Homogenization of reactive flows in porous media

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Outline

* Why study Reactive Flows in porous media?
* Periodic porous media and Model description
* Two-scale Expansion with Drift Method
* Numerical Study with FreeFem++
* Conclusions

Why study Reactive Flows in porous media?

* Oil reservoir simulation (Enhanced Recovery Mechanisms)
* CO_2 storage (Natural Gas Extraction)
* Geothermal energy extraction
* Underground coal gasification
* Stockage of Nuclear Wastes
* Ground water contaminant transport (Drinking and Irrigation)
* Soil Chemistry (Movement of moisture, nutrients, pollutants in soil)

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Σ^0 solid part

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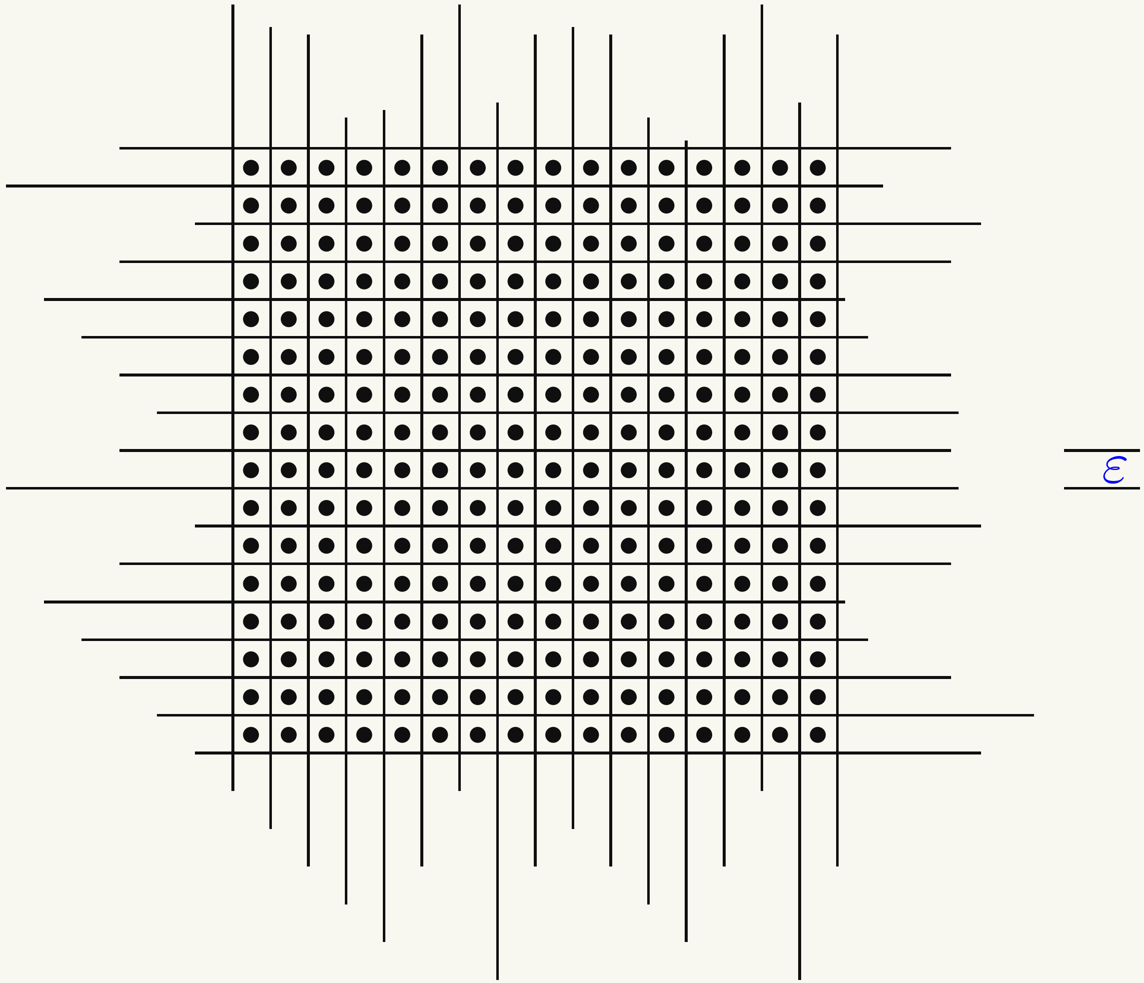
Assumptions:
Σ^0 smooth, connected set strictly included in Y or forms a connected set in $\mathbb{R}^n$ by Y-periodicity.
Ω_ε smooth, connected set in $\mathbb{R}^n$

2-D schematics



2-D schematic of an unbounded porous media

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For simplicity, we study Reactive Transport of a single solute.

