A free boundary model describing corrosion process

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Gradient Flows Face-to-Face 3

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Plan

Outline

Framework, Motivations

Considered problem : the burial of radioactive waste

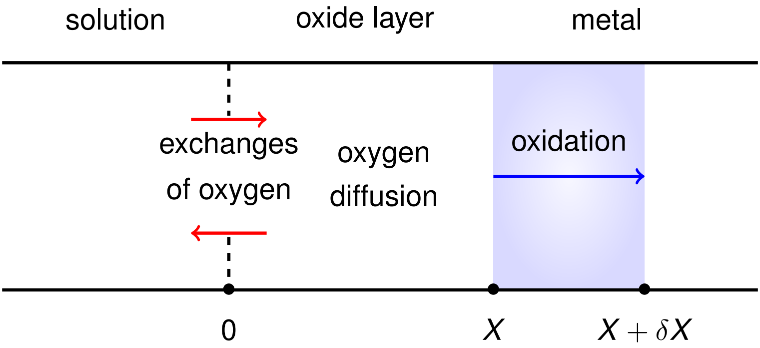
• metallic barrel containing radioactive waste stored in a clay soil.

• the barrel is in contact with an aqueous solution

• on the surface, an oxide layer forms and protects the metal.

• thickness of the layer is small in relation to the size of the barrel $\Rightarrow$ 1D model

Three areas in the model



In the oxide layer

$\rightsquigarrow$ unknown ρ : concentration of oxygen vacancies

Assumption : linear diffusion of oxygen vacancies

$$\partial_t \rho(x,t) - \partial_x^2 \rho(x,t) = 0, \ \textit{for } x \in (0, X(t))$$

Fixed interface

Let us consider two constant concentrations ρ_- , ρ_+ :

• if $\rho = \rho_-$ then oxygen vacancies reach the oxide layer ($\rightarrow$)

• if $\rho = \rho_+$ then oxygen vacancies leave from the oxide layer ($\leftarrow$)

• if $\rho_- < \rho < \rho_+$ then there is no exchange

$\rightsquigarrow$Unknown M ($\dot{M}$ represents the flux of oxygen vacancies from the solution into the oxide layer)

Mobile interface

- metal = constant source of oxygen vacancies ($\rho = 1$)
- $\forall x > X(t), \quad \rho(t,x) = 1$
- the metal reforms if the concentration ρ is 1

$\rightsquigarrow$ Unknown X (position of the mobile interface between the oxide layer and the metal)

Outline

Model

Let us consider $T > 0$, $X^0 > 0$, an initial density ρ^0, we are looking for a solution (ρ, X, M) of :

$$\partial_t \rho(x,t) - \partial_x^2 \rho(x,t) = 0 \qquad (x,t) \in (0, X(t)) \times (0,T)$$

$$\rho(x,t) = 1 \qquad (x,t) \in (X(t), +\infty) \times (0,T)$$

$$\partial_x \rho(X(t)^-, t) + \dot{X}(t) \left(\rho(X(t)^-, t) - 1\right) = 0 \qquad t \in (0,T)$$

$$\partial_x \rho(0,t) = -\dot{M}(t) \qquad t \in (0,T)$$

$$\rho(x,0) = \rho^0(x) \qquad x \in (0, X^0)$$

$$X(0) = X^0$$

$$M(0) = 0$$

Moving interface

$$\partial_x \rho(X(t)^-, t) + \dot{X}(t) \left(\rho(X(t)^-, t) - 1 \right) = 0 \quad \text{pour} \quad t \in (0, T)$$

$\rightsquigarrow$ Neumann boundary condition in a moving domain

The evolution of the moving interface is prescribed by :

For $t \in (0, T)$,

$$\lambda \dot{X}(t) = \alpha - \left(1 - \rho(X(t)^-, t)\right) - \left(\log \rho(X(t)^-, t)\right)$$

Fixed interface

Let us define

$$\rho_+ = \exp\left(\beta + \theta - 1\right) \quad \text{and} \quad \rho_- = \exp\left(\beta - \theta - 1\right),$$

with $\beta, \theta \in \mathbb{R}^+$ verifying $\beta + \theta < 1 \quad (\Rightarrow \rho_- < \rho_+ < 1)$.

