Investigating the role of tortuosity in the Kozeny-Carman equation

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The objective of this work is to evaluate the role of tortuosity on fitting simulation data to the Kozeny-Carman equation.

Outline:

- Review of Kozeny-Carman eqn.
- Review of different tortuosity definitions
- Obtaining permeability and tortuosity from pore-scale modeling
- Example geometries: in-line array, staggered-array, overlapping squares
- Fitting simulation data to Kozeny-Carman eqn.
- Conclusion

Kozeny-Carman equation

- derived from theory by treating porous media as comprised of parallel and uniform channels
- relates permeability to pore-structure properties:

$$k = \frac{\phi^3}{cS^2} = \frac{\phi^3}{\beta\tau^2 S^2} \quad (1)$$

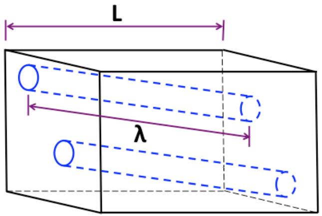

Figure: Tortuosity: $\tau = \lambda/L$

Carman, 1937 & 1939:

Shape of cross-section	Kozeny constant, c
Circle	2
Ellipse (major/minor = 2)	2.13
Ellipse (major/minor = 10)	2.45
Rectangle (width/height = 1)	1.78
Rectangle (width/height = 2)	1.94
Rectangle (width/height = 10)	2.65
Rectangle (width/height = ∞)	3

In granular beds, how can we compute tortuosity? Is it a function of porosity?

Past work on measuring tortuosity

Many authors have theoretically or empirically derived tortuosity as a function of porosity.

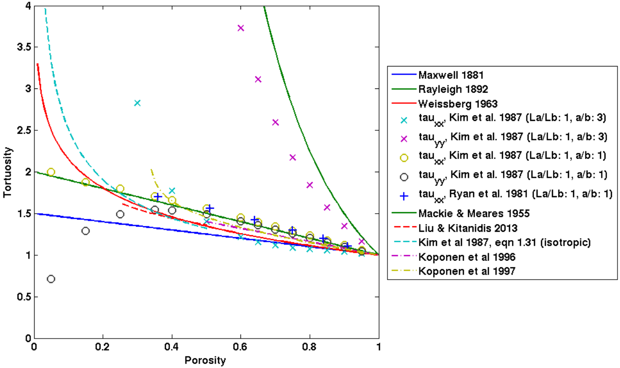

Figure: Porosity vs tortuosity trends from literature: generally, $\tau \geq 1$, and $\tau \rightarrow 1$ as $\phi \rightarrow 1$.

Study	Samples Considered	Tortuosity vs Porosity Fit	Tortuosity Type
Maxwell, 1881*	array of spheres (3D), dilute suspension, non-conducting	$\tau = 1 + \frac{1}{2}(1-\phi)$	electrical conductivity
Rayleigh, 1892*	array of cylinders (2D)	$\tau = 2 - \phi$	diffusion?
Mackie & Meares, 1955**	diffusion of electrolytes in membrane	$\tau = (\frac{2-\phi}{\phi})^2$	diffusion
Weissberg, 1963	bed of uniform spheres (applicable to overlapping, non-uniform spheres)	$\tau = 1 - \frac{1}{2} ln\phi$	diffusion
Kim et al, 1987	isotropic system, $0 < \phi < 0.5$	$\tau = \phi^{-0.4}$	diffusion
Koponen et al, 1996	2D random overlapping mono-sized squares, $0.5 < \phi < 1$	$\tau = 1 + 0.8(1-\phi)$	hydraulic
Koponen et al, 1997	2D random overlapping mono-sized squares, $0.4 < \phi < 1$	$\tau = 1 + a\frac{1-\phi}{(\phi-\phi_c)^m}$, $a = 0.65,\ m = 0.19$	hydraulic
Matyka et al, 2008	2D random overlapping mono-sized squares	$\tau - 1 \propto R\frac{S}{\phi}$	hydraulic
Duda et al, 2011	2D freely overlapping squares	$\tau - 1 \propto (1-\phi)^\gamma$, $\gamma = 1/2$	hydraulic
Pisani, 2011	random, partial overlapping shapes	$\tau = \frac{1}{1-\alpha(1-\phi)}$, α=shape factor	diffusion
Liu & Kitanidis, 2013	isotropic grain (spherical), staggered $0.25 < \phi < 0.5$	$\tau = \phi^{1-m} + 0.15$, $m = 1.28$	electrical conductivity

* as referenced in Ochoa-Tapia et al 1994

** as referenced in Shen & Chen 2007, and Boudreau 1996

However recent work states that *any* definition of tortuosity (i.e., hydraulic and diffusive) is *not* a function of porosity but rather a **function of the pore geometry only** and is a **tensorial property** (*Valdes-Parada et al. 2011*, *Liu & Kitanidis 2013*).