Also, we assume that the reactive interactions are present only on the pore surfaces (Linear Adsorption).

Model Description contd.

The model is described as follows:

$$\begin{cases} \partial_t u_\varepsilon + \dfrac{1}{\varepsilon} b_\varepsilon \cdot \nabla_x u_\varepsilon - div_x(D_\varepsilon \nabla_x u_\varepsilon) = 0 \text{ in } (0,T) \times \Omega_\varepsilon \\ u_\varepsilon(0,x) = u^0(x), \;\; x \in \Omega_\varepsilon \\ \partial_t v_\varepsilon + \dfrac{1}{\varepsilon} b_\varepsilon^S \cdot \nabla_x^S v_\varepsilon - div_x^S(D_\varepsilon^S \nabla_x^S v_\varepsilon) = \dfrac{1}{\varepsilon^2}\kappa \left(u_\varepsilon - \dfrac{1}{K} v_\varepsilon \right) \\ \qquad\qquad = -\dfrac{1}{\varepsilon} D_\varepsilon \nabla_x u_\varepsilon \cdot \gamma \text{ on } (0,T) \times \partial\Omega_\varepsilon \\ v_\varepsilon(0,x) = v^0(x), \;\; x \in \partial\Omega_\varepsilon \end{cases} \tag{1}$$

$u_\varepsilon(t,x)$ respresents the concentration of the solute in the bulk.

$v_\varepsilon(t,x)$ represents the concentration of the solute on the pore surfaces.

model description

κ Rate constant
K Linear adsorption eq. const.

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$\nabla_x^S v = G \nabla_x v$ tangential gradient

$div_x^S \Psi = div_x(G\Psi)$ tangential divergence

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$b_\varepsilon(x) = b\left(\frac{x}{\varepsilon}\right)$ Stationary incompressible periodic flow
$div_y b = 0$ in Y^0
$b \cdot \gamma = 0$ on $\partial\Sigma^0$

$b_\varepsilon^S(x) = b^S(\frac{x}{\varepsilon})$ Stationary incompressible periodic flow
$div_y^S b^S = 0$ on $\partial\Sigma^0$

Main Result

Theorem 1 *The solution* $(u_\varepsilon, v_\varepsilon)$ *of (1) satisfies*

$$u_\varepsilon(t,x) \approx u_0(t, x - \frac{b^*}{\varepsilon} t) \ \ \textit{and} \ \ v_\varepsilon(t,x) \approx K u_0(t, x - \frac{b^*}{\varepsilon} t)$$

with the effective drift

$$b^* = \frac{\int_{Y^0} b(y)\, dy + K \int_{\partial\Sigma^0} b^S(y)\, d\sigma(y)}{|Y^0| + K|\partial\Sigma^0|_{n-1}}$$

and u_0 *the solution of the homogenized problem*

$$\begin{cases} K_d\, \partial_t u_0 = div_x\,(A^* \nabla_x u_0) \ \ \textit{in} \ \ (0,T) \times \mathbb{R}^n \\ K_d\, u_0(0,x) = |Y^0| u^0(x) + |\partial\Sigma^0|_{n-1} v^0(x), \quad x \in \mathbb{R}^n \end{cases}$$

Where, $K_d = |Y^0| + K|\partial\Sigma^0|_{n-1}$*, the dispersion tensor* A^* *will be described later.*

Two-scale Asymptotic Expansion

The usual Two-scale Expansion method suggests us to

- Take the ansatz for $u_\varepsilon(t,x)$ and $v_\varepsilon(t,x)$ in slow and fast variables as
$$u_\varepsilon = \sum_{i=0}^{\infty} \varepsilon^i u_i\left(t, x, \frac{x}{\varepsilon}\right) \text{ and } v_\varepsilon = \sum_{i=0}^{\infty} \varepsilon^i v_i\left(t, x, \frac{x}{\varepsilon}\right)$$
- Plug-in the two asymptotic expansions in (1).
- Identify the co-efficients of identical powers of ε and get a cascade of equations.
- solve those system of equations to arrive at the homogenized equation.

