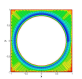
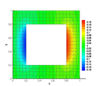
Nonlocal models of transport in multiscale porous media: something old and something new, something borrowed ...





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Outline

1. Introduction and motivation
   - Flow and transport in subsurface, nomenclature
   - Multiscale flow and transport in subsurface, experimental results
2. Something old: double porosity models
   - Literature review
   - Double porosity models, diffusion+advection
3. Something new: building a new model
   - Ideas and steps
   - Computational experiments
   - Construct affine approximations
   - Model calculations
   - Computational experiments with elements of upscaled model

NSF 0511190 “Model adaptivity in porous media”, DOE 98089 “Modeling, Analysis, and Simulation of Multiscale Preferential Flow”.
Also, see presentations at NSF-CMBS Nevada 5/20-25, DOE Multiscale workshop Tacoma, 5/25-30 (links from my webpage)

Flow coupled to transport $\mathcal{F}(\Theta) = 0$ with $\Theta = (\mathbf{u}, p, c)$

Flow

$$\mathbf{u} = -\mathbf{K}\nabla p, \quad \nabla \cdot \mathbf{u} = 0$$

Diffusive-dispersive transport

$$\phi \frac{\partial c}{\partial t} \quad + \quad \nabla \cdot (\mathbf{u} c - \mathbf{D}(\mathbf{u}) \nabla c) = 0$$

Definitions

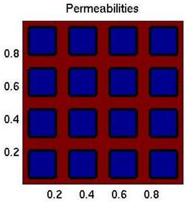
$$\begin{aligned}
\mathbf{D}(\mathbf{u}) &:= \text{diffusion} + \text{dispersion} \\
&:= d_{mol}\mathbf{I} + |\mathbf{u}|(d_{long}\mathbf{E}(\mathbf{u}) + d_{transv}(\mathbf{I} - \mathbf{E}(\mathbf{u}))). \\
\mathbf{E}(\mathbf{u}) &= \frac{1}{|\mathbf{u}|^2} u_i u_j \\
\mathbf{D}(\mathbf{u}) &\approx d_{mol}\mathbf{I} + d_{long}|\mathbf{u}|\mathbf{E}(\mathbf{u})
\end{aligned}$$

Multiscale flow and transport, set-up

Model $\mathcal{F}(\Theta) = 0$ with $\Theta = (p, \mathbf{u}, c)$

$$\mathbf{u} = -\mathbf{K}\nabla p, \quad \nabla \cdot \mathbf{u} = 0$$

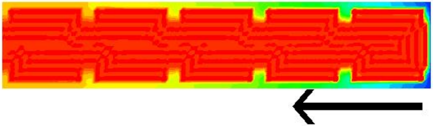
$$\phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{u})\nabla c) = 0$$

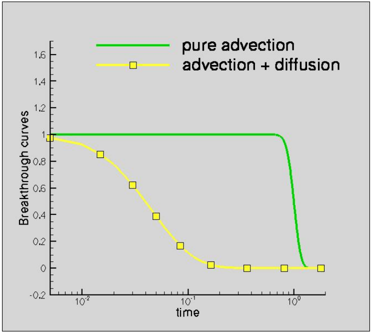


K_{fast}, K_{slow} give $\mathbf{u}_{fast}, \mathbf{u}_{slow}$ give $\mathbf{D}_{fast}, \mathbf{D}_{slow}$

Advection+diffusion in multiscale media: tailing

Breakthrough curves = total concentration at outlet

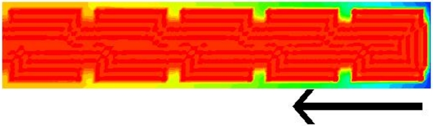


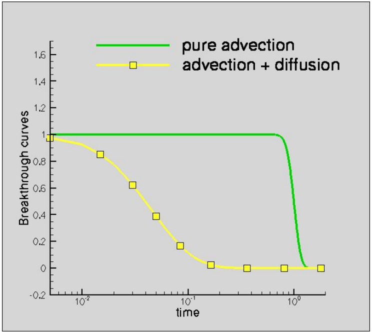


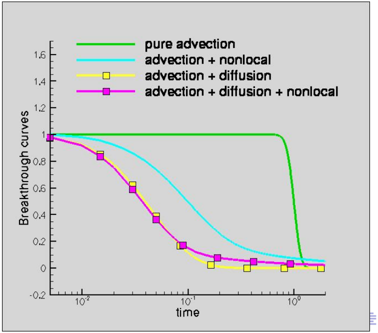
MOVIE

Advection+diffusion in multiscale media: tailing

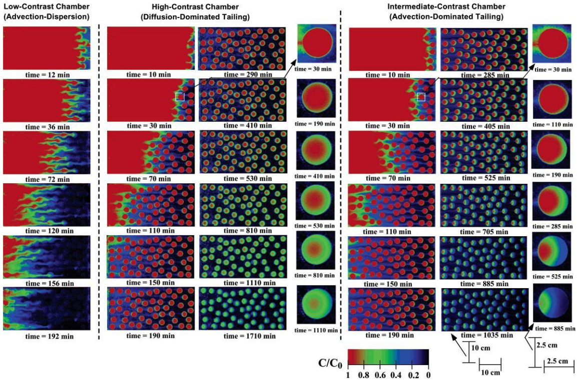
Breakthrough curves = total concentration at outlet







