Past and present approaches to calculate hydrodynamic parameters in evolving porous media

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Past and present approaches to calculate hydrodynamic parameters in evolving porous media

Nadja Ray, Raphael Schulz, Andreas Rupp, Peter Knabner*

Core ideas

- Review of well established relations between porosity and hydrodynamic parameters
- Calculation and comparison with results from homogenization theory for 2D and 3D an-/isotropic geometries
- Discussion of mathematical bounds on hydrodynamic parameters
- Discussion of the relation between porosity and tortuosity

Abstract

The evolution of a porous medium’s underlying geometrical structure caused, for instance, by various heterogeneous reactions and biological processes significantly affects its hydrodynamic parameters, in particular its effective permeability and diffusivity. We review well-established relations between these hydrodynamic parameters and the medium’s porosity, such as the Kozeny-Carman equation. In order to capture the underlying geometric structure of the porous medium, geometric, shape, or tortuosity factors are often included into these relations. Contrarily, the method of homogenization directly enables to calculate the hydrodynamic parameters taking the underlying and evolving geometric structure into account. To this end flux solutions of supplementary cell problems that are defined on a representative elementary volume are integrated. We compare the results of this approach to the well-established relations and the well-known Voigt-Reiss or Hashin-Shtrikman bounds in the saturated case and illustrate them numerically. Finally, we discuss the relation between the porosity and tortuosity and briefly outline areas of possible future work.

1 Introduction

Flow and transport processes through porous media have an incredible long research history. Nevertheless, even the basic and most commonly used model equations and their parameters are still under investigation. In this paper, we review and compare well-established relations (experimentally, heuristically, theoretically, and mathematically derived) of the hydrodynamic parameters that are important components in the modeling of flow and transport in porous media.

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To start, we shortly review the underlying model equations: Fluid flow through a porous medium is classically described by Darcy’s law \( \mathbf{v} = -\frac{1}{\mu} K \nabla p \) with Darcy velocity \( \mathbf{v} \), pressure \( p \), viscosity \( \mu \) and effective hydraulic conductivity/permeability \( K \). Electric, thermal, and diffusive transport of chemical species are - in their simplest form - described by the following transport equation:

\[
- \nabla \cdot (D \nabla \psi) = 0
\]

with \( \psi \) describing the electric potential, the temperature, or the species’ concentration and the coefficient \( D \) representing the effective electric permittivity, effective thermal conductivity, or effective diffusion tensor for a chemical species, respectively.

The effective tensors \( K \) and \( D \) are in general very difficult to characterize, even if it is assumed that they are represented by scalars \( K_p \) and \( D_p \). Consequently, formulae in terms of simple features of the microstructure, e.g. the porosity are frequently used. Although giving often quite good approximations, in particular for models including parameters that are fitted by experimental data, changes in the composition and structure of the porous medium cannot be accounted for by porosity variations only. This is due to the fact that the effective tensors depend also on the detailed microstructure of the porous medium which is challenging to measure. Moreover, changes in particle distribution and grain shape and size modify the tortuosity and connectivity of the pore-space and therefore the bulk response of the medium.

Alternatively to explicit formulae for the tensors or their scalar representatives, (sharp) bounds on the effective tensors are used including the arithmetic or harmonic mean, Voigt-Reiss bounds, or Hashin-Shtrikman bounds.

## 2 Review of well-established relations

### 2.1 Dependency of the hydrodynamic parameters on the porosity

Finding suitable functional relations between the porosity and the effective tensors \( K, D \) or rather their scalar representatives \( K_p, D_p \) has been the topic of research for several decades. The most commonly used relation for the permeability \( K \) is the Kozeny-Carman equation (1). Kozeny [1] originally proposed \( K_p = \frac{c_0 \theta^3}{\sigma_1^2} \) as a functional dependence between the permeability and the porosity for a porous medium with straight tubes as pores with \( c_0 \) the so-called Kozeny’s constant depending slightly on the geometrical cross-section of the tubes, \( \theta \) the porosity of the porous medium, and \( \sigma_1 \) its specific surface per unit bulk volume. Replacing \( \sigma_1 \) by the specific surface \( \sigma \) with respect to the unit volume of the porous matrix, it holds \( \sigma_1 = (1 - \theta) \sigma \) [2, (2.6.3)] and Carman [3] reformulated the Kozeny equation as

\[
K_p = \frac{c_0}{\sigma^2} \frac{\theta^3}{(1 - \theta)^2}.
\]