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- solve those system of equations to arrive at the homogenized equation.
- Convection term in microscale results in strong convection term dominating the diffusion. So, we cannot expect to prove the convergence of $u_\varepsilon(t,x)$ in a fixed spatial frame x but in a moving frame $x + b^* t$

Two-scale Asymptotic Expansion with DRIFT

$$u_\varepsilon = \sum_{i=0}^{\infty} \varepsilon^i u_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \tag{2}$$

$$v_\varepsilon = \sum_{i=0}^{\infty} \varepsilon^i v_i \left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon} \right) \tag{3}$$

Where b^* is the drift which shall be computed along the process. Consider $y = \frac{x}{\varepsilon}$. Then we have:

$$\begin{aligned} \frac{\partial}{\partial t}\left[\phi\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right] &= \left[\frac{\partial \phi}{\partial t} - \sum_{j=1}^{n} \frac{b_j^*}{\varepsilon}\frac{\partial \phi}{\partial x_j}\right]\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \\ \frac{\partial}{\partial x_j}\left[\phi\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right)\right] &= \left[\frac{\partial}{\partial x_j}\phi + \frac{1}{\varepsilon}\frac{\partial}{\partial y_j}\phi\right]\left(t, x - \frac{b^* t}{\varepsilon}, \frac{x}{\varepsilon}\right) \end{aligned} \tag{4}$$

$\forall j \in \{1, \cdots, n\}$

Fredholm type result

Before listing the cascade of equations, we shall state a Fredholm type result that helps us solve them.

Lemma 2 *For* $f \in L^2(Y^0)$, $g \in L^2(\partial\Sigma^0)$ *and* $h \in L^2(\partial\Sigma^0)$*, the following system of p.d.e.'s admit a solution* $(u, v) \in H^1_{per}(Y^0) \times H^1(\partial\Sigma^0)$*, unique up to the addition of a constant multiple of* $(1, K)$*,*

$$\begin{cases} b(y) \cdot \nabla_y u - div_y(D(y)\nabla_y u) = f & \textit{in } Y^0, \\ -D(y)\nabla_y u \cdot \gamma + g = k\left(u - \frac{1}{K}v\right) & \textit{on } \partial\Sigma^0, \\ b^S(y) \cdot \nabla_y^S v_0 - D^S div_y^S(D^S(y)\nabla_y^S v_0) - h = k\left(u - \frac{1}{K}v\right) & \textit{on } \partial\Sigma^0, \\ y \to (u(y), v(y)) & Y - \textit{periodic}, \end{cases} \tag{5}$$

if and only if

$$\int_{Y_0} f\, dy + \int_{\partial\Sigma_0} (g + h)\, d\sigma(y) = 0 \tag{6}$$

Co-efficients of ε^{-2}

$$\begin{cases} b(y)\cdot\nabla_y u_0 - div_y(D(y)\nabla_y u_0) = 0 & \text{in } Y^0, \\ \\ -D\nabla_y u_0\cdot\gamma = b^S(y)\cdot\nabla_y^S v_0 - D^S div_y^S(D^S(y)\nabla_y^S v_0) & \\ \qquad\qquad = k\left[u_0 - \frac{1}{K}v_0\right] & \text{on } \partial\Sigma^0, \\ \\ y \to (u_0(y), v_0(y)) & Y-\text{periodic}, \end{cases} \tag{7}$$

The compatibilty condition is trivially satisfied.

Hence the existence and uniqueness of (u_0, v_0).

Substituting the test functions by (u_0, v_0) in the variational formulation of (7), we can deduce that

$$v_0 = Ku_0 \quad \text{and} \quad u_0 = u_0(t, x)$$

Cascade of Systems Contd.

Co-efficients of ε^{-1}

$$\begin{cases} -b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - div_y(D(y)(\nabla_x u_0 + \nabla_y u_1)) = 0 & \text{in} Y^0, \\ -b^* \cdot \nabla_x v_0 + b^S(y) \cdot (\nabla_x^S v_0 + \nabla_y^S v_1) - div_y^S(D^S(y)(\nabla_x^S v_0 + \nabla_y^S v_1)) & \\ \qquad = -D(y)(\nabla_x u_0 + \nabla_y u_1) \cdot \gamma = k\left[u_1 - \frac{v_1}{K}\right] & \text{on} \partial\Sigma^0 \\ y \to (u_1(y), v_1(y)) & Y - \text{periodic}, \end{cases} \tag{8}$$

The linearity helps us deduce that

$$u_1(t, x, y) = \chi(y) \cdot \nabla_x u_0$$

and

$$v_1(t, x, y) = \omega(y) \cdot \nabla_x u_0$$

The above representation of (u_1, v_1) results in the following coupled cell problem, for $i \in \{1, \cdots, n\}$