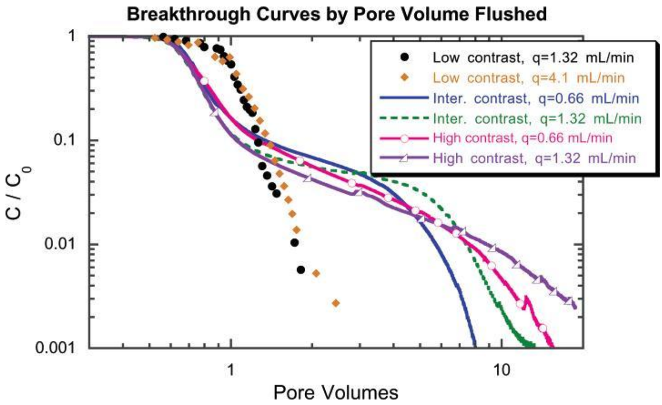
Experimental visualization by Haggerty et al



Presentation at SIAM Annual 2004 by Haggerty

[ZMH+04] Brendan Zinn, Lucy C. Meigs, Charles F. Harvey, Roy Haggerty, Williams J. Peplinski, and Claudius Freiherr von Schwerin, *Experimental visualization of solute transport and mass transfer processes in two-dimensional conductivity fields with connected regions of high conductivity*, Environ Sci. Technol. **38** (2004), 3916–3926.

Experimental breakthrough curves



Results from [ZMH+04]

Challenge in view of the experimental results

- Not-well separated scales:
  - *double porosity* diffusion model does not fit in low/intermediate contrast regime
  - $\epsilon_0 > 0$ is fixed (perhaps the homogenized model not good enough ? need a corrector ?)
  - $\frac{\mathbf{K}_{fast}}{\mathbf{K}_{slow}}$ small, moderate, intermediate, or large
- Evidence of advection-diffusion-dispersion in Ω_{slow} and advection-dispersion in Ω_{fast}
- Related project (Wood, Haggerty, Waymire, Thomann, Ramirez, OSU) on Taylor-Aris dispersion/skew diffusion models
- other results on tailing *[HG95, HMM00, HFMM01]*

Formidable challenge: find an upscaled model similar to double-porosity which can capture all of the above

Todd Arbogast, Jim Douglas, Jr., and Ulrich Hornung, *Derivation of the double porosity model of single phase flow via homogenization theory*, SIAM J. Math. Anal. **21** (1990), no. 4, 823–836. MR 91d:76074

Todd Arbogast, *Analysis of the simulation of single phase flow through a naturally fractured reservoir*, SIAM J. Numer. Anal. **26** (1989), no. 1, 12–29. MR 90e:76122

______, *On the simulation of incompressible, miscible displacement in a naturally fractured petroleum reservoir*, RAIRO Modél. Math. Anal. Numér. **23** (1989), no. 1, 5–51. MR MR1015918 (91d:76073)

______, *Computational aspects of dual-porosity models*, Homogenization and porous media (U. Hornung, ed.), Interdiscip. Appl. Math., vol. 6, Springer, New York, 1997, pp. 203–215. MR 1 434 324

John D. Cook and R. E. Showalter, *Microstructure diffusion models with secondary flux*, J. Math. Anal. Appl. **189** (1995), no. 3, 731–756. MR 96j:76138

J. Jr. Douglas and T. Arbogast, *Dual-porosity models for flow in naturally fractured reservoirs*, Dynamics of Fluids in Hierarchical Porous Media (J. H. Cushman, ed.), Academic Press, 1990, pp. 177–221.

J. Douglas, Jr., M. Peszyńska, and R. E. Showalter, *Single phase flow in partially fissured media*, Transp. Porous Media **28** (1997), 285–306.

Jim Douglas, Jr. and Anna M. Spagnuolo, *The transport of nuclear contamination in fractured porous media*, J. Korean Math. Soc. **38** (2001), no. 4, 723–761, Mathematics in the new millennium (Seoul, 2000). MR MR1838095 (2002g:76111)

Mark N. Goltz and Paul Roberts, *Using the method of moments to analyze three-dimensional diffusion-limited solute transport from temporal and spatial perspectives*, Water Res. Research **23** (1987), no. 8, 1575–1585.

R. Haggerty, S.W. Fleming, L.C. Meigs, and S.A. McKenna, *Tracer tests in a fractured dolomite 2. analysis of mass transfer in single-well injection-withdrawal tests*, Water Resources Research **37** (2001), no. 5, 1129–1142.

R. Haggerty and S.M. Gorelick, *Multiple-rate mass transfer for modeling diffusion and surface reactions in media with pore-scale heterogeneity*, Water Resources Research **31** (1995), no. 10, 2383–2400.

R. Haggerty, S.A. McKenna, and L.C. Meigs, *On the late-time behavior of tracer test breakthrough curves*, Water Resources Research **36** (2000), no. 12, 3467–3479.