Different forms of tortuosity

The tortuous nature of fluid flow through porous media:

$$\tau_h = \frac{\text{path traveled by fluid}}{\text{domain unit length}}$$

The tortuous nature of a solute diffusing through porous media:

$$\tau_d = \frac{\text{path traveled by diffusing solute}}{\text{domain unit length}}$$

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The Kozeny-Carman equation uses hydraulic tortuosity:

$$k = \frac{\phi^3}{c{\tau_h}^2 S^2} = \frac{\phi^3}{\beta S^2}$$

Effective diffusivity is the binary diffusion scaled by diffusive tortuosity

$$\mathbf{D_{eff}} = \frac{D}{\boldsymbol{\tau}_\mathbf{d}} = D\boldsymbol{\tau}_\mathbf{d}'$$

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Past Work on measuring τ_h and/or fitting simulated data to KC-eqn:

- overlapping squares (Koponen et al 1996/7, Matyka et al 2008, Duda et al 2011)
- 3D body-centered-cubic unit cells (Ebrahimi Khabbazi et al 2013)

Past Work on measuring $\boldsymbol{\tau}_{\mathbf{d}}$ or $\mathbf{D_{eff}}$:

- in cellular geometry (Ochoa et al. 1987)
- in porous wick (Beyhaghi & Pillai 2011)
- in packed beds and unconsolidated porous media (Kim et al. 1987, Quintard 1993)

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$$\boxed{\tau_h \neq \tau_d}$$

Work flow of this research

- represent porous media in domain, using simple geometries
- do **pore-scale modeling**:
  - solve Stokes flow $\Rightarrow$ obtain pressure and velocity fields $\Rightarrow$ compute permeability tensor and hydraulic tortuosity
  - solve Closure Variable problem $\Rightarrow$ obtain diffusive tortuosity tensor
- compare the hydraulic and diffusive tortuosity results
- fit simulation results (permeability, hydraulic tortuosity) to Kozeny-Carman equation

Solve Stokes flow → obtain velocities, permeability

Wang et al. 2013.

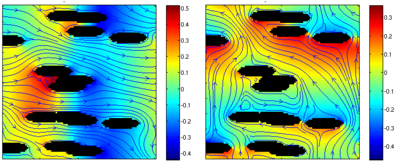
1. Solve Stokes flow in pore space of media ⇒ obtain p and $\mathbf{v}$.

$$\mu\nabla^2\mathbf{v} - \nabla p + \rho\mathbf{g} = 0 \quad (2)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (3)$$

2. Assuming Darcy's equation is valid ($\mathbf{u} = -\frac{\mathbf{K}}{\mu}(\nabla p + \rho\mathbf{g})$), compute $\mathbf{K}$ from $\mathbf{u} = \phi\langle\mathbf{v}\rangle$ ($\nabla p = 0$ in REV).

Pressure and flow fields in 0.05mm x 0.05mm REV,



(a) Flux in X-direction (b) Flux in Y-direction

and the resulting $\mathbf{K}$ in m^2 is

$$\begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix} = \begin{bmatrix} 6.03x10^{-12} & -1.15x10^{-12} \\ -1.15x10^{-12} & 2.86x10^{-12} \end{bmatrix}.$$

Solve Stokes flow → obtain velocities, hydraulic tortuosity

The hydraulic tortuosity can be computed from fluid velocity fields*,

$$\tau_{h_x} = \frac{\langle\sqrt{v_x^2 + v_y^2}\rangle}{\langle|v_x|\rangle}, \quad \tau_{h_y} = \frac{\langle\sqrt{v_x^2 + v_y^2}\rangle}{\langle|v_y|\rangle} \tag{4}$$

In other words,

$$\tau_{h_x} = \frac{\sum_{i,j} \sqrt{v_x(i,j)^2 + v_y(i,j)^2}}{\sum_{i,j} |v_x(i,j)|}, \quad \tau_{h_y} = \frac{\sum_{i,j} \sqrt{v_x(i,j)^2 + v_y(i,j)^2}}{\sum_{i,j} |v_y(i,j)|}$$

* Koponen et al 1997, Duda et al 2011.

Solve closure problem* → obtain diffusive tortuosity

- diffusive transport at pore-scale:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D_m \nabla c) \tag{5}$$

- use theory of volume averaging to define $\langle c \rangle^f$
- local spatial deviation $\tilde{c} = c - \langle c \rangle^f$
- $\tilde{c}$ is a linear function of $\langle c \rangle^f$, so is given by

$$\tilde{c} = \mathbf{b} \cdot \nabla \langle c \rangle^f \tag{6}$$

- $\mathbf{b}$ is a vector field that maps $\nabla \langle c \rangle^f$ onto $\tilde{c}$
- closed form of local volume average transport eqn.,

$$\phi \frac{\partial \langle c \rangle^f}{\partial t} = \nabla \cdot \left(\phi \mathbf{D_{eff}} \cdot \nabla \langle c \rangle^f \right) \tag{7}$$

where

$$\mathbf{D_{eff}} := D_m \left(\mathbf{I} + \frac{1}{V_f} \int_{A_{fs}} \mathbf{n} \cdot \mathbf{b} dA \right) \tag{8}$$

- by convention, $\mathbf{D}_{eff} / D_m = 1/\boldsymbol{\tau}$

Solve closure problem* $\rightarrow$ obtain diffusive tortuosity

The closure problem* is given by:

$$\nabla^2 \mathbf{b} = 0 \tag{9}$$

$$\mathbf{n}_{fs} \cdot \nabla \mathbf{b} = -\mathbf{n}_{fs} \quad \text{at } A_{fs} \tag{10}$$

$$\mathbf{b}(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}(\mathbf{r}) \quad i = 1, 2 \tag{11}$$

$$\langle \mathbf{b} \rangle^f = 0 \tag{12}$$

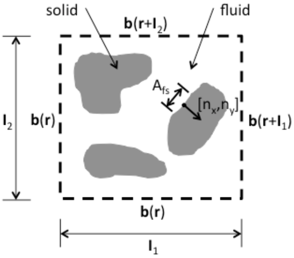


Figure: Closure Problem

The tortuosity (factor) tensor is

$$\boldsymbol{\tau}' = \mathbf{I} + \frac{1}{V_f} \int_{A_{fs}} \mathbf{n}_{fs} \cdot \mathbf{b} dA \tag{13}$$

* Valdes-Parada et al. 2011, Beyhaghi & Pillai 2011, Quintard 1993, Kim et al. 1987, Ochoa et al. 1987.