Cell Problem

$$\begin{cases} b(y) \cdot \nabla_y \chi_i - div_y(D(y)(\nabla_y \chi_i + e_i)) = (b^* - b(y)) \cdot e_i & \text{in } Y^0, \\ b^S(y) \cdot \nabla_y^S \omega_i - div_y^S(D^S(y)(\nabla_y^S \omega_i + K e_i)) & \\ = K(b^* - b^S(y)) \cdot e_i + \kappa \left(\chi_i - \frac{1}{K}\omega_i\right) & \text{on } \partial\Sigma^0, \\ -D(y)(\nabla_y \chi_i + e_i) \cdot \gamma = \kappa \left(\chi_i - \frac{1}{K}\omega_i\right) & \text{on } \partial\Sigma^0, \\ y \to (\chi_i(y), \omega_i(y)) & Y - \text{periodic}, \end{cases} \tag{9}$$

Using the Fredholm result, we get the existence of (χ_i, ω_i) provided

$$b^* = \frac{\int\limits_{Y^0} b(y)\, dy + K \int\limits_{\partial\Sigma^0} b^S(y)\, d\sigma(y)}{|Y^0| + K|\partial\Sigma^0|_{n-1}} \tag{10}$$

Cascade of Systems contd.

Co-efficients of ε^0

$$\begin{cases} \partial_t u_0 - b^* \cdot \nabla_x u_1 + b(y) \cdot (\nabla_x u_1 + \nabla_y u_2) \\ -div_x(D(y)(\nabla_x u_0 + \nabla_y u_1)) - div_y(D(y)(\nabla_x u_1 + \nabla_y u_2)) = 0 & \text{in } Y^0, \\ \partial_t v_0 - b^* \cdot \nabla_x v_1 + b^S(y) \cdot (\nabla_x^S u_1 + \nabla_y^S u_2) \\ -div_x(GD^S(y)(G\nabla_x v_0 + \nabla_y^S v_1)) - div_y^S(D^S(y)(G\nabla_x v_1 + \nabla_y^S v_2)) \\ = -D(y)(\nabla_y u_2 + \nabla_x u_1) \cdot \gamma = \kappa \left[u_2 - \frac{1}{K} v_2\right] & \text{on } \partial\Sigma^0, \\ y \to (u_2(y), v_2(y)) & Y - \text{periodic}, \end{cases} \tag{11}$$

Homogenized equation

The compatibility condition for (u_2, v_2) yields the homogenized equation.

$$\begin{cases} K_d\, \partial_t u_0 = div_x \left(A^* \nabla_x u_0\right) \ \text{ in } \ (0,T) \times \mathbb{R}^n \\ \\ K_d\, u_0(0,x) = |Y^0| u^0(x) + |\partial \Sigma^0|_{n-1} v^0(x), \quad x \in \mathbb{R}^n \end{cases} \tag{12}$$

Where, $K_d = |Y^0| + K |\partial \Sigma^0|_{n-1}$, the dispersion tensor A^* is given by

$$\begin{aligned} A^*_{ij} = & \int_{Y^0} D \left(\nabla_y \chi_i + e_i\right) \cdot \left(\nabla_y \chi_j + e_j\right) \, dy \\ & + \kappa \int_{\partial \Sigma^0} \left(\chi_i - K^{-1} \omega_i\right) \left(\chi_j - K^{-1} \omega_j\right) \, d\sigma(y) \\ & + K \int_{\partial \Sigma^0} D^S \left(G e_i + K^{-1} \nabla^S_y \omega_i\right) \cdot \left(G e_j + K^{-1} \nabla^S_y \omega_j\right) \, d\sigma(y) \end{aligned} \tag{13}$$

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It should be noted that we have used the information we know of (u_1, v_1) in terms of (χ, ω). A^* is symmetrized as anti-symmetric part doesn't contribute.

Equivalent homogenized equation

Define $\tilde{u}_\varepsilon(t,x) = u_0(t, x - \frac{b^*}{\varepsilon}t)$. Then, it is solution of

$$\begin{cases} \partial_t \tilde{u}_\varepsilon + \frac{1}{\varepsilon} b^* \cdot \nabla \tilde{u}_\varepsilon = {K_d}^{-1} div_x \left(A^* \nabla_x \tilde{u}_\varepsilon \right) \text{ in } (0,T) \times \mathbb{R}^n \\ \\ K_d \, \tilde{u}_\varepsilon(0,x) = |Y^0| u^0(x) + |\partial \Sigma^0|_{n-1} v^0(x), \quad x \in \mathbb{R}^n \end{cases} \quad (14)$$

Numerical Study using FreeFem++

Numerical tests were done using FreeFem++.