Furthermore, Carman 1939 estimated the Kozeny constant \( c_0 \) to be equal to \( \frac{1}{5} \) giving the best agreement with experiments. Moreover, experiments suggest that the Kozeny coefficient \( c_0 = c_0(\theta) \) depends on the porosity \( \theta \) itself. Thus, Carman concludes that the equation (1) is not satisfied for very small porosities, e.g. clays [4].

Well known models for the gas diffusion \( D_p \) are reviewed in [5–7], see also (2) and the discussion below. An exclusive dependence on the gas diffusion coefficient in free air \( D_0 \) and the air filled porosity \( \theta \) is presumed by the following models:

\[
\begin{align*}
\frac{D_p}{D_0} &= \theta^2 \quad \text{(Buckingham 1904)}, \\
\frac{D_p}{D_0} &= \theta^{1.5} \quad \text{(Marshall 1959)}, \\
\frac{D_p}{D_0} &= 0.66 \theta \quad \text{(Penman 1940)}, \\
\frac{D_p}{D_0} &= 2.8 \theta^3 \quad \text{(Papendick/Campbell 1980)}.
\end{align*}
\]
Due to the general complexity of porous media, the same porosities may nevertheless induce different effective tensors, cf. [8] for the permeability. Hence, there is already numerous research taking additionally the geometric structure such as the specific surface, the mean particle size, or the tortuosity (see below) into account. Such extensions were mostly determined empirically, e.g. [9] for the permeability. In some models the permeability coefficient is described, for instance, in terms of the hydraulic radius \( R = \frac{d}{\tau} \) or of the mean particle size \( d \) [10], e.g. \( d = \frac{6}{\sigma} \) for spherical grains of constant size leading to \( K_p = \frac{d^2}{180 (1-\theta)} \). In more general geometrical settings it is reasonable to introduce a shape factor \( f(s) \) with \( f(s) d^2 = \frac{\sigma^2}{6} \) and hence \( k = f(s) d^2 \frac{\sigma^3}{(1-\theta)^2} \), cf. [2].

There are also several approaches for the diffusivity taking further information into account, cf. [5–7] and references cited in. First in terms of the soil total porosity \( \Phi \) proposed by Millington and Quirck 1961 \( \left( \frac{D_p}{D_0} = \frac{\theta^{10/3}}{\Phi^2} \right. \) reducing to \( \theta^{4/3} \) for \( \theta = \Phi \), or Olesen 1996 \( \left( \frac{D_p}{D_0} = \theta \left( \frac{\Phi}{\theta} \right)^{4/3} \right) \). Moldrup 1999 and Moldrup 2000 included the Campbell soil-water characteristic curve parameter \( b \) ranging from 2 to 11 \( \left( \frac{D_p}{D_0} = \Phi^2 \left( \frac{\theta}{\Phi} \right)^{2+3b} \right) \) and the air filled porosity \( \theta_{100} \) at -100 cm \( H_2O \) of soil water matrix potential into their models to obtain the so-called Buckingham-Burdon-Campbell (BBC) model \( \frac{D_p}{D_0} = (2\theta_{100}^2 + 0.04\theta_{100}) \left( \frac{\theta}{\Phi} \right)^{2+3b} \), respectively. Finally, Olesen 2001 included the volumetric soil surface area \( S A_{vol} \) into their model: \( \frac{D_p}{D_0} = 1.1\theta(\theta - 0.039SA_{vol}^{3.52}) \). Furthermore, combinations of the models are used.

Nowadays, there is an unmanageable number of formulae for the effective hydrodynamic parameters depending not only on the porosity but also on numerous parameters and physical variables. However, in terms of applicability low parameter models being particularly independent of hard to measure input are most desirable. Many of the cited models are derived from fitting to data and are often only valid in a restricted range of the porosity.