Ulrich Hornung and Ralph E. Showalter, *Diffusion models for fractured media*, J. Math. Anal. Appl. **147** (1990), no. 1, 69–80. MR MR1044687 (91d:76072)

Małgorzata Peszyńska, *Fluid flow through fissured media. mathematical analysis and numerical approach*, Ph.D. thesis, University of Augsburg, Augsburg, Germany, 1992.

Małgorzata Peszyńska, *Analysis of an integro-differential equation arising from modelling of flows with fading memory through fissured media*, J. Partial Differential Equations **8** (1995), no. 2, 159–173. MR MR1331523 (96a:45007)

______, *Finite element approximation of diffusion equations with convolution terms*, Math. Comp. **65** (1996), no. 215, 1019–1037. MR MR1344620 (96j:65104)

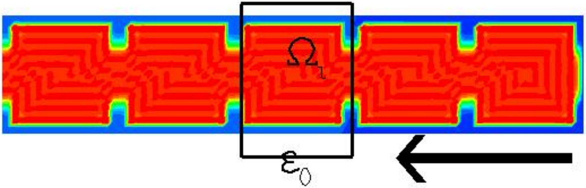
M. Peszyńska, *Mortar adaptivity in mixed methods for flow in porous media*, International Journal of Numerical Analysis and Modeling **2** (2005), no. 3, 241–282.

M. Peszyńska, M. F. Wheeler, and I. Yotov, *Mortar upscaling for multiphase flow in porous media*, Computational Geosciences **6** (2002), 73–100.

Sanchez-Villa X. and J. Carrera, *On the striking similarity between the moments of breakthrough curves for a heterogeneous medium and a homogeneous medium with a matrix diffusion term*, Journal of Hydrology **294** (2004), 164–175.

Brendan Zinn, Lucy C. Meigs, Charles F. Harvey, Roy Haggerty, Williams J. Peplinski, and Claudius Freiherr von Schwerin, *Experimental visualization of solute transport and mass transfer processes in two-dimensional conductivity fields with connected regions of high conductivity*, Environ Sci. Technol. **38** (2004), 3916–3926.

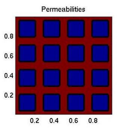
Notation



$\Omega = \bigcup_i \hat{\Omega}_i$, $\Omega_{slow} = \bigcup_{i=1} \Omega_i$,
$\partial\Omega_{slow} \cap \partial\Omega_{fast} \equiv \bigcup_i \Gamma_i$
$\Omega = \Omega_{slow} \cup \Omega_{fast} \cup \bigcup_i \Gamma_i$
$|\hat{\Omega}_i| \approx \epsilon_0$

Averaged (single porosity) model

Exact model at microscale

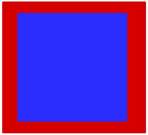


$\mathbf{D} = \mathbf{D}_{slow}, \mathbf{D}_{fast}$

replaced by homogenized model

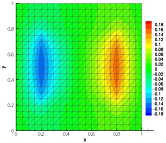
with $\tilde{\mathbf{D}}$

Compute homogenized coefficients $\tilde{\mathbf{D}}$



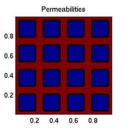
$$\tilde{D}_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_0} D_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y}))dA$$

$$\begin{cases} -\nabla \cdot \mathbf{D}\nabla\omega_j(\mathbf{y}) & = \nabla \cdot (\mathbf{D}\mathbf{e}_j), \quad \mathbf{y} \in \Omega_0 \\ \omega_j & \Omega_0 - \text{ periodic} \end{cases}$$



Averaged (single porosity) model

Exact model at microscale



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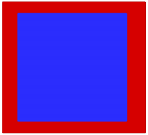
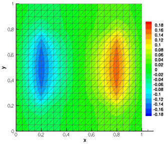


$$\tilde{D}_{jk} = \frac{1}{|\Omega_0|}\int_{\Omega_0} D_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y}))dA$$

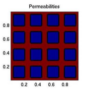
$$\begin{cases} -\nabla \cdot \mathbf{D}\nabla\omega_j(\mathbf{y}) & = \nabla \cdot (\mathbf{D}\mathbf{e}_j), \quad \mathbf{y} \in \Omega_0 \\ \omega_j & \Omega_0 - \text{ periodic} \end{cases}$$



But this doesn't work very well for time-dependent problems with large contrast $\mathbf{D}_{fast}/\mathbf{D}_{slow}$

Double porosity model: main idea I

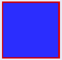
Exact model at microscale



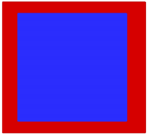
$\mathbf{D} = \mathbf{D}_{slow}, \mathbf{D}_{fast}$

replaced by homogenized model with two sheets

with $\tilde{\mathbf{D}}$ plus cell model

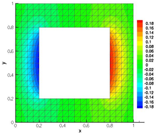


Compute homogenized coefficients $\tilde{\mathbf{D}}$



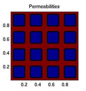
$$\tilde{D}_{jk} = \frac{1}{|\Omega_0|}\int_{\Omega_0} D_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y}))dA$$

$$\begin{cases} -\nabla \cdot \mathbf{D}\nabla\omega_j(\mathbf{y}) & = \nabla \cdot (\mathbf{D}\mathbf{e}_j), \quad \mathbf{y} \in \Omega_{0,fast} \\ \omega_j & \Omega_0 - \text{ periodic} \end{cases}$$