Solve closure problem* $\rightarrow$ obtain diffusive tortuosity

In 2D, the tensor components are

$$\boldsymbol{\tau'} = \begin{bmatrix} \tau'_{xx} & \tau'_{xy} \\ \tau'_{yx} & \tau'_{yy} \end{bmatrix} = \begin{bmatrix} 1 + \frac{1}{V_f}\int_{A_{fs}} n_x b_x dA & \frac{1}{V_f}\int_{A_{fs}} n_x b_y dA \\ \frac{1}{V_f}\int_{A_{fs}} n_y b_x dA & 1 + \frac{1}{V_f}\int_{A_{fs}} n_y b_y dA \end{bmatrix} \tag{14}$$

The Laplace equation $\nabla^2 \mathbf{b} = 0$ is used to solve the closure variable $\mathbf{b}$, where $\mathbf{b} = b_x \mathbf{i} + b_y \mathbf{j}$. In 2D, these spatial derivatives are

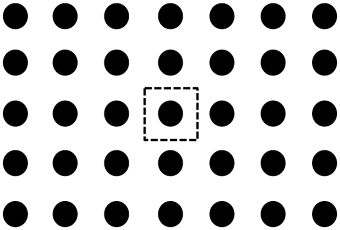
$$\nabla^2 b_x = \frac{\partial}{\partial x}\left(\frac{\partial b_x}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial b_x}{\partial y}\right) = 0 \tag{15}$$

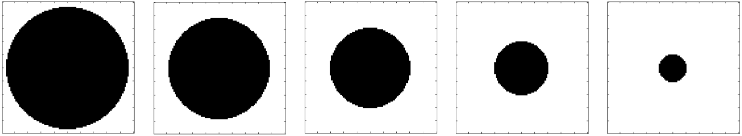
$$\nabla^2 b_y = \frac{\partial}{\partial x}\left(\frac{\partial b_y}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial b_y}{\partial y}\right) = 0 \tag{16}$$

In this work, we solve these PDEs using finite difference.

* Valdes-Parada et al. 2011, Beyhaghi & Pillai 2011, Quintard 1993, Kim et al. 1987, Ochoa et al. 1987.

Example 1: In-line array of uniform shapes

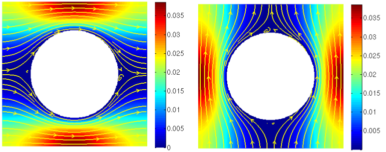




(a) $\phi = 0.32$ (b) $\phi = 0.54$ (c) $\phi = 0.71$ (d) $\phi = 0.87$ (e) $\phi = 0.97$

In-line array of circles; $\phi = 0.71$

Hydraulic tortuosity:



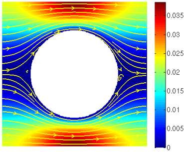
(a) Flow in x-dir. (b) Flow in y-dir.

Figure: Magnitude of pressure gradients (i.e., velocities) with hydraulic flow lines

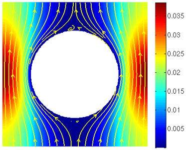
Diffusive tortuosity:

In-line array of circles; $\phi = 0.71$

Hydraulic tortuosity:



(a) Flow in x-dir.



(b) Flow in y-dir.

Figure: Magnitude of pressure gradients (i.e., velocities) with hydraulic flow lines

$$\tau_{hx} = \langle\sqrt{v_x^2 + v_y^2}\rangle / \langle|v_x|\rangle = \mathbf{1.02}$$

$$\tau_{hy} = \langle\sqrt{v_x^2 + v_y^2}\rangle / \langle|v_y|\rangle = \mathbf{1.02}$$

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In-line array of circles; $\phi = 0.71$

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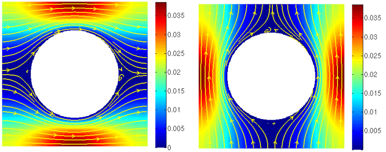

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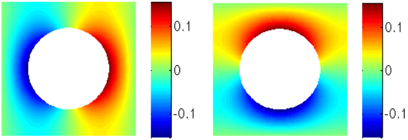

(a) b_x (b) b_y

Figure: Closure variable fields used to obtain surface intergrals

$$\tau_{hx} = \langle \sqrt{v_x^2 + v_y^2} \rangle / \langle |v_x| \rangle = \mathbf{1.02}$$

$$\tau_{hy} = \langle \sqrt{v_x^2 + v_y^2} \rangle / \langle |v_y| \rangle = \mathbf{1.02}$$

In-line array of circles; $\phi = 0.71$

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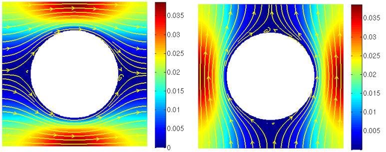

(a) Flow in x-dir. (b) Flow in y-dir.

