Theoretical and numerical analysis of a diffusion problem on a moving domain

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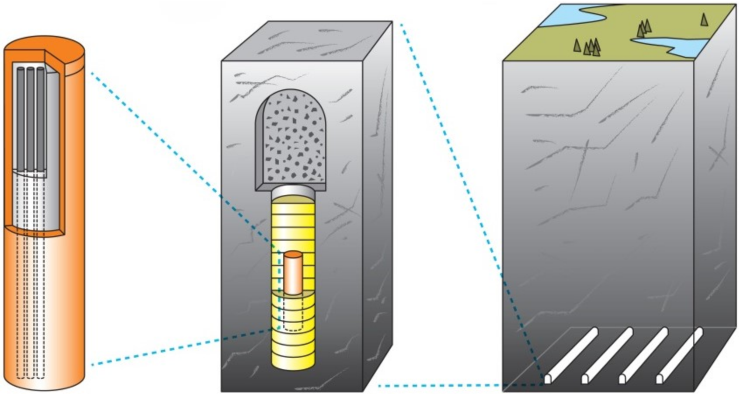
Nuclear waste storage



- ▷ Steel canister, buried in clay soil
- ▷ Main concern: the **corrosion** of the steel layer

1D model

$X_0(t)$ $X_1(t)$

soil | oxide layer | metal

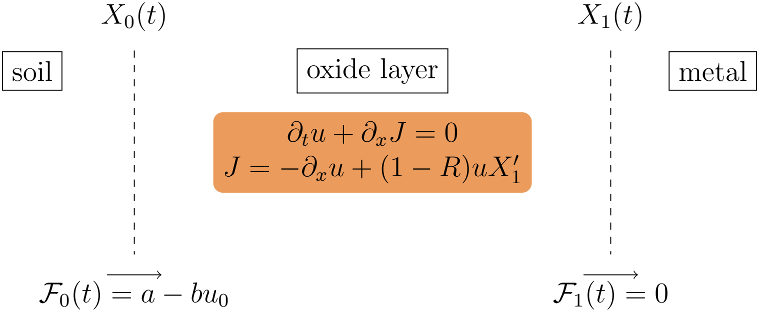
$$\partial_t u + \partial_x J = 0$$
$$J = -\partial_x u + (1 - R)uX_1'$$

$\mathcal{F}_0(t) = a - bu_0$ $\mathcal{F}_1(t) = 0$

Notations $\ell \in \{0, 1\}$

- $u_\ell(t) = u(t, X_\ell(t))$
- $J_\ell(t) = J(t, X_\ell(t))$
- $\mathcal{F}_\ell(t) = J_\ell(t) - u_\ell(t)X_\ell'(t)$
- $u^{init} = u(0, \cdot) \geq 0.$

1D model



Equations on the boundaries

- ▷ $X_0'(t) = \alpha_0 - \beta_0 u_0(t) + (1 - R)X_1'(t)$
- ▷ $X_1'(t) = -\alpha_1 + \beta_1 u_1(t)$
- ▷ $L(t) = X_1(t) - X_0(t)$

Objectives

Continuous problem

- Existence of a particular **travelling wave solution**
- Dissipation of an **energy** along time
  - A priori estimates

Numerical analysis

- Construction of a numerical method
  - Preserving the travelling wave profile
  - Dissipative energy

Main goal

- **Existence of a solution** to the continuous problem by taking the limit in the numerical scheme

Travelling wave

Travelling wave

One looks for a solution of the form:

$$u(t,x) = \hat{u}(x - \hat{c}t), \quad X_0' = X_1' = \hat{c}.$$

Explicit profile

$$\xi \in [0,1],\ \hat{u}(\xi) = \frac{a}{b} e^{-R\hat{c}\xi\hat{L}}.$$

- ▷ length: $\hat{L} = -\frac{1}{R\hat{c}} \log\left(\frac{b}{\beta_1 a}(\alpha_1 + \hat{c})\right) > 0$
- ▷ velocity: $\hat{c} = \frac{1}{R}\left(\alpha_0 - \beta_0 \frac{a}{b}\right) > 0$