Using Lagrange P1 finite elements.

Number of vertices = 23894.

The solid obstacles are isolated circular disks of radius 0.2

The velocity field $b(y)$ is generated by solving the following filtration problem in the fluid part Y^0 of the unit cell Y. For simplicity, we have taken the surface convection b^S to be zero.

$$\begin{cases} \nabla_y p - \Delta_y b = e_i & \text{in } Y^0, \\ div_y b = 0 & \text{in } Y^0, \\ b = 0 & \text{on } \partial\Sigma^0, \\ p, b & Y^0 - periodic \end{cases} \tag{15}$$

Calculations were done to see the effect of the variation in κ and D^S on the effective co-efficients. They are seen to show a stable asymptotic behaviour.

Behavior of the cell solution

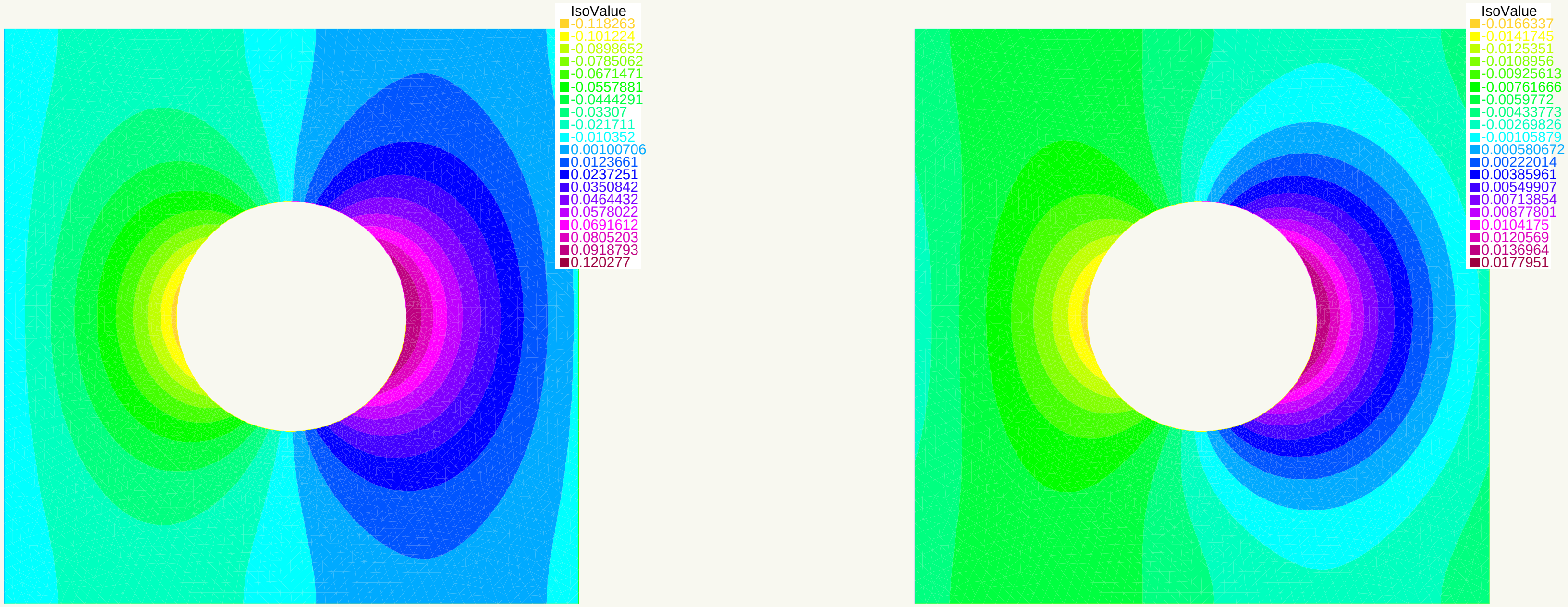


Figure 1: The cell solution χ_1: Left, reference value $\kappa = \kappa^0$; Right, $\kappa = 5\kappa^0$

Behavior of the cell solution contd.

