Models for capturing the penetration of a diffusant concentration into rubber: Numerical analysis and simulation

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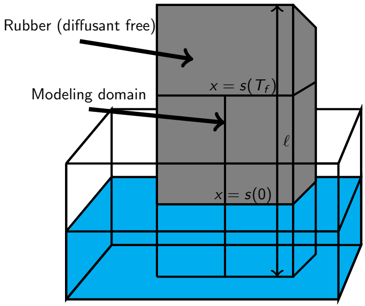
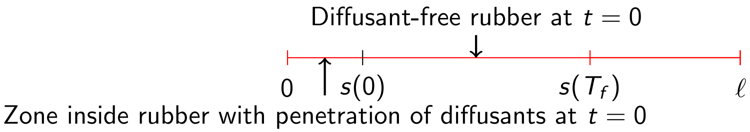
Motivation and geometry

Q) *How far does the concentration of a diffusant species penetrate into a rubber?*

Our goal is to:

1. approximate numerically the diffusant concentration profile and the penetration front that reflect the lab experiment results.
2. investigate the effectiveness of the numerical method (order of convergence).





Model equations

Find the concentration profile $m(t,x)$ and the position of moving boundary $s(t)$ such that

$$
\begin{aligned}
\frac{\partial m}{\partial t} - D\frac{\partial^2 m}{\partial x^2} &= 0 \quad \text{in} \quad (t,x) \in (0, T_f) \times (0, s(t)),\\
-D\frac{\partial m}{\partial x}(t,0) &= \beta(b(t) - \mathrm{H}m(t,0)),\\
-D\frac{\partial m}{\partial x}(t,s(t)) &= s'(t)m(t,s(t)),\\
s'(t) &= a_0(m(t,s(t)) - \sigma(s(t))),\\
m(0,x) &= m_0(x) \quad \text{for} \quad x \in [0, s(0)],\\
s(0) &= s_0 \text{ with } \ 0 < s_0 < s(t) < \ell,
\end{aligned}
$$

where

- D is a diffusion constant,
- σ represents the swelling behaviour of the rubber,
- $s_0 > 0$ and m_0 are initial data,
- β is mass transfer coefficient,
- H is Henry's constant.

Assumptions

We assume the following restrictions on the parameters:

(A1) $a_0 > 0,\ \mathrm{H} > 0,\ D > 0,\ s_0 > 0,\ T_f > 0$;

(A2) $b \in W^{1,2}(0, T_f)$ with $0 < b_* \leq b \leq b^*$ on $(0, T_f)$;

(A3) $\beta \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ such that $\beta = 0$ on $(-\infty, 0]$, and there exists $r_\beta > 0$ such that $\beta' > 0$ on $(0, r_\beta)$ and $\beta = k_0$ on $[r_\beta, +\infty)$, where $k_0 > 0$;

(A4) $\sigma \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ such that $\sigma = 0$ on $(-\infty, 0)$, and there exist r_σ such that $\sigma' > 0$ on $(0, r_\sigma)$ and $\sigma = c_0$ on $[r_\sigma, +\infty)$, where c_0 satisfying

$$0 < c_0 < \min\{2\sigma(0), b^*\mathrm{H}^{-1}\};$$

(A5) $0 < s_0 < r_\sigma$ and $m_0 \in H^1(0, s_0)$ such that $\sigma(0) \leq u_0 \leq b^*\mathrm{H}^{-1}$ on $[0, s_0]$.

K. Kumazaki and A. Muntean. Global weak solvability, continuous dependence on data, and large time growth of swelling moving interfaces. *Interfaces and Free Boundaries*, 2020.

Non-dimensionalization

Find $u(\tau, z)$ and $h(\tau)$ such that

$$
\begin{aligned}
\frac{\partial u}{\partial \tau} - \frac{\partial^2 u}{\partial z^2} &= 0 \quad \text{in} \quad (\tau, z) \in (0, T) \times (0, h(\tau)), \\
-\frac{\partial u}{\partial z}(\tau, 0) &= \mathrm{Bi}\left(\frac{b(\tau)}{m_{ref}} - \mathrm{H} u(\tau, 0)\right), \\
-\frac{\partial u}{\partial z}\left(\tau, h(\tau)\right) &= h'(\tau) u\left(\tau, h(\tau)\right), \\
h'(\tau) &= A_0\left(u\left(\tau, h(\tau)\right) - \frac{\sigma(h(\tau))}{m_{ref}}\right), \\
u(0, z) &= u_0(z) \quad \text{for} \quad z \in [0, h(0)], \\
h(0) &= h_0 \ \text{ with } \ 0 < h_0 < h(\tau) < L,
\end{aligned}
$$

where $u_0(z) := m_0/m_{ref}$, $h_0 := s_0/x_{ref}$ and $L := \ell/x_{ref}$.
Bi $:= \beta x_{ref}/D$ is the standard mass transfer *Biot number*.
$A_0 := x_{ref}\, m_{ref}\, a_0/D$ is a sort of *Thiele modulus*.