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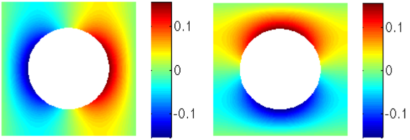
Diffusive tortuosity:



(a) b_x (b) b_y

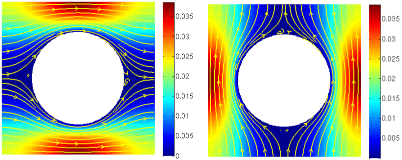
Figure: Closure variable fields used to obtain surface intergrals

$$\tau_{dx} = \left(1 + \frac{1}{V_f}\int_{A_{fs}} n_x b_x dA\right)^{-1} = \mathbf{1.29}$$

$$\tau_{dy} = \left(1 + \frac{1}{V_f}\int_{A_{fs}} n_y b_y dA\right)^{-1} = \mathbf{1.29}$$

In-line array of circles; $\phi = 0.71$

Hydraulic tortuosity:

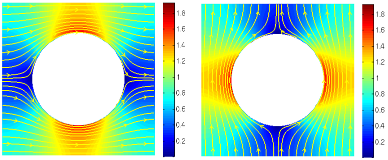


(a) Flow in x-dir. (b) Flow in y-dir.

Figure: Magnitude of pressure gradients (i.e., velocities) with hydraulic flow lines

$$\tau_{hx} = 1.0185$$
$$\tau_{hy} = 1.0185$$

Diffusive tortuosity:

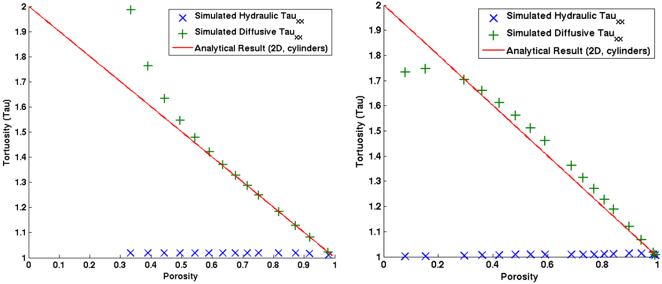


(a) $\sqrt{\frac{\partial c_x}{\partial x}^2 + \frac{\partial c_x}{\partial y}^2}$ (b) $\sqrt{\frac{\partial c_y}{\partial x}^2 + \frac{\partial c_y}{\partial y}^2}$

Figure: Magnitude of concentration gradients with diffusive flow lines

$$\tau_{dx} = 1.2866$$
$$\tau_{dy} = 1.2866$$

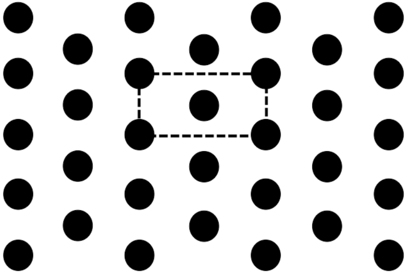
In-line array of circles and squares; $0 < \phi < 1$

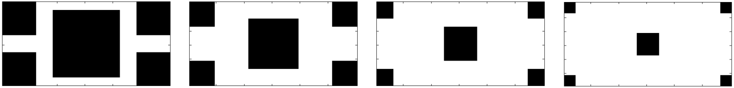


(a) Circle (b) Square

Figure: Porosity vs. tortuosity: diffusive tortuosity trend follows analytical solution from Rayleigh 1892 until inadequate mesh refinement, while hydraulic tortuosity is independent of porosity for this geometry.

Example 2: Staggered-array of uniform shapes

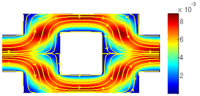




(a) $\phi = 0.36$ (b) $\phi = 0.64$ (c) $\phi = 0.84$ (d) $\phi = 0.93$

Staggered-array of squares; $\phi = 0.716$

Hydraulic tortuosity:

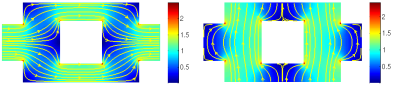


(a) Flow in x-dir. (b) Flow in y-dir.

Figure: Magnitude of pressure gradients (i.e., velocities) with hydraulic flow lines

$$\tau_{hx} = 1.37$$
$$\tau_{hy} = 1.06$$

Diffusive tortuosity:

