A study of optimal control problems for transport processes in porous media: analysis and homogenization

KAAS Seminar

by
Arghya Kundu

Department of Mathematics
Indian Institute of Technology Kharagpur
Kharagpur, India

29th January, 2026

Outline of presentation

Introduction

Optimal Control problem

- An optimal control problem (OCP) seeks a control function that minimizes a given performance criterion, while satisfying the governing equations of the system.
- Mathematically,

$$\min_{\theta} J(\theta) = J(u(\theta), \theta)\,, \text{ subject to } A(u, \theta) = 0,$$

where

- u: state variable, describes the system's behavior.
- θ: control variable.
- $A(u, \theta) = 0$: State (governing) equation, often an ODE or PDE.
- $J(u, \theta)$: cost functional, measures system's performance.

Homogenization

Microscopic Scale

- describes the heterogeneties
- size of nm-mm
- not suited for numerical simulations

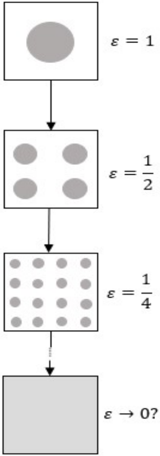
Macroscopic Scale

- describes the global behavior
- size of cm-km
- better suited for numerical simulations

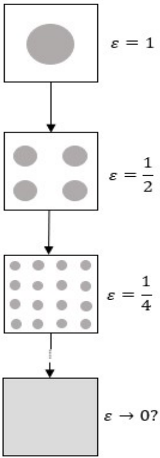
- Mathematically, homogenization is an averaging process that replaces heterogeneities in microscopic description with effective macroscopic ones.
- $$\begin{cases} A^{\varepsilon}(u^{\varepsilon}) = f & \text{inside the material,} \\ u^{\varepsilon} = g & \text{on the boundary,} \end{cases}$$

  what if ε (heterogeneity) $\to 0$?

Periodic Setting



- $\Omega \subset \mathbb{R}^n$- bounded domain and $Y := [0,1)^n$- representative cell.
- Y^p is the pore space and Y^s is the solid parts such that $Y := Y^p \cup Y^s$.
- $\partial\Omega$ and Γ- are the boundaries of Ω and Y^s.



- $\Omega \subset \mathbb{R}^n$- bounded domain and $Y := [0,1)^n$- representative cell.
- Y^p is the pore space and Y^s is the solid parts such that $Y := Y^p \cup Y^s$.
- $\partial\Omega$ and Γ- are the boundaries of Ω and Y^s.
- Choose a sequence of scale parameter $\varepsilon > 0$. For $y \in Y$, we set $x = \varepsilon y$.
- For fixed $\varepsilon, \Omega \subset \bigcup_{k \in \mathbb{Z}^n} \varepsilon(Y + k)$.
- $\Omega_p^\varepsilon := \bigcup_{k \in \mathbb{Z}^n} \varepsilon(Y^p + k)$, $\Omega_s^\varepsilon := \bigcup_{k \in \mathbb{Z}^n} \varepsilon(Y^s + k)$, $\Gamma_\varepsilon^* := \bigcup_{k \in \mathbb{Z}^n} \varepsilon(\Gamma + k)$, $\partial\Omega_p^\varepsilon := \partial\Omega \cup \Gamma_\varepsilon^*$.

ε-scaling

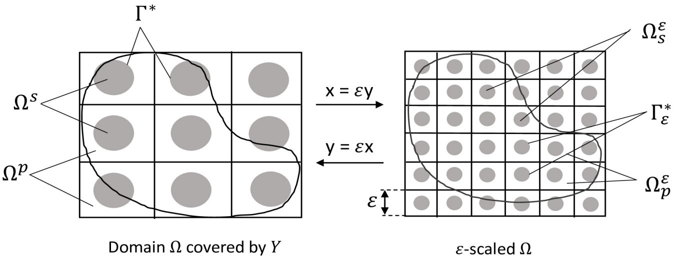


Figure : ε-periodic scaling of Ω.

Assumptions:

- Ω_p^ε is connected.
- Ω_s^ε is disconnected.

Homogenization of an OCP

$(\mathcal{OP})^{\varepsilon}$

$$\min_{\theta^{\varepsilon}} J^{\varepsilon}(\theta^{\varepsilon}) = J^{\varepsilon}(u^{\varepsilon}(\theta^{\varepsilon}), \theta^{\varepsilon})$$

subject to the constraint

$$A(u^{\varepsilon}, \theta^{\varepsilon}) = 0.$$

$(\mathcal{OP})$

$$\min_{\theta_0} J_0(\theta_0) = J_0(u_0(\theta_0), \theta_0)$$

subject to the constraint

$$A(u_0, \theta_0) = 0.$$

Homogenization

- If $\theta^{\varepsilon *}$ and θ_0^* be optimal controls for $(\mathcal{OP})^{\varepsilon}$ and $(\mathcal{OP})$, respectively, then what is the convergence relation between them?

Literature Survey and Proposed Work

Nandakumaran et al., 2015 [16]

An OCP associated to a bvp in a two dimensional oscillatory domain is considered and homogenization of the optimal solution is discussed.

Ayappan et al., 2019 [1]

considered OCP on a rapidly oscillating circular domain and homogenization.

S. Ayappan and A.k Nandakumaran, 2017 [2]

discussed a homogenization of an OCP in a multibranched oscillating domain.

Diaj et al., 2022 [12, 11]

- studied convergence analysis of an OCP for adsorption chemical phenomena in a perforated domain.
- homogenization problem in a perforated domain with holes of critical size and arbitrary shape.

.

cabarrubias, 2016 [9]

limiting behaviors of OCP based on an elliptic boundary value problem with highly oscillating coefficients in a periodically perforated domain.

Literature Survey and Proposed Work

Biswas et al., 2020[8]

Studied OCP governed by 2D nonlocal Cahn-Hillard-Navier-Stokes equations.

Bag et al., 2023, [7]

Optimal boundary control for the CHNS equations.

Hintermuller 2014, [13]

Optimal control of a semidiscrete CHNS system.

Colli et al., 2021, [10]

Well-posedness and optimal control for a Cahn-Hilliard-Oono system with control in the mass term.

Proposed Work

- Homogenization of OCP for chemical reactions in porous medium governed by a system of diffusion-reaction equations.
- Homogenization of a system of diffusion-reaction-precipitation-dissolution equations.
- An OCP for Stokes-Cahn-Hilliard-Oono system in a smooth domain.

Mathematical Preliminaries

- Let $1 < \mu < \infty$, $r \in \mathbb{N}_0$ and $\Theta \in \{\Omega, \Omega_p^\varepsilon\}$. Then Sobolev space $H^{r,\mu}(\Theta)$ is defined with the norm

$$||g||_{H^{r,\mu}(\Theta)} := \begin{cases} \left[\sum_{|\alpha|\le r} \int_\Theta |D^\alpha g|^\mu \, dx\right]^{\frac{1}{\mu}} & \text{for} \quad 1 \le \mu < \infty \\ \sum_{|\alpha|\le r} \operatorname*{ess\,sup}_{\Theta} |D^\alpha g| & \text{for} \quad \mu = \infty, \end{cases}$$

  where $\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_n)$, $D^\alpha g = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \frac{\partial^{\alpha_2}}{\partial x_2^{\alpha_2}} \cdots \frac{\partial^{\alpha_n}}{\partial x_1^{\alpha_n}} g$ and $|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_n$.

- Extension Theorem: Let $g \in H^{1,\mu}(\Omega_p^\varepsilon)$, then there exists a bounded linear operator $E^\varepsilon : H^{1,\mu}\left(\Omega_p^\varepsilon\right) \to H^{1,\mu}(\Omega)$ such that

$$\text{(a)} \ E^\varepsilon g := g \text{ in } \Omega_p^\varepsilon,$$
$$\text{(b)} \ \|E^\varepsilon g\|^\mu_{H^{1,\mu}(\Omega)} \le C\|g\|^\mu_{H^{1,\mu}\left(\Omega_p^\varepsilon\right)}$$

  where the constant C is independent of ε and g but depends on μ.