Fixed domain transformation

Landau Transformation: $y = z/h(\tau)$.

$$(0, T) \times (0, h(\tau)) \Longrightarrow (0, T) \times (0, 1) =: Q(T).$$

In dimensionless form, the transformed problem read as follows:

$$\begin{aligned}
\frac{\partial u}{\partial \tau} - y\frac{h'(\tau)}{h(\tau)}\frac{\partial u}{\partial y} - \frac{1}{(h(\tau))^2}\frac{\partial^2 u}{\partial y^2} = 0 \quad \text{in} \quad Q(T),& \\
-\frac{1}{h(\tau)}\frac{\partial u}{\partial y}(\tau, 0) = \mathrm{Bi}\left(\frac{b(\tau)}{m_0} - \mathrm{H}u(\tau, 0)\right) \quad \text{for} \ \ \tau \in (0, T),& \\
-\frac{1}{h(\tau)}\frac{\partial u}{\partial y}(\tau, 1) = h'(\tau)u(\tau, 1),& \\
h'(\tau) = A_0\left(u(\tau, 1) - \frac{\sigma(h(\tau))}{m_0}\right)& \\
u(0, y) = u_0(y) \quad \text{for} \ \ y \in [0, 1],& \\
h(0) = h_0.&
\end{aligned}$$

We call the problem described above as (P).

S. Nepal, R. Meyer, N. H. Kröger, T. Aiki, A. Muntean, Y. Wondmagegne, and U. Giese. A moving boundary approach of capturing diffusants penetration into rubber: FEM approximation and comparison with laboratory measurements. *Kautschuk Gummi Kunststoffe*, 2021

Weak solution to (P)

We call (u, h) a weak solution to problem (P) on $S_T := (0, T)$ if and only if

$h \in W^{1,\infty}(S_T)$ with $h_0 < h(T) \leq L$, and

$u \in W^{1,2}(Q(T)) \cap L^\infty(S_T, H^1(0,1)) \cap L^2(S_T, H^2(0,1))$, such that for all $\tau \in S_T$

and for all $\varphi \in H^1(0,1)$ the following relations hold:

$$\left(\frac{\partial u}{\partial \tau}, \varphi\right) - \frac{h'(\tau)}{h(\tau)}\left(y\frac{\partial u}{\partial y}, \varphi\right) + \frac{1}{(h(\tau))^2}\left(\frac{\partial u}{\partial y}, \frac{\partial \varphi}{\partial y}\right)$$

$$- \frac{1}{h(\tau)}\mathrm{Bi}\left(\frac{b(\tau)}{m_0} - \mathrm{H}u(\tau, 0)\right)\varphi(0) + \frac{h'(\tau)}{h(\tau)}u(\tau,1)\varphi(1) = 0,$$

$$h'(\tau) = A_0\left(u(\tau,1) - \frac{\sigma(h(\tau))}{m_0}\right),$$

$$u(0,y) = u_0(y) \text{ for } y \in [0,1], \quad h(0) = h_0.$$

Theorem (K. Kumazaki and A. Muntean (2020))

If (A1)–(A5) hold, then the problem (P) has a unique solution (u, h) on S_T.

Weak solution to semi-discrete form

Define $V_k := \{\psi \in C[0,1] : \psi|_{I_j} \in \mathbb{P}_1\} \subset H^1(0,1)$, where $I_j := [y_j, y_{j+1}]$.

We call the couple (u_k, h_k) a weak solution to a semi-discrete problem if and only if there is a $S_T := (0, T)$ such that

$$
\begin{aligned}
& h_k \in W^{1,\infty}(S_T) \ \text{ with } \ h_0 < h_k(T) \leq L \\
& u_k \in H^1(S_T, V_k) \cap L^2(S_T, H^1(0,1)) \cap L^\infty(S_T, L^2(0,1))
\end{aligned}
$$

and for all $\tau \in S_T$ and for all $\varphi_k \in V_k$, it holds

$$
\begin{aligned}
& \left(\frac{\partial u_k}{\partial \tau}, \varphi_k\right) - \frac{(h_k)'(\tau)}{h_k(\tau)} \left(y \frac{\partial u_k}{\partial y}, \varphi_k\right) + \frac{1}{(h_k(\tau))^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial \varphi_k}{\partial y}\right) \\
& \qquad - \frac{1}{h_k(\tau)} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} u_k(\tau, 0)\right) \varphi_k(0) + \frac{h_k'(\tau)}{h_k(\tau)} u_k(\tau, 1) \varphi_k(1) = 0, \\
& h_k'(\tau) = A_0 \left(u_k(\tau, 1) - \frac{\sigma(h_k(\tau))}{m_0}\right), \\
& u_k(0) = u_{0,k}(y), \quad h_k(0) = h_0.
\end{aligned}
$$

We call the problem described above for semi-discrete form (P_k).