Double porosity model: main idea I

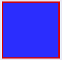
Exact model at microscale



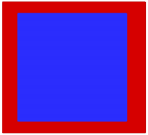
$\mathbf{D} = \mathbf{D}_{slow}, \mathbf{D}_{fast}$

replaced by homogenized model with two sheets

with $\tilde{\mathbf{D}}$ plus cell model

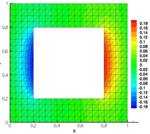


Compute homogenized coefficients $\tilde{\mathbf{D}}$



$$\tilde{D}_{jk} = \frac{1}{|\Omega_0|}\int_{\Omega_0} D_{jk}(\mathbf{y})(\delta_{jk} + \partial_k \omega_j(\mathbf{y}))dA$$

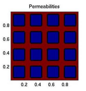
$$\begin{cases} -\nabla \cdot \mathbf{D}\nabla\omega_j(\mathbf{y}) & = \nabla \cdot (\mathbf{D}\mathbf{e}_j), \quad \mathbf{y} \in \Omega_{0,fast} \\ \omega_j & \Omega_0 - \text{ periodic} \end{cases}$$



This formulation introduces nonlocal effects and works very well for time-dependent problems with large contrast $\mathbf{D}_{fast}/\mathbf{D}_{slow}$

Double porosity model: main idea II

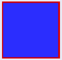
Exact model at microscale



$\mathbf{D} = \mathbf{D}_{slow}, \mathbf{D}_{fast}$

replaced by homogenized model with two sheets

with $\tilde{\mathbf{D}}$ plus cell model



Global equation, $x \in \Omega$

$$\tilde{\phi}\frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{\mathbf{D}} \nabla \tilde{c} = 0$$

$$q_i(t) = \Pi^*_{0,i}(\Pi_{0,i}(\tilde{c}))$$

Cell problem, $x \in \Omega_i$

$$\phi_{slow}\frac{\partial c_i}{\partial t} - \nabla \cdot \mathbf{D}_{slow} \nabla c_i = 0$$

$$c_i|_{\Gamma_i} = \Pi_{0,i}(\tilde{c})$$

This formulation works well for single & multi-phase multicomponent problems and has been implemented in commercial reservoir simulators

Recall double porosity models for diffusion

Exact ϵ_0 model $\mathcal{F}_{\epsilon_0}(\Theta_{\epsilon_0}) = 0$

$$\phi_\alpha \frac{\partial c_\alpha}{\partial t} - \nabla \cdot \mathbf{D}_\alpha \nabla c_\alpha = 0, \quad x \in \Omega_\alpha, \quad \alpha = fast, slow$$

plus interface conditions on $\partial\Omega_{slow} \cap \partial\Omega_{fast}$:

$$c_{fast} = c_{slow}, \quad \mathbf{D}_{fast} \nabla c_{fast} \cdot \nu = \mathbf{D}_{slow} \nabla c_{slow} \cdot \nu$$

Approximate microstructure model [Arb89a, Arb97] $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

$$\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{\mathbf{D}} \nabla \tilde{c} = 0$$

$$q_i(t) = \Pi^*_{0,i}(\Pi_{0,i}(\tilde{c}))$$

- also for multiphase problems[DA90]

Homogenized model [ADH90, HS90, Pes92] $\mathcal{F}_\epsilon(\Theta_\epsilon) \to \mathcal{F}_0(\Theta_0) = 0$

$$\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} + \tau * \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot \tilde{\mathbf{D}} \nabla \tilde{c} = 0,$$

- analysis and convergence
- computational approach[Pes95, Pes96, DPS97]

Local (cell) problem and averages Π_0, Π_0^*

Local averages $\Pi_{0,i}, \Pi_{0,i}^*$

$$\Pi_{0,i}\xi := \frac{1}{|\hat{\Omega}_i|}\int_{\hat{\Omega}_i} \xi(\mathbf{x})dA$$

$$\Pi_{0,i}^*\gamma := \frac{1}{|\hat{\Omega}_i|}\int_{\Gamma_i} \mathbf{D}_{slow}\nabla c_i(\gamma)(\mathbf{x},t)\cdot\nu ds = \Pi_{0,i}(\phi_{slow}\frac{\partial c_i(\gamma)}{\partial t})$$

where $c_i = c_i(\gamma)$ solves the local (cell) problem

$$\phi_{slow}\frac{\partial c_i}{\partial t} - \nabla\cdot\mathbf{D}_{slow}\nabla c_i = 0, x \in \Omega_i,$$

$$c_i = \gamma(\mathbf{x},t), \mathbf{x} \in \partial\Omega_i$$

Double porosity models for diffusion-advection

Exact ϵ_0 model $\mathcal{F}_{\epsilon_0}(\Theta_{\epsilon_0}) = 0$

$$\phi \frac{\partial c_\alpha}{\partial t} - \nabla \cdot (\mathbf{D}_\alpha \nabla c_\alpha - \mathbf{u}_\alpha c_\alpha) = 0, \quad x \in \Omega_\alpha, \; \alpha = fast, slow$$

plus interface conditions on $\partial\Omega_{slow} \cap \partial\Omega_{fast}$

Approximate microstructure model [Arb89b] $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

$$\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i - \nabla \cdot (\tilde{\mathbf{D}} \nabla \tilde{c} - \tilde{\mathbf{u}} \tilde{c}) = 0,$$

$$q_i(t) = \Pi_{1,i}^*(\Pi_{1,i}(\tilde{c}))$$

Π_1 =local L_2 projections onto linears, Π_1^* its dual.
Numerical model only.