- Let Γ_ε^* be defined as in domain description, then $\lim_{\varepsilon\to 0}|\Gamma_\varepsilon^*| = |\Gamma|\dfrac{|\Omega|}{|Y|}$. The surface area of Γ_ε^* increases proportionally to $\frac{1}{\varepsilon}$, i.e, $|\Gamma_\varepsilon^*| \to \infty$ as $\varepsilon \to 0$, this leads us to define the duality pairing between $L^\rho(\Gamma_\varepsilon^*)$ and $L^\mu(\Gamma_\varepsilon^*)$ as

$$\langle g_1, g_2\rangle := \varepsilon \int_{\Gamma_\varepsilon^*} g_1 g_2 \, d\sigma_x \quad \text{for } g_1 \in L^\rho(\Gamma_\varepsilon^*) \text{ and } g_2 \in L^\mu(\Gamma_\varepsilon^*)$$

and norm of the space $L^r(S \times \Gamma_\varepsilon^*)$ is defined by

$$||g||^r_{L^r(S\times\Gamma_\varepsilon^*)} = \begin{cases} \varepsilon \int_{S\times\Gamma_\varepsilon^*} g^r(t,x)\, \mathrm{d}(t,\sigma_x) & \text{for } 1 \le r < \infty, \\ \text{ess sup}_{(t,x)\in S\times\Gamma_\varepsilon^*} |g(t,x)| & \text{for } r = \infty. \end{cases}$$

- Trace Theorem: For $1 \le \mu < \infty$, there exists a bounded linear operator $T^\varepsilon : H^{1,\mu}\left(\Omega_p^\varepsilon\right) \to L^\mu\left(\Gamma_\varepsilon^*\right)$ such that

(a) $T^\varepsilon g = g|_{\Gamma_\varepsilon^*}$ for $g \in H^{1,\mu}(\Omega_p^\varepsilon) \cap C\left(\bar{\Omega}_p^\varepsilon\right)$

(b) $$\varepsilon \int_{\Gamma_\varepsilon^*} |T^\varepsilon g(x)|^p \, d\sigma_x \le C\left(\int_{\Omega_p^\varepsilon} |g(x)|^p dx + \varepsilon^p \int_{\Omega_p^\varepsilon} |\nabla_x g(x)|^p \, dx\right),$$

where the constant C is independent of ε and g. [14]

- Let $U \subset \mathbb{R}^n$ be a bounded domain with Lipschitz boundary ∂U. Suppose further that $r \in (1, n]$ and $p \in [2 - \frac{1}{r}, \frac{2(n-1)}{n-r}]$, $q = r^*(p-1)$ with $\frac{1}{r} + \frac{1}{r^*} = 1$. Then for $g \in H^{1,r}(U)$,

$$\int_{\partial U} |g|^p \, ds \leq C_1 \int_U |g|^p \, dx + p \; C_2 \; ||g||_{L^q(U)}^{p-1} ||\nabla g||_{L^r(U)},$$

hence

$$\varepsilon \int_{\Gamma_\varepsilon^*} |g|^4 \, d\sigma_x \leq C_1 \int_{\Omega_p^\varepsilon} |g|^4 \, dx + 4\varepsilon C_2 ||g||_{L^6(\Omega_p^\varepsilon)}^3 ||\nabla g||_{L^2(\Omega_p^\varepsilon)},$$

where constants C_1, C_2 are independent of both ε and g. [6]

- A sequence of functions $(u^\varepsilon)_{\varepsilon>0}$ in $L^2(S\times\Omega)$ is said to be two-scale convergent to a limit $u\in L^2(S\times\Omega\times Y)$ if

$$\lim_{\varepsilon\to 0}\int_{S\times\Omega} u^\varepsilon(t,x)\eta(t,x,\frac{x}{\varepsilon})\ \mathrm{d}(x,t)=\int_{S\times\Omega\times Y} u(t,x,y)\eta(t,x,y)\ \mathrm{d}(x,y,t)$$

for all $\eta\in L^2(S\times\Omega;C_\#(Y))$. [4, 5]

- A sequence $(u^\varepsilon)_{\varepsilon>0}$ in $L^2(S\times\Gamma_\varepsilon^*)$ is said to two-scale convergent to a limit $u\in L^2(S\times\Omega\times\Gamma)$ if

$$\lim_{\varepsilon\to 0}\varepsilon\int_0^T\int_{\Gamma_\varepsilon^*} u^\varepsilon(t,x)\phi(t,x,\frac{x}{\varepsilon})\ \mathrm{d}(\sigma_x,t)=\int_0^T\int_\Omega\int_\Gamma u(t,x,y)\phi(t,x,y)\ \mathrm{d}(x,\sigma_y,t).$$

for any $\phi\in C(S\times\Omega;C_\#(Y))$. [3]

- Let $(u^\varepsilon)_{\varepsilon>0}$ be a sequence in $L^2(S\times\Gamma_\varepsilon^*)$ such that

$$\varepsilon\int_0^T\int_{\Gamma_\varepsilon^*}|u^\varepsilon(t,x)|^2\ \mathrm{d}(\sigma_x,t)\le C,$$

where C is independent of ε. Then there exists a subsequence (still denoted by ε) and a function $u\in L^2(S\times\Omega\times\Gamma)$ such that u^ε is two-scale convergent to u in the sense of the above definition.

Homogenization of an Optimal Control Problem for a Diffusion-Reaction System

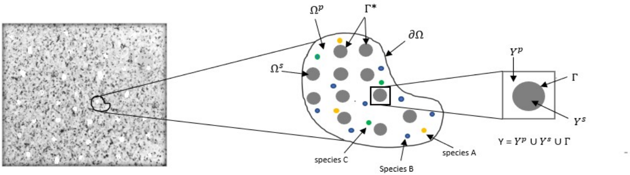


Figure 1: Chemical species A, B and C in Ω^p.

- Chemical species A, B and C has microscopic concentrations u_1^ε, u_2^ε and u_3^ε, respectively.
- A, B and C are chemically involved in such a way that
  - source terms:

$$A: \quad k_1^2 u_3^\varepsilon, \quad B: \quad k_2^1 u_3^\varepsilon, \quad C: \quad k_1^1 f_1(u_1^\varepsilon) + k_2^2 f_2(u_2^\varepsilon),$$

  - sink terms:

$$A: \quad k_1^1 f_1(u_1^\varepsilon), \quad B: \quad k_2^2 f_2(u_2^\varepsilon), \quad C: \quad (k_1^2 + k_2^1) u_3^\varepsilon.$$

Problem Description

An OCP $(\mathcal{OP}^{\varepsilon})$

$$\inf_{\theta^{\varepsilon}} \mathcal{J}^{\varepsilon}(\theta^{\varepsilon}) = \frac{1}{2}\sum_{i=1}^{3}\left\{ \int_{S\times\Omega_p^{\varepsilon}} |u_i^{\varepsilon} - u_{d_i}|^2 \,\mathrm{d}(x,t) + \int_{\Omega_p^{\varepsilon}} |u_i^{\varepsilon}(T,x) - u_{d_i}(T,x)|^2 \, dx \right\} + \frac{\beta}{2}\int_{S\times\Omega_p^{\varepsilon}} |\theta^{\varepsilon}|^2 \,\mathrm{d}(x,t),$$

subject to $(\mathcal{P}^{\varepsilon})$

$$\begin{aligned}
\frac{\partial u_1^{\varepsilon}}{\partial t} - D_1 \Delta u_1^{\varepsilon} &= k_1^2 u_3^{\varepsilon} - k_1^1 f_1(u_1^{\varepsilon}) && \text{in } S \times \Omega_p^{\varepsilon},\\
\frac{\partial u_2^{\varepsilon}}{\partial t} - D_2 \Delta u_2^{\varepsilon} &= k_2^1 u_3^{\varepsilon} - k_2^2 f_2(u_2^{\varepsilon}) && \text{in } S \times \Omega_p^{\varepsilon},\\
\frac{\partial u_3^{\varepsilon}}{\partial t} - D_3 \Delta u_3^{\varepsilon} &= k_1^1 f_1(u_1^{\varepsilon}) + k_2^2 f_2(u_2^{\varepsilon}) - (k_1^2 + k_2^1) u_3^{\varepsilon} + \theta^{\varepsilon} && \text{in } S \times \Omega_p^{\varepsilon},\\
D_i \nabla u_i^{\varepsilon} \cdot \vec{n} &= 0 && \text{on } S \times \partial\Omega \cup \Gamma_{\varepsilon}^{*},\\
u_i^{\varepsilon}(0,x) &= u_{i_0}(x) && \text{in } \Omega_p^{\varepsilon}.
\end{aligned}$$

Problem Description, Function Spaces and Assumptions

- $i = 1, 2, 3.$
- u_1^ε, u_2^ε and u_3^ε microscopic concentrations of A, B and C.
- D_i is the diffusion coefficient.
- θ^ε control variable.
- $\beta > 0$.
- k_1^1, k_2^2, k_1^2 and k_2^1 are reaction rate terms.