A priori and a posteriori error estimate [1]

Theorem

Assume (A1)–(A5) and $u_0 \in H^2(0,1)$. *Let* (u, h) *and* (u_k, h_k) *be the corresponding weak solutions to problems* (P) *and* (P_k).

1) Then there exists a constant $c > 0$ *(not depending on* k*) such that*

$$\|u - u_k\|^2_{L^\infty(S_T, L^2(0,1)) \cap L^2(S_T, H^1(0,1))} + \|h - h_k\|^2_{H^1(S_T)} \le ck^2.$$

2) Then there exists constants $c_1, c_2, c_3 > 0$ *(independent of* k *and* u*) it holds*

$$\|u - u_k\|^2_{L^2(0,1)} + c_1 |h - h_k|^2 + c_2 \int_0^\tau \left\| \frac{\partial}{\partial x}(u - u_k) \right\|^2_{L^2(0,1)} ds$$

$$\le c_3 \left(|h(0) - h_k(0)|^2 + \sum_{i=0}^{N-2} k_i^2 \left\{ \|R(u_k)\|^2_{L^2(S_T, L^2(I_i))} + k_i^2 \|u_0\|^2_{H^2(I_i)} \right\} \right),$$

where the residual $R(u_k)$ *is defined by*

$$R(u_k) := \frac{h_k'}{h_k} y \frac{\partial u_k}{\partial y} + \frac{1}{h_k} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} u_k(\tau, 0) \right) - \frac{h_k'}{h_k} u_k(\tau, 1) - \frac{\partial u_k}{\partial \tau}.$$

[1] S. Nepal, Y. Wondmagegne, A. Muntean, Error estimates for semi-discrete finite element approximations for a moving boundary problem capturing the penetration of diffusants into rubber. *International Journal of Numerical Analysis & Modeling*, 2022.

Fully discrete Euler-Galerkin scheme

Let $M \in \mathbb{N}$. Let $\Delta\tau := T/M$ be a time step size. Define $\tau^n := n\Delta\tau$ for $n \in \{0, 1, 2, \cdots, M\}$. Given (U^n, W^n), we want to find the pair $(U^{n+1}, W^{n+1}) \in V_k \times \mathbb{R}^+$ such that the following system holds for all $n \in \{0, \cdots, M-1\}$ and for all $\varphi_k \in V_k$:

$$
\begin{aligned}
(\Delta_\tau U^n, \varphi_k) - \frac{\Delta_\tau W^n}{W^{n+1}} \left(y \frac{\partial U^{n+1}}{\partial y}, \varphi_k \right) + \frac{1}{(W^{n+1})^2} \left(\frac{\partial U^{n+1}}{\partial y}, \frac{\partial \varphi_k}{\partial y} \right) \\
- \frac{1}{W^{n+1}} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} U^n(0) \right) \varphi_k(0) + \frac{\Delta_\tau W^n}{W^{n+1}} U^n(1) \varphi_k(1) = 0,
\end{aligned}
$$

$$
\Delta_\tau W^n = A_0 \left(U^n(1) - \frac{\sigma(W^n)}{m_0} \right),
$$

$$
U^0 = U_0, \quad W^0 = h_0,
$$

where U_0 is an appropriate approximation of the initial condition $u_0 \in V_k$ and

$$
\Delta_\tau U^n := \frac{U^{n+1} - U^n}{\Delta\tau} \quad \text{and} \quad \Delta_\tau W^n := \frac{W^{n+1} - W^n}{\Delta\tau}.
$$

Theorem (Solvability of the fully discrete problem)

Assume (A1)–(A5) hold. Then there exists a unique solution to the fully discrete problem.

A priori error estimate [2]

Denote $h^n := h(\tau^n)$ and $u^n := u(\tau^n, y)$. Let $e_1^n := W^n - h^n$ and $e^n := U^n - u^n = \psi^n + \rho^n$, with $\psi^n := U^n - I_k u^n$ and $\rho^n := I_k u^n - u^n$.