Limit $\epsilon \longrightarrow 0$ model[DS01] $\mathcal{F}_0(\Theta_0) = 0$

$$\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} + \phi_{slow} \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot (\tilde{\mathbf{D}} \nabla \tilde{c} - \tilde{\mathbf{u}} \tilde{c}) = 0$$

$$\phi_{slow} \frac{\partial \tilde{c}}{\partial t} \approx \Pi_{0,i}^*(\Pi_{1,i}(\tilde{c}))$$

Π_1 =local Taylor. Cell problem: $\mathbf{u}_{slow} \approx 0$, symmetry exploited.

Why these are not enough ... and other related results

Approximate microstructure model [Arb89b] $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

Numerical model only.

Limit $\epsilon \to 0$ model [DS01] $\mathcal{F}_0(\Theta_0) = 0$

Cell problem: $\mathbf{u}_{slow} \approx 0$. Use Π_0^* for flux.

Want to have $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

constructed with “global” (upscaled) flavor (akin diffusion model $\tilde{\phi}\frac{\partial \tilde{c}}{\partial t} + \tau * \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot (\tilde{\mathbf{D}}\nabla \tilde{c} - \tilde{\mathbf{u}}\tilde{c}) = 0$,) or secondary diffusion as in [CS95]

- account for (lack of) separation of scales $\epsilon_0 > 0$ and advection-dispersion
- track transition between different regimes of phenomena

Why these are not enough ... and other related results

Approximate microstructure model [Arb89b] $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

Numerical model only.

Limit $\epsilon \to 0$ model[DS01] $\mathcal{F}_0(\Theta_0) = 0$

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- account for (lack of) separation of scales $\epsilon_0 > 0$ and advection-dispersion
- track transition between different regimes of phenomena

Other models known in hydrology/ applied math and geosciences

- Gerke van Genuchten 1993 (for Richards’ equation)
- nonlocal models of dispersion (Cushman et al)

Building the upscaled model $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

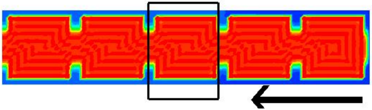
Want to have $\tilde{\mathcal{F}}_{\epsilon_0}(\tilde{\Theta}_{\epsilon_0}) = 0$

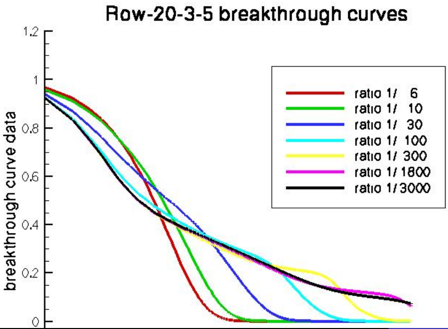
constructed with “global” flavor.

- Computational experiments on microscale
- Building the model
  - use the model *á la* *[Arb89b]* but with different Π_1, Π_1^*,
  - construct convolution approximations of all terms *á la* *[Pes92]* with a family of kernels
- simulate the upscaled nonlocal model for a continuum of regimes of phenomena
  - kernels reflect the regimes

Computational experiments at microscale

GOAL: reproduce qualitatively experimental results, understand significance of different regimes of flow and trasport





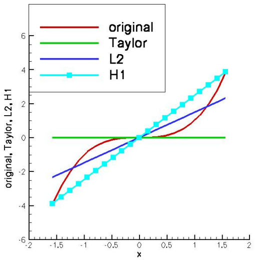
MOVIES

Choice of ffine approximations Π_1

Recall $\Pi_0 f := \frac{1}{|\Omega_0|}\int_{\Omega_0} f(\mathbf{x})dA$, assume here $|\Omega_0| = 1$.
Denote $\mathbf{x}^C$ - center of mass of Ω_0.
General affine approximation $f(\mathbf{x}) \approx \Pi_1 f := m + \mathbf{n}\cdot\mathbf{x}, \;\; \mathbf{x}\in\Omega_0$

Choice of $m, \mathbf{n}$

- Taylor ($f \in C^1(\Omega_0)$) about midpoint
  $f(\mathbf{x}) \approx f(\mathbf{x}^C) + \nabla f(\mathbf{x}^C)(\mathbf{x} - \mathbf{x}^C)$
- $L_2(\Omega_0)$-projection onto affines that is:
  $(f, v)_{\Omega_0} = (m + \mathbf{n}\cdot\mathbf{x}, v)_{\Omega_0}, \forall \text{ affine } v$
- $H^1(\Omega_0)$ projection:
  $f(\mathbf{x}) \approx \Pi_1 f := \Pi_0 f + \Pi_0 \nabla f \cdot (\mathbf{x} - \mathbf{x}^C)$
  Basis functions not necessarily orthogonal.