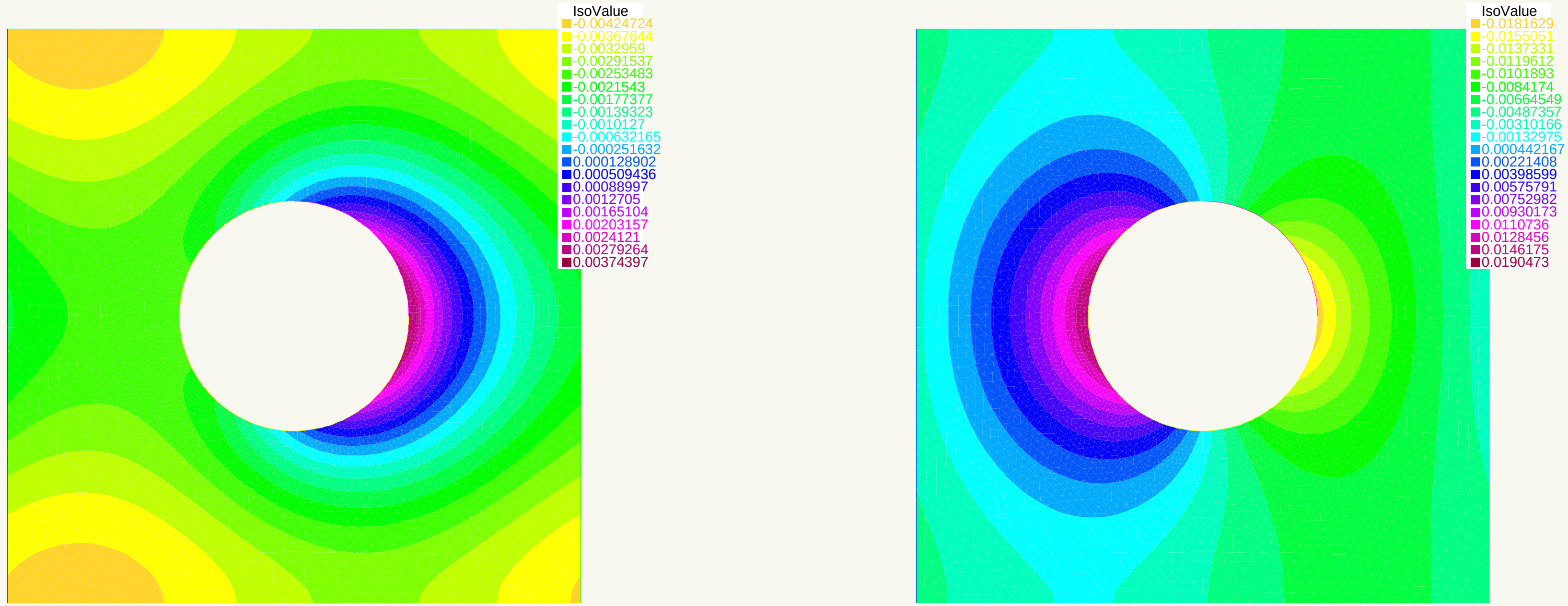
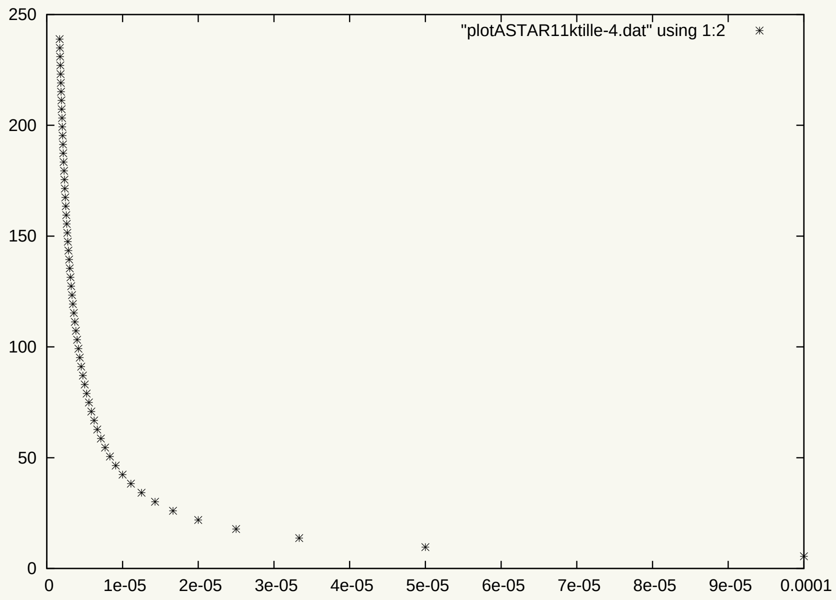