Theorem

Assume (A1)–(A5) and $u_0 \in H^2(0,1)$. Let (u, h) be the corresponding regular solution to the problem (P). Let (U^n, W^n) be the solution to the fully discrete formulation. Then there exists a constant $K > 0$ such that the following holds for sufficiently small $\Delta\tau$:

$$\|\psi^{n+1}\|^2 + |e_1^{n+1}|^2 + \alpha\Delta\tau \sum_{i=1}^{n+1} \left\| \frac{\partial \psi^j}{\partial y} \right\|^2 \leq K\{\Delta\tau^2 + k^2\}.$$

Theorem (A priori error estimate)

Assume (A1)–(A5) and $u_0 \in H^2(0,1)$. Then there exists a constant $K > 0$ such that

$$\max_{0\leq n\leq M} \|U^n - u^n\|^2 + \max_{0\leq n\leq M} |W^n - h^n|^2 \leq K\{\Delta\tau^2 + k^2\}.$$

[2] S. Nepal, Y. Wondmagegne, A. Muntean. Analysis of a fully discrete approximation to a moving-boundary problem describing rubber exposed to diffusants. *Applied Mathematics and Computation*, 2023

Numerical illustration

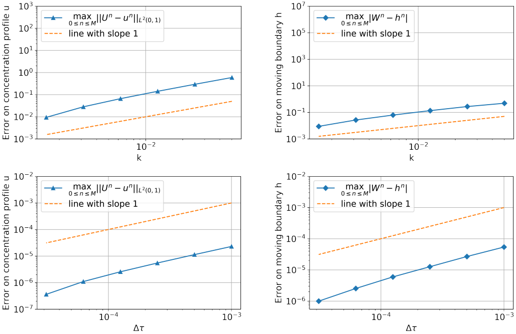


Figure: Log log scale plot of an error on the concentration profile and the moving-boundary. Top: convergence order in space when time step size $\Delta t = 10^{-4}$ is fixed. Bottom: convergence order in time when space mesh size is fixed with $N = 320$.

Simulation results

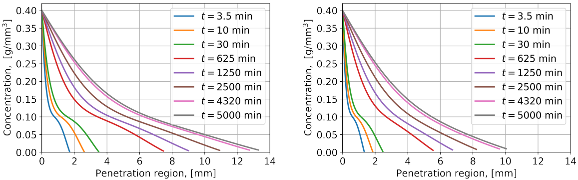


Figure: Dense rubber case: Concentration *vs.* space with $\sigma(s(t)) = \frac{s(t)}{20}$ (left), $\sigma(s(t)) = \frac{s(t)}{10}$ (right).

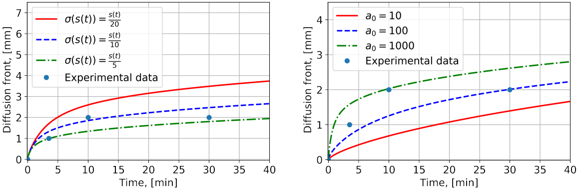


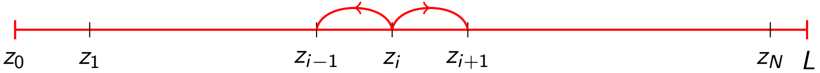
Figure: Comparison of the experimental diffusant front with numerical diffusant front. Left: $a_0 = 500$ and for different choices of $\sigma(s(t))$. Right: $\sigma(s(t)) = \frac{s(t)}{10}$ and for different choices of a_0.

Random walk method

Can we approximate the moving front and concentration profile by using a finite number of randomly driven diffusant particles?

Space discretization: $0 = z_0 < z_1 < \cdots < z_N \leq L$ with $\Delta z = z_i - z_{i-1}$.
Time discretization: $0 = \tau_0 < \tau_1 < \cdots < \tau_M = T$ with $\Delta \tau = \tau_i - \tau_{i-1}$.

Consider a walker represents a unit concentration.
Each walker chooses randomly $p \in \{-1, 1\}$ and decides the direction to move.



Let N_i^j denote the number of walkers at $z = z_i$ and $\tau = \tau_j$. Then

$$N_i^{j+1} = N_i^j - PN_i^j - PN_i^j + PN_{i+1}^j + PN_{i-1}^j$$
$$\implies \frac{N_i^{j+1} - N_i^j}{\Delta\tau} = d\,\frac{(N_{i-1}^j - 2N_i^j + N_{i+1}^j)}{(\Delta z)^2},$$

where $d = (P/\Delta\tau)(\Delta z)^2$, $P = 1/2 \implies \Delta z = \sqrt{2\Delta\tau}$

S. Nepal, M. Ögren, Y. Wondmagegne, A. Muntean. Random walks and moving boundaries: Estimating the penetration of diffusants into dense rubbers. *Probabilistic Engineering Mechanics*, 2023.