Dual affine approximations Π_1^* to Π_1

- $L_2(\Omega_0)$-projection onto affines, use an orthonormal basis (ϕ_0, ϕ_1, ϕ_2)

$$\Pi_1 f(\mathbf{x}) = \sum_k f_k \phi_k(\mathbf{x})$$

Flux calculations

$$\Pi_1^* q = \sum_k q_k \phi_k(\mathbf{x}), \quad q_k = \Pi_0(q\phi_k)$$

- $H^1(\Omega_0)$ projection:

$$f(\mathbf{x}) \approx \Pi_0 f + \Pi_0 \nabla f \cdot (\mathbf{x} - \mathbf{x}^C)$$

Note $(1, (\mathbf{x} - \mathbf{x}^C)_1, (\mathbf{x} - \mathbf{x}^C)_2)$ are not necessarily orthogonal !

$$\Pi_1^* q = q_0 \xi_0(\mathbf{x}) + q_1 \xi_1(\mathbf{x}) + q_2 \xi_2(\mathbf{x})$$

We use $H^1(\Omega_i)$-projection denoted $\Pi_{1,i} \equiv \Pi_i$ and $Pi^*_{1,i} \equiv \Pi^*_i$

Calculate Π_i and Π_i^*

Recall Π_i: $H^1(\Omega) \mapsto H^1(\hat{\Omega}_i)$

$$\Pi_i(w)(\mathbf{x}) \equiv \frac{1}{|\hat{\Omega}_i|}\left(\int_{\hat{\Omega}_i} w(\mathbf{y})\,dA + \sum_{k=1}^{2}\left[\int_{\hat{\Omega}_i} \partial_k w(\mathbf{y})\,dA\right](x_k - (\hat{\mathbf{x}}_i^C)_k)\right)$$

Dual Π_i^*: $(H^1(\hat{\Omega}_i))^* \mapsto (H^1(\Omega))^*$ affine approximation of flux $q \in H^{-1/2}(\Gamma_i)$

$$\langle \Pi_i^*(q), w\rangle = \langle q, \Pi_i(w)\rangle, \forall w \in C_0^\infty(\Omega)$$

with $\langle q, v\rangle := \sum_i \int_{\Gamma_i} q(s)v(s)ds$ uses moments M_i^0,$\mathbf{M}_i^1$

$$\langle q, \Pi_i(w)\rangle = \frac{1}{|\hat{\Omega}_i|}\int_{\Gamma_i} q(s)\left[\int_{\hat{\Omega}_i} wdA + (s - \mathbf{x}_i^c)\int_{\hat{\Omega}_i} \nabla w ds\right]$$

$$= \int_\Omega \bar{\chi}_i(\mathbf{x})\frac{1}{|\hat{\Omega}_i|}\int_{\Gamma_i} q(s)ds w(\mathbf{x})dA + \int_\Omega \bar{\chi}_i(\mathbf{x})\frac{1}{|\hat{\Omega}_i|}\int_{\Gamma_i} q(s)(\mathbf{s} - \mathbf{x}^C)ds \cdot \nabla w(\mathbf{x})dA$$

$$= \int_\Omega \bar{\chi}_i(\mathbf{x})M_i^0(q)w(\mathbf{x})dA - \int_\Omega \nabla\cdot(\bar{\chi}_i(\mathbf{x})\mathbf{M}_i^1(q))\,w(\mathbf{x})dA = \langle \Pi_i^*(q), w\rangle$$

Calculations Π_i and Π_i^* summary

Affine approximation $\Pi_i : H^1(\Omega) \mapsto H^1(\hat{\Omega}_i)$

$$\Pi_i(w)(x) \equiv \Pi_0 w + \Pi_0(\nabla w) \cdot (\mathbf{x} - \mathbf{x}^C)$$

Its dual $\Pi_i^* : H^1(\hat{\Omega}_i)^* \mapsto H^1(\Omega)^*$ pointwise

$$\Pi_i^*(q)(\mathbf{x}) = \bar{\chi}_i(\mathbf{x}) M_i^0(q) - \nabla \cdot \bar{\chi}_i(\mathbf{x}) \mathbf{M}_i^1(q)$$

Note the last term is a scaled line source !

Application of Green's theorem to moments

For any smooth region D, smooth $\mathbf{v} = (v_1, v_2)$ and $\hat{\mathbf{x}}^C \in D$,

$$\int_D (\nabla \cdot \mathbf{v})(x_k - (\hat{\mathbf{x}}^C)_k) dA = \int_{\partial D} \mathbf{v} \cdot \nu (x_k - (\hat{\mathbf{x}}^C)_k) ds - \int_D v_k dA$$

hence for the flux from the cell $q(s) = (\mathbf{D}_i \nabla c_i(s) - \mathbf{v}_i c_i(s)) \cdot \nu$

$$\mathbf{M}_i^1(q)$$

$$= \int_{\Omega_i} \Big(\nabla \cdot (\mathbf{D}_i \nabla c_i(\mathbf{y},t) - \mathbf{v}_i c_i(\mathbf{y},t)) (\mathbf{y} - \hat{\mathbf{x}}_i^C) + \mathbf{D}_i \nabla c_i(\mathbf{y},t) - \mathbf{v}_i c_i(\mathbf{y},t) \Big) dA \,.$$

$$= - \sum_i \bar{\chi}_i(\mathbf{x}) \int_{\Omega_i} (\phi_i \frac{\partial c_i}{\partial t}(\mathbf{y},t)(\mathbf{y} - \hat{\mathbf{x}}_i^C) + \mathbf{D}_i \nabla c_i(\mathbf{y},t) - \mathbf{v}_i c_i(\mathbf{y},t)) \, dA$$