Finally, we emphasize the fundamental drawback that the Kozeny-Carman equation (1) and all models listed in (2) and their modifications or extensions refer to scalar coefficients rather than to the full tensors. This simplification is only verified for isotropic porous media, compare also discussion in Section 3.2.1 and numerical illustrations in Section 4. However, porous media and hence also the effective tensors are often anisotropic, cf. [11] for the permeability.

### 2.2 Dependency on the tortuosity

It is evident that within a porous medium paths are no straight lines. One possibility to overcome this drawback is to relate the effective hydrodynamic parameters to the tortuosity which is defined as the ratio of the average traveling length per unit length. Incorporating the tortuosity the Kozeny-Carman equation (1) changes to \( K_p = \frac{d^2}{\tau_{vol} (1-\theta)} \) cf. [8, 12]. The following basic relations potentially including the porosity for the diffusivity are often presupposed: \( \frac{D_p}{D_0} = \frac{\theta}{1-\theta}, \frac{D_p}{D_0} = \frac{\theta}{\tau}, \) cf. [13]. Finally, relations potentially also including the constrictivity \( c \), resistivity factor \( F \) or model parameters that may be calibrated with experimental data are available for the tortuosity. Archies law \( F = \frac{A}{\rho_m} \) (with parameters \( A, m \)) and further findings for instance suggest to relate the theoretical models for tortuosity to some geometric shape factor or the porosity, e.g. via \( c^2 = (F\theta)^n = (A\theta^{(1-m)})^n \). In the context of permeability, the empirical coefficient \( A^{n/2} \in (0.6, 2) \) and the tortuosity factor \( (1 - m)n/2 \in (-3, 0) \), see [14]. A review of different available expressions for the tortuosity \( \tau \) and possible choices of parameters is given in [13], e.g. \( \tau = \theta + B(1 - \theta) \).
and \( \tau^2 = 1 - C \ln(\theta) \). Considering the second constitutive relations with \( C = 2 \), it is argued in [13] that \( \tau^2 \approx \frac{1}{\theta^2} \) so that both formulations for the diffusion are equivalent for this choice.

3 Mathematical models

If the underlying geometry of a representative elementary volume \( Y \) is prescribed, cf. Figure 1 and Figure 2, some mathematical theory is available that makes it possible to calculate the full tensors \( K, D \). Starting from mathematical models at the pore scale which describe fluid flow or transport, an averaging procedure is performed in order to derive effective models. For the fluid flow, incompressible Stokes equations and for the transport equation, e.g. a diffusion equation with molecular/free diffusion \( D_0 \) are the starting point. Two-scale asymptotic expansion [15] or mathematically more rigorously, two-scale convergence [16, 17] may be applied to these equations, cf. [18] for an application oriented introduction. Lately, also two-scale asymptotic expansion in a level set framework has been developed in [19] to account for an evolving underlying microstructure. As a result of the averaging procedure, Darcy’s law and the averaged transport equation as introduced in Section 1 are derived. The effective tensors \( K, D \) are given explicitly as the integral over flux solutions of auxiliary cell problems which are defined on a potentially evolving representative elementary volume.

3.1 Review of homogenization potentially including an evolving geometry

The porosity \( \theta = \frac{|Y_f|}{|Y|} \) is defined as the volume of the pore space \( Y_f = Y \setminus Y_s \) with respect to the total volume of the representative elementary volume \( Y \). Further, according to [18] we hypothesize that the permeability tensor \( K \) may be determined via

\[
K_{ij} := \frac{1}{|Y|} \int_{Y_f} (w_j)^i dy
\]  

with supplementary cell problems in \( w_j, \pi_j, j = 1, \ldots, n \)

\[
\begin{align*}
-\Delta_y w_j + \nabla_y \pi_j &= -e_j & \text{in } Y_f, \\
-\nabla_y \cdot w_j &= 0 & \text{in } Y_f, \\
w_j &= 0 & \text{on } \partial Y_s, \\
w_j, \pi_j \text{ periodic in } y.
\end{align*}
\]  