Initial condition and boundary conditions at $z = z_0$

Let h_j and $u(\tau_j, z_i)$ be the RW approximation of h at $\tau = \tau_j$ and of u at $\tau = \tau_j$ and $z = z_i$.

Define

$$k_j := \left\lfloor \frac{h_j}{\Delta z} \right\rfloor, \quad j \in \{0, 1, \cdots, M-1\},$$

where $\lfloor x \rfloor$ rounds x down towards the nearest integer.

Let $N(\tau_j, z_i)$ denote the number of walkers at $\tau = \tau_j$ and $z = z_i$.

Initial condition: $N(\tau_0, z_i) = n u_0(z_i), n$ is a large number, $i \in \{0, 1, \cdots, k_0\}$.

Boundary condition at $z = z_0$:

Using the forward difference gives

$$\frac{u(\tau_j, z_0) - u(\tau_j, z_1)}{\Delta z} = \mathrm{Bi}\left(\frac{b(\tau_j)}{m_0} - \mathrm{H} u(\tau_j, z_0)\right).$$

$$N(\tau_j, z_0) = \left\lfloor \frac{n \Delta z \mathrm{Bi}\, b(\tau_j)/m_0 + u(\tau_j, z_1)}{1 + \Delta z \mathrm{Bi}\, \mathrm{H}} \right\rceil \quad \text{for } j \in \{1, 2, \cdots, M\},$$

where $\lfloor x \rceil$ rounds x to the nearest integer.

Treatment of the moving boundary

Recall that

$$h'(\tau) = A_0 \left(u\left(\tau, h(\tau)\right) - \frac{\sigma(h(\tau))}{m_{ref}} \right).$$

Update formula

$$h_{j+1} = h_j + \frac{\Delta h_j}{n}, \quad j \in \{0, 1, 2, \cdots, M-1\},$$

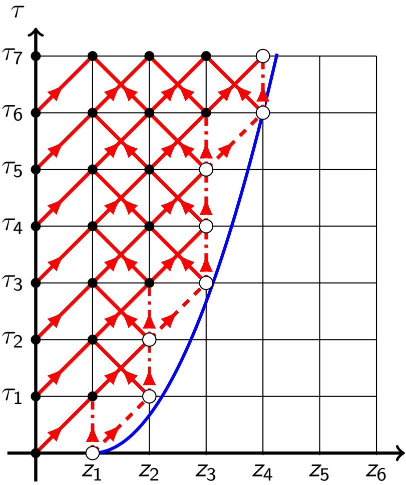
where

$$\frac{\Delta h_j}{n} = N_j \left[\frac{\Delta\tau A_0}{n} \left(N\left(\tau_j, h_j\right) - \frac{\sigma(h_j)}{m_{ref}} \right) \right].$$

- N_j is the total number of walkers contributing to the increment of the moving boundary.
- $\frac{\Delta\tau A_0}{n} \left(N\left(\tau_j, h_j\right) - \frac{\sigma(h_j)}{m_{ref}} \right)$ is the increment of the boundary for a walker at time $\tau = \tau_j$.

Boundary condition at the moving boundary $z = h(\tau)$

- For walkers at the boundary $z = z_{k_j}$, they move to the left if $p = -1$.
- and if $p = 1$,
  1. Compute
     $$P_b(\tau_j) = \frac{\sqrt{2\Delta\tau}A_0}{n}\left(N\left(\tau_j, z_{k_j}\right) - \frac{\sigma(h_j)}{m_{ref}}\right).$$
  2. Generate a random number r between $(0, 1)$.
  3. If $r < P_b(\tau_j)$, the boundary will be increased. We update h_{j+1} and
     $$N(\tau_{j+1}, z_{k_j}) = N(\tau_{j+1}, z_{k_j}) + 1.$$
  4. If $r \geq P_b(\tau_j)$, the walker is reflected and moves to the left, i.e.
     $$N(\tau_{j+1}, z_{k_j-1}) = N(\tau_{j+1}, z_{k_j-1}) + 1.$$



Simulation results

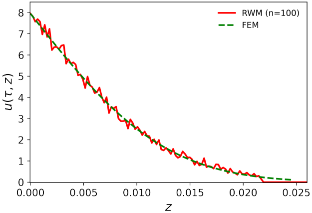


Figure: Concentration profile at $\tau = 0.00005$ with $\Delta\tau = 2.5 \times 10^{-8}$.