Cell problem: elementary solutions

Cell problem solved for $u_i^j, j = 0, 1, 2$

$$\phi_{slow}\frac{\partial u_i^j}{\partial t} - \nabla\cdot(\mathbf{D}_{slow}\nabla u_i^j - \mathbf{u}_{slow}u_i^j) = 0, \mathbf{x}\in\Omega_i,$$

$$u_i^j(\mathbf{x}, 0) = 0, \mathbf{x}\in\Omega_i$$

$$\begin{cases} u_i^0|_{\Gamma_i} = 1, \\ u_i^1|_{\Gamma_i} = (\mathbf{x}-\mathbf{x}_i^C)_1, \\ u_i^2|_{\Gamma_i} = (\mathbf{x}-\mathbf{x}_i^C)_2 \end{cases}$$

Represent the solution to the cell problem

$$\phi_{slow}\frac{\partial c_i}{\partial t} - \nabla\cdot(\mathbf{D}_{slow}\nabla c_i - \mathbf{u}_{slow}c_i) = 0, \mathbf{x}\in\Omega_i,$$

$$c_i(\mathbf{x}, 0) = 0, \mathbf{x}\in\Omega_i$$

$$c_i|_{\Gamma_i} = \Pi_{1,i}(c_*)(\mathbf{x}, t)$$

$$\equiv A_i^0(t) + (A_i^1, A_i^2)\cdot(\mathbf{x}-\mathbf{x}_i^C),$$

By linearity $c_i(\mathbf{x}, t) = \int_0^t \sum_{j=0}^2 \frac{\partial u_i^j}{\partial t}(\mathbf{x}, t-s)A_i^j(s)ds = \sum_{j=0}^2 \frac{\partial u_i^j(\mathbf{x},\cdot)}{\partial t} * A_i^j$

Putting it together

Solution to the cell problem $c_i(\mathbf{x},t) = \sum_{j=0}^{2} \frac{\partial u_i^j(\mathbf{x},\cdot)}{\partial t} * A_i^j$

$$\begin{aligned} \phi_{slow}\frac{\partial c_i}{\partial t} - \nabla\cdot(\mathbf{D}_{slow}\nabla c_i - \mathbf{u}_{slow}c_i) &= 0, \mathbf{x}\in\Omega_i, \\ c_i(\mathbf{x},0) &= 0, \mathbf{x}\in\Omega_i \end{aligned}$$

$$c_i|_{\Gamma_i} = \Pi_{1,i}(c_*)(\mathbf{x},t) \equiv A_i^0(t) + (A_i^1, A_i^2)\cdot(\mathbf{x}-\hat{x}_i^C), \mathbf{x}\in\Gamma_i$$

Use u_i^j and A_j so that $\Pi_{1,i}(c_*)(\mathbf{x},t) \equiv A_i^0(t) + (A_i^1, A_i^2)\cdot(\mathbf{x}-\hat{x}_i^C)$

Compute the normal flux

$$q(s) \equiv (\mathbf{D}_{slow}\nabla c_i - \mathbf{u}_{slow}c_i)\cdot\eta, s\in\Gamma_i$$

... and its affine approximations $\Pi_{1,i}^* q$ using A_j, u_i^j
... and the moments $M_i^0(q), \mathbf{M}_i^1(q)$.

Convolution kernels

Write the moments $M_i^0(q), \mathbf{M}_i^1(q)$ in terms of A_k and u_i^j

Define the kernels for each i and each function $u_i^j, j = 0, 1, 2$ by

$$\begin{aligned}
\mathcal{S}_i^{j0}(t) &\equiv \int_{\Omega_i} \phi_i \frac{\partial u_i^j}{\partial t}(\mathbf{x}, t)\, dA, \quad 0 \le j \le 2. \\
\mathcal{S}_i^{jk}(t) &\equiv \int_{\Omega_i} \phi_i \frac{\partial u_i^j}{\partial t}(\mathbf{x}, t)(x_k - (\hat{\mathbf{x}}_i^C)_k)\, dA, \quad 1 \le k \le 2. \\
\mathbf{T}_i^j(t) &\equiv (T_i^{j1}, T_i^{j2}) \equiv \int_{\Omega_i} (\mathbf{D}_i \nabla - \mathbf{v}_i) \frac{\partial u_i^j}{\partial t}(\mathbf{x}, t)\, dA.
\end{aligned}$$

Together we have 15 scalar kernels, some of which will be zero due to symmetry/lack of thereof

Computational experiments

Model summary (suppress $i, \bar{\chi}_i$ etc.)