For $t \in (0, T)$,

$$\begin{cases} \partial_x \rho(0,t) & \geq 0 \quad \text{if } \rho(0,t) = \rho_+, \\ \partial_x \rho(0,t) & \leq 0 \quad \text{if } \rho(0,t) = \rho_-, \\ \partial_x \rho(0,t) & = 0 \quad \text{if } \rho_- < \rho(0,t) < \rho_+. \end{cases}$$

Theorem

Let us consider (X^0, ρ^0) such that $X^0 > 0$,

$\rho^0(x) = 1 \quad$ for all $x \in (X^0, +\infty)$,

$\rho^0_{|[0,X^0]} \in C^{1,1}([0, X^0])$, $\rho^0(0) \in [\rho_-, \rho_+]$ and

$0 < \rho_{min} \leq \rho^0(x) \leq \rho_{max} \leq 1, \quad$ for all $x \in (0, X^0)$.

Note that $\rho_{min} \leq \rho_- < \rho_+ \leq \rho_{max}$.

Then there exits (at least) one weak solution (ρ, M, X) to the previous problem.

Weak solution

(ρ, M, X) is a weak solution if

1) $\rho \in L^2_{\text{loc}}(\mathbb{R}_+ \times (0,T)) \cap L^\infty(\mathbb{R}_+ \times (0,T))$ and $\partial_x \rho \in L^2(D_T)$
$\rho(0,t) \in [\rho_-, \rho_+]$ for a.e. $t \in (0,T)$
$\rho(x,t) = 1$ for a.e. $x > X(t)$ and $t \in (0,T)$

2) X is a nondecreasing function in $H^1(0,T)$

3) $M \in BV(0,T)$

4) for all $\varphi \in C_0^\infty([0,+\infty) \times [0,T))$

$$-\int_0^T \int_{\mathbb{R}_+} \rho(x,t)\,\partial_t\varphi(x,t)dx\,dt - \int_{\mathbb{R}_+} \rho^0(x)\,\varphi(x,0)\,dx$$

$$-\int_0^T \varphi(0,t)\,dDM(t) + \int_0^T \int_{\mathbb{R}_+} \partial_x\rho(x,t)\,\partial_x\varphi(x,t)\,dx\,dt = 0,$$

5) for all $\xi \in \mathcal{C}(0,T)$

$$\lambda \int_0^T \dot{X}(t)\,\xi(t)\,dt = \alpha \int_0^T \xi(t)\,dt$$

$$-\int_0^T \left(1 - \rho(X^-(t),t)\right)\,\xi(t)\,dt - \int_0^T \log\rho(X^-(t),t)\,\xi(t)\,dt.$$

Variational Inequality

6) for all nonnegative $\phi \in C_0^\infty([0,T))$ and every $\eta \in C^\infty(\mathbb{R}_+ \times [0,T))$ with $\eta(0,t) \in [\rho_-, \rho_+]$ for every $0 \leq t \leq T$.

$$
\begin{aligned}
&-\int_0^T \dot{\phi} \int_0^{X^0} \left(\frac{u^2}{2} - \eta\, u\right) dxdt + \int_0^T \int_0^{X^0} \phi\, u\, \partial_t \eta\, dxdt \\
&\qquad + \int_0^T \int_0^{X^0} \phi \partial_x u \partial_x (u-\eta)\, dxdt \\
&\leq \phi(0) \int_0^{X^0} \left(\frac{u^2}{2} - \eta u\right)(x,0)\, dx + \int_0^T \int_0^{X^0} \phi g(u-\eta)\, dxdt.
\end{aligned}
$$

Outline

Minimizing scheme

To obtain the existence of the solutions, we introduce a JKO (Jordan, Kinderlehrer and Otto) minimizing scheme, which allows to interpret the problem as a steepest descent of some energy functional with respect to the Wasserstein distance.

