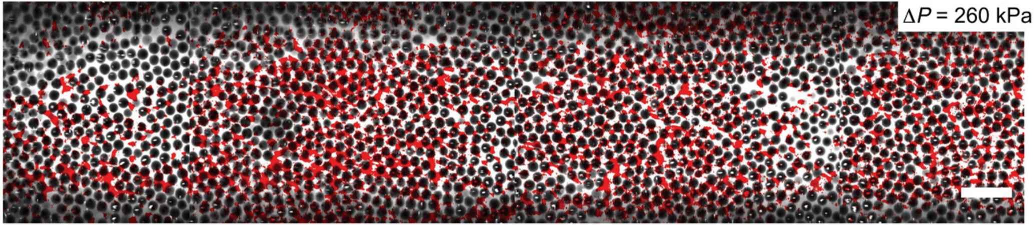
A Stokes-Reaction System with Evolving Microstructure

Michael Eden
joint work with Richard M. Höfer

University of Regensburg
(Free Boundary Problems: Theory and Applications)

Preprint: Reactive Flow around Spherically Evolving Particles in Critical and Supercritical Dilute Regimes (arXiv:2608.28489)

Motivation: Reactive transport inside porous media



- A fluid transports a dissolved chemical species through a porous medium.
- The species can be adsorbed or desorbed at microscopic inclusions.
- This changes the size of the inclusions and hence the flow domain itself.

Main question: What macroscopic model describes this feedback when the inclusions are *very small* and *numerous*?

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[1] N. Bizmark, J. Schneider, R. Priestley, S. Datta, *Multiscale dynamics of colloidal deposition and erosion in porous media*, *Sci. Adv.*

Mathematical idealization: many small evolving inclusions

Geometry ($N_\varepsilon = \varepsilon^{-3}$, $\alpha \in (1,3]$)

$$\Omega_\varepsilon(t) = \Omega \setminus \bigcup_{i=1}^{N_\varepsilon} B_{\varepsilon^\alpha r_{\varepsilon,i}(t)}(z_{\varepsilon,i}).$$

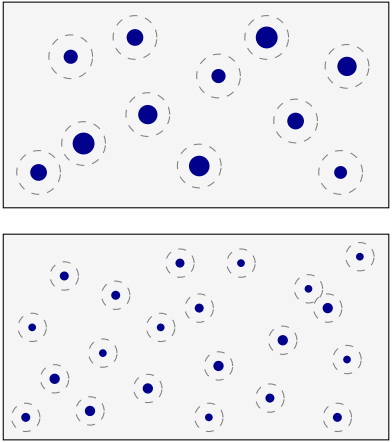
- The centers are separated on the scale ε:

$$|z_{\varepsilon,i} - z_{\varepsilon,j}| \geq d\varepsilon \ (i \neq j), \ \mathrm{dist}(z_{\varepsilon,i}, \partial\Omega) \geq d\varepsilon.$$

- Initial particle radii $r_{\varepsilon,i,0}$ satisfy for some $\overline{r} > 1$

$$\overline{r}^{-1} \leq r_{\varepsilon,i,0} \leq \overline{r} \quad (\varepsilon > 0, \ i \in \{1, \dots, N_\varepsilon\})$$

- No lattice structure and no representative periodic cell.



2D crosssection of 3D domain $\Omega_\varepsilon(t)$

Fluid problem and moving no-slip condition

Quasi-steady, incompressible Stokes system in the evolving domain

$$
\begin{aligned}
-\varepsilon^{3-\alpha}\Delta u_\varepsilon + \nabla p_\varepsilon &= h_\varepsilon, & \operatorname{div} u_\varepsilon &= 0 & &\text{in } \Omega_\varepsilon(t),\\
u_\varepsilon &= \varepsilon^\alpha \dot{r}_{\varepsilon,i}\nu_{\varepsilon,i} & & & &\text{on } \Gamma_{\varepsilon,i}(t),\\
\sigma_\varepsilon[u_\varepsilon, p_\varepsilon]n &= 0 & & & &\text{on } \Sigma_1,\\
u_\varepsilon &= 0 & & & &\text{on } \Sigma_2.
\end{aligned}
$$

- The scaling $\varepsilon^{3-\alpha}$ balances the drag generated by $N_\varepsilon = \varepsilon^{-3}$ particles of radius ε^α.
- The particle centers are fixed, but they are allowed to grow/shrink.
- This corresponds to the typical Brinkman/Darcy-setup.
- The Neumann condition $\sigma_\varepsilon[u_\varepsilon, p_\varepsilon]n = 0$ on Σ_1 allows incompressibility.