Function Spaces

$$\mathcal{F}^\varepsilon = \{u^\varepsilon : u^\varepsilon \in L^2(S; H^1(\Omega_p^\varepsilon)),\, \partial_t u^\varepsilon \in L^2(S; H^1(\Omega_p^\varepsilon)^*)\},$$
$$\mathcal{F} = \{u : u \in L^2(S; H^1(\Omega)),\, \partial_t u \in L^2(S; H^1(\Omega)^*)\}.$$

Assumptions

A1. $u_{i_0} \in L^2(\Omega_p^\varepsilon)$ such that $\sup_{\varepsilon>0} ||u_{i_0}||_{L^2(\Omega_p^\varepsilon)} < \infty$.

A2. $u_{d_i} \in L^2(S \times \Omega)$ and $u_{d_i}(T) \in L^2(\Omega)$.

A3. Constants k_1^1, k_1^2, k_2^2, k_2^1, D_i, $\beta > 0$.

A4. $f_i : \mathbb{R} \to \mathbb{R}$ is a real-valued smooth function such that $0 < C_1 \le f_i'(x) \le C_2$, $f_i(0) = 0$ and f'' is bounded.

Estimates

Lemma 1 (A-priori estimate)

Let the assumptions A1 - A4 be satisfied, then there exists a weak solution $(u_1^\varepsilon, u_2^\varepsilon, u_3^\varepsilon) \in \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon$ of $(\mathcal{P}^\varepsilon)$ which satisfies the following estimate

$$||u_1^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon))} + ||\partial_t u_1^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon)^*)} + ||u_2^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon))} + ||\partial_t u_2^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon)^*)} \\ + ||u_3^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon))} + ||\partial_t u_3^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon)^*)} \leq C(||u_{1_0}||_{L^2(\Omega_p^\varepsilon)} + ||u_{2_0}||_{L^2(\Omega_p^\varepsilon)} \\ + ||u_{3_0}||_{L^2(\Omega_p^\varepsilon)} + ||\theta^\varepsilon||_{L^2(S\times\Omega_p^\varepsilon)}),$$

where the constant C is independent of ε.

Theorem 1

Let θ_1^ε, θ_2^ε be two controls, then the asociated solutions $((u_1^\varepsilon)_1, (u_2^\varepsilon)_1, (u_3^\varepsilon)_1)$ and $((u_1^\varepsilon)_2, (u_2^\varepsilon)_2, (u_3^\varepsilon)_2)$ to the state equations $(\mathcal{P}^\varepsilon)$ satisfy

$$||(u_1^\varepsilon)_1 - (u_1^\varepsilon)_2||_{\mathcal{F}^\varepsilon} + ||(u_2^\varepsilon)_1 - (u_2^\varepsilon)_2||_{\mathcal{F}^\varepsilon} + ||(u_3^\varepsilon)_1 - (u_3^\varepsilon)_2||_{\mathcal{F}^\varepsilon} \leq C||\theta_1^\varepsilon - \theta_2^\varepsilon||_{L^2(S\times\Omega_p^\varepsilon)},$$

where the constant C is independent of ε.

Optimality Condition

Lemma 2 (Existence of optimal solution)

Assume that assumptions A1-A4 hold, then for a fixed $\varepsilon > 0$, $(\mathcal{OP}^\varepsilon)$ admits a solution.

proof.

- Let $m = \inf_{\theta^\varepsilon} \mathcal{J}^\varepsilon(\theta^\varepsilon)$ with $0 \leq m < \infty$. Then there exists a sequence $\{\theta_n^\varepsilon\}_n$ such that $\lim_{n\to\infty} \mathcal{J}^\varepsilon(\theta_n^\varepsilon) = m$.
- WOLG taking $\mathcal{J}^\varepsilon(\theta_n^\varepsilon) \leq \mathcal{J}^\varepsilon(0)$ implies $(\theta_n^\varepsilon)_n$ is bounded in $L^2(S \times \Omega_p^\varepsilon)$.
- There exists subsequences $\{\theta_n^\varepsilon\}_n, \{(u_i^\varepsilon)_n\}_n$ and $\{\partial_t(u_i^\varepsilon)_n\}_n$, s.t.

(i) $\theta_n^\varepsilon \xrightarrow{w} \theta^\varepsilon$ in $L^2(S \times \Omega_p^\varepsilon)$,

(ii) $(u_i^\varepsilon)_n \xrightarrow{w} u_i^\varepsilon$ in $L^2(S; H^1(\Omega_p^\varepsilon))$,

(iii) $\partial_t(u_i^\varepsilon)_n \xrightarrow{w} \partial_t u_i^\varepsilon$ in $L^2(S; H^1(\Omega_p^\varepsilon)^*)$,

(iv) $(u_i^\varepsilon)_n \to u_i^\varepsilon$ in $L^2(S \times \Omega_p^\varepsilon)$,

(v) $f_1((u_1^\varepsilon)_n) \to f_1(u_1^\varepsilon)$ in $L^2(S \times \Omega_p^\varepsilon)$,

(vi) $f_2((u_2^\varepsilon)_n) \to f_2(u_2^\varepsilon)$ in $L^2(S \times \Omega_p^\varepsilon)$.

- Weakly lower semicontinuity of $\mathcal{J}^\varepsilon$ implies that θ^ε is an optimal control for $(\mathcal{OP}^\varepsilon)$ and $\mathcal{S}(\theta^\varepsilon) = (u_1^\varepsilon, u_2^\varepsilon, u_3^\varepsilon)$ is the associate state, where $\mathcal{S} : L^2(S \times \Omega_p^\varepsilon) \to \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon$ is control to state mapping.

Optimality Condition

Theorem 2

For any optimal control $\theta^{\varepsilon *} \in L^2(S \times \Omega_p^\varepsilon)$, control to state mapping $\mathcal{S}$ is Fréchet differentiable. Moreover, the Fréchet derivative $\mathcal{DS}(\theta^{\varepsilon *})$ in the direction h is given by

$$\mathcal{DS}(\theta^{\varepsilon *})(h) = (\varphi_1, \varphi_2, \varphi_3),$$

where $(\varphi_1, \varphi_2, \varphi_3)$ is the unique weak solution to the following linearized system associated with h

$$\begin{aligned}
\frac{\partial \varphi_1}{\partial t} - D_1 \Delta \varphi_1 &= k_1^2 \varphi_3 - k_1^1 f_1'(u_1^{\varepsilon *})\varphi_1 && \text{in} \quad S \times \Omega_p^\varepsilon, \\
\frac{\partial \varphi_2}{\partial t} - D_2 \Delta \varphi_2 &= k_2^1 \varphi_3 - k_2^2 f_2'(u_2^{\varepsilon *})\varphi_2 && \text{in} \quad S \times \Omega_p^\varepsilon, \\
\frac{\partial \varphi_3}{\partial t} - D_3 \Delta \varphi_3 &= k_1^1 f_1'(u_1^{\varepsilon *})\varphi_1 + k_2^2 f_2'(u_2^{\varepsilon *})\varphi_2 - (k_2^1 + k_1^2)\varphi_3 + h && \text{in} \quad S \times \Omega_p^\varepsilon, \\
D_i \nabla \varphi_i \cdot \vec{n} &= 0 && \text{on} \quad S \times \partial\Omega \cup \Gamma_\varepsilon^*, \\
\varphi_i(0, x) &= 0 && \text{in} \quad \Omega_p^\varepsilon.
\end{aligned}$$

- Since $\theta^{\varepsilon *}$ is an optimal control, we have $\mathcal{D}J^{\varepsilon}(\theta^{\varepsilon *})\theta^{\varepsilon} = 0$ for all $\theta^{\varepsilon} \in L^2(S \times \Omega_p^{\varepsilon})$.
- Hence,

$$
\begin{aligned}
0 &= \mathcal{D}J^{\varepsilon}(\theta^{\varepsilon *})\theta^{\varepsilon} \\
&= \sum_{i=1}^{3} \left\{ \int_{S \times \Omega_p^{\varepsilon}} (u_i^{\varepsilon *} - u_{d_i})\, \varphi_i \,\mathrm{d}(x,t) + \int_{\Omega_p^{\varepsilon}} (u_i^{\varepsilon *}(T) - u_{d_i}(T))\, \varphi_i(T) dx \right\} \\
&\qquad + \beta \int_{S \times \Omega_p^{\varepsilon}} \theta^{\varepsilon *} \theta^{\varepsilon} \,\mathrm{d}(x,t),
\end{aligned}
$$

where $(\varphi_1, \varphi_2, \varphi_3) = \mathcal{D}\mathcal{S}(\theta^{\varepsilon *})\theta^{\varepsilon}$ is the unique weak solution to the linearized system with $h = \theta^{\varepsilon}$.