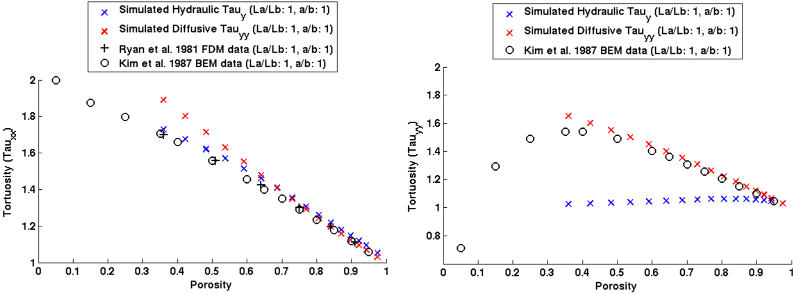


(a) X-Prob (b) Y-Prob

Figure: Magnitude of concentration gradients with diffusive flow lines

$$\tau_{dxx} = 1.37$$
$$\tau_{dyy} = 1.32$$

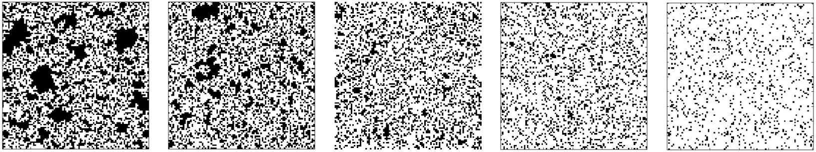
Staggered-array of squares; $0.35 < \phi < 1$



(a) τ_{xx} (b) τ_{yy}

Figure: Tortuosity vs. porosity trends for staggered-array of squares: hydraulic flow is predominantly parallel to driving force, unless an obstacle prevents a linear flow path.

Example 3: Randomly distributed, freely overlapping squares

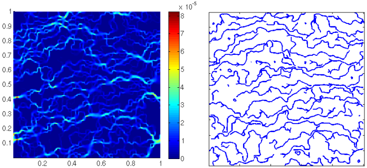


(a) $\phi = 0.53$ (b) $\phi = 0.61$ (c) $\phi = 0.70$ (d) $\phi = 0.80$ (e) $\phi = 0.90$

Figure: Various pore-structure geometries. Notice isolated fluid sites are filled in, causing larger, non-uniform shapes. Square length = 0.01 x domain length (Koza et al 2000, Duda et al 2011).

Overlapping Squares; $\phi = 0.7$

Hydraulic tortuosity:

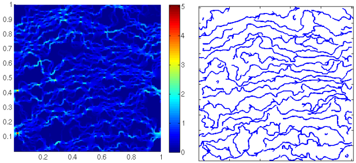


(a) $\sqrt{\frac{\partial p_x}{\partial x}^2 + \frac{\partial p_x}{\partial y}^2}$ (b) Hydr. lines

Figure: Magnitude of pressure gradients (i.e., velocities) and hydraulic flow lines for X-problem

$$\tau_{hx} = 1.3228$$

Diffusive tortuosity:

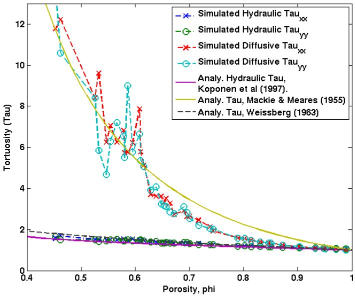


(a) $\sqrt{\frac{\partial c_x}{\partial x}^2 + \frac{\partial c_x}{\partial y}^2}$ (b) Diff. lines

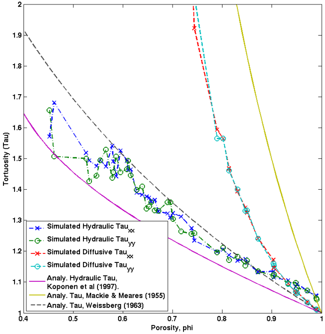
Figure: Magnitude of concentration gradients and diffusive flow lines for X-problem

$$\tau_{dx} = 2.6596$$

Overlapping Squares; $0.45 < \phi < 1$



(a) Plot of full simulated data



(b) Close-up plot of simulated data

Figure: Porosity vs tortuosity for pore-structures of overlapping squares: diffusive tortuosity $>>$ than hydraulic tortuosity at low porosities

Overlapping Squares: Anisotropy of τ_h and τ_d

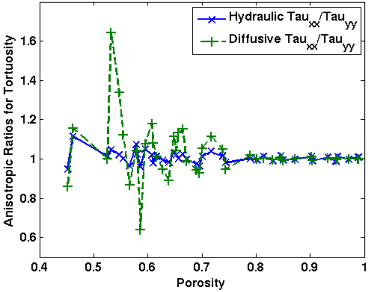
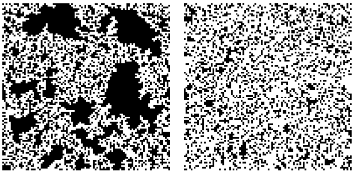


Figure: Anisotropic ratio for hydraulic and diffusive tortuosity: the degree of anisotropy for hydraulic flow and diffusive flow ≈ 1 for higher porosities, while the diffusive flow is anisotropic at lower porosities.

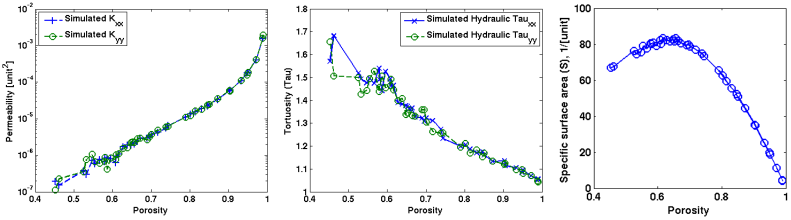


(a) $\phi = 0.4525$ (b) $\phi = 0.7005$

Figure: Pore-structures of lower porosity exhibit more isolated fluid site that are filled it, thus creating non-uniform distribution of solids in overlapping squares configuration. This impacts degree of anisotropy.