Similarly, following [18], for the diffusion tensor \( D \), it holds

\[
D_{ij} := \frac{1}{|Y|} \int_{Y_f} D(y)(\partial_y \zeta_j + \delta_{ij}) dy
\]  

with supplementary cell problems in \( \zeta_j, j = 1, \ldots, n \)

\[
\begin{align*}
-\nabla_y \cdot (\nabla_y \zeta_j + e_j) &= 0 & \text{in } Y_f, \\
(\nabla_y \zeta_j + e_j) \cdot \nu &= 0 & \text{on } \partial Y_s, \\
\zeta_j \text{ periodic in } y \text{ and } (\zeta_j, 1)_{L^2} &= 0.
\end{align*}
\]
Hereby, \( \nu \) denotes the unit outer normal, \( e_j \) the unit vector in direction \( j \), and \( \delta_{ij} \) the Kronecker delta.

If the geometry is non stationary, the fluid domain \( Y_f \) on which the cell problems are defined are changing in time. In this sense a functional relation between the porosity and the effective tensors may be derived.

### 3.2 Special cases and analytical bounds

#### 3.2.1 Isotropic media

For isotropic media, the effective tensors reduce to scalars, i.e. \( K = K_p E \) and \( D = D_p E \) with unity matrix \( E \). Such settings are numerically illustrated in Section 4.1, Figure 3 and also comparisons with the formulae cited in Section 2.1 and the bounds stated in Section 3.2.3 and Section 3.2.4 below are conducted.

#### 3.2.2 Layered medium

As described in [18, Chapt. 1, Prop. 3.3], for a \( n \)-dimensional layered medium, characterized by \( D(y) = D(y_1, \ldots, y_n) = \tilde{D}(y_n) \), the cell problems’ solutions of (6) may be calculated explicitly:

\[
\zeta_n = \frac{\int_0^{y_n} \frac{1}{D(\eta)} \, d\eta}{\int_0^1 \frac{1}{D(\eta)} \, d\eta} - y_n \quad \text{and} \quad \zeta_j = 0 \quad \text{for} \ j \neq n.
\]

and the effective tensor according to (5) is given by

\[
D_{nn} = \hat{D} = \left( \int_0^1 \frac{1}{\tilde{D}(\eta)} \, d\eta \right)^{-1} \quad \text{and} \quad D_{ij} = \bar{D} \delta_{ij} = \frac{1}{k} \left( \sum_{\ell=1}^{k} D_\ell \right) \delta_{ij} \quad \text{for} \ i \neq n \land j \neq n.
\]

These are the harmonic mean \( \hat{D} \) and the arithmetic mean \( \bar{D} \) vertical and parallel to the layers, respectively.

If the medium has for instance \( k \) layers of equal thickness \( 1/k \) and the diffusion is constant and equal to \( D_\ell, \ \ell = 1, 2, \ldots, k \) in each of the \( k \) layers, we have

\[
D_{nn} = \hat{D} = \left( \frac{1}{k} \sum_{\ell=1}^{k} D_\ell \right)^{-1} \quad \text{and} \quad D_{ij} = \bar{D} \delta_{ij} = \frac{1}{k} \left( \sum_{\ell=1}^{k} D_\ell \right) \delta_{ij} \quad \text{for} \ i \neq n \land j \neq n.
\]

As a second example, we consider a two-dimensional porous medium with porosity \( \theta \) consisting of a system of tubes with diffusivity \( D \) and impermeable porous matrix. Then, it holds

\[
D_{22} = \hat{D} = 0 \quad \text{and} \quad D_{ij} = \bar{D} \delta_{ij} = \theta D \delta_{ij} \quad \text{for} \ i \neq 2 \land j \neq 2.
\]

Hence, in this setting, the method of homogenization states a linear dependency of the diffusivity on the porosity, cf. Equation (2) (Penman 1940).

