L e^{-a_2^L(V-\Psi_{I+1})} N_m.$$

Scheme for Ψ : $-\lambda^2(d\Psi_{i+\frac{1}{2}} - d\Psi_{i-\frac{1}{2}}) = h_i(3P_i - N_i - 5),\ 1 \le i \le I$

$$\Psi_0 - \alpha_0 d\Psi_{\frac{1}{2}} = U_0, \qquad d\Psi_{i+\frac{1}{2}} = \frac{\Psi_{i+1} - \Psi_i}{h_{i+\frac{1}{2}}}$$

$$\Psi_{I+1} + \alpha_1 d\Psi_{I+\frac{1}{2}} = U_1.$$

Presentation of the scheme : the fluxes

$$J_P = -\partial_x P - 3P\partial_x \Psi, \quad J_N = -\partial_x N + N\partial_x \Psi$$

$$\mathcal{F}_{i+\frac{1}{2}} = \frac{B(3(\Psi_{i+1} - \Psi_i))P_i - B(-3(\Psi_{i+1} - \Psi_i))P_{i+1}}{h_{i+\frac{1}{2}}} \quad 0 \le i \le I$$

$$\mathcal{G}_{i+\frac{1}{2}} = \frac{B(-(\Psi_{i+1} - \Psi_i))N_i - B(\Psi_{i+1} - \Psi_i)N_{i+1}}{h_{i+\frac{1}{2}}} \quad 0 \le i \le I$$

Choices for B

- Classical upwind scheme

$$B(x) = 1 + (-x)^+$$

- Scharfetter-Gummel scheme

$$B(x) = \frac{x}{e^x - 1} \text{ for } x \neq 0, \quad B(0) = 1.$$

Presentation of the scheme : the Slotboom variables

Change the variables

$$u_i = e^{3\Psi_i} P_i, \quad v_i = e^{-\Psi_i} N_i$$

$$\Downarrow$$

$$\mathcal{F}_{i+\frac{1}{2}} = \frac{1}{\mathbf{f}(\Psi_i, \Psi_{i+1})} \frac{u_i - u_{i+1}}{h_{i+\frac{1}{2}}}, \quad \mathcal{G}_{i+\frac{1}{2}} = \frac{1}{\mathbf{g}(\Psi_i, \Psi_{i+1})} \frac{v_i - v_{i+1}}{h_{i+\frac{1}{2}}}$$

$\Longrightarrow$ $\mathbf{u}$ and $\mathbf{v}$ expressed as a function of $\mathbf{\Psi}$

Nonlinear system of equations on Ψ

$$-\lambda^2 (\frac{\Psi_{i+1} - \Psi_i}{h_{i+\frac{1}{2}}} - \frac{\Psi_i - \Psi_{i-1}}{h_{i-\frac{1}{2}}}) = h_i (3u_i e^{-3\Psi_i} - v_i e^{\Psi_i} - 5),$$

$$\Psi_0 - \alpha_0 d\Psi_{\frac{1}{2}} = U_0,$$

$$\Psi_{I+1} + \alpha_1 d\Psi_{I+\frac{1}{2}} = U_1.$$

Numerical analysis

Theorem 1

Under hypothesis : $a_i^0 + b_i^0 = a_i^L + b_i^L = 1$, $i = 1, 2$, we have :

- **Existence of a solution** to the scheme :

  $\mathbf{u} = (u_i)_{0 \le i \le I+1}$, $\mathbf{v} = (v_i)_{0 \le i \le I+1}$, $\mathbf{\Psi} = (\Psi_i)_{0 \le i \le I+1}$,

- with L^∞ **and discrete** H^1**-estimates** :

$$0 \le u_i \le \frac{k_1^L}{m_1^L} e^{3V} P_m, \quad 0 \le v_i \le \frac{k_2^L}{m_2^L} e^{-V} N_m$$

$$|\Psi_i| \le M \text{ and } \quad \sum_{i=0}^{I} \frac{(\Psi_{i+1} - \Psi_i)^2}{h_{i+\frac{1}{2}}} + \Psi_0^2 + \Psi_{I+1}^2 \le M$$

$$\sum_{i=0}^{I} \frac{(u_i - u_{i+1})^2}{h_{i+\frac{1}{2}}} \le M, \quad \sum_{i=0}^{I} \frac{(v_i - v_{i+1})^2}{h_{i+\frac{1}{2}}} \le M.$$