Computing Kozeny constant for Ex. 3: overlapping squares

Overlapping Squares: Kozeny constant



(a) Permeability k (b) Hydraulic tortuosity τ (c) Spec. surface S

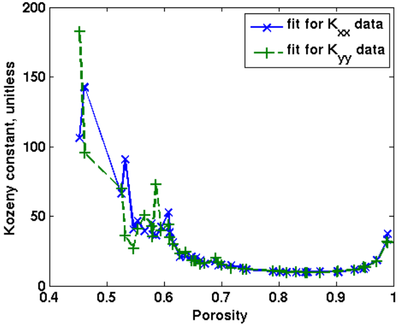
Figure: Simulated data

The Kozeny constant c, or shape factor β, can be computed by

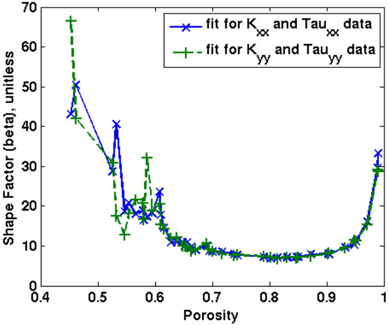
$$k = \frac{\phi^3}{cS^2} = \frac{\phi^3}{\beta\tau^2 S^2} \tag{17}$$

where $S = \frac{A_{f-s}}{V_{tot}}$ (i.e., V_{tot} is the fluid and solid space combined).

Overlapping Squares: Kozeny constant



(a) Kozeny constant, c



(b) Shape factor, β

Figure: Parameters that fit simulated data to Kozeny-Carman equation. Kozeny constant and shape factor do not change within a porosity interval of $0.65 < \phi < 0.95$.

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- The diffusive tortuosity is able to capture the anisotropic nature of pore geometry more readily that hydraulic tortuosity
- The Kozeny-Carman eqn. proposes a relationship between permeability, porosity, specific surface area, and *hydraulic* tortuosity

Questions?

Appendix

Obtaining full permeability tensor

The compute the full permeability tensor, consider the pore structure:

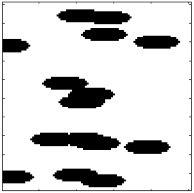


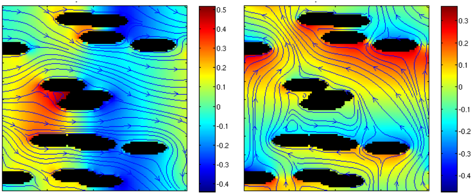
Figure: Pore structure example, $\phi = 0.82$

We assume this pore structure is a representative elementary volume (REV), which implies the properties measured from this sample represents the properties of the porous media the sample came from. The rest of the domain is made up of repeating structures of this figure. As such, we use periodic boundary conditions on all external sides.

Slow and steady flow is modeled through the pore space by Stokes equation,

$$0 = \rho g_i + \frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 v_i}{\partial x_j \partial x_j} \tag{18}$$

where the solution for pressure p and velocity v_i are obtained for a specified flow driving force, g_i. The spatial average pore-space velocity $\hat{v}_i$ can be computed for each flow scenario.



(a) Driving force in X-direction: $(g_x, g_y) = (1, 0)$. $(\hat{v}_x, \hat{v}_y) = (?, ?)$

(b) Driving force in Y-direction: $(g_x, g_y) = (0, 1)$. $(\hat{v}_x, \hat{v}_y) = (?, ?)$

Figure: Pressure and velocity solutions after solving Stokes flow through

Then, we use Darcy's equation to describe flow at the macro-scale,

$$u_i = -\frac{k_{ij}}{\mu}\left(\frac{\partial P}{\partial x_i} + \rho g_i\right) \tag{19}$$

where u_i is the Darcy's velocity of the pore structure ($u_i = \hat{v}_i/\phi$), and where k_{ij} and $\partial P/\partial x_i$ are with respect to the whole structure (i.e., the REV). In 2D, Darcy's equation is

$$\begin{bmatrix} u_x \\ u_y \end{bmatrix} = -\frac{1}{\mu}\begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix}\left(\begin{bmatrix} \frac{\partial P}{\partial x} \\ \frac{\partial P}{\partial y} \end{bmatrix} + \rho\begin{bmatrix} g_x \\ g_y \end{bmatrix}\right) \tag{20}$$

and since we assume periodic boundaries on all external sides of the pore structure, the pressure gradients are

$$\frac{\partial P}{\partial x}|_{REV} = 0, \quad \frac{\partial P}{\partial y}|_{REV} = 0 \tag{21}$$

thus equation 20 becomes

$$\begin{bmatrix} u_x \\ u_y \end{bmatrix} = -\frac{\rho}{\mu}\begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix}\begin{bmatrix} g_x \\ g_y \end{bmatrix} \tag{22}$$

When $(g_x, g_y) = (1, 0)$, equation 22 is

$$\boxed{\begin{bmatrix} \hat{v}_x/\phi \\ \hat{v}_y/\phi \end{bmatrix} = -\begin{bmatrix} k_{xx} \\ k_{yx} \end{bmatrix}} \tag{23}$$

and when $(g_x, g_y) = (0, 1)$, equation 22 is

$$\boxed{\begin{bmatrix} \hat{v}_x/\phi \\ \hat{v}_y/\phi \end{bmatrix} = -\begin{bmatrix} k_{xy} \\ k_{yy} \end{bmatrix}} \tag{24}$$

where $\rho/\mu = 1$, and $u_i = \hat{v}_i/\phi$.
In our pore structure example, the resulting permeability tensor is

$$\begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix} = \begin{bmatrix} 0.0025612 & -0.00045863 \\ -0.00045862 & 0.00099666 \end{bmatrix} \tag{25}$$

To conclude, the full permeability tensor can be computed by using the spatial average pore-space velocity $\hat{v}_i$ obtained by solving Stokes flow for two different driving force scenarios.

