Diffusion in periodic porous media: the large deviation regime

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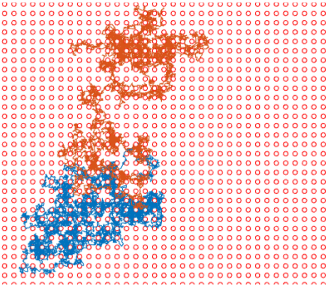

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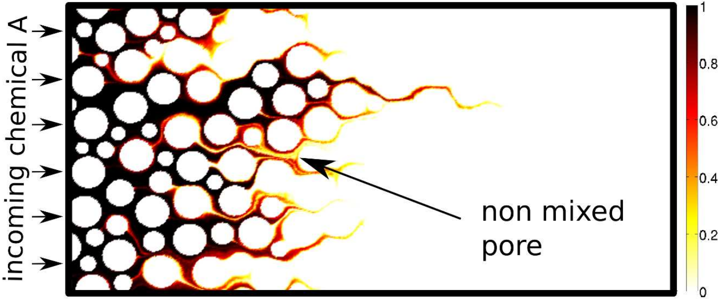
Reactions spreading in porous media

- The spread of the reactions depends on dispersion=advection+molecular diffusion at large times.



de Anna (2012)

Reactions spreading in porous media

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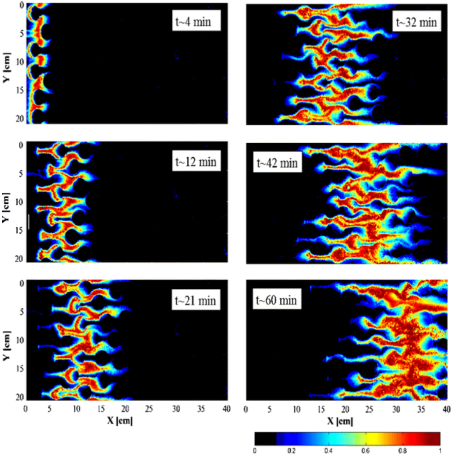


Oates and Harvey (2006)

The basic problem: diffusion in the presence of obstacles

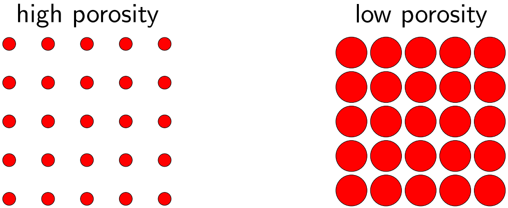


Figure: An example of a periodic porous environment composed of void (white) and solid (red) phases.

Ω_v is the void or fluid phase, C is the solute concentration

$$
\begin{aligned}
\frac{\partial C}{\partial t} &= \nabla^2 C, \quad \boldsymbol{x} \in \Omega_v \\
0 &= \boldsymbol{n} \cdot \nabla C, \quad \boldsymbol{x} \in \partial\Omega_v,
\end{aligned}
$$

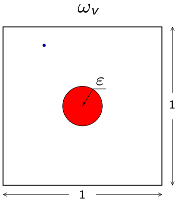
where $\boldsymbol{n}$ is the unit normal to Ω_v.

Effective description in terms of a diffusion equation

At long times, using multiple scales,

$$\frac{\partial c}{\partial t} = \nabla_{\boldsymbol{x}} \cdot (D_e \cdot \nabla_{\boldsymbol{x}} c),$$

where the effective diffusive tensor is given by a microscale model.



For a sudden localised release, predicts Gaussian evolution:

$$c(\boldsymbol{x}, t) \sim t^{-d/2} e^{-|\boldsymbol{x}|^2/(4D_e t)}.$$

(initial work by Maxwell/Lord Raleigh, put on a solid footing by e.g. Aris & Brenner (1988), see also Bruna & Chapman (2015))

Effective description in terms of large deviations

An alternative description is based on large deviation theory in which case

$$c(\boldsymbol{x}, t) \sim t^{-d/2} e^{-tg(\boldsymbol{x}/t)}.$$

- g is the rate function associated with the probability for the position of particles that have been displaced by $|\boldsymbol{x}|$ at $t \gg 1$.
- $g(\boldsymbol{x}/t) \sim |\boldsymbol{x}|^2/(4D_e t) + \dots$ for $|\boldsymbol{x}| \ll t$, thus recovering the picture given by the effective diffusion equation.
- employed in periodic fluid (Haynes & Vanneste, JFM (2014a,b)) and network (Tzella & Vanneste, PRL (2016)) environments.

Effective description in terms of large deviations

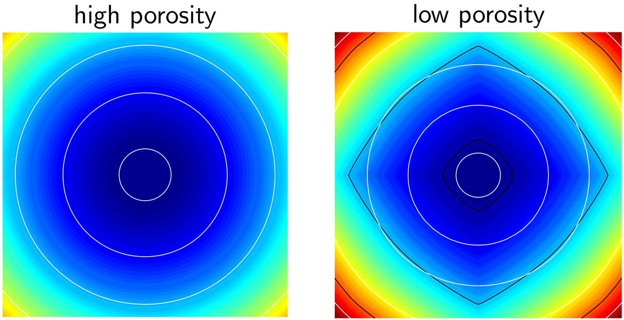


Figure: Snapshots of coarse-grained concentration of solute diffusing inside the porous environment.

- **High porosity**: effective diffusion is good.
- **Low porosity**: effective diffusion fails to capture a more complex anisotropic behaviour. The diffusion approximation underestimates c – bad if c is toxic!

Farah, Loghin, Tzella & Vanneste (2019) in preparation.