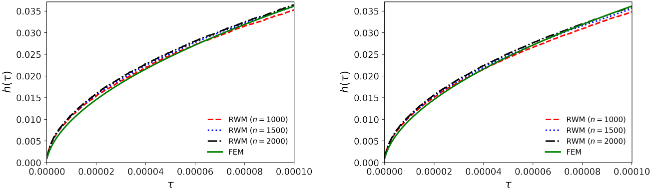


Figure: Moving front by RWM for different values of n and FEM, with $\Delta\tau = 5 \times 10^{-8}$ (left), and $\Delta\tau = 2.5 \times 10^{-8}$ (right).

Simulation results

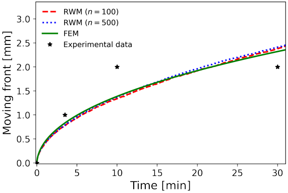


Figure: Comparison of FEM and RWM solution in the experimental range.

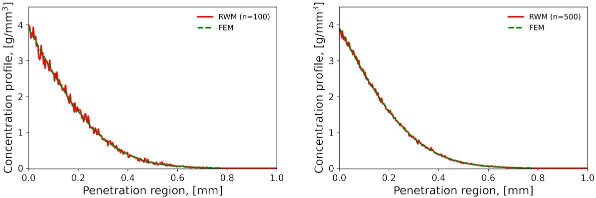


Figure: Concentration profile at $t = 3$ min with $\Delta t = 0.0005$ min.

Conclusions

- We discussed a one-dimensional moving boundary approach to model the penetration of a diffusant into rubber.
- We constructed a finite element scheme to solve the moving boundary problem and proved *a priori* and *a posteriori* error estimates.
- We constructed a random walk algorithm and presented simulation results for the moving boundary problem.

S. Nepal, R. Meyer, N. H. Kröger, T. Aiki, A. Muntean, Y. Wondmagegne, and U. Giese. A moving boundary approach of capturing diffusants penetration into rubber: FEM approximation and comparison with laboratory measurements. *Kautschuk Gummi Kunststoffe*, 2021.

S. Nepal, Y. Wondmagegne, and A. Muntean. Error estimates for semi-discrete finite element approximations for a moving boundary problem capturing the penetration of diffusants into rubber. *International Journal of Numerical Analysis & Modeling*, 2022.

S. Nepal, Y. Wondmagegne, and A. Muntean. Analysis of a fully discrete approximation to a moving-boundary problem describing rubber exposed to diffusants. *Applied Mathematics and Computation*, 2023.

S. Nepal, M. Ögren, Y. Wondmagegne, A. Muntean. Random walks and moving boundaries: Estimating the penetration of diffusants into dense rubbers. *Probabilistic Engineering Mechanics*, 2023.

The laboratory experiment was conducted at the Deutsches Institut für Kautschuktechnologie (DIK) e. V. in Hannover, Germany by R. Meyer, N. H. Kröger, and U. Giese.

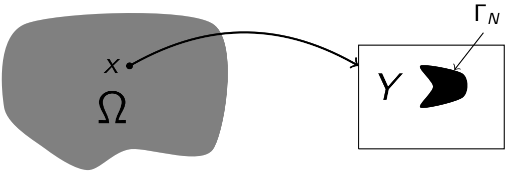
Two-scale elliptic-parabolic system

Find (u, W) (with $W = (w_1, w_2)$) satisfying

$$\begin{cases} \partial_t u + \mathrm{div}(-D^*(W)\nabla u) = f & \text{in } (0,T)\times\Omega, \\ u = 0 & \text{on } (0,T)\times\partial\Omega, \\ u(0) = u_0 & \text{in } \overline{\Omega}, \\ \mathrm{div}_y\left(-D\nabla_y w_i + G(u)Bw_i\right) = \mathrm{div}_y(De_i) & \text{in } Y, \\ (-D\nabla_y w_i + G(u)Bw_i)\cdot n_y = (De_i)\cdot n_y & \text{on } \Gamma_N, \\ w_i \text{ is } Y\text{–periodic.} & \end{cases}$$

where

$$D^*(W) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1} \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2} \end{bmatrix}\right) \mathrm{d}y.$$



S. Nepal, V. Raveendran, M. Eden, R. Lyons, A. Muntean. Numerical study of a strongly coupled two-scale system with nonlinear dispersion. *arXiv:2402.09607*, 2024.