Transport, adsorption, and desorption

Advection–diffusion–reaction

$$
\begin{aligned}
\partial_t c_\varepsilon - \operatorname{div}(\nabla c_\varepsilon - u_\varepsilon c_\varepsilon) &= F(c_\varepsilon) && \text{in } \Omega_\varepsilon(t),\\
-(\nabla c_\varepsilon - u_\varepsilon c_\varepsilon)\cdot \nu_{\varepsilon,i} &= \varepsilon^\alpha \dot r_{\varepsilon,i} c_\varepsilon + \varepsilon^{3-2\alpha} G(c_\varepsilon, r_{\varepsilon,i}) && \text{on } \Gamma_{\varepsilon,i}(t),\\
c_\varepsilon &= 0 && \text{on } \Sigma_1,\\
-(\nabla c_\varepsilon - u_\varepsilon c_\varepsilon)\cdot n &= 0 && \text{on } \Sigma_2.
\end{aligned}
$$

- F is locally Lipschitz with at most linear growth.
- We take a dissipative exchange law

$$
G(c,r) = g(r)\big(c^{\mathrm{eq}}(r) - c\big), \qquad g(r) \geq 0
$$

  with g, c^{eq} locally Lipschitz and non-negative.
- Since $N_\varepsilon |\Gamma_{\varepsilon,i}(t)| \sim \varepsilon^{-3}\varepsilon^{2\alpha}$, the prefactor $\varepsilon^{3-2\alpha}$ gives an order-one total surface contribution.

The local change of the geometry

Radius evolution $(G(c,r) = g(r)\big(c^{\mathrm{eq}}(r) - c\big))$

$$\dot{r}_{\varepsilon,i}(t) = -\frac{1}{|\Gamma_{\varepsilon,i}(t)|} \int_{\Gamma_{\varepsilon,i}(t)} G(c_\varepsilon, r_{\varepsilon,i}) \,\mathrm{d}\sigma, \qquad i = 1, \ldots, N_\varepsilon.$$

- The radius is driven by the averaged exchange flux on the particle boundary.
- The averaging keeps the inclusions spherical.
- To prevent collapse or unbounded growth of the radii, we assume

$$\int_0^1 \frac{1}{g(r)c^{\mathrm{eq}}(r)} \,\mathrm{d}r = \infty, \qquad \int_1^\infty \frac{1}{g(r)} \,\mathrm{d}r = \infty.$$

These conditions make $r = 0$ and $r = \infty$ unreachable in finite time.

Summary: The microscopic model at a glance

Quasi-steady Stokes for the fluid

$$-\varepsilon^{3-\alpha}\Delta u_\varepsilon + \nabla p_\varepsilon = h_\varepsilon,\ \operatorname{div} u_\varepsilon = 0$$

Diffusion equation

$$\partial_t c_\varepsilon - \operatorname{div}(\nabla c_\varepsilon - u_\varepsilon c_\varepsilon) = F(c_\varepsilon)$$

Interfacial exchange

$$-(\nabla c_\varepsilon - u_\varepsilon c_\varepsilon)\cdot\nu_{\varepsilon,i} = \varepsilon^\alpha \dot{r}_{\varepsilon,i} c_\varepsilon + \varepsilon^{3-2\alpha} G(c_\varepsilon, r_{\varepsilon,i})$$

Evolution of each particle

$$\dot{r}_{\varepsilon,i} = -\frac{1}{|\Gamma_{\varepsilon,i}(t)|}\int_{\Gamma_{\varepsilon,i}(t)} G(c_\varepsilon, r_{\varepsilon,i})\,\mathrm{d}\sigma$$

- Unknowns: $(u_\varepsilon, p_\varepsilon, c_\varepsilon, r_\varepsilon)$.
- The system is posed on the unknown, evolving domain $\Omega_\varepsilon(t)$.
- Goals: well-posedness for fixed ε and identify the limit for $\varepsilon \to 0$.
- The critical case is $\alpha = 3$, where the particles produce a Brinkman-type effect.