Figure 2: The cell solution χ_1: Left, $\kappa = 6\kappa^0$; Right, $\kappa = 8\kappa^0$

Behavior of logitudinal dispersion with variation in reaction rate



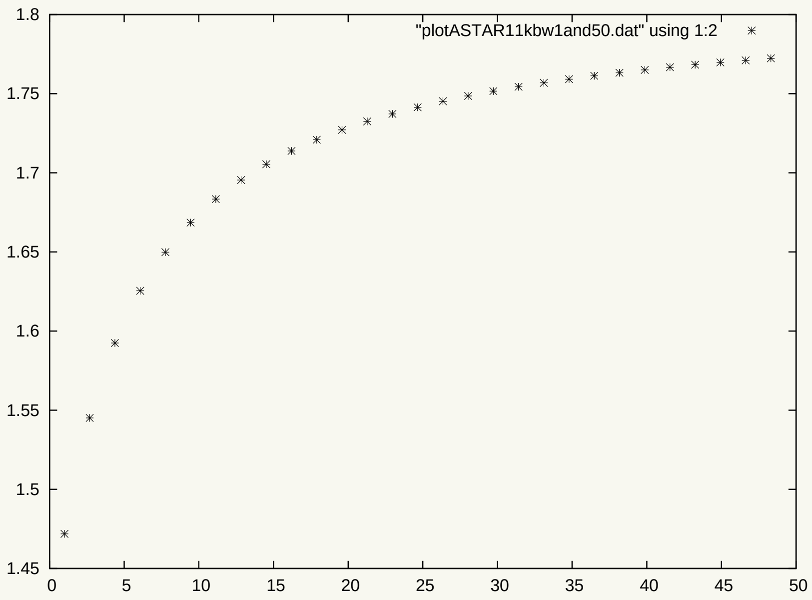


Figure 3: The variation of effective longitudinal diffusion: Left, κ tending to 0; Right, κ increasing in magnitude

Behavior of transverse dispersion with variation in reaction rate

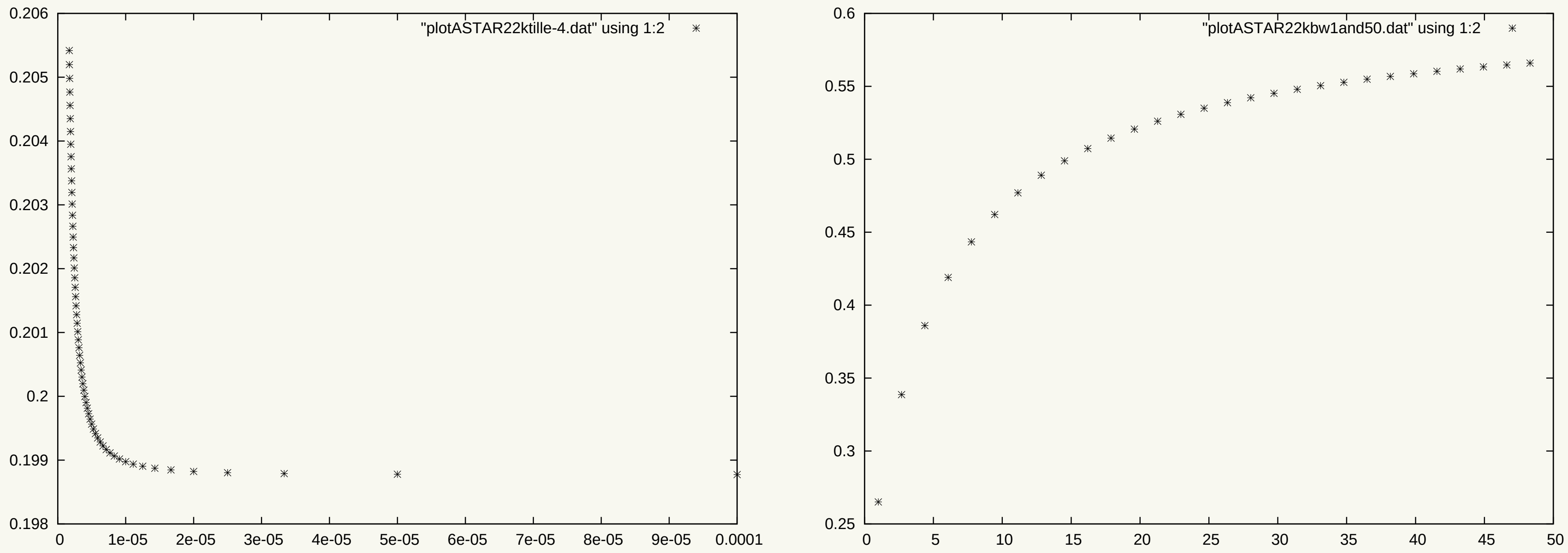
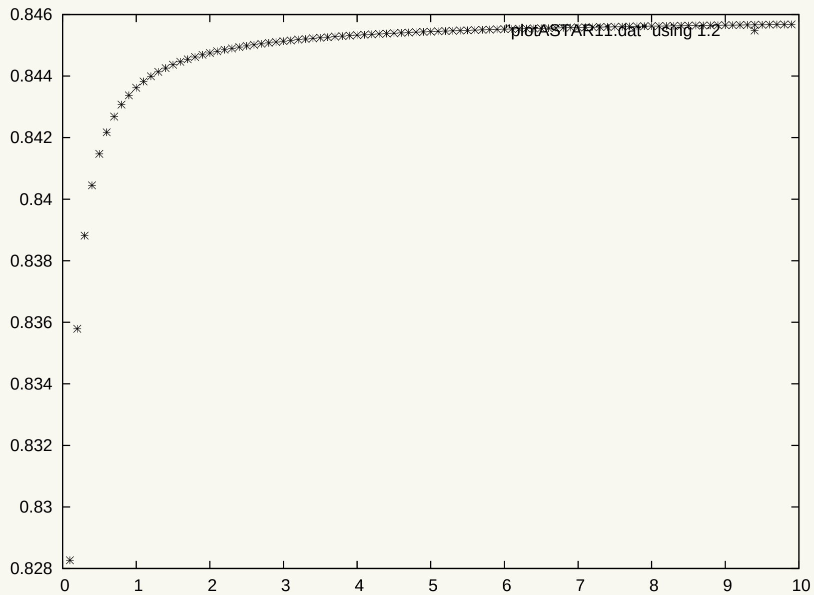