First difficulty : our measures will have unequal masses because of exchange in 0 and $X(t)$. Second difficulty : by the way, the mass is infinite here !

Mass in 0

Let us define the space $\mathbb{A}$ given by

$$\mathbb{A} := \Big\{(X, \rho) \in (0, \infty) \times L^1_{loc}(\mathbb{R}_+; \mathbb{R}_+) \ : \ \rho(x) = 1 \text{ for a.e. } x \geq X\Big\}$$

Now starting from the initial configuration $(X^0, \rho^0) \in \mathbb{A}$, for any $(X, \rho) \in \mathbb{A}$, we construct the measures

$$\mu(\rho, \rho^0) := \rho\mathcal{L}\llcorner\mathbb{R}_+ + (-M(\rho, \rho^0))_+\delta_0,$$

and

$$\mu^0(\rho, \rho^0) := \rho^0\mathcal{L}\llcorner\mathbb{R}_+ + (M(\rho, \rho^0))_+\delta_0,$$

where

$$M(\rho, \rho^0) := \int_{\mathbb{R}_+} (\rho - \rho^0)\, dx = \int_0^{\Lambda} (\rho - \rho^0)\, dx < \infty,$$

with $\Lambda = \max(X, X^0)$

Infinite mass

In order to bypass this difficulty, we rewrite these measures as

$$\mu = \nu + \mathcal{L}\llcorner(\Lambda, \infty)$$
$$\mu^0 = \nu^0 + \mathcal{L}\llcorner(\Lambda, \infty)$$

with

$$\nu = \rho\mathcal{L}\llcorner(0, \Lambda) + (-M(\rho, \rho^0))_+\delta_0$$
$$\nu^0 = \rho^0\mathcal{L}\llcorner(0, \Lambda) + (M(\rho, \rho^0))_+\delta_0$$

ν and ν^0 are positive measures in $([0, \Lambda))$ with equal mass.

Final distance d

With classical results, we define the unique optimal transport plan $\hat{\gamma} \in \Gamma(\nu, \nu^0)$ and

$$\gamma = \hat{\gamma} + (Id, Id)_{\#}\, \mathcal{L} \llcorner (\Lambda, \infty) \in \Gamma(\mu, \mu^0),$$

Thus

$$\mathbf{W}_2^2(\mu, \mu^0) = \int_{(0,\Lambda)\times(0,\Lambda)} (x-y)^2 d\hat{\gamma}(x,y).$$

Finally we define **d** the tensorized metric given by

$$\mathbf{d}^2\Big((X,\rho),(X^0,\rho^0)\Big) := \mathbf{W}_2^2(\mu,\mu^0) + \lambda\,(X - X^0)^2.$$

Function E

Let us now introduce the energy functional. Consider $f : \mathbb{R} \to \mathbb{R}$ with

$$f(r) = r\,(\log(r) - \beta) + \beta.$$

For a given $(X^0, \rho^0) \in \mathbb{A}$, we define the functional $\mathbf{E}_{(X^0,\rho^0)} : \mathbb{A} \to \mathbb{R}$ as

$$\begin{aligned} \mathbf{E}_{(X^0,\rho^0)}(X,\rho) &:= \int_{\mathbb{R}_+} f(\rho(x))\,dx + \theta|M(\rho,\rho^0)| - \alpha X. \\ &= \int_0^X f(\rho(x))\,dx + \theta|M(\rho,\rho^0)| - \alpha X. \end{aligned}$$

Function J

Finally, for all $(X^0, \rho^0) \in \mathbb{A}$ we introduce the functional $\mathbf{J}_{(X^0,\rho^0)} : \mathbb{A} \to \mathbb{R}$ defined as

$$\mathbf{J}_{(X^0,\rho^0)}(X, \rho) = \frac{1}{2\tau}\mathbf{d}^2((X, \rho), (X^0, \rho^0)) + \mathbf{E}_{(X^0,\rho^0)}(X, \rho) + p_\tau(M(\rho, \rho^0)),$$

