Numerical solution of a two-scale system for concrete corrosion in sewer pipes

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Abstract

In this poster we summarize the results presented in our recent paper [2], where we consider two multiscale reaction-diffusion (RD) systems modeling sulfate attack in concrete structures (here: sewer pipes). The systems are posed on two different spatially separated scales. The only difference between them is the choice of the *micro-macro transmission condition*. We explore numerically the way the macroscopic Biot number Bi^M connects the two reaction-diffusion scenarios. We indicate connections between the solution of the "regularized" system (with moderate size of Bi^M) and the solution to the "matched" system (with blowing up size of Bi^M), where Henry's law plays the role of the micro-macro transmission condition.

Introduction

In [2] we deal with the problem of corrosion of concrete sewer pipes that sustain the attack of aggressive compounds like sulfuric acid.

Concrete is a material with porous structure – it can be viewed as consisting of a solid matrix and a system of interconnected pores and fissures, which are partly filled with water. There are two scales related inherently to the size of the air and water phase. The network of pores allows for a fast diffusion of gaseous compounds throughout the air phase on the macroscopic scale while diffusion in the water phase is limited by the size of pores and thus takes place at a much smaller, microscopic scale. This scenario indicates that one really needs to get a sound understanding of *structured transport* – since this is the main mechanism responsible for a significant interplay between micro (pore level) and macro (pipe level) scales. These considerations motivate our multiscale approach to this corrosion process.

Chemistry Active anaerobic bacteria existing in the waste water produce gaseous H_2S which moves in the air space of the pipe and goes up towards the pipe wall. Gaseous H_2S enters the concrete pores (microstructures) via both air and water parts. Once arrived inside the microstructure, H_2S diffuses within the available air space and dissolves in the thin (stationary) water film clinging on the wall of the fabric. In sewer pipes with increased temperature, sulfate-rich environments rapidly lead to the formation of sulfuric acid by the action of aerobic bacteria. This aggressive acid reacts with calcium carbonate (i.e., with our concrete sample) and produces gypsum.

We pay special attention to the following aspects:

- exchange of H_2S from water to the air phase and vice versa (modeled by Henry's law);
- production of gypsum at micro solid-water interfaces (non-standard non-linear reaction rate).

Problem geometry We consider a sewer pipe made of partially wet concrete. We consider a single critical macroscopic region $\Omega := (0, L)$ where corrosion initiates. The boundary Γ of Ω is composed of two disjoint parts $\Gamma^D := \{0\}$ (the inner surface of the pipe) and $\Gamma^N := \{L\}$, the Dirichlet and the Neumann boundaries. We assume that the medium Ω is made by periodically repeating the *same* microstructure (or standard cell [5]) $Y := (0, \ell)$ representing the wet part of the pore. See [4] for more comments regarding x-dependent cells Y_x.

Let S be the time interval $(0, T)$ during which we consider the process. By subscript y we denote differentiation only w.r.t. the variable $y \in Y$ and similarly for subscript x.

Two-scale model (P) for sulfate attack

We consider the following two-scale system of PDEs and one ODE for unknown functions $w_k : \Omega \times Y \times S \to \mathbb{R}$, $k \in \{1, 2, 4\}$, $w_3 : \Omega \times S \to \mathbb{R}$, and $w_5 : \Omega \times \{y = \ell\} \times S \to \mathbb{R}$ such that

$$\begin{aligned}
\beta_1 \partial_t w_1 - \beta_1 d_1 \Delta_y w_1 &= -\Phi_1^2 k_1 w_1 + \Phi_2^2 k_2 w_2, \ \text{in } \Omega \times Y \times S,\\
\beta_2 \partial_t w_2 - \beta_2 d_2 \Delta_y w_2 &= \Phi_1^2 k_1 w_1 - \Phi_2^2 k_2 w_2, \ \text{in } \Omega \times Y \times S,\\
\partial_t w_3 - d_3 \Delta_x w_3 &= -Bi^M \left(H w_3 - w_2|_{y=0} \right), \ \text{in } \Omega \times S,\\
\beta_4 \partial_t w_4 - \beta_4 d_4 \Delta_y w_4 &= k_1 w_1, \ \text{in } \Omega \times Y \times S,\\
\beta_5 \partial_t w_5 &= +\Phi_3^2 \eta(w_1, w_5), \ \text{in } \Omega \times \{y = \ell\} \times S,
\end{aligned}$$

where $\beta_k > 0$, $k \in \{1, 2, 4, 5\}$, are parameters, $d_k > 0$, $k \in \{1, 2, 3, 4\}$, are the diffusion coefficients, Bi^M is a dimensionless Biot number, and $k_k : Y \to \mathbb{R}$, $k \in \{1, 2, 3\}$, are functions modeling the rate "constants". We assume the reaction rate η takes the form