Some related literature (not exhaustive)

- **Fixed geometry,** $\alpha \in (1,3]$
  - Stokes: Allaire (1991); Giunti–Höfer (2019)
  - Chemistry: Berlyand–Goncharenko (1990); Jäger–Neuss-Radu–Shaposhnikova (2011); Borisov (2024)
- **Geometry changes, periodic regime** $\alpha = 1$
  - Prescribed changes: Cioranescu–Piatnitski (2003); E.–Muntean (2017); Gahn–Neuss-Radu–Pop (2021)
  - Evolving microstructures: Wiedemann–Peter (2023); Gahn–Pop (2023); E.–Muntean (2024); Gahn–Peter–Pop–Wiedemann (2025)

This work

Solution-dependent evolving microstructure in a non-periodic dilute regime:

$$\mathrm{dist}(z_{\varepsilon,i}, z_{\varepsilon,j}) \sim \varepsilon, \qquad \text{radius} \sim \varepsilon^{\alpha}, \qquad \alpha \in (1,3].$$

A-priori maximum principle

Theorem: A priori estimates directly in the moving geometry

Let $(c_\varepsilon, u_\varepsilon, p_\varepsilon, r_\varepsilon)$ be a weak solution on $S = (0, T)$ and $\sup_\varepsilon \|c_{\varepsilon,0}\|_\infty < \infty$ with $c_{\varepsilon,0} \geq 0$. Then, directly on $\Omega_\varepsilon(t)$,

$$0 \leq c_\varepsilon(t, x) \leq C_T \qquad \text{for a.e. } (t, x),$$

and there are ε-independent bounds

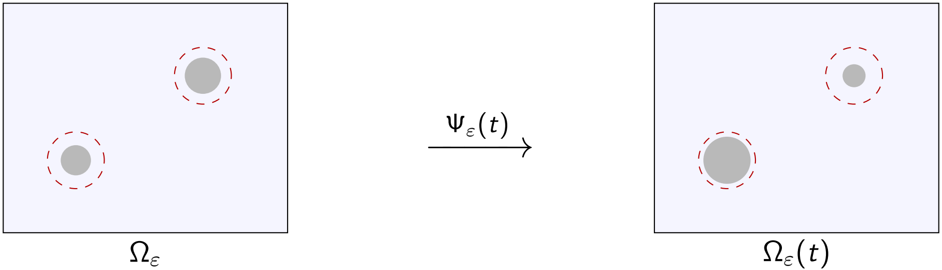
$$0 < \underline{\xi}(t) \leq r_{\varepsilon,i}(t) \leq \overline{\xi}(t) < \infty, \qquad |\dot{r}_{\varepsilon,i}(t)| \leq C_T.$$

- The dissipative exchange law

$$G(c, r) = g(r)\big(c^{\mathrm{eq}}(r) - c\big)$$

  gives the sign needed to control the boundary contribution.
- Consequence: no collapse and no blow-up (in finite time).

Step 1: transform to a fixed reference geometry



- A local radial diffeomorphism is constructed around each particle.
- Separation and $\varepsilon^\alpha \ll \varepsilon$ make the supports disjoint.
- Uniform estimates, e.g.,

$$\|D\Psi_\varepsilon\|_{L^\infty} + \|D\Psi_\varepsilon^{-1}\|_{L^\infty} \leq C, \qquad \det D\Psi_\varepsilon \geq c > 0.$$

Step 2: solve for prescribed radii

Fix an *admissible* radius path $r = (r_i)_i \in W^{1,\infty}(0,T)^{N_\varepsilon}$.