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- velocity: $\hat{c} = \frac{1}{R}\left(\alpha_0 - \beta_0 \frac{a}{b}\right) > 0$
  - existence iff: $R > 0,\ 0 < \frac{\alpha_0 + R\alpha_1}{\beta_0 + R\beta_1} < \frac{a}{b} \leq \frac{\alpha_0}{\beta_0}$

Free energy

Free energy

- $\phi : \mathbb{R} \to \mathbb{R}$ convex, $\mathcal{H}_\phi(t) = \displaystyle\int_{X_0(t)}^{X_1(t)} \phi(u)$.
- pressure: $\pi(u) = u\phi'(u) - \phi(u)$; $\pi'(u) = u\phi''(u) \geq 0$ for $u \geq 0$.

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Derivative of $\mathcal{H}$

$$\frac{d}{dt}\mathcal{H}_\phi(t) = -\int_{X_0(t)}^{X_1(t)} |\partial_x u|^2 \phi''(u) + (a - bu_0)\phi'(u_0) + R(\alpha_1 - \beta_1 u_1)\pi(u_1) + (\alpha_0 - \beta_0 u_0)\pi(u_0)\,.$$

Decreasing total energy

Total energy

$$\mathcal{H}_\phi^{tot}(t) = \mathcal{H}_\phi(t) + R\pi\left(\frac{\alpha_1}{\beta_1}\right)(X_1(t) - X_1(0)) \\ - \pi\left(\frac{\alpha_0}{\beta_0}\right)\int_0^t (\alpha_0 - \beta_0 u_0) - \phi'\left(\frac{a}{b}\right)\int_0^t (a - bu_0).$$

Proposition

$$\forall t > 0,\ \frac{d}{dt}\mathcal{H}_\phi^{tot}(t) = -\mathcal{D}_\phi(t) \leq 0.$$

Dissipation term

$$\mathcal{D}_\phi(t) = \int_{X_0(t)}^{X_1(t)} |\partial_x u|^2 \phi''(u) - R(\alpha_1 - \beta_1 u_1)\left(\pi(u_1) - \pi\left(\frac{\alpha_1}{\beta_1}\right)\right) \\ - (\alpha_0 - \beta_0 u_0)\left(\pi(u_0) - \pi\left(\frac{\alpha_0}{\beta_0}\right)\right) - (a - bu_0)\left(\phi'(u_0) - \phi'\left(\frac{a}{b}\right)\right).$$

A priori bounds

L^∞-bounds

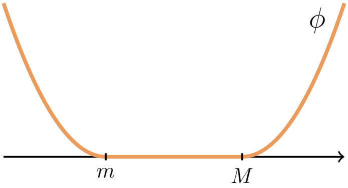
Any solution u satisfies

$$m \leq u \leq M$$

with

$$m = \min\left\{\inf u^{init}, \frac{\alpha_1}{\beta_1}\right\}, \; M = \max\left\{\sup u^{init}, \frac{\alpha_0}{\beta_0}\right\}.$$

Proof



- $\frac{d}{dt}\mathcal{H}_\phi^{tot}(t) \leq 0$
- $\mathcal{H}_\phi^{tot}(0) = 0$

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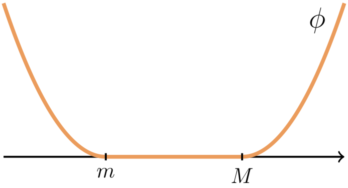

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  - $\mathcal{H}_\phi = 0$

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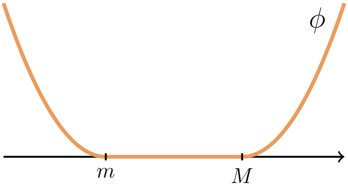


- $\frac{d}{dt}\mathcal{H}_\phi^{tot}(t) \leq 0$
- $\mathcal{H}_\phi^{tot}(0) = 0$
  - $\mathcal{H}_\phi = 0$