Optimality Condition

Theorem 3

Let $(u_1^{\varepsilon *}, u_2^{\varepsilon *}, u_3^{\varepsilon *}, \theta^{\varepsilon *})$ be an optimal solution for $(\mathcal{OP}^{\varepsilon})$, then we have the following optimality condition:

$$\theta^{\varepsilon *} = -\frac{1}{\beta}\gamma_3^{\varepsilon},$$

where $(\gamma_1^{\varepsilon}, \gamma_2^{\varepsilon}, \gamma_3^{\varepsilon})$ is the solution of the following adjoint equations

$$\begin{aligned}
&-\frac{\partial \gamma_1^{\varepsilon}}{\partial t} - D_1 \Delta \gamma_1^{\varepsilon} + k_1^1 f_1'(u_1^{\varepsilon *})\gamma_1^{\varepsilon} - k_1^1 f_1'(u_1^{\varepsilon *})\gamma_3^{\varepsilon} = u_1^{\varepsilon *} - u_{d_1} && \text{in} \quad S \times \Omega_p^{\varepsilon},\\
&-\frac{\partial \gamma_2^{\varepsilon}}{\partial t} - D_2 \Delta \gamma_2^{\varepsilon} + k_2^2 f_2'(u_2^{\varepsilon *})\gamma_2^{\varepsilon} - k_2^2 f_2'(u_2^{\varepsilon *})\gamma_3^{\varepsilon} = u_2^{\varepsilon *} - u_{d_2} && \text{in} \quad S \times \Omega_p^{\varepsilon},\\
&-\frac{\partial \gamma_3^{\varepsilon}}{\partial t} - D_3 \Delta \gamma_3^{\varepsilon} + (k_2^1 + k_1^2)\gamma_3^{\varepsilon} - k_1^2 \gamma_1^{\varepsilon} - k_2^1 \gamma_2^{\varepsilon} = u_3^{\varepsilon *} - u_{d_3} && \text{in} \quad S \times \Omega_p^{\varepsilon},\\
&D_i \nabla \gamma_i^{\varepsilon} \cdot \vec{n} = 0 && \text{on} \quad S \times \partial\Omega \cup \Gamma_{\varepsilon}^{*},\\
&\gamma_i^{\varepsilon}(T, x) = u_i^{\varepsilon *}(T) - u_{d_i}(T) && \text{in} \quad \Omega_p^{\varepsilon}.
\end{aligned}$$

Theorem 4

Suppose $(u_1^{\varepsilon*}, u_2^{\varepsilon*}, u_3^{\varepsilon*})$ is the optimal solution of $(\mathcal{OP}^\varepsilon)$ and let $(\gamma_1^\varepsilon, \gamma_2^\varepsilon, \gamma_3^\varepsilon)$ be the solution of the adjoint equations. Then, for $i = 1, 2, 3$, there exists a constant C (independent of ε) such that

$$||u_i^{\varepsilon*}||_{L^2(S;H^1(\Omega_p^\varepsilon))} + ||\partial_t u_i^{\varepsilon*}||_{L^2(S;H^1(\Omega_p^\varepsilon)^*)} + ||\gamma_i^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon))} + ||\partial_t \gamma_i^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon))} \leq C < \infty.$$

Lemma 3 (Extension Lemma)

For all $i = 1, 2, 3$; we get an extension of $u_i^{\varepsilon*}$, γ_i^ε and $\theta^{\varepsilon*}$ into all $S \times \Omega$ (still denoted by same symbol) such that

$$||u_i^{\varepsilon*}||_{L^2(S,H^1(\Omega))} + ||\partial_t u_i^{\varepsilon*}||_{L^2(S,H^1(\Omega)^*)} + ||\gamma_i^\varepsilon||_{L^2(S,H^1(\Omega))} + ||\partial_t \gamma_i^\varepsilon||_{L^2(S,H^1(\Omega)^*)} + ||\theta^{\varepsilon*}||_{L^2(S\times\Omega)} \leq C,$$

where C is independent of ε.

Lemma 4

Assuming that $(u_i^{\varepsilon *})_{\varepsilon>0}$, $(\gamma_i^{\varepsilon})_{\varepsilon>0}$ and $(\theta^{\varepsilon *})_{\varepsilon>0}$ satisfy the Extension Lemma, then there exist subsequences, still indexed by ε, the following convergence results are obtained:

(i) $(u_i^{\varepsilon *})_{\varepsilon>0} \overset{w}{\rightharpoonup} u_i^0$ in $L^2(S; H^1(\Omega))$,

(ii) $(\gamma_i^{\varepsilon})_{\varepsilon>0} \overset{w}{\rightharpoonup} \gamma_i^0$ in $L^2(S; H^1(\Omega))$,

(iii) $(u_i^{\varepsilon *})_{\varepsilon>0} \overset{2}{\rightharpoonup} u_i^0$ in $L^2(S; H^1(\Omega))$,

(iv) $(\nabla_x u_i^{\varepsilon *})_{\varepsilon>0} \overset{2}{\rightharpoonup} \nabla_x u_i^0 + \nabla_y u_i^1$,

(v) $(\gamma_i^{\varepsilon})_{\varepsilon>0} \overset{2}{\rightharpoonup} \gamma_i^0$ in $L^2(S; H^1(\Omega))$,

(vi) $(\nabla_x \gamma_i^{\varepsilon})_{\varepsilon>0} \overset{2}{\rightharpoonup} \nabla_x \gamma_i^0 + \nabla_y \gamma_i^1$,

(vii) $(u_i^{\varepsilon *})_{\varepsilon>0} \to u_i^0$ in $L^2(S \times \Omega)$,

(viii) $(\gamma_i^{\varepsilon})_{\varepsilon>0} \to \gamma_i^0$ in $L^2(S \times \Omega)$,

(ix) $f_j((u_j^{\varepsilon *})_{\varepsilon>0}) \to f_j(u_j^0)$ in $L^2(S \times \Omega_p^{\varepsilon})$,

(x) $f_j'((u_j^{\varepsilon *})_{\varepsilon>0}) \to f_j'(u_j^0)$ in $L^2(S \times \Omega_p^{\varepsilon})$,

(xi) $(\theta^{\varepsilon *})_{\varepsilon>0} \to \theta^0$ in $L^2(S \times \Omega)$.

where $u_i^0, \gamma_i^0 \in L^2(S; H^1(\Omega))$, $u_i^1, \gamma_i^1 \in L^2(S \times \Omega; H^1_{per}(Y)/\mathbb{R})$, $i = 1, 2, 3$ and $j = 1, 2$.

Convergence Analysis

Limit optimal control problem $(\mathcal{OP})$:

$$\inf_{\theta \in L^2(S\times\Omega)} \mathcal{J}(\theta) = \frac{1}{2}\sum_{i=1}^{3}\left\{ \int_{S\times\Omega} |u_i - u_{d_i}|^2 \,\mathrm{d}(x,t) + \int_{\Omega} |u_i(T,x) - u_{d_i}(T,x)|^2 dx \right\} + \frac{\beta}{2}\int_{S\times\Omega} |\theta|^2 \,\mathrm{d}(x,t),$$

subject to

$$\begin{aligned}
\frac{\partial u_1}{\partial t} - A_1 \Delta u_1 &= k_1^2 u_3 - k_1^1 f_1(u_1) && \text{in } S\times\Omega,\\
\frac{\partial u_2}{\partial t} - A_2 \Delta u_2 &= k_2^1 u_3 - k_2^2 f_2(u_2) && \text{in } S\times\Omega,\\
\frac{\partial u_3}{\partial t} - A_3 \Delta u_3 &= k_1^1 f_1(u_1) + k_2^2 f_2(u_2) - (k_1^2 + k_2^1) u_3 + \theta && \text{in } S\times\Omega,\\
D_i \nabla u_i \cdot \vec{n} &= 0 && \text{on } S\times\partial\Omega,\\
u_i(0,x) &= u_{i_0}(x) && \text{in } \Omega,
\end{aligned}$$

where

$$A_i = (a^i_{lm})_{1\le l,m\le n}, \text{ with } a^i_{lm} = \int_{Y^p} \frac{D_i}{|Y^p|}\left(\delta_{lm} + \frac{\partial k_l(y)}{\partial y_m}\right) dy$$

and k_l solves the cell problem

$$\nabla_y \cdot (\nabla_y k_l + e_l) = 0 \quad \forall\, y \in Y^p,$$
$$(\nabla_y k_l + e_l) \cdot \vec{n} = 0 \quad \text{on } \Gamma,$$
$$y \to k_l(y) \text{ is } Y - \text{ periodic.}$$