Stokes subsystem

After lifting the moving Dirichlet data, a saddle-point problem yields

$$(u_r, p_r) \quad \text{with estimates in terms of } \dot{r}.$$

Transport subsystem

The transformed parabolic problem with fluid velocity u_r yields

$$c_r \geq 0, \qquad \|c_r\|_{L^\infty} + \|c_r\|_{L^2(H^1)} \leq C.$$

The surface average of $G(c_r, r_i)$ defines a new radius path:

$$\mathcal{L}_\varepsilon(r)_i(t) = r_{\varepsilon,i,0} - \int_0^t \frac{1}{|\Gamma_{\varepsilon,i}|} \int_{\Gamma_{\varepsilon,i}} G(c_r, r_i)\,\mathrm{d}\sigma\,\mathrm{d}s.$$

A solution of the coupled problem is precisely a fixed point $\mathcal{L}_\varepsilon(r) = r$.

Step 3: local lipschitz control

Fix two *admissible* radius paths $r^{(1)}, r^{(2)}$ with $\frac{1}{\lambda} \leq r_i^{(j)}(t) \leq \lambda$ ($\lambda > 1$) and let

$$(u_\varepsilon^{(j)}, p_\varepsilon^{(j)}, c_\varepsilon^{(j)}), \qquad j = 1, 2,$$

be the corresponding Stokes–transport solutions.

Local Lipschitz dependence

On a sufficiently short time interval $(0, \tau)$,

$$\|c_\varepsilon^{(1)} - c_\varepsilon^{(2)}\|_{L^\infty(0,\tau;L^2)\cap L^2(0,\tau;H^1)} \leq C_\varepsilon(\tau, \lambda)\, \|\dot{r}^{(1)} - \dot{r}^{(2)}\|_{L^2(0,\tau)^{N_\varepsilon}}.$$

Moreover,

$$C_\varepsilon(\tau, \lambda) \to 0 \qquad \text{as } \tau \to 0.$$

- This gives the contraction estimate for the radius update map.

Well-posedness result

Theorem

For every $T > 0$, the microscopic problem is well posed on $[0, T]$ for all sufficiently small ε

1. Solve the Stokes and transport systems for a prescribed radius path.
2. Show that $\mathcal{L}_\varepsilon$ maps an admissible set into itself.
3. On a sufficiently short interval $(0, t_\varepsilon)$, prove

$$\|\mathcal{L}_\varepsilon(r^{(1)}) - \mathcal{L}_\varepsilon(r^{(2)})\| \leq \frac{1}{2}\|r^{(1)} - r^{(2)}\|$$

   using the local Lipschitz estimates.
4. Obtain a unique local fixed point by Banach's theorem.
5. Use the radius and concentration barriers to restart the construction repeatedly up to any fixed T (once ε is small enough).

Homogenization: From many radii to a radius distribution

Empirical radius distribution

$$f_\varepsilon(t) := \frac{1}{N_\varepsilon} \sum_{i=1}^{N_\varepsilon} \delta_{z_{\varepsilon,i}} \otimes \delta_{r_{\varepsilon,i}(t)}.$$

- The homogenization result identifies a limit $f = f(t, x, \sigma)$ uniformly in time, in Wasserstein distance:

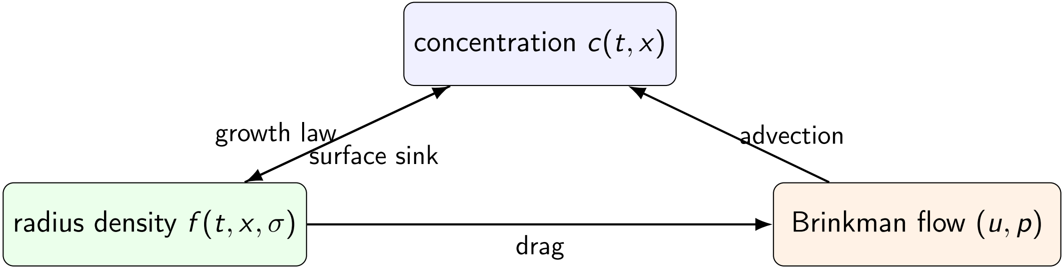
$$W_2\big(f_\varepsilon(0), f_0\big) \to 0 \quad \Longrightarrow \quad \sup_{t\in[0,T]} W_2\big(f_\varepsilon(t), f(t)\big) \to 0.$$

- Thus $f(t, x, \sigma)$ becomes an additional macroscopic unknown which is included in the well-known *strange terms*

$$\int_0^\infty 4\pi\sigma f(t, x, \sigma)\, \mathrm{d}\sigma \quad \text{reaction/capacity}, \qquad \int_0^\infty 6\pi\sigma f(t, x, \sigma)\, \mathrm{d}\sigma \quad \text{drag}.$$

Critical regime $\alpha = 3$: the coupled limit

The microscopic problem converges to three coupled macroscopic equations:



The limit retains the full local radius distribution; replacing it only by a mean radius would generally lose information.