Scheme 1 (Iterative scheme)

We set $u^0 = u_0$, and, for any $k \in \mathbb{N} \cup \{0\}$, we denote as u^{k+1}, w_1^k, and w_2^k the solutions to the following decoupled system:

$$\begin{aligned} \operatorname{div}_y\left(-D\nabla_y w_i^k + G(u^k)Bw_i^k\right) &= \operatorname{div}_y(De_i) && \text{in } \ Y, \\ \left(-D\nabla_y w_i^k + G(u^k)Bw_i^k\right)\cdot n_y &= (De_i)\cdot n_y && \text{on } \ \Gamma_N, \\ w_i^k \ \text{ is } Y\text{−periodic}, & && i \in \{1,2\} \end{aligned}$$

$$\begin{aligned} \partial_t u^{k+1} + \operatorname{div}(-D^*(W^k)\nabla_x u^{k+1}) &= f && \text{in } \ (0,T)\times\Omega, \\ u^{k+1}(0) &= u_0 && \text{in } \ \overline{\Omega}, \\ u^{k+1} &= 0 && \text{on } \ (0,T)\times\partial\Omega, \end{aligned}$$

where the dispersion tensor $D^*(W^k)$ is given by

$$D^*(W^k) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_1^k}{\partial y_1} & \frac{\partial w_2^k}{\partial y_1} \\ \frac{\partial w_1^k}{\partial y_2} & \frac{\partial w_2^k}{\partial y_2} \end{bmatrix}\right)\mathrm{d}y.$$

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Scheme 1 (Iterative scheme)

Given u_{n-1}^k and u_{n-1}^{k+1}, find (W_{n-1}^k, u_n^{k+1}) such that the following holds for $n \in \{1, 2, \cdots, M\}$:

$$
\begin{aligned}
\mathrm{div}_y\left(-D\nabla_y w_{i,n-1}^k + G(u_{n-1}^k)Bw_{i,n-1}^k\right) &= \mathrm{div}_y(De_i) && \text{in } \; Y,\\
\left(-D\nabla_y w_{i,n-1}^k + G(u_{n-1}^k)Bw_{i,n-1}^k\right)\cdot n_y &= (De_i)\cdot n_y && \text{on } \; \Gamma_N,\\
w_{i,n-1}^k \; \text{is } Y&\text{-periodic}, && i \in \{1,2\},
\end{aligned}
$$

$$
\begin{aligned}
\frac{u_n^{k+1} - u_{n-1}^{k+1}}{\Delta t} + \mathrm{div}(-D^*(W_{n-1}^k)\nabla_x u_n^{k+1}) &= f_n && \text{in } \; \Omega,\\
u_n^{k+1}(0) &= u_0 && \text{in } \; \overline{\Omega},\\
u_n^{k+1} &= 0 && \text{on } \; \partial\Omega,
\end{aligned}
$$

where the dispersion tensor $D^*(W_{n-1}^k)$ is given by

$$
D^*(W_{n-1}^k) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_{1,n-1}^k}{\partial y_1} & \frac{\partial w_{2,n-1}^k}{\partial y_1} \\ \frac{\partial w_{1,n-1}^k}{\partial y_2} & \frac{\partial w_{2,n-1}^k}{\partial y_2} \end{bmatrix}\right)\mathrm{d}y.
$$

Scheme 2 (Time stepping scheme)

Given u_{n-1}, find (W_{n-1}, u_n) such that the following holds for $n \in \{1, 2, \cdots, M\}$:

$$\begin{aligned}
\mathrm{div}_y\left(-D\nabla_y w_{i,n-1} + G(u_{n-1})Bw_{i,n-1}\right) &= \mathrm{div}_y(De_i) && \text{in } Y,\\
\left(-D\nabla_y w_{i,n-1} + G(u_{n-1})Bw_{i,n-1}\right)\cdot n_y &= (De_i)\cdot n_y && \text{on } \Gamma_N,\\
w_{i,n-1} \text{ is } Y\text{–periodic}, & && i \in \{1,2\}
\end{aligned}$$

$$\begin{aligned}
\frac{u_n - u_{n-1}}{\Delta t} + \mathrm{div}(-D^*(W_{n-1})\nabla_x u_n) &= f_n && \text{in } \Omega,\\
u_n(0) &= u_0 && \text{in } \overline{\Omega},\\
u_n &= 0 && \text{on } \partial\Omega,
\end{aligned}$$

where the dispersion tensor $D^*(W_{n-1})$ is given by

$$D^*(W_{n-1}) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_{1,n-1}}{\partial y_1} & \frac{\partial w_{2,n-1}}{\partial y_1} \\ \frac{\partial w_{1,n-1}}{\partial y_2} & \frac{\partial w_{2,n-1}}{\partial y_2} \end{bmatrix}\right) \mathrm{d}y.$$

Precomputing strategy

$$\begin{aligned} \mathrm{div}_y\left(-D\nabla_y w_{i,p} + pBw_{i,p}\right) &= \mathrm{div}_y(De_i) && \text{in } Y, \\ \left(-D\nabla_y w_{i,p} + pBw_{i,p}\right)\cdot n_y &= (De_i)\cdot n_y && \text{on } \Gamma_N, \\ w_i \text{ is } Y\text{–periodic,} & \end{aligned}$$

where $i \in \{1,2\}$ and $p \in [-L, L] \subset \mathbb{R}$.