Theorem 5

Let $(u_1^{\varepsilon*}, u_2^{\varepsilon*}, u_3^{\varepsilon*}, \theta^{\varepsilon*}) \in \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon \times L^2(S \times \Omega_p^\varepsilon)$ be the optimal solution of $(\mathcal{OP}^\varepsilon)$ and $(u_1^*, u_2^*, u_3^*, \theta^*) \in \mathcal{F} \times \mathcal{F} \times \mathcal{F} \times L^2(S \times \Omega)$ be the optimal solution of $(\mathcal{OP})$, then the following convergence results hold:

(i) $\theta^{\varepsilon*} \to \theta^*$ in $L^2(S \times \Omega)$,

(ii) $u_i^{\varepsilon*} \xrightarrow{w} u_i^*$ in $L^2(S; H^1(\Omega))$,

(iii) $u_i^{\varepsilon*} \to u_i^*$ in $L^2(S \times \Omega)$,

(iv) $\gamma_i^\varepsilon \xrightarrow{w} \gamma_i$ in $L^2(S; H^1(\Omega))$,

(v) $\gamma_i^\varepsilon \to \gamma_i$ in $L^2(S \times \Omega)$

for $i = 1, 2, 3$.

continued· · ·

where $(\gamma_1, \gamma_2, \gamma_3)$ satisfies the following adjoint system

$$
\begin{aligned}
&\frac{\partial \gamma_1}{\partial t} + A_1 \Delta \gamma_1 + k_1^1 f_1'(u_1^*)(\gamma_3 - \gamma_1) = u_{d_1} - u_1^* && \text{in} \quad S \times \Omega, \\
&\frac{\partial \gamma_2}{\partial t} + A_2 \Delta \gamma_2 + k_2^2 f_2'(u_2^*)(\gamma_3 - \gamma_2) = u_{d_2} - u_2^* && \text{in} \quad S \times \Omega, \\
&\frac{\partial \gamma_3}{\partial t} + A_3 \Delta \gamma_3 - (k_2^1 + k_1^2)\gamma_3 + k_1^2 \gamma_1 + k_2^1 \gamma_2 = u_{d_3} - u_3^* && \text{in} \quad S \times \Omega, \\
&D_i \nabla \gamma_i \cdot \vec{n} = 0 && \text{on} \quad S \times \partial\Omega, \\
&\gamma_i(T, x) = u_i^*(T) - u_{d_i}(T) && \text{in} \quad \Omega,
\end{aligned}
$$

with the charaterization $\theta^* = -\frac{1}{\beta}\gamma_3$.

Homogenization of a Diffusion-Reaction-Precipitation-Dissolution System

Chemical Reaction

$$A + B \rightleftharpoons C \text{ on } \Gamma_\varepsilon^*.$$

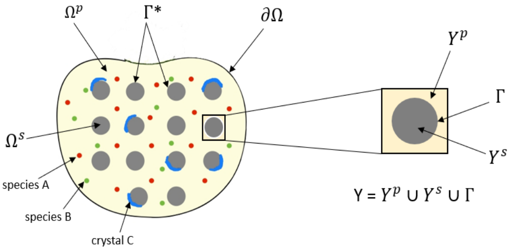


Figure 2: mobile species A and B in Ω^p with crystal C on Γ^*.

The Model ($\mathcal{P}^\varepsilon$):

$$\frac{\partial u_i^\varepsilon}{\partial t} + \nabla \cdot (-D_i \nabla u_i^\varepsilon) = 0 \quad \text{in} \quad S \times \Omega_p^\varepsilon,$$

$$-D_i \nabla u_i^\varepsilon \cdot \vec{n} = 0 \quad \text{on} \quad S \times \partial\Omega,$$

$$-D_i \nabla u_i^\varepsilon \cdot \vec{n} = \varepsilon \frac{\partial w_\varepsilon}{\partial t} \quad \text{on} \quad S \times \Gamma_\varepsilon^*,$$

$$u_i^\varepsilon(0, x) = u_{i_0}(x) \quad \text{in} \quad \Omega_p^\varepsilon,$$

Problem Description

$$\begin{aligned} \frac{\partial w_\varepsilon}{\partial t} &= k_p u_1^\varepsilon u_2^\varepsilon - k_d z_\varepsilon && \text{on} \quad S \times \Gamma_\varepsilon^*, \\ z_\varepsilon &\in \psi(w_\varepsilon) && \text{on} \quad S \times \Gamma_\varepsilon^*, \\ w_\varepsilon(0,x) &= w_0(x) && \text{in} \quad \Gamma_\varepsilon^*. \end{aligned}$$

- $i = 1, 2$.
- D_i diffusion coefficient.
- u_i^ε, w_ε microscopic concentrations.
- [17] The dissolution process is described by a multi-valued function: when the crystal/mineral is present in the solid matrix, the dissolution rate is constant; in its absence, the rate is adjusted to ensure a net zero dissolution. In summary, if the dissolution term is $r_d(x)$, then it can be represented as $r_d(x) \in k_d\psi(x)$, where

$$\psi(x) = \begin{cases} \{0\} & \text{if } x < 0 \\ [0,1] & \text{if } x = 0 \\ \{1\} & \text{if } x > 0. \end{cases}$$

Function Spaces and Assumptions

Function Spaces:

$$\mathcal{F}^{\varepsilon} = \{u^{\varepsilon} : u^{\varepsilon} \in L^2(S; H^1(\Omega_p^{\varepsilon})), \partial_t u^{\varepsilon} \in L^2(S; H^1(\Omega_p^{\varepsilon})^*)\},$$
$$\mathcal{F} = \{u : u \in L^2(S; H^1(\Omega)), \partial_t u \in L^2(S; H^1(\Omega)^*)\},$$
$$\mathcal{W}_{\varepsilon} = \{w_{\varepsilon} : w_{\varepsilon} \in L^2(S \times \Gamma_{\varepsilon}^*), \partial_t w_{\varepsilon} \in L^2(S \times \Gamma_{\varepsilon}^*)\},$$
$$\mathcal{W} = \{w : w \in L^2(S \times \Omega \times \Gamma), \partial_t w \in L^2(S \times \Omega \times \Gamma)\}.$$

Assumptions:

A1. $u_{i_0}(x) \geq 0$ and $w_0(x) \geq 0$.

A2. $u_{i_0} \in H^1(\Omega)$, $w_0 \in L^2(\Omega \times \Gamma)$ such that $\sup_{\varepsilon > 0} ||u_{i_0}||_{H^1(\Omega)} < \infty$ and $\sup_{\varepsilon > 0} ||w_0||_{L^2(\Omega \times \Gamma)} < \infty$.

A3. $k_p u_1^{\varepsilon} u_2^{\varepsilon} = 0$ if u_1^{ε} or $u_2^{\varepsilon} \leq 0$.

A4. k_p, k_d, D_i, $\beta > 0$.

Well-posedness of $(\mathcal{P}^\varepsilon)$

Theorem

Let the assumptions A1 - A4 be satisfied, then for $i = 1, 2$, there exists a unique positive weak solution $(u_1^\varepsilon, u_2^\varepsilon, w_\varepsilon) \in \mathcal{F}^\varepsilon \times \mathcal{F}^\varepsilon \times \mathcal{W}_\varepsilon$ of $(\mathcal{P}^\varepsilon)$ which satisfies

$$
\begin{aligned}
&||u_i^\varepsilon(t)||_{L^2(\Omega_p^\varepsilon)} \leq M_i \quad \text{in} \quad \Omega_p^\varepsilon, \\
&||w_\varepsilon(t)||_{L^2(\Gamma_\varepsilon^*)} \leq M_3 \quad \text{on} \quad \Gamma_\varepsilon^*, \\
&||u_i^\varepsilon(t)||_{L^2(\Omega_p^\varepsilon)} + ||\nabla u_i^\varepsilon(t)||_{L^2(\Omega_p^\varepsilon)} + ||\partial_t u_i^\varepsilon||_{L^2(S;H^1(\Omega_p^\varepsilon)^*)} < \infty, \\
&||w_\varepsilon(t)||_{L^2(\Gamma_\varepsilon^*)} + ||\partial_t w_\varepsilon||_{L^2(S\times\Gamma_\varepsilon^*)} < \infty
\end{aligned}
$$

for a.e. $t \in S$, and constants M_i's are independent of ε.