Brinkman equation from many small particles ($\alpha = 3$)

Macroscopic flow (Brinkman regime)

$$-\Delta u + \nabla p + \underbrace{\left(\int_0^\infty 6\pi\sigma f(t,x,\sigma)\,\mathrm{d}\sigma \right)}_{\text{local drag coefficient}} u = h,$$

$$\operatorname{div} u = 0.$$

- Each small sphere contributes the classical Stokes drag $6\pi \times$ radius.
- Summation over ε^{-3} particles produces a finite zeroth-order resistance term.
- Because f evolves, the effective permeability is time- and space-dependent.

Effective reaction and evolution of the radius density ($\alpha = 3$)

In the critical regime, a local boundary-layer correction is encoded by H, defined implicitly by

$$H(b,\sigma) = \sigma G\big(b + H(b,\sigma), \sigma\big).$$

Macroscopic concentration

$$\partial_t c - \operatorname{div}(\nabla c - uc) = F(c) + \int_0^\infty 4\pi\sigma H(c,\sigma) f(t,x,\sigma)\,\mathrm{d}\sigma.$$

Transport in radius space

$$\partial_t f - \partial_\sigma\left(\frac{H(c,\sigma)}{\sigma} f\right) = 0.$$

The same microscopic exchange determines both the bulk sink/source and the velocity of particles in radius space.

Quantitative homogenization result

Let (u, p, c, f) be a *sufficiently regular* solution of the critical limit system and let

$$f_\varepsilon(t) = \frac{1}{N_\varepsilon} \sum_i \delta_{z_{\varepsilon,i}} \otimes \delta_{r_{\varepsilon,i}(t)}.$$

Then, for sufficiently small ε,

Convergence result including error estimate

$$\|u_\varepsilon - u\|_{L^\infty(0,T;L^2(\Omega_\varepsilon(t)))} + \|c_\varepsilon - c\|_{L^\infty(0,T;L^2(\Omega_\varepsilon(t)))} + \sup_{t\in[0,T]} \mathrm{W}_2(f_\varepsilon(t), f(t))$$
$$\leq C\Big(\varepsilon + \|h_\varepsilon - h\|_{H^{-1}} + \|c_{\varepsilon,0} - c_0\|_{L^2} + \mathrm{W}_2(f_\varepsilon(0), f_0)\Big).$$

This gives simultaneous convergence of flow, chemistry, and evolving particle statistics.

Proof idea: correctors and relative energy

The main difficulty is that neither u nor c satisfies the microscopic boundary conditions.

1. Build local correctors around every particle:
$$c_\varepsilon^{\mathrm{app}} = c + \sum_i c_{\varepsilon,i}^{\mathrm{app}}.$$
2. Couple the concentration error to an optimal transport plan between f_ε and f:
$$\mathcal{E}_\varepsilon(t) = \|c_\varepsilon - c_\varepsilon^{\mathrm{app}}\|^2_{L^2(\Omega_\varepsilon(t))} + \mathrm{W}_2(f_\varepsilon(t), f(t))^2.$$
3. Establish
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_\varepsilon + \|\nabla(c_\varepsilon - c_\varepsilon^{\mathrm{app}})\|^2_{L^2} \leq C\mathcal{E}_\varepsilon + C\varepsilon^2 + C\|h_\varepsilon - h\|^2_{H^{-1}}.$$
4. Apply Gronwall and recover the velocity estimate from the quasi-static Stokes problem.

Some future questions

- Moving particles (rotation & translation)
- Weaker assumption on separation of particles (allowing *some* clustering).
- More complicated geometries with local changes
- Particle size variable w.r.t. ε scale

Thank you.