Figure 4: The variation of effective transverse diffusion: Left, κ tending to 0; Right, κ increasing in magnitude

Behavior of effective dispersion with variation in surface diffusion



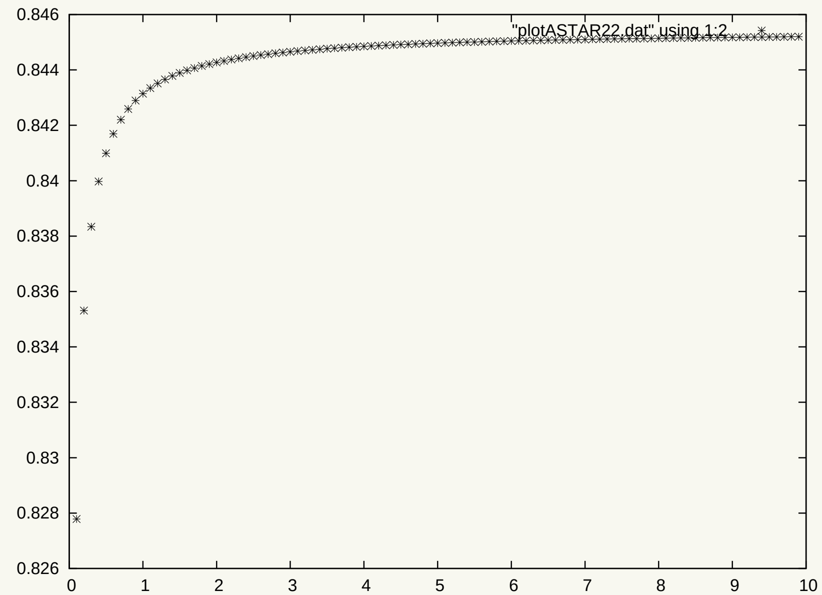


Figure 5: The variation of effective diffusion with D^S increasing in magnitude: Left, longitudinal diffusion; Right, transverse diffusion

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- Study of the effective behaviour of the model with the variation in the surface diffusion D^S. The case $D^S = 0$ exactly matches with the previous results on effective dispersion with no surface diffusion. When $D^S \to \infty$, the transverse and longitudinal dispersion exhibit a stable asymptotic behaviour with transverse dispersion remaining almost equal to longitudinal dispersion.
- The Mathematical justification of the upscaling using two-scale convergence with drift upon introducing 2-scale convergence with drift on surfaces.

References

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