Step 1: Obtaining the a-priori estimates by choosing suitable test functions.
Step 2: Introducing Lipschitz regularization $\delta > 0$ such that

$$\psi_\delta(w_\varepsilon) = \begin{cases} 0 & \text{if } \; w_\varepsilon < 0, \\ \frac{w_\varepsilon}{\delta} & \text{if } \; w_\varepsilon \in (0, \delta), \\ 1 & \text{if } \; w_\varepsilon > \delta. \end{cases}$$

Corresponding integral formulation is

$$\int_S \left\langle \frac{\partial u_i^\varepsilon(t)}{\partial t}, \eta_i(t) \right\rangle_{H^1(\Omega_p^\varepsilon)^* \times H^1(\Omega_p^\varepsilon)} dt + \int_{S \times \Omega_p^\varepsilon} D_i \nabla u_i^\varepsilon \cdot \nabla \eta_i \, \mathrm{d}(t, x) + \varepsilon \int_{S \times \Gamma_\varepsilon^*} \partial_t w_\varepsilon \, \eta_i \, \mathrm{d}(t, \sigma_x) = 0, \quad (4.1)$$

$$\int_{S \times \Gamma_\varepsilon^*} \partial_t w_\varepsilon \, \phi \, \mathrm{d}(t, \sigma_x) = k_p \int_{S \times \Gamma_\varepsilon^*} u_1^\varepsilon \, u_2^\varepsilon \, \phi \, \mathrm{d}(t, \sigma_x) - k_d \int_{S \times \Gamma_\varepsilon^*} \psi_\delta(w_\varepsilon) \, \phi \, \mathrm{d}(t, \sigma_x). \quad (4.2)$$

Step 3:Forming the closed convex sets to apply Banach Fixed point theorem. The closed sets are

$$S^1_{\mathcal{F}^\varepsilon} = \{u_1^\varepsilon \in \mathcal{F}^\varepsilon : ||u_1^\varepsilon(t)||_{L^2(\Omega_p^\varepsilon)} \leq M_1 \quad \text{a.e. in} \quad S\},$$

$$S^2_{\mathcal{F}^\varepsilon} = \{u_2^\varepsilon \in \mathcal{F}^\varepsilon : ||u_2^\varepsilon(t)||_{L^2(\Omega_p^\varepsilon)} \leq M_2 \quad \text{a.e. in} \quad S\},$$

$$S_{\mathcal{W}_\varepsilon} = \{w_\varepsilon \in \mathcal{W}_\varepsilon : ||w_\varepsilon(t)||_{L^2(\Gamma_\varepsilon^*)} \leq M_3 \quad \text{a.e. in} \quad S\}.$$

Step 4: For $(u_1^\varepsilon, u_2^\varepsilon) \in S^1_{\mathcal{F}^\varepsilon} \times S^2_{\mathcal{F}^\varepsilon}$, consider the equation (4.2) with $w_\varepsilon(0,x) = w_0(x)$, then the Lipschitzness of r.h.s. of (4.2) implies that there exists a unique solution $w_\varepsilon \in S_{\mathcal{W}_\varepsilon}$ of (4.2).
Step 5: Again, for $u_1^\varepsilon \in S^1_{\mathcal{F}^\varepsilon}$ and considering the equation (4.1) for $i = 2$ with the initial condition, there exists a unique solution $\mathcal{G}_1 u_2^\varepsilon \in S_{\mathcal{F}^\varepsilon}$. Here, $\mathcal{G}_1$ s a contraction mapping from $S^2_{\mathcal{F}^\varepsilon}$ to $S^2_{\mathcal{F}^\varepsilon}$, ensuring the existence of a unique fixed point. Consequently, for $u_1^\varepsilon \in S_{\mathcal{F}^\varepsilon}$; the equation (4.1) for $i = 1$ has solution $\mathcal{G}_2 u_1^\varepsilon$ where $\mathcal{G}_2 : S^1_{\mathcal{F}^\varepsilon} \to S^1_{\mathcal{F}^\varepsilon}$ is a contraction map and possesses a fixed point in $S^1_{\mathcal{F}^\varepsilon}$.
Step 6: Passing limit $\delta \to 0$.

Limiting Analysis

Lemma

There exists extensions of the solutions u_i^ε into all of $S \times \Omega$ (still denoted by same symbols), such that $\forall\ i = 1, 2, 3$ and $\forall\ \varepsilon$

$$||u_i^\varepsilon||_{L^2(S\times\Omega)} + ||\nabla u_i^\varepsilon||_{L^2(S\times\Omega)} + ||\partial_t u_i^\varepsilon||_{L^2(S;H^1(\Omega)^*)} \leq C < \infty,$$

where the constant C is independent of ε.

Lemma

There exists functions $u_i^0 \in L^2(S; H^1(\Omega))$, $u_i^1 \in L^2(S \times \Omega; H^1_{per}(Y)/\mathbb{R})$ and $w_0 \in L^2(S \times \Omega \times \Gamma)$ such that upto a subsequence (still denoted by same symbol), the following convergence results hold:

- $(u_i^\varepsilon)_{\varepsilon>0} \xrightharpoonup{w} u_i^0$ *in* $L^2(S; H^1(\Omega))$.
- $(u_i^\varepsilon)_{\varepsilon>0} \xrightharpoonup{2} u_i^0$ *in* $L^2(S; H^1(\Omega))$.
- $(\nabla_x u_i^\varepsilon)_{\varepsilon>0} \xrightharpoonup{2} \nabla_x u_i^0 + \nabla_y u_i^1$.
- $(u_i^\varepsilon)_{\varepsilon>0} \to u_i^0$ *strongly in* $L^2(S \times \Omega)$.
- $(w_\varepsilon)_{\varepsilon>0}, (\partial_t w_\varepsilon)_{\varepsilon>0} \xrightharpoonup{2} w_0, \partial_t w_0$ *in* $L^2(S \times \Omega \times \Gamma)$.

Lemma

The following convergence results hold:

(i) $(u_i^\varepsilon)_{\varepsilon>0} \to u_i^0$ *strongly in* $L^2(S \times \Gamma_\varepsilon^*)$ *for* $i = 1, 2$.

(ii) $(u_1^\varepsilon u_2^\varepsilon)_{\varepsilon>0} \xrightharpoonup{2} u_1^0 u_2^0$ *in* $L^2(S \times \Omega \times \Gamma)$.

(iii) $(z_\varepsilon)_{\varepsilon>0} \xrightharpoonup{2} z_i^0$ *in* $L^2(S \times \Omega \times \Gamma)$.

(iv) *The unfolded sequence* $\{\mathcal{T}_b^\varepsilon(w_\varepsilon)\}_{\varepsilon>0} \to w_0$ *in* $L^2(S \times \Omega \times \Gamma)$.

Upscaled model:

$$\begin{aligned}
\partial_t u_i^0 + \nabla\cdot(-A_i \nabla u_i^0) + P(t,x) &= 0 && \text{in} \quad S\times\Omega,\\
-A_i\nabla u_i^0\cdot\vec{n} &= 0 && \text{on} \quad S\times\partial\Omega\cup\Gamma,\\
\frac{\partial w_0}{\partial t} &= k_p u_1^0 u_2^0 - k_d z_0 && \text{in} \quad S\times\Omega\times\Gamma,\\
z_0 &\in \psi(w_0) && \text{on} \quad S\times\Omega\times\Gamma,\\
u_i^0(0,x) &= u_{i_0}(x) && \text{in} \quad \Omega,\\
w_0(0,x,\sigma_y) &= w_0(x,\sigma_y) && \text{on} \quad \Omega\times\Gamma,
\end{aligned}$$

where $\bar{\theta}_i^0 = \frac{1}{|Y^p|}\int_Y \theta_i^0\,dy$, $P(t,x) = \frac{1}{|Y^p|}\int_\Gamma \frac{\partial w_0}{\partial t}\,d\sigma_y$, $A_i = (a_{lm}^i)_{1\le l,m\le n}$, with $a_{lm}^i = \int_{Y^p}\frac{D_i}{|Y^p|}\left(\delta_{lm} + \frac{\partial k_l(y)}{\partial y_m}\right)dy$ and k_l solves the cell problem

$$\begin{aligned}
\nabla_y\cdot(\nabla_y k_l + e_l) &= 0 \quad \forall\, y\in Y^p,\\
(\nabla_y k_l + e_l)\cdot\vec{n} &= 0 \quad \text{on } \Gamma,\\
y \to k_l(y) &\text{ is } Y - \text{ periodic.}
\end{aligned}$$