Solve closure problem* $\longrightarrow$ obtain diffusive tortuosity

- diffusive transport at pore-scale:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D_m \nabla c) \tag{26}$$

- use theory of volume averaging to define $\langle c \rangle^f$
- local spatial deviation $\tilde{c} = c - \langle c \rangle^f$
- transport of local volume average, $\langle c \rangle^f$:

$$\phi \frac{\partial \langle c \rangle^f}{\partial t} = \nabla \cdot \left(\phi D_m \left(\nabla \langle c \rangle^f + \frac{1}{V_f} \int_{A_{fs}} \mathbf{n} \tilde{c} dA \right) \right) \tag{27}$$

- $\tilde{c}$ is a linear function of $\langle c \rangle^f$, so is given by

$$\tilde{c} = \mathbf{b} \cdot \nabla \langle c \rangle^f \tag{28}$$

- $\mathbf{b}$ is a vector field that maps $\nabla \langle c \rangle^f$ onto $\tilde{c}$

* Valdes-Parada et al. 2011, Beyhaghi & Pillai 2011, Quintard 1993, Kim et al. 1987, Ochoa et al. 1987.

- take the surface integral of $\tilde{c} = \mathbf{b} \cdot \nabla \langle c \rangle^f$
- substitute it into the local volume average transport eqn. to get its closed form,

$$\phi \frac{\partial \langle c \rangle^f}{\partial t} = \nabla \cdot \left(\phi \mathbf{D_{eff}} \cdot \nabla \langle c \rangle^f \right) \tag{29}$$

where

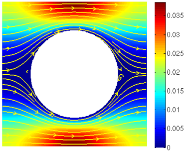
$$\mathbf{D_{eff}} := D_m \left(\mathbf{I} + \frac{1}{V_f} \int_{A_{fs}} \mathbf{n} \cdot \mathbf{b} dA \right) \tag{30}$$

- by convention, $D_{eff} / D_m = 1/\tau$, thus the tortuosity (or tortuosity factor) is computed by

$$\frac{1}{\boldsymbol{\tau}} = \boldsymbol{\tau}' = \left(\mathbf{I} + \frac{1}{V_f} \int_{A_{fs}} \mathbf{n} \cdot \mathbf{b} dA \right) \tag{31}$$

In-line array of circles; $\phi = 0.71$

Hydraulic tortuosity:



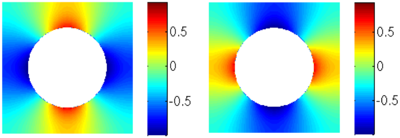
(a) Flow in x-dir. (b) Flow in y-dir.

Figure: Magnitude of pressure gradients (i.e., velocities) with hydraulic flow lines

$$\tau_{hx} = \langle \sqrt{v_x^2 + v_y^2} \rangle / \langle |v_x| \rangle = \mathbf{1.02}$$

$$\tau_{hy} = \langle \sqrt{v_x^2 + v_y^2} \rangle / \langle |v_y| \rangle = \mathbf{1.02}$$

Diffusive tortuosity:



(a) $\partial b_x / \partial x$ (b) $\partial b_y / \partial y$

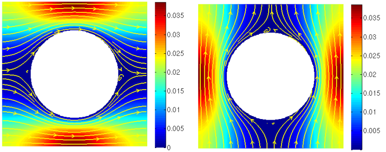
Figure: Closure variable gradients used to obtain volume integrals

$$\tau_{dx} = \left(1 + \frac{1}{V_f} \int_{V_f} \frac{\partial b_x}{\partial x} dV \right)^{-1}$$

$$\tau_{dy} = \left(1 + \frac{1}{V_f} \int_{V_f} \frac{\partial b_y}{\partial y} dV \right)^{-1}$$

In-line array of circles; $\phi = 0.71$

Hydraulic tortuosity:



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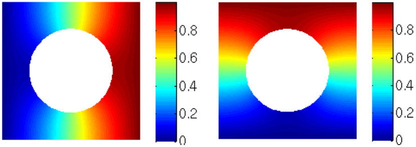
Diffusive tortuosity:



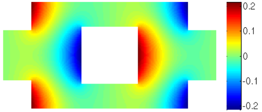
(a) $c_x = b_x + xs$ (b) $c_y = b_y + ys$

Figure: Concentration fields

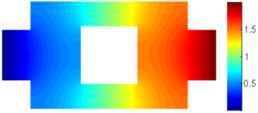
$$\tau_{dx} = \left(\frac{1}{V_f} \int_{V_f} \frac{\partial c_x}{\partial x} dV \right)^{-1}$$

$$\tau_{dy} = \left(\frac{1}{V_f} \int_{V_f} \frac{\partial c_y}{\partial y} dV \right)^{-1}$$