The minimization problem is the following :

Starting from $(X^0, \rho^0) \in \mathbb{A}$
determine the existence of at least one $(X, \rho) \in \mathbb{A}$ such that

$$(X, \rho) = \operatorname{argmin}_{(Y,\tilde{\rho}) \in \mathbb{A}} \mathbf{J}_{(X^0, \rho^0)}(Y, \tilde{\rho}).$$

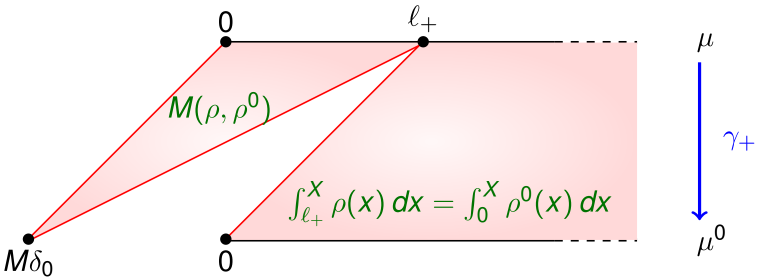
Existence of a minimizer

Theorem

For $0 < \tau < 1$ the previous minimizing problem admits at least one solution $(X, \rho) \in \mathbb{A}$ where X satisfies $X \geq X^0$.

Calculation of $\mathbf{W}_2(\mu, \mu^0)$

Case $M(\rho, \rho^0) \geq 0$



$$\int_0^{\ell_+} \rho(x)\,dx = M(\rho, \rho^0).$$

$$T_{+\#}\, \rho\mathcal{L}\llcorner(\ell_+, X) = \rho^0\mathcal{L}\llcorner(0, X).$$

Calculation of $\mathbf{W}_2(\mu, \mu^0)$

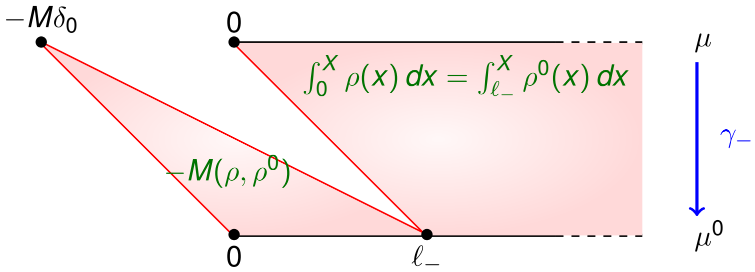
Case of $M(\rho, \rho^0) \geq 0$

$$\mathbf{W}_2^2(\mu, \mu^0) = \int_0^X (x - T_+(x))^2 \, \rho(x) \, dx$$

$$\gamma_+ := (Id, T_+)_\# \, \rho \, \mathcal{L} \llcorner (0, X) + (Id, Id)_\# \, \mathcal{L} \llcorner (X, \infty)$$

Calculation of $\mathbf{W}_2(\mu, \mu^0)$

Case $M(\rho, \rho^0) < 0$



$$\int_0^{\ell_-} \rho^0(x)\,dx = -M(\rho, \rho^0)$$

$$T_- \# \rho\, \mathcal{L}_{|(0,+\infty)} = \rho^0\, \mathcal{L}_{|(\ell_-,+\infty)}, \quad S_- \# \rho^0\, \mathcal{L}_{|(0,\ell_-)} = -M(\rho, \rho^0)\, \delta_0$$

Calculation of $\mathbf{W}_2(\mu, \mu^0)$

Case $M(\rho, \rho^0) < 0$

$$\mathbf{W}_2^2(\mu, \mu^0) = \int_0^X (x - T_-(x))^2 \rho(x)\, dx + \int_0^{\ell_-} y^2 \rho^0(y)\, dy.$$

$$\gamma_- = (Id, T_-)\#\rho\,\mathcal{L}_{|(0,+\infty)} + (S_-, Id)\#\rho^0\,\mathcal{L}_{|(0,\ell_-)} + (Id, Id)_\#\,\mathcal{L}\llcorner(X, \infty)$$