$\Rightarrow \phi(u) = 0$ in $[X_0(t), X_1(t)]$

$\Rightarrow m \leq u \leq M$

Mesh and notations

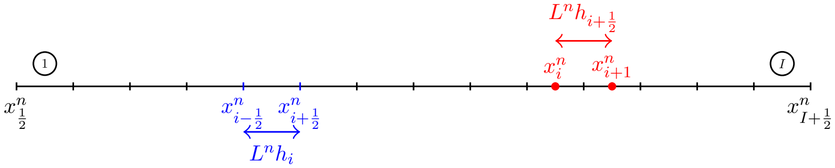
Time-dependent mesh

- initial mesh of $[0,1]$:

$$0 = \xi_{\frac{1}{2}} < \xi_{\frac{3}{2}} < \dots < \xi_{I-\frac{1}{2}} < \xi_{I+\frac{1}{2}} = 1.$$

- mesh of $[X_0^n, X_1^n]$:

$$x_{i+\frac{1}{2}}^n = X_0^n + L^n \xi_{i+\frac{1}{2}}.$$



- velocity related to the moving of the mesh and the transport term:

$$v_{i+\frac{1}{2}}^n = (1-R)\frac{X_1^n - X_1^{n-1}}{\Delta t} - \xi_{i+\frac{1}{2}} \frac{L^n - L^{n-1}}{\Delta t} - \frac{X_0^n - X_0^{n-1}}{\Delta t}.$$

Numerical scheme

Given $(u^{n-1}, X_0^{n-1}, X_1^{n-1})$, for $1 \leq i \leq J$:

$$h_i \frac{L^n u_i^n - L^{n-1} u_i^{n-1}}{\Delta t} + \mathcal{F}_{i+\frac{1}{2}}^n - \mathcal{F}_{i-\frac{1}{2}}^n = 0$$

- Scharfetter-Gummel fluxes:

$$\mathcal{F}_{i+\frac{1}{2}}^n = \frac{1}{L^n h_{i+\frac{1}{2}}} \left(B\left(-L^n h_{i+\frac{1}{2}} v_{i+\frac{1}{2}}^n \right) u_i^n - B\left(L^n h_{i+\frac{1}{2}} v_{i+\frac{1}{2}}^n \right) u_{i+1}^n \right)$$

  - Bernoulli function : $B(x) = \dfrac{x}{e^x - 1}$
- boundaries:
  - $$\frac{X_0^n - X_0^{n-1}}{\Delta t} - \alpha_0 + \beta_0 u_0^n - (1-R) \frac{X_1^n - X_1^{n-1}}{\Delta t} = 0$$
  - $$\frac{X_1^n - X_1^{n-1}}{\Delta t} + \alpha_1 - \beta_1 u_{J+1}^n = 0$$

Discrete free energy

Total discrete energy

$$\mathcal{H}_{\phi}^{tot,n} = \sum_{i=1}^{I} L^n h_i \phi(u_i^n) + \pi\left(\frac{\alpha_0}{\beta_0}\right)\sum_{k=0}^{n}\Delta t(\alpha_0 - \beta_0 u_0^k)$$
$$+ \phi'\left(\frac{a}{b}\right)\sum_{k=0}^{n}\Delta t(a - b u_0^k) + R\pi\left(\frac{\alpha_1}{\beta_1}\right)\sum_{k=0}^{n}\Delta t(\alpha_1 - \beta_1 u_{I+1}^k).$$

Proposition

For any $n > 0$, there exists a non-negative diffusion term $\mathcal{D}_{\phi}^{n}$ such that:

$$\frac{\mathcal{H}_{\phi}^{tot,n} - \mathcal{H}_{\phi}^{tot,n-1}}{\Delta t} + \mathcal{D}_{\phi}^{n} \leq 0.$$

Existence of a solution

Theorem

The ALE scheme admits a solution, that satisfies:

- $\forall 0 \leq i \leq J,\ \forall n \geq 0,\ m \leq u_i^n \leq M$.
- $\forall n \geq 0,\ \exists \varepsilon^n, \mathcal{L}^n > 0$ s.t. $\varepsilon^n \leq L^n \leq \mathcal{L}^n$.

Proof

- **a priori bounds** thanks to decreasing energy,
- **existence** by Brouwer's topological degree.