$$\eta(\alpha, \beta) = \begin{cases} k_3 \alpha^p (\bar{c} - \beta)^q, & \text{if } \alpha \geq 0,\ \beta \geq 0,\\ 0, & \text{otherwise,} \end{cases} \tag{1}$$

where $\bar{c}$ is a known equilibrium constant concentration and $p \geq 1, q \geq 1$ are the partial orders of reaction. The Φ_k^2, $k \in \{1, 2, 3\}$, are Damköhler numbers corresponding to three distinct chemical mechanisms. It is worth noting that terms like

$$Bi^M \left(H w_3(t, x) - w_2(t, x, y = 0) \right) \tag{2}$$

are usually referred to in the literature as production terms by Henry's or Raoult's law. $H > 0$ is the Henry's constant. The special feature of our scenario is that now the term (2) *bridges* two distinct spatial scales: one macro with $x \in \Omega$ and one micro with $y \in Y$.

The system is supplemented with initial and boundary conditions, which read as

$$\begin{aligned}
-d_1 \partial_y w_1 &= 0, && \text{on } \Omega \times \{y = 0\} \times S,\\
-d_1 \partial_y w_1 &= \Phi_3^2 \eta(w_1, w_5), && \text{on } \Omega \times \{y = \ell\} \times S,\\
-d_2 \partial_y w_2 &= -Bi^M (H w_3 - w_2), && \text{on } \Omega \times \{y = 0\} \times S,\\
-d_2 \partial_y w_2 &= 0, && \text{on } \Omega \times \{y = \ell\} \times S,\\
w_3 &= w_3^D, && \text{on } \Gamma^D \times S,\\
-d_3 \partial_x w_3 &= 0, && \text{on } \Omega \setminus \Gamma^D \times S,\\
-d_4 \partial_y w_4 &= 0, && \text{on } \Omega \times \{y = 0, \ell\} \times S,
\end{aligned}$$

Lemma 1. *Under suitable assumptions the weak solutions are positive and bounded a.e. in Ω or, following the case, in $\Omega \times Y$.*

Theorem 2 (Global existence and uniqueness). *Let $\tau > 0$ be arbitrarily chosen. Then under suitable assumptions problem (P) admits a unique positive and bounded (weak) solution such that*

$$\begin{aligned}
w_3 &\in w_3^D + L^2(0, \tau; H_0^1(\Omega)),\\
\partial_t w_3 &\in L^2((0, \tau) \times \Omega),\\
(w_1, w_2, w_4) &\in \left[L^2(0, \tau; L^2(\Omega, H^1(Y))) \right]^3,\\
(\partial_t w_1, \partial_t w_2, \partial_t w_4) &\in \left[L^2((0, \tau) \times \Omega \times Y) \right]^3,\\
w_5 &\in H^1(0, \tau; L^\infty(\Omega \times \{y = \ell\})).
\end{aligned}$$

Fast-transfer two-scale model $(\tilde{P})$ for sulfate attack

We are interested in understanding the behavior of solutions to problem (P) as the mass-transfer Biot number Bi^M goes to infinity: we expect the solution $(w_1^\epsilon, w_2^\epsilon, w_3^\epsilon, w_4^\epsilon, w_5^\epsilon)$ of problem (P) to converge as

$$\epsilon := \frac{1}{Bi^M} \to 0 \tag{3}$$

to the solution $(u_1, u_2, u_3, u_4, u_5)$ of the following problem, say $(\tilde{P})$:

$$\begin{aligned}
\beta_1 \partial_t u_1 - \beta_1 d_1 \Delta_y u_1 &= -\Phi_1^2 k_1 u_1 + \Phi_2^2 k_2 u_2, \ \text{in } \Omega \times Y \times S,\\
\beta_2 \partial_t u_2 - \beta_2 d_2 \Delta_y u_2 &= \Phi_1^2 k_1 u_1 - \Phi_2^2 k_2 u_2, \ \text{in } \Omega \times Y \times S,\\
\partial_t u_3 - d_3 \Delta_x u_3 &= d_2 \partial_y u_2|_{y=0}, \ \text{in } \Omega \times S,\\
\beta_4 \partial_t u_4 - \beta_4 d_4 \Delta_y u_4 &= k_1 u_1, \ \text{in } \Omega \times Y \times S,\\
\beta_5 \partial_t u_5 &= \Phi_3^2 \eta(u_1, u_5), \ \text{in } \Omega \times \{y = \ell\} \times S,
\end{aligned}$$