Behaviour in the oxide layer

ρ satisfies the following equation

$$\int_0^X \xi(x)\,\frac{(x - T(x))}{\tau}\,\rho(x)\,dx - \int_0^X \rho(x)\,\xi'(x)\,dx = 0 \qquad \forall \xi \in C_0^\infty(0, X),$$

where T denotes the optimal transport map ($T = T_+$ or T_-).

Behaviour at the fixed interface

ρ satisfies

$$\rho(0) = \rho_+ \exp(-p'_\tau(M(\rho,\rho^0))), \quad \text{if } M(\rho,\rho^0) < 0,$$

$$\rho(0) = \rho_-, \quad \text{if } M(\rho,\rho^0) > 0,$$

$$\rho_- \leq \rho(0) \leq \rho_+, \quad \text{if } M(\rho,\rho^0) = 0.$$

Behaviour at the free interface

X satisfies the following equation

$$\lambda \frac{X - X^0}{\tau} = \alpha - (1 - \rho(X)) - \log(\rho(X)).$$

Outline

Scheme

Let $\tau \in (0,1)$, $(X^0, \rho^0) \in \mathbb{A}$, we define

$$(X^{n+1}, \rho^{n+1}) = \operatorname{argmin}_{(Y,\tilde{\rho})\in\mathbb{A}} \mathbf{J}_{(X^n, \rho^n)}(Y, \tilde{\rho})$$

with

$$\mathbf{J}_{(X^n, \rho^n)}(Y, \tilde{\rho}) =$$

$$\frac{1}{2\tau}\mathbf{d}^2((Y,\tilde{\rho}),(X^n,\rho^n)) + \mathbf{E}_{(X^n,\rho^n)}(Y,\tilde{\rho}) + p_\tau(M(\tilde{\rho},\rho^n))$$

Theorem

There exists $X \in H^1(0,T)$ such that, up to a subsequence,

$$\tilde{X}^\tau \to X \quad \text{strongly in } L^2(0,T), \quad \text{as } \tau \downarrow 0,$$
$$\dot{\tilde{X}}^\tau \rightharpoonup \dot{X} \quad \text{weakly in } L^2(0,T), \quad \text{as } \tau \downarrow 0.$$

It also exists $M \in BV(0,T)$ such that, up to a subsequence,

$$M^\tau \to M \quad \text{strongly in } L^1(0,T), \quad \text{as } \tau \downarrow 0,$$
$$DM^\tau \rightharpoonup DM \quad \text{weakly in } \mathcal{M}(0,T), \quad \text{as } \tau \downarrow 0.$$

Moreover, there exists $\rho \in L^2_{\mathrm{loc}}(\mathbb{R}_+ \times (0,T)) \cap L^\infty(\mathbb{R}_+ \times (0,T)) \cap H^1(0,T;H^*)$ with $\partial_x \rho \in L^2(\mathbb{R}_+ \times (0,T))$ where $\rho(x,t) = 1$ for a.e. $(x,t) \in (X(t), +\infty) \times (0,T)$ such that, up to a subsequence, as $\tau \downarrow 0$

$$\rho^\tau \to \rho \quad \text{strongly in } L^p(0,T;L^q_{\mathrm{loc}}(\mathbb{R}_+)), \quad \forall 1 \leq p,q < \infty$$

$$\partial_x \rho^\tau \rightharpoonup \partial_x \rho \quad \text{weakly in } L^2(\mathbb{R}_+ \times (0,T)),$$
$$\tau^{-1}(\sigma_\tau \rho^\tau - \rho^\tau) \rightharpoonup \partial_t \rho \quad \text{weakly in } L^2(0,T;H^*).$$

Thank you for your attention !