

# <sup>1</sup> **Pedotransfer Functions for Permeability: A** <sup>2</sup> **Computational Study at Pore Scales**

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3 **Abstract.** Three phenomenological power law models for the permeabil-  
4 ity of porous media are derived from computational experiments with flow  
5 through explicit pore spaces. The pore spaces are represented by three di-  
6 mensional pore networks in sixty-three virtual porous media along with fif-  
7 teen physical pore networks. The power laws relate permeability to (i) poros-  
8 ity, (ii) squared mean hydraulic radius of pores, and (iii) their product. Their  
9 performance is compared to estimates derived via the Kozeny equation, which  
10 also uses the product of porosity with squared mean hydraulic pore radius  
11 to estimate permeability. The power laws provide tighter estimates than the  
12 Kozeny equation even after adjusting for the extra parameter they each re-  
13 quire. The best fit is with the power law based on the Kozeny predictor, that  
14 is, the product of porosity with the square of mean hydraulic pore radius.

## 1. Introduction

15 Flows of fluid through a porous medium are distinguished from flows through open  
16 bodies by spatially variable resistance arising from variations in the medium's pore space  
17 geometry and topology that yields a steady flow. At pore-resolving scales a porous medium  
18 is a network of explicit, interconnected channels embedded in a solid medium. Critical  
19 parameters affecting resistance in pore spaces include typical radius of the pores, the  
20 length of a streamline between two points relative to the distance between the points,  
21 and the density of pores. Sample volumes ranging from 0.01-1000 cm<sup>3</sup> are typical of  
22 laboratory pore space experiments with most at the lower end of the range. At macroscopic  
23 scales, porous media are usually represented as volumes with system states, e.g. velocity  
24 and hydraulic head, and parameters, e.g. permeability and porosity, defined piece-wise  
25 continuously at every point in the volume. Macroscopic resistance to flow is quantified  
26 by its approximate inverse, permeability, which is defined via Darcy's law in terms of the  
27 ratio of fluid flux to the gradient of pressure within the fluid. Darcy's law was established  
28 experimentally [*Darcy*, 1856] and later derived analytically by upscaling pore-network  
29 flows through homogenization, or volume averaging [*Shvidler*, 1964; *Whitaker*, 1999].  
30 Alternatives based on ensemble averaging have also been used to estimate permeability  
31 from pore-scale properties of porous media [*Rubinstein*, 1986].

32 Although permeability is a well-established property of most relatively uniform porous  
33 media, its actual dependence on specific geometric and topological properties of porous  
34 networks is not fully understood. Phenomenological transfer functions have been devel-  
35 oped by soil physicists, hydrologists, chemical and petroleum engineers, and materials

36 scientists to estimate permeability from properties of porous media that are relatively  
 37 easy to observe. A natural starting point is to suppose that a sample volume's perme-  
 38 ability is proportional to its porosity since the latter indicates pore density and is a good  
 39 measure of the medium's capacity to hold fluid. Yet this is not entirely satisfactory, since  
 40 two porous media can have the same porosity but one may be entirely impermeable while  
 41 the other offers minimal resistance to flow.

42 Perhaps the best known phenomenological transfer functions are the Kozeny equa-  
 43 tion [*Kozeny*, 1932; *Carman*, 1956; *Bear*, 1988] and the Kozeny-Carman equation [*Car-*  
 44 *man*, 1939]. Kozeny derived his equation,

$$45 \quad k = c_0 n R^2, \quad (1)$$

46 by reasoning about flow through an idealized pore network: he equated the velocity given  
 47 by Poiseuille's law for flow through a bundle of capillary tubes to the specific discharge  
 48 obtained from Darcy's law and thus solved for permeability. He concluded that perme-  
 49 ability,  $k$ , is proportional to the product of porosity,  $n$ , with the square of mean hydraulic  
 50 radius,  $R$ , a measure of typical pore size. Hence, the Kozeny predictor,  $nR^2$ , combines a  
 51 factor,  $n$ , depending on the capacity of a medium to hold fluid with another,  $R$ , depending  
 52 on the ability of the medium to transmit it. The dimensionless constant,  $c_0$ , is known as  
 53 the Kozeny coefficient. *Carman* [1939] extended (1) by including a factor of tortuosity,  $\tau$ ,  
 54 an index of the complexity of streamlines in the medium, and derived the Kozeny-Carman  
 55 equation

$$56 \quad k = c'_0 n R^2 / \tau^2. \quad (2)$$

57 Since permeability is a characteristic of a porous medium, (1) and (2) need to be properly  
58 scaled by fluid viscosity and density to relate a medium's permeability to its saturated  
59 hydraulic conductivity with respect to a particular fluid.

60 We follow *Smolarkiewicz and Winter* [2010], [SW10] for brevity, and determine per-  
61 meability computationally by simulating the basic elements of Darcy's original experi-  
62 ment [*Darcy*, 1856] in three-dimensional networks of pores, allowing pore-scale processes  
63 to be observed in detail. *Hyman et al.* [2012], hereafter [HSW12], employed the techniques  
64 of [SW10] to study the influence of porosity on the degree of heterogeneity in steady state  
65 flows within stochastically generated three dimensional pore networks. [HSW12] reports  
66 technical aspects of modeling flow in explicit pore spaces and provides a Lagrangian per-  
67 spective of the pore space via particle tracking. That paper focuses on heterogeneity of  
68 microscopic flow field and its relationship to porosity, while this paper focuses on the  
69 continuum scale properties of permeability. They quantify the degree of heterogeneity in  
70 the flow and identify coherent heterogeneities in the flow field by tracking fluid particles  
71 and recording various attributes including tortuosity, trajectory length, and first passage  
72 time in media with porosities between 0.2 and 0.7.

73 Here, the techniques of [SW10] are used to estimate overall permeability for each of  
74 seventy-eight small,  $O(1\text{cm}^3)$ , sample volumes of porous media. Sixty-three realizations  
75 are drawn from ensembles of virtual pore spaces with porosities ranging from 0.19 to  
76 0.84, while the others are a volcanic tuff [*Wildenschild et al.*, 2004], a column of glass  
77 beads [*Culligan et al.*, 2004], and thirteen unique sandpacks, sandstones, and carbonate  
78 from *Mostaghimi et al.* [2013]. Virtual pore spaces are isotropic and statistically station-  
79 ary in space with permeabilities corresponding to a well-sorted gravel or sand [SW10];

80 [HSW12] demonstrated that the virtual media are large enough to constitute representa-  
81 tive elementary volumes. Their material properties appear consistent with those of the  
82 glass beads and tuff. Owing to the high resolution of the seventy-eight pore space samples,  
83 porosity and hydraulic radius can be directly evaluated.

84 The computed permeability, porosity, and hydraulic radii of the virtual media are used  
85 to empirically estimate the Kozeny coefficient,  $c_0$ . The estimate  $\hat{c}_0 = 0.19$  is in excellent  
86 agreement with Carman's original value,  $c_0 = 0.2$ , indicating the representativeness of the  
87 virtual pore spaces. Additionally, over a restricted range of porosities,  $0.2 < n < 0.7$ , the  
88 analytically derived Kozeny and Kozeny-Carman laws are both reproduced reasonably  
89 well. The Kozeny equation (1) fits results from media with porosities in  $0.2 < n < 0.7$   
90 fairly well and the Kozeny coefficient is within an interval later noted by noted by *Carman*  
91 [1956]. The Kozeny-Carman equation (2) also predicts permeability adequately within this  
92 limited range and the computed coefficient,  $c'_0$ , is near that suggested by Carman.

93 Yet the Kozeny equation is