#### 3.2.3 Voigt-Reiss bounds

Unfortunately, in the most cases (including even isotropic ones) it is not possible to calculate the homogenized parameters via (3) and (5) analytically. Analytical solutions to a cell problem similar to (6) with different boundary conditions on \( \partial Y \) are explicitly
Assuming that the initial matrix $D(x)$ describing the diffusivity at the pore scale is symmetric and periodic with respect to the representative elementary volume $Y := [0, 1]^n$, the following estimate holds:

$$\left( \int_Y \frac{1}{D(\eta)} d\eta \right)^{-1} \leq D \leq \int_Y D(\eta) d\eta.$$  

(7)

These bounds are sharp in the case of a layered medium, cf. Section 3.2.2 and cf. [21, Sec. 6.1, (6.8)]. In the case of a porous media, we assume $\theta < 1$ and that the above inequality holds:

$$\frac{n(1-\theta)(D_2-D_1)}{nD_2+\theta(D_1-D_2)} \leq D_p \leq \frac{D_2}{D_1}.$$  

(8)

This estimate yields a very good approximation, cf. the simulations in Section 4 where the excluded area is visualized in gray in Figure 3 (middle) and in Figure 4 (right, bottom). We emphasize that in two dimensions the functional relation $\theta^{4/3}$ proposed by Millington and Quirk and $\theta^{1.5}$ proposed by Marshall 1959 insects this upper bound whereas is not necessarily the case in three dimensions.

### 3.2.4 Hashin-Shtrikman bounds

However, the bounds provided by the Voigt-Reiss inequality are often not sharp enough. For isotropic two-phase materials the best bounds that do not take into account particular geometric properties are given by the so-called Hashin-Shtrikman bounds: Let $D(x) = D_1 \chi(x) + D_2(1-\chi(x))$ be the scalar diffusivity of an isotropic two-phase material, where $D_1$, $D_2$ are the two values of diffusivity and $\chi$ is the characteristic function of $\{ x \in [0, 1]^n : D(x) = D_1 \}$. If $D_1 < D_2$ and $\theta = 1 - \int_Q \chi(x) dx$ denotes the respective volume fraction of the material with diffusivity $D_2$, we have $D_1 \left( 1 + \frac{n\theta(D_2-D_1)}{nD_2+\theta(D_1-D_2)} \right) \leq D_p \leq D_2 \left( 1 - \frac{n(1-\theta)(D_2-D_1)}{nD_2+\theta(D_1-D_2)} \right)$, cf. [21, Sec. 6.1, (6.8)]. In the case of a porous media, we assume that one material representing the porous matrix is impermeable, i.e. $D_1 = 0$ and $D_2 = D_0$. Then $\theta$ describes the porosity and the above inequality holds $\frac{D_p}{D_0} \in [0, \frac{n-1}{n-\theta}]$. This estimate yields a very good approximation, cf. the simulations in Section 4 where the excluded area is visualized in gray in Figure 3 (middle) and in Figure 4 (right, bottom). We emphasize that in two dimensions the functional relation $\theta^{4/3}$ proposed by Millington and Quirk and $\theta^{1.5}$ proposed by Marshall 1959 insects this upper bound whereas is not necessarily the case in three dimensions.

### 4 Evaluation and numerical simulations

Assumption on the hard to access microstructure have to be made to apply the mathematical theory introduced in Section 3.1. However, having modern imaging techniques at hand, that become better and better, it is to be expected that rapid progress may be made. Already several attempts have been made in the past to solve problems as stated in 3.1 on real data sets. In Figure 1 and Figure 2, several geometries that are considered for the numerical simulations in Section 4.1 are depicted. The evolution of the porous matrix represented by the inclusions is prescribed in such a way that its general shape...
is maintained. For the square/cube and circle/sphere the evolution is uniform in radial direction and in direction of the axis, respectively. For rectangles of different thickness uniform evolution in width is considered (type 1). Moreover, rectangles of type 2 and ellipse evolve uniformly in width and also in height. For the cross two different evolutions are taken into account. First a pure lengthening of the cross arms along their axes (type 1) and second an additional thickening of the cross arms while lengthening (type 2). Likewise, the more sophisticated and random geometries as depicted in Figure 1 are evolving.