with

$$\begin{aligned}
-d_1 \partial_y u_1 &= 0, && \text{on } \Omega \times \{y = 0\} \times S,\\
-d_1 \partial_y u_1 &= \Phi_3^2 \eta(u_1, u_5), && \text{on } \Omega \times \{y = \ell\} \times S,\\
u_2 &= H u_3, && \text{on } \Omega \times \{y = 0\} \times S,\\
-d_2 \partial_y u_2 &= 0, && \text{on } \Omega \times \{y = \ell\} \times S,\\
u_3 &= u_3^D, && \text{on } \Gamma^D \times S,\\
-d_3 \partial_x u_3 &= 0, && \text{on } \Omega \setminus \Gamma^D \times S,\\
-d_4 \partial_y u_4 &= 0, && \text{on } \Omega \times \{y = 0, \ell\} \times S,
\end{aligned}$$

Following the terminology of [3], problem $(\tilde{P})$ is a *matched microstructure model*.

Numerical results for problem (P)

We assume zero constant initial conditions for $w_h^k(0)$, $k = 2, 4, 5$, while we assume $w_h^1(0) = 0.01$. The value of the initial concentration $w_h^3(0)$ is chosen to be compatible with the Dirichlet boundary condition $w_3^D = 0.011$. The values of the remaining parameters are summarized in the following table:

β_i	k_1	k_2	k_3	$d_{1,2,4}$	d_3	$\bar{c}$	H	p	q	Φ_2^i
1	0.84	7.2	1.0	0.00864	0.864	0.9	2.5	1	1	1

Illustration of the convergence scenario: $\epsilon \to 0$ In this paragraph we are concerned with the behavior of solutions to (P) as $\epsilon \to 0$. The main result here is that we show numerically that

$$\| H w_3 - w_2|_{y=0} \|_{L^2(\Omega)} \to 0 \text{ as } \epsilon \to 0,$$

i.e., as $Bi^M \to \infty$. We show this by simply measuring the experimental order of convergence. We plan to prove rigorously this behavior elsewhere. We proceed as follows: We compute solutions of (P) at $T = 800$ for gradually increasing values of $Bi^M = 4^i$, $i \in \{1, \dots, 6\}$. For each choice of ϵ, we measure the quantity $E_\epsilon := \| H w_h^3(T) - w_h^2(T)|_{\Omega_h} \|_2$ in terms of a discrete L^2-norm. Finally, we define the experimental order of convergence of E_ϵ as

$$EOC_{E_\epsilon} := \frac{\log(E_{\epsilon_1}) - \log(E_{\epsilon_2})}{\log(\epsilon_1) - \log(\epsilon_2)}. \tag{4}$$

The results shown in the following table indicate that E_ϵ behaves as $O(\epsilon)$:

$\log_4 Bi^M$	$\| H w_h^3 - w_h^2|_{\Omega_h} \|_2$	EOC_{E_ϵ}
1	$1.12728 \cdot 10^{-3}$	0.99896
2	$2.82225 \cdot 10^{-4}$	0.99973
3	$7.05819 \cdot 10^{-5}$	0.99993
4	$1.76471 \cdot 10^{-5}$	0.99998
5	$4.41187 \cdot 10^{-6}$	0.99999
6	$1.10297 \cdot 10^{-6}$	

Conclusion

The results of EOC analysis encourage us to ask the questions:

- Do the concentration profiles corresponding to (P) approach those corresponding to $(\tilde{P})$ as ϵ goes to zero? If yes, then in which sense?
- For suitable parameter regimes, have the solutions to problems (P) and $(\tilde{P})$ have the *same* large-time behavior?

Trusting the analysis reported in [3], we expect a positive answer to the first question. However, we need to take into account the specifics of (P) and check which regularity of data and parameters is required for the limit $Bi^M \to \infty$ to make sense.

To reply to the second question, we would need to do more numerical experiments. From the analysis point of view, we expect the existence of constant steady states. Again, it remains to investigate what are the necessary and sufficient conditions that both problems have the same constants as steady states.