Optimal Control Problem for Stokes-Cahn-Hilliard-Oono Equations

An OCP$(\mathcal{OP})$

$$\inf \mathcal{J}(\theta) = \frac{1}{2}\int_{S\times\Omega} |v - v_d|^2 \, \mathrm{d}(x,t) + \frac{1}{2}\int_{S\times\Omega} |u - u_d|^2 \, \mathrm{d}(x,t) + \frac{\beta}{2}\int_{S\times\Omega} |\theta|^2 \, \mathrm{d}(x,t)$$

Subject to$(\mathcal{P})$

$$\begin{aligned}
\partial_t v - \mu\Delta v + \nabla p &= -\lambda u \nabla w + \theta && \text{in} \quad S\times\Omega,\\
\nabla\cdot v &= 0 && \text{in} \quad S\times\Omega,\\
v &= 0 && \text{on} \quad S\times\partial\Omega,\\
v(0,x) &= v_0(x) && \text{in} \quad \Omega,\\
\partial_t u + v\cdot\nabla u + \alpha u &= \Delta w && \text{in} \quad S\times\Omega,\\
w &= -\Delta u + f(u) && \text{in} \quad S\times\Omega,\\
\nabla u\cdot\vec{n} &= 0 && \text{on} \quad S\times\partial\Omega,\\
\nabla w\cdot\vec{n} &= 0 && \text{on} \quad S\times\partial\Omega,\\
u(0,x) &= u_0(x) && \text{in} \quad \Omega.
\end{aligned}$$

- μ viscosity
- v velocity
- u concentrations
- $\alpha, \beta > 0$ constants
- $F = \frac{1}{4}(u^2 - 1)^2$
- $f(u) = F'(u)$
- λ interfacial length
- v_d, u_d desired state
- θ control variable
- $\Omega \subset \mathbb{R}^n \, (n = 2, 3)$
- $S = [0, T)$

- Free energy E

$$E(u) = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 + F(u)\right) dx + \int_\Omega \int_\Omega u(x')g(x', x)u(x) \, dx' \, dx,$$

where $g(x', x)$ describes the long ranged interactions [15].

- Function Spaces

$$\mathcal{V} = \{\eta : \eta \in H_0^1(\Omega)^n, \nabla \cdot \eta = 0\},$$
$$\mathcal{H} = \{\phi : \phi \in L^2(\Omega)^n\}.$$

Weak Formulation

Assumptions

A1. $v_0 \in \mathcal{V}$ and $u_0 \in H^1(\Omega)$.

A2. $v_d \in L^2(S;\mathcal{V})$ and $u_d \in L^2(S \times \Omega)$.

A3. $\beta > 0$.

Weak Formulation

Let the assumptions A1-A3 hold true, then $(v, u, w) \in L^2(S;\mathcal{V}) \cap H^1(S;\mathcal{V}^*)$ $\times H^1(S; H^1(\Omega)^*) \cap L^2(S; H^3(\Omega)) \times L^2(S; H^1(\Omega))$ is called a weak solution of $\mathcal{P}$, if it satisfies $v(0,x) = v_0(x)$ and $u(0,x) = u_0(x)$ for all $x \in \Omega$ and

$$\int_S \langle \partial_t v, \psi \rangle \, dt + \mu \int_{S\times\Omega} \nabla v : \nabla \psi \; \mathrm{d}(x,t) = -\lambda \int_{S\times\Omega} u \nabla w \cdot \psi \; \mathrm{d}(x,t) + \int_{S\times\Omega} \theta \cdot \psi \; \mathrm{d}(x,t),$$

$$\int_S \langle \partial_t u, \phi \rangle \, dt + \int_{S\times\Omega} \nabla w \cdot \nabla \phi \; \mathrm{d}(x,t) + \alpha \int_{S\times\Omega} u\phi \; \mathrm{d}(x,t) = \int_{S\times\Omega} uv \cdot \nabla \phi \; \mathrm{d}(x,t),$$

$$\int_{S\times\Omega} w\varphi \; \mathrm{d}(x,t) = \int_{S\times\Omega} \nabla u \cdot \nabla \varphi \; \mathrm{d}(x,t) + \int_{S\times\Omega} f(u)\varphi \; \mathrm{d}(x,t),$$

for all $\psi \in L^2(S;\mathcal{V})$ and $\phi, \varphi \in L^2(S; H^1(\Omega))$.

Estimates

Lemma 1 (A-priori estimate)

Let the assumptions A1-A3 hold true, then weak solution (v, u, w) of $\mathcal{P}$ satisfies the following a-priori estimate:

$$||u||_{L^\infty(S;L^4(\Omega))} + ||\partial_t u||_{L^2(S;H^1(\Omega)^*)} + ||\nabla u||_{L^\infty(S,L^2(\Omega))} + ||w||_{L^2(S;H^1(\Omega))} + ||\nabla w||_{L^2(S\times\Omega)}$$
$$+||u||_{L^2(S;H^3(\Omega))} + ||v||_{L^2(S;L^2(\Omega)^n)} + ||\nabla v||_{L^2(S\times\Omega)^{n\times n}} + ||\partial_t v||_{L^2(S;\mathcal{V}^*)} \leq C < \infty,$$

where C is a constant.

Theorem 1

Let (v_1, u_1, w_1) and (v_2, u_2, w_2) be two week solutions of $\mathcal{P}$ for θ_1 and θ_2, respectively. Then the following estimates hold

$$||u_1 - u_2||_{L^2(S;H^3(\Omega))} + ||\partial_t u_1 - \partial_t u_2||_{L^2(S;H^1(\Omega)^*)} + ||\nabla w_1 - \nabla w_2||_{L^2(S\times\Omega)} + ||v_1 - v_2||_{L^2(S;\mathcal{V})}$$
$$+ ||\nabla u_1 - \nabla u_2||_{L^2(S\times\Omega)} + ||\partial_t v_1 - \partial_t v_2||_{L^2(S;\mathcal{V}^*)} \leq C_1||\theta_1(t) - \theta_2(t)||_{L^2(\Omega)}$$

for t a.e in S and C_1 is a constant depending on initial conditions. $\mathcal{S} : \theta \to (v, u, w)$ is a Lipschitz continuous from $L^2(S, \mathcal{H})$ onto $\mathcal{F} = L^2(S; \mathcal{V}) \cap H^1(S, \mathcal{V}^*) \times H^1(S; H^1(\Omega)^*)$ $\cap C([0, T]; H^1(\Omega)) \cap L^2(S; H^3(\Omega)) \times L^2(S; H^1(\Omega))$.

Optimality condition

Lemma 2 (Existence of optimal solution)

Assume that assumptions A1-A3 hold, then $\mathcal{OP}$ admits a solution.

Proof.

- Let $m = \inf_{\theta} \mathcal{J}(\theta)$. Since $0 \leq m < \infty$, then, there exists a sequence $\{\theta_n\}_n$ s.t. $\lim_{n\to\infty} \mathcal{J}(\theta_n) = m$.
- WOLG $\mathcal{J}(\theta_n) \leq \mathcal{J}(0)$ implies $(\theta_n)_n$ is bounded in $L^2(S;\mathcal{H})$.
- There exists subsequences $\{\theta_n\}_n$, $\{v_n\}_n$, $\{\partial_t v_n\}_n$, $\{u_n\}_n$, $\{\partial_t u_n\}_n$, $\{w_n\}_n$ s.t.

  (i) $\theta_n \overset{w}{\rightharpoonup} \hat{\theta}$ in $L^2(S,\mathcal{H})$,
  (ii) $v_n \overset{w}{\rightharpoonup} v$ in $L^2(S,\mathcal{V})$,
  (iii) $\partial_t v_n \overset{w}{\rightharpoonup} \partial_t v$ in $L^2(S,\mathcal{V}^*)$,
  (iv) $u_n \overset{w}{\rightharpoonup} u$ in $L^2(S;H^3(\Omega))$,
  (v) $u_n \overset{w^*}{\rightharpoonup} u$ in $L^\infty(S;H^1(\Omega))$,
  (vi) $\partial_t u_n \overset{w}{\rightharpoonup} \partial_t u$ in $L^2(S,H^1(\Omega)^*)$,
  (vii) $w_n \overset{w}{\rightharpoonup} w$ in $L^2(S;H^1(\Omega))$,
  (viii) $u_n \to u$ in $L^2(S;H^2(\Omega)) \cap C([0,T];H^1(\Omega))$.

- Next, the weakly lower semicontinuity of $\mathcal{J}$ implies that $\hat{\theta}$ is an optimal control for $\mathcal{OP}$.