Homogenization theory has already been applied to derive functional relations between effective tensors and porosity: In [22] rectangular and triangular geometries are considered and the effective tensor (5) over the porosity is evaluated. Similarly, in [19] a circular geometry is considered and the calculated functional relations between diffusion, permeability, and porosity are fitted to second and third order polynomials, respectively. In [23] the permeability depending on the saturation for fixed porosity is computed for 2D rectangular cell geometries. In [24] the permeability is computed for some simple geometries, where the underlying cell problem is considered for several boundary conditions (periodic, uniform, confined). Numerical simulations and computations for the permeability in geometries with textile microstructures are considered in [25]. A numerical procedure for the evaluation of equivalent permeability for fractured vuggy porous media is investigated in [26]. In [27], a perturbed straight channel is considered in the representative elementary volume and the cell problems (6) and the effective tensor (5) are evaluated. In [28] the same setting is considered and interpreted in the context of tortuosity. In [29] effective diffusion and tortuosity are related for bentonite with laminar montmorillonite structures. Thereby, a comparison of straight and winding paths or their combination is considered. In [30], a more complex situation is considered: In an anisotropic rectangular geometry, the permeability and electrodiffusion tensors over the porosity are calculated, which finally lead to a non-monotonic functional relations for the cations. Similarly in [31], different interaction potentials relating rather to van-der Waals-interaction than electric ones are considered and the effective permeability and diffusion tensors over the porosity are evaluated. Finally, in [32] diffusion tensors based on randomly generated geometries have been investigated.
All simulations in this paper were conducted in MATLAB 2016a\textsuperscript{1} [33] and M++ [34]. For the discretization the Mixed Finite Elements Method and the Local Discontinuous Galerkin method have been used.

### 4.1 Evaluation of effective tensors over porosity

We evaluate the effective tensors given in (3) and (5). Their scalar representations or eigenvalues over the porosity are depicted for isotropic geometries in Figure 3 and for simple anisotropic geometries in Figure 4 (left) and Figure 4 (middle). In addition to these quite regular geometries, more sophisticated as well as three dimensional setting are considered in Figure 4 (right).

We emphasize that depending on the chosen geometry significantly different values are obtained for the effective tensors for the same porosity values. It is evident from Figure 3 (degenerating cross) and Figure 4 (left, thin rectangle) that the diffusion tensor may also degenerate for non vanishing porosity both in the isotropic and anisotropic case. In such cases the drop to zero may even occur for comparable high values of the porosity. It is remarkable to note that the connectivity is much better in the three dimensional situation and consequently the degeneration of the tensors is less prominent, cf. randomly generated geometries in Figure 4 (right).

The investigations depicted in Figure 4 (left) demonstrate that the behavior of the two eigenvalues may be significantly different. While one of the two eigenvalues shows a linear dependence on the porosity (compare the functional relation (2) proposed by Penman 1940), the second eigenvalue evidently shows a monotonic but nonlinear behavior. In Figure 4 (middle), the respective eigenvalues of the rectangle and the ellipse show very similar behavior. However, it is remarkable to note that the eigenvalues diverge for vanishing porosity.

[Figure 3: Scalar representatives $K_p$ (left) and $D_p$ (middle) over porosity for isotropic geometries in 2D: square, circle, and cross (type 1 and 2); Hashin-Shtrikman bound $\theta^2$ (exclusion of gray area) (middle); comparison to Kozeny-Carman (for square based geometry, left) and functional relations $\theta^{1.5}$ (Marshall 1959) and $\theta^2$ (Buckingham 1904) in 2D (right).]

A quantitative functional dependence of $K_p$ and $D_p$ on the porosity is determined via an approximation with polynoms $ax^y + b$ with parameters $a, b, y$, cf. Table 1 and Table 2.
Figure 4: LEFT: Eigenvalues of \( K \) (top) and \( D \) (bottom) over porosity for anisotropic geometries in 2D: Rectangles with different varying width but fixed heights. MIDDLE: Eigenvalues of \( K \) (top) and \( D \) (bottom) over porosity for anisotropic geometries in 2D: Rectangles and ellipses with varying widths and heights. RIGHT: Eigenvalues of \( D \) over porosity for sophisticated and random geometries in 2D (top) and for isotropic (cube, sphere) and random geometries in 3D (bottom); comparison to functional relations \( \theta^{1.5} \) (Marshall 1959) and \( \theta^2 \) (Buckingham 1904) in 3D (bottom).