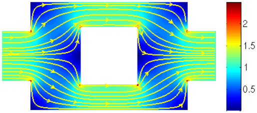
Staggered-array of squares; $\phi = 0.716$



(a) b_x

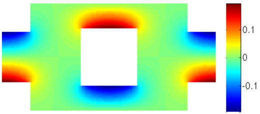


(b) $c_x = b_x + xs$

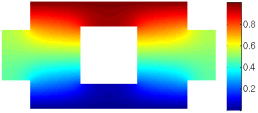


(c) $\sqrt{\frac{\partial c_x}{\partial x}^2 + \frac{\partial c_x}{\partial y}^2}$ with diffusive flow lines

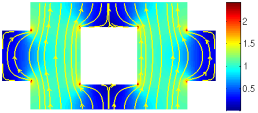
Figure: Diffusive tortuosity, τ_{xx}



(a) b_y



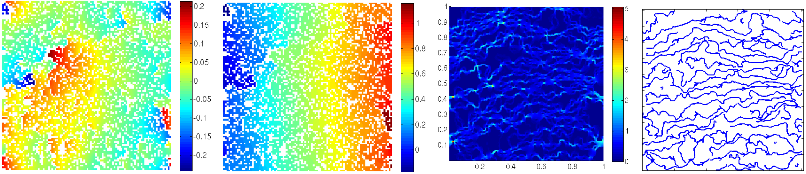
(b) $c_y = b_y + ys$



(c) $\sqrt{\frac{\partial c_y}{\partial x}^2 + \frac{\partial c_y}{\partial y}^2}$ with diffusive flow lines

Figure: Diffusive tortuosity, τ_{yy}

Overlapping Squares; $\phi = 0.7$



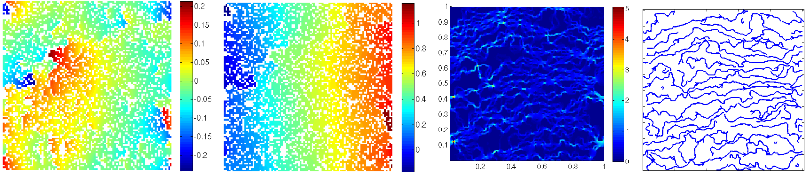
(a) b_x (b) $c_x = b_x + xs$ (c) $\sqrt{\frac{\partial c_x}{\partial x}^2 + \frac{\partial c_x}{\partial y}^2}$ (d) Diffu. lines

Figure: Scalar fields (closure variable b_x, concentration c_x), magnitude of concentration gradients, and diffusive flow lines for X-problem

$$\begin{bmatrix} \tau'_{xx} & \tau'_{xy} \\ \tau'_{yx} & \tau'_{yy} \end{bmatrix} = \mathbf{I} + \frac{1}{V_f}\int_{V_f} \nabla \mathbf{b} dV_f = \frac{1}{V_f}\int_{V_f} \nabla \mathbf{c} dV_f$$

$$\tau'_{xx} = \frac{1}{\tau_{dx}} = 1 + \frac{1}{V_f}\int_{V_f} \frac{\partial b_x}{\partial x} dV_f = \frac{1}{V_f}\int_{V_f} \frac{\partial c_x}{\partial x} dV_f$$

Overlapping Squares; $\phi = 0.7$



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$$\begin{bmatrix} 1 + \frac{1}{V_f}\sum_{i,j}\frac{\partial b_x}{\partial x}\delta V_f & \frac{1}{V_f}\sum_{i,j}\frac{\partial b_y}{\partial x}\delta V_f \\ \frac{1}{V_f}\sum_{i,j}\frac{\partial b_x}{\partial y}\delta V_f & 1 + \frac{1}{V_f}\sum_{i,j}\frac{\partial b_y}{\partial y}\delta V_f \end{bmatrix} = \begin{bmatrix} \frac{1}{V_f}\sum_{i,j}\frac{\partial c_x}{\partial x}\delta V_f & \frac{1}{V_f}\sum_{i,j}\frac{\partial c_y}{\partial x}\delta V_f \\ \frac{1}{V_f}\sum_{i,j}\frac{\partial c_x}{\partial y}\delta V_f & \frac{1}{V_f}\sum_{i,j}\frac{\partial c_y}{\partial y}\delta V_f \end{bmatrix}$$

Overlapping Squares: Anisotropy of k and τ_h

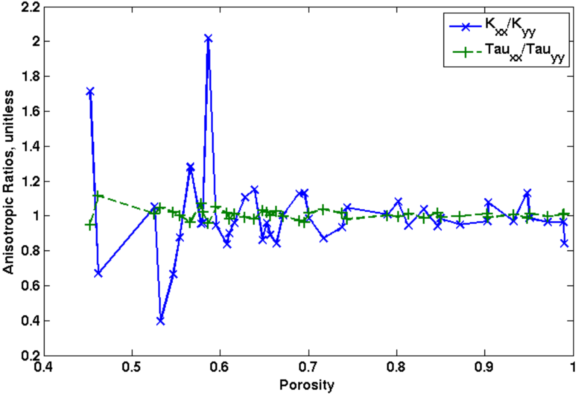

Figure: Comparison between the degree of anisotropy of permeability and hydraulic tortuosity: permeability is more anisotropic than hydraulic tortuosity at lower porosities