Optimality Condition

Theorem 2

For any $\hat{\theta} \in L^2(S;\mathcal{H})$, control to state mapping $\mathcal{S}$ is Fréchet differentiable. Moreover, the Fréchet derivative $D\mathcal{S}(\hat{\theta})$ is given by

$$D\mathcal{S}(\hat{\theta})(h) = (\varphi_3, \varphi_1, \varphi_2),$$

where $(\varphi_3, \varphi_1, \varphi_2)$ is the weak solution to the following linearized system associated with h.

$$\begin{aligned}
&\frac{\partial \varphi_3}{\partial t} - \mu\Delta\varphi_3 + \nabla\bar{p} = -\lambda\varphi_1\nabla\hat{w} - \lambda\hat{u}\nabla\varphi_2 + h && \text{in} \quad S\times\Omega,\\
&\frac{\partial \varphi_1}{\partial t} - \Delta\varphi_2 + \varphi_3\cdot\nabla\hat{u} + \hat{v}\cdot\nabla\varphi_1 + \alpha\varphi_1 = 0 && \text{in} \quad S\times\Omega,\\
&\varphi_2 = -\Delta\varphi_1 + f'(\hat{u})\varphi_1 && \text{in} \quad S\times\Omega,\\
&\nabla\cdot\varphi_3 = 0 && \text{in} \quad S\times\Omega,\\
&\varphi_3(x,t) = 0,\ \nabla\varphi_1\cdot\vec{n} = \nabla\varphi_2\cdot\vec{n} = 0 && \text{on} \quad S\times\partial\Omega,\\
&\varphi_3(x,0) = 0,\ \varphi_1(x,0) = 0 && \text{in} \quad \Omega.
\end{aligned}$$

Optimality Condition

- Since $\hat{\theta}$ is an optimal control, we have $\mathcal{DJ}(\hat{\theta})\theta = 0$ for all $\theta \in L^2(S; \mathcal{H})$.
- Hence,

$$
\begin{aligned}
0 &= \mathcal{DJ}(\hat{\theta})\theta \\
&= \int_{S\times\Omega} (\hat{u} - u_d)\varphi_1 \,\mathrm{d}(x,t) + \int_{S\times\Omega} (\hat{v} - v_d)\cdot\varphi_3 \,\mathrm{d}(x,t) \\
&\qquad + \beta \int_{S\times\Omega} \theta\cdot\hat{\theta} \,\mathrm{d}(x,t)
\end{aligned}
$$

where $\mathcal{DS}(\hat{\theta})\theta = (\varphi_3, \varphi_1, \varphi_2)$ is the unique weak solution to the linearized system for $h = \theta$.

First Order Optimality Condition

Let $(\hat{v}, \hat{u}, \hat{w})$ be an optimal solution for $(\mathcal{OP})$, then we have the following optimality condition:

$$\hat{\theta} = -\frac{1}{\beta}\gamma_1,$$

where $(\gamma_1, \gamma_2, \gamma_3)$ is the solution of the following adjoint equations

$$\begin{aligned}
&-\frac{\partial \gamma_1}{\partial t} - \mu\Delta\gamma_1 + \nabla q = -\gamma_2 \nabla \hat{u} + (\hat{v} - v_d) && \text{in } S \times \Omega \\
&-\frac{\partial \gamma_2}{\partial t} - \hat{v} \cdot \nabla\gamma_2 + \alpha\gamma_2 + \lambda\nabla\hat{w} \cdot \gamma_1 + f'(\hat{u})\gamma_3 = (\hat{u} - u_d) + \Delta\gamma_3 && \text{in } S \times \Omega \\
&\gamma_3 = -\Delta\gamma_2 - \lambda\nabla\hat{u} \cdot \gamma_1 && \text{in } S \times \Omega \\
&\nabla \cdot \gamma_1 = 0 && \text{in } S \times \Omega \\
&\gamma_1(x, t) = \nabla\gamma_2 \cdot \vec{\eta} = \nabla\gamma_3 \cdot \vec{\eta} = 0 && \text{on } S \times \partial\Omega \\
&\gamma_1(x, T) = \gamma_2(x, T) = 0 && \text{in } \Omega
\end{aligned}$$

Future Scopes

- The homogenization analysis can be extended by considering arbitrary domains instead of assuming a periodic microstructure.
- Instead of considering a fixed domain, an evolving microstructure could be explored (i.e., $\Omega_p^\varepsilon(t)$, $\Omega_s^\varepsilon(t)$, $\Gamma^\varepsilon(t)$).
- For the phase-field model, several meaningful extensions can be explored:
  - One can extend the current problem by incorporating homogenization techniques to capture the multiscale effects.
  - Instead of Stokes equations, damped Navier-Stokes equations (convective Brinkman-Forchheimer equations) can be considered to model flow through porous media more realistically.
  - Replacing the double well free energy functional, one can choose a more general energy functional, such as a Logarithmic functional.
  - Extending the analysis to compressible, miscible, or non-Newtonian fluid systems to address a wider range of physical phenomena.
- Conducting detailed numerical studies of the optimal control problem to validate the theoretical results and to explore the behavior of optimal states and controls.
- In this study, we assumed constant diffusion coefficients for the chemical species. As a future work, we can explore models where the diffusion coefficients depend on the concentration.

S Aiyappan, Editha C Jose, Ivy Carol B Lomerio, and AK Nandakumaran.
Control problem on a rough circular domain and homogenization.
Asymptotic Analysis, 115(1-2):19–46, 2019.

S Aiyappan and AK Nandakumaran.
Optimal control problem in a domain with branched structure and homogenization.
Mathematical Methods in the Applied Sciences, 40(8):3173–3189, 2017.

G. Allaire, A. Damlamian, and U. Hornung.
Two-scale convergence on periodic structures and applications.
Proceedings of the International Conference on Mathematical Modelling of Flow through Porous Media, pages 15–25, World Scientific Publication, Singapore, 1996.

Grégoire Allaire.
Homogenization and two-scale convergence.
SIAM Journal on Mathematical Analysis, 23(6):1482–1518, 1992.

Grégoire Allaire.
Two-scale convergence and homogenization of periodic structures.
School on homogenization, ICTP, Trieste, 1993.

References II

G. Auchmuty.
Sharp boundary trace inequalities.
Proceedings of the Royal Society of Edinburgh A, 144(1):1–12, 2014.

Manika Bag, Tania Biswas, and Sheetal Dharmatti.
Optimal boundary control for the cahn-hilliard-navier-stokes equations.
arXiv preprint arXiv:2305.02501, 2023.

Tania Biswas, Sheetal Dharmatti, and Manil T Mohan.
Maximum principle for some optimal control problems governed by 2d nonlocal cahn–hillard–navier–stokes equations.
Journal of Mathematical Fluid Mechanics, 22:1–42, 2020.

B. Cabarrubias.
Homogenization of optimal control problems in perforated domains via periodic unfolding method.
Applicable Analysis, 95(11):2517–2534, 2016.

References III

Pierluigi Colli, Gianni Gilardi, Elisabetta Rocca, and Jürgen Sprekels.
Well-posedness and optimal control for a cahn-hilliard-oono system with control in the mass term.
arXiv preprint arXiv:2108.03165, 2021.

J.I. Díaz, A. Podolskiy, and T.A. Shaposhnikova.
On the homogenization of an optimal control problem in a domain perforated by holes of critical size and arbitrary shape.
In *Doklady Mathematics*, volume 105, pages 6–13. Springer, 2022.

J.I. Díaz, A.V. Podolskiy, and T.A. Shaposhnikova.
On the convergence of controls and cost functionals in some optimal control heterogeneous problems when the homogenization process gives rise to some strange terms.
Journal of Mathematical Analysis and Applications, 506(1):125559, 2022.

M Hintermuller and Donat Wegner.
Optimal control of a semidiscrete cahn–hilliard–navier–stokes system.
SIAM Journal on Control and Optimization, 52(1):747–772, 2014.

References IV

Ulrich Hornung and Willi Jäger.
Diffusion, convection, adsorption, and reaction of chemicals in porous media.
Journal of differential equations, 92(2):199–225, 1991.

Alain Miranville and Roger Temam.
On the cahn-hilliard-oono-navier-stokes equations with singular potentials.
Applicable Analysis, 95(12):2609–2624, 2016.

AK Nandakumaran, Ravi Prakash, and Bidhan Chandra Sardar.
Periodic controls in an oscillating domain: controls via unfolding and homogenization.
SIAM Journal on Control and Optimization, 53(5):3245–3269, 2015.

CJ Van Duijn and Iuliu Sorin Pop.
Crystal dissolution and precipitation in porous media: pore scale analysis.
2003.

Thank You

Thanks for your attention