Table 1: Quantitative relations of \( K_p \) and \( D_p \) on porosity.

<table>
<thead>
<tr>
<th></th>
<th>( K_p )</th>
<th>( D_p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Square</td>
<td>0.1345 ( \theta^{1.5170} ) - 0.0145</td>
<td>0.9561 ( \theta^{1.2207} ) - 0.0551</td>
</tr>
<tr>
<td>Circle</td>
<td>0.1496 ( \theta^{5.8448} ) - 0.0132</td>
<td>0.9676 ( \theta^{1.7135} ) + 0.0148</td>
</tr>
<tr>
<td>Cross (type 2)</td>
<td>0.1380 ( \theta^{1.8537} ) - 0.0141</td>
<td>0.9519 ( \theta^{1.4116} ) + 0.0497</td>
</tr>
</tbody>
</table>

If the specific surface \( \sigma \) is proportional to \( \frac{1}{\sqrt{1-\theta}} \), the Kozeny-Carman’s equation (1) transfers to \( K_p = c_0 \frac{\theta^3}{(1-\theta)^2(n-1)/n} \). For a two-dimensional square and \( c_0 = \frac{1}{5} \) we obtain \( K_p = \frac{1}{80} \frac{\theta^3}{1-\theta} \), cf. Figure 3 (left). Consequently, for \( \theta \) close to 1 exponents larger than 3 are reasonable. It is evident that the functional relations \( \theta^{4/3} \) (Millington & Quirck 1961), \( \theta^{1.5} \) (Marshall 1959), and \( \theta^2 \) (Buckingham 1904), and for the diffusion yield very good approximations for these geometries, cf. also Figure 3 (right) and Figure 4 (right, bottom). It is evident that higher exponents as proposed by Papendick and Campell 1980 (cf. (2)) are also reasonable for specific geometries, cf. Table 2.

4.2 Evaluation of the tortuosity

Considering the geometry on the left in Figure 5, with respect to the number of hills \( \ell \), the porosity is given by \( \theta = 1/32 + \ell \cdot 58/1024 \) and the tortuosity lies in between the shortest and the longest traveling length, i.e. \( \tau \in [1 + 1, 8135\ell, 1 + 1, 875\ell] \). In summary, the linear relation \(-0,000 + 32,0176\theta\) between the tortuosity and porosity is obtained, cf.
Table 2: Quantitative relations of $D_p$ on porosity.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>$D_p$</th>
<th>Geometry</th>
<th>$D_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cube 3D</td>
<td>$1.0025 \theta^{1.2167} - 0.0292$</td>
<td>Random 2D</td>
<td>$1.0083 \theta^{4.057/3} + 0.0497$</td>
</tr>
<tr>
<td>Sphere 3D</td>
<td>$1.0008 \theta^{1.5535} + 0.0130$</td>
<td>Random 3D</td>
<td>$1.0130 \theta^{4.1111} + 0.1652$</td>
</tr>
</tbody>
</table>

Section 2.2.

For the second and third geometrical setting as depicted in Figure 5 the porosity remains constant, while the tortuosity increases and the porosity and tortuosity increases simultaneously, respectively. The three examples show that the relation between tortuosity and the porosity may show significantly different behavior, as is also indicated by the relations stated in Section 2.2. Likewise, the diffusion inherits this behavior.

5 Conclusion

In this paper, we presented a review of well-established functional relations between the porosity and hydrodynamic parameters. These relations were compared to results from homogenization theory and also well-known bounds for various two- and three-dimensional geometries.

Quantitative relation were also established from homogenization results by means of fitting the parameters of polynomials $ax^y + b$. In further studies fits with more general polynomials $\sum a_k x^k$ may certainly be addressed.

Finally, further research including extension of homogenization results is needed to
similarly approach the unsaturated case.

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