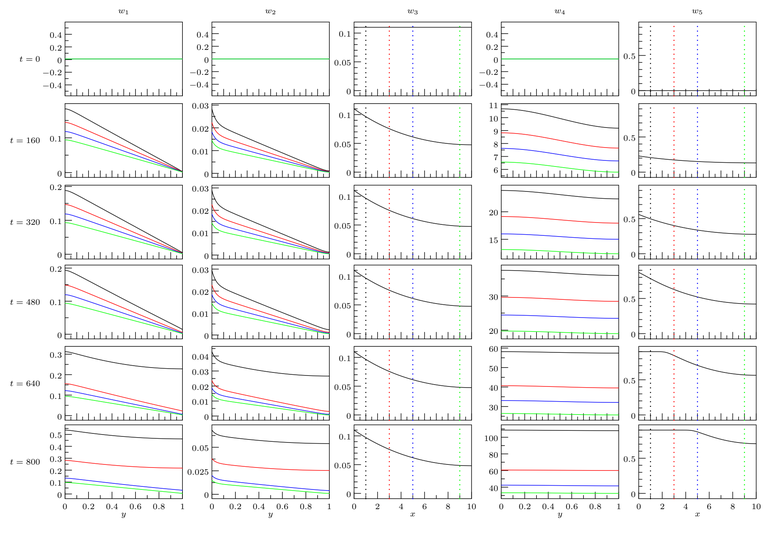

Figure 1: Plot of a the semi-discrete solution to problem (P) for intermediate value of $Bi^M = 0.00864$. Note the concentration of gypsum in the fifrth column – the w_5 grows until it reaches a critical value $\bar{c} = 0.9$ which can be interpreted as an *indication of complete conversion of concrete into gypsum*. As the time increases, the corrosion tends to be complete and apparently the system wants to reach a constant steady state.

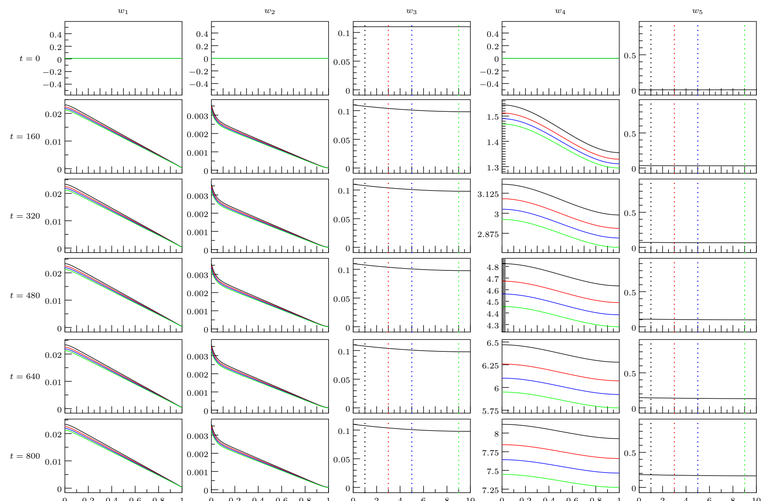

Figure 2: Plot of a semi-discrete solution to problem (P) for a low value of $Bi^M = 0.000864$. The coupling between the equations for w_3 and w_2 is looser due to a *barrier* for H_2S in the air hindering its entrance into the water phase. Hence w_2 and w_1 attain lower values and their profiles tend to be uniform along the x-axis. Eventually, this leads to a slow, gradual corrosion of the pipe wall along the whole domain and we do not observe the same progress of the corroding front as in Fig 1.

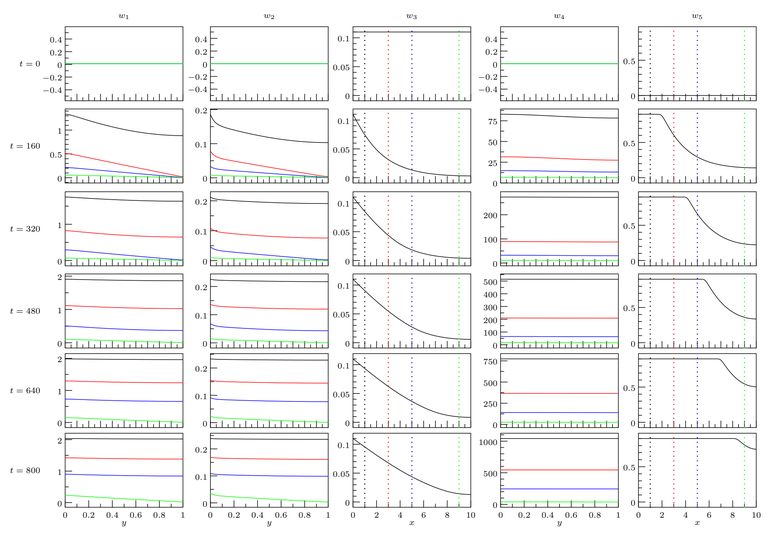

Figure 3: Plot of a semi-discrete solution to problem (P) for a large value of $Bi^M = 864$. The boundary condition for w_2 at $y = 0$ is essentially a Dirichlet one. We can observe that the concentrations of w_2 and w_3 are higher than in Fig. 1 and Fig. 2. Additionally, the corrosion process seems to be much faster exhibiting a prominent corroding front advancing into the concrete.

References

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