Numerical analysis

Theorem 2

- $a_i^0 + b_i^0 = a_i^L + b_i^L = 1,\ i = 1, 2$
- $(\mathbf{u}^h, \mathbf{v}^h, \mathbf{\Psi}^h)_{h>0}$ sequence of approximate solutions

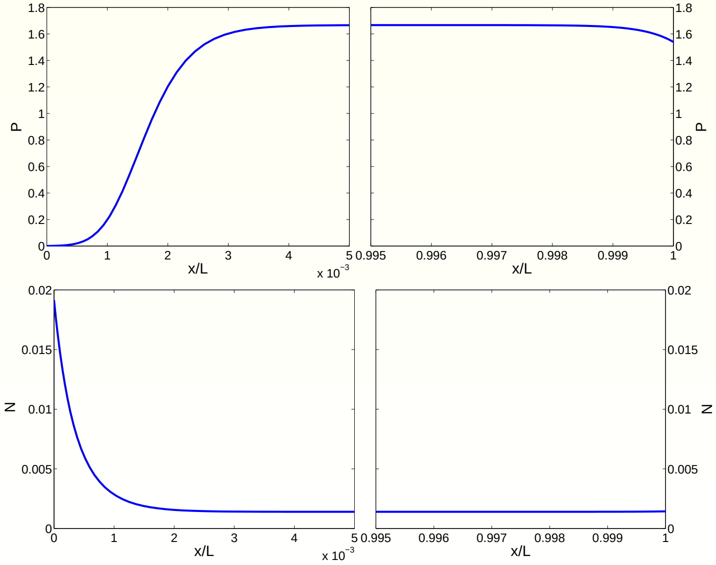
Then, up to a subsequence,

$$\mathbf{u}^h \to u, \quad \mathbf{v}^h \to v, \quad \mathbf{\Psi}^h \to \Psi \text{ as } h \to 0 \text{ in } C([0,1]).$$

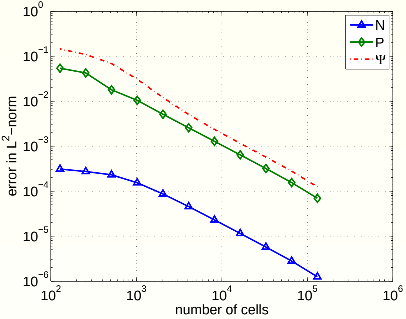
and

$$(N = e^{\Psi} v, P = e^{-3\Psi} u, \Psi) \text{ is a weak solution}$$
to the corrosion model.

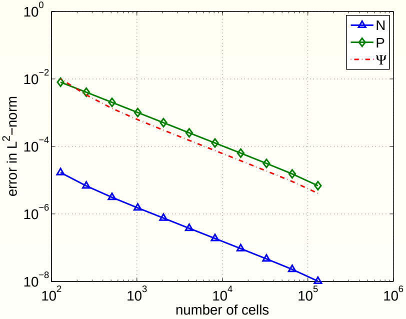
Numerical experiments : profiles



Numerical experiments : convergence



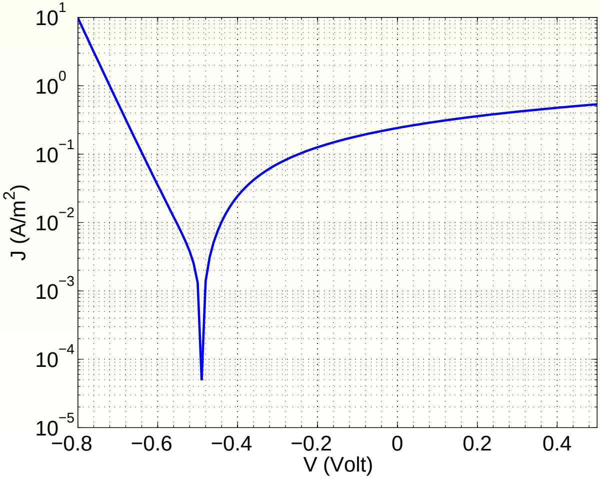
Uniform mesh



Tchebychev mesh

Numerical experiments

Current-voltage curve



Prospects

- More numerical simulations and comparison to the experiments :

  $$\Longrightarrow \text{Help for the choice of all parameters}$$

- Addition of a third charge carrier : the oxygen vacancies
- Evolution in time of the oxide layer :
  - Scheme for the non stationary system of equations
  - Free boundary problem
- Computation of the corrosion speed