Convergence of the scheme

Theorem

The sequence $(u_\nu, X_{0,\nu}, X_{1,\nu})_\nu$ converges to a limit (u, X_0, X_1) with

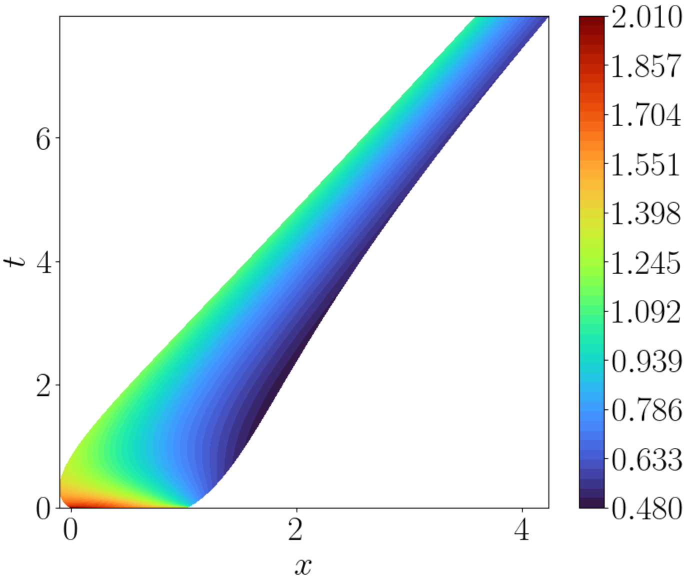
$$\begin{gathered} X_{\ell,\nu} \to X_\ell \text{ in } \mathcal{C}(0,T), \text{ for } \ell \in \{0,1\}, \\ \partial_{t,\Delta t} X_{\ell,\nu} \overset{*}{\rightharpoonup} X'_\ell \text{ in } L^\infty(0,T), \text{ for } \ell \in \{0,1\}, \\ u_\nu \to u \text{ in } L^2(0,T;L^2(\mathbb{R})), \\ \partial_{x,h} u_\nu \rightharpoonup \partial_x u \text{ in } L^2(0,T;L^2(\mathbb{R})), \end{gathered}$$

and (u, X_0, X_1) is a solution to the continuous problem.

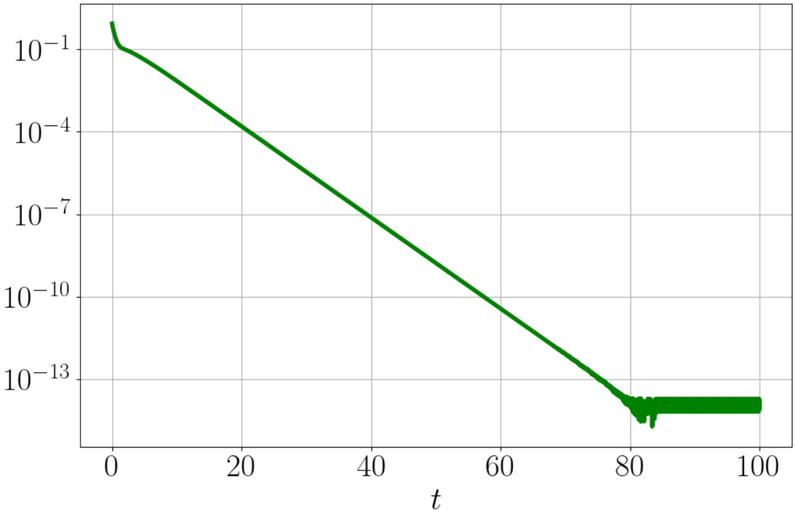
Proof

- **compactness** via rescaling and Aubin Simon lemma,
- convergence of the traces,
- **discrete estimates** thanks to decreasing energy.

Numerical results



Convergence towards the TW profile



Conclusion and perspectives

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- a priori bounds on the solution
- existence of a solution to the numerical scheme
- convergence towards a solution to the continous problem
- numerical convergence towards the travelling wave profile

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Perspectives

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- extend to a more complete model

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Thanks for your attention!