$$\frac{\partial}{\partial t}\{\phi_* c_* + \mathcal{S}^{00} * c_* + (\mathcal{S}^{01}, \mathcal{S}^{02}) * \nabla c_* - \nabla \cdot (\mathcal{S}^{10} * c_* + (\mathcal{S}^{11}, \mathcal{S}^{12}) * \nabla c_*)\}$$
$$-\nabla \cdot \{\mathbf{D}_* \nabla c_* - \mathbf{v}_* c_* + \mathbf{T}^0 * c_* + (\mathbf{T}^1, \mathbf{T}^2) * \nabla c_*\} = 0$$

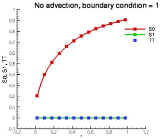
- Convolution kernels for different regimes of diffusion vs advection
  - no advection
  - with advection
  - with signficant advection
- Upscaled problem with nonlocal terms
- Comparison between exact model and upscaled model with nonlocal terms and computed kernels

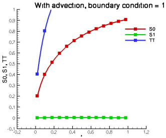
Convolution kernels: regimes of $Pe = \frac{advection}{diffusion}$

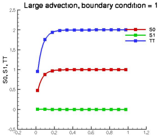
Solution u^j and the associated kernels S^{j0}, S^{j1}, T^{j1}

$j = 0$

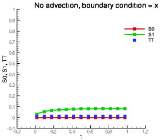
No advection	With advection	Large advection

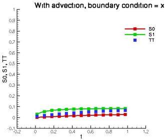


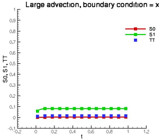




$j = 1$

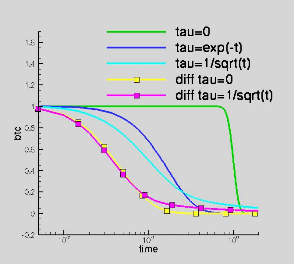






Upscaled model: numerical treatment

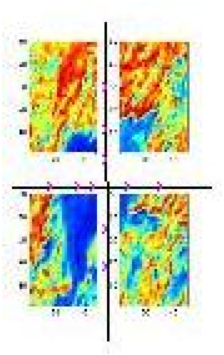
- nonlocal diffusion (FE+time-stepping on c_t) *[Pes95]* stable, convergence $O(\triangle t + h^2)$, singular kernels
- nonlocal diffusion with secondary diffusion terms (as in viscoelasticity) (*[Thomee,Lin,Ewing'91-'01]*) with nonsingular kernels
- nonlocal advection (FD+time-stepping): stable, convergent $O(\triangle t + h)$ *[P06]*, singular kernels
- nonlocal advection+diffusion+secondary diffusion+secondary advection:
  - issues of memory storage, need adaptive treatment
  - relative importance of the terms ∇c_*, $\nabla^2 c_*$: adaptivity a must

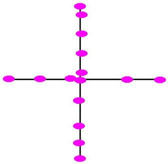


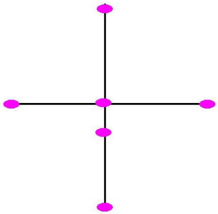
- pore-scale modeling (with K. Augustson)
- unsaturated flow models
- use experimental results by Wildenschild et al

Connection to mortar upscaling

[PWY02, Pes05]







Summary: the upscaled model

$$
\begin{aligned}
\frac{\partial}{\partial t}\Bigg(\phi_* c_*(x,t) &+ \sum_{i=1}^{N} \bar{\chi}_i(\mathbf{x}) \int_0^t \mathcal{S}_i^{00}(t-\tau)\frac{1}{|\hat{\Omega}_i|}\int_{\hat{\Omega}_i} c_*(\mathbf{y},\tau)\,dA\,d\tau \\
&+ \sum_{i=1}^{N} \bar{\chi}_i(\mathbf{x}) \int_0^t \sum_{j=1}^{2} \mathcal{S}_i^{j0}(t-\tau)\frac{1}{|\hat{\Omega}_i|}\int_{\hat{\Omega}_i} \partial_j c_*(\mathbf{y},\tau)\,dA\,d\tau \\
-\nabla\cdot \sum_{i=1}^{N} \bar{\chi}_i(\mathbf{x}) \int_0^t \sum_{j=0}^{2} &(\mathcal{S}_i^{j1}(t-\tau),\mathcal{S}_i^{j2}(t-\tau))\frac{1}{|\hat{\Omega}_i|}\int_{\hat{\Omega}_i} \partial_j c_*(\mathbf{y},\tau)\,dA\,d\tau \Bigg) \\
&- \nabla\cdot\left(\mathbf{D}_*\nabla c_*(x,t) - \mathbf{v}_* c_*(x,t)\right. \\
+ \sum_{i=1}^{N} \bar{\chi}_i(\mathbf{x}) \int_0^t \sum_{j=0}^{2} &(T_i^{j1}(t-\tau),T_i^{j2}(t-\tau))\frac{1}{|\hat{\Omega}_i|}\int_{\hat{\Omega}_i} \partial_j c_*(\mathbf{y},\tau)\,dA\,d\tau\Bigg) \\
&= 0,\ \mathbf{x}\in\Omega,\ t\geq 0.
\end{aligned}
$$