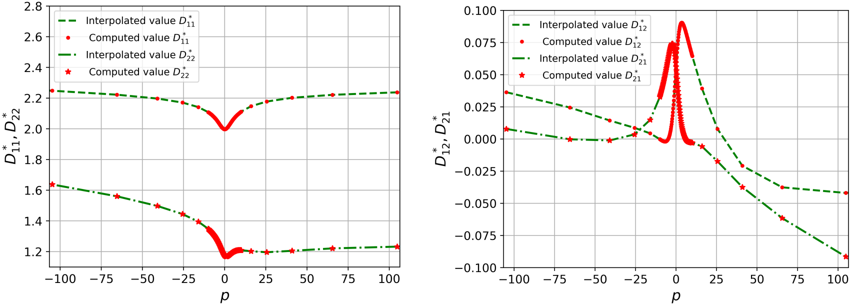

Figure: Computed values for the entries of the dispersion tensor D^* for different values of p and its interpolated values.

Simulation results

Macro DOFs	Scheme 1		Scheme 1 (precomputing)	
	Errors	Computational time (s)	Errors	Computational time (s)
16	4.8023658	396.91	4.804463	2.25
64	1.6308094	1781.25	1.632296	4.42
256	0.4155008	7059.71	0.416212	11.70
1024	0.1678484	28417.18	0.1671295	53.35
4096		113488.39		189.84
Macro DOFs	Scheme 2		Scheme 2 (precomputing)	
	Errors	Computational time (s)	Errors	Computational time (s)
16	4.8023659	70.52	4.804463	0.36
64	1.6308094	278.65	1.632296290	0.48
256	0.4141075	1112.10	0.416212306	1.30
1024	0.1667797	4345.78	0.16712954	4.64
4096		17013.41		20.92

Table: Errors and computational time of the schemes for $T = 2$ with $M = 20$.

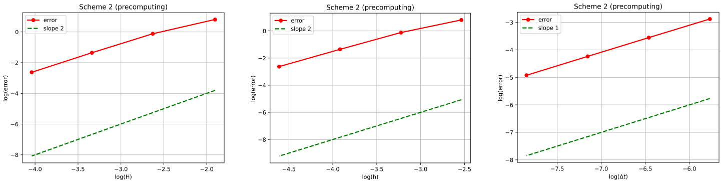

Figure: Log-log plot of L^2 error versus H, h and Δt with scheme 2 precomputing.

Simulation results

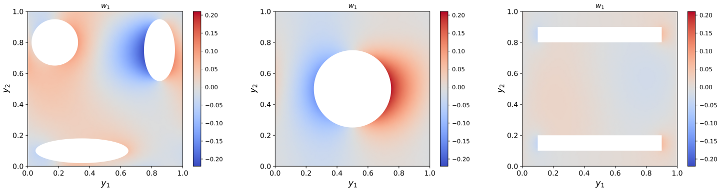

Figure: Microscopic solutions w_1 with different microscopic geometries.

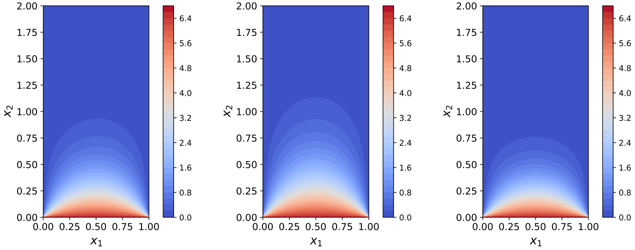

Figure: Macroscopic solutions with scheme 2 (precomputing) for different microscopic geometries.

Conclusion

- We discussed a two-scale elliptic-parabolic coupled problem, describing the transport of particles into a porous media.
- We constructed two numerical schemes and presented simulation results.
- We introduced a precomputing strategy that reduces the computation time of both schemes.

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Outline for future work

- We plan to extend the current moving boundary model to a multiscale framework and perform numerical simulation to understand the macroscopic swelling driven by the microscopic absorption of diffusants, model equation based on T. Aiki, N. H. Kröger, A. Muntean (2021).
- We plan to study the convergence behaviour of the constructed random walk method in the same framework proposed by O. H. Hald (1981) and W. Lu (1998).
- We plan to study the wellposedness and convergence of scheme 2 for the two-scale elliptic-parabolic problem, ideas follows from M. Lind, A. Muntean, O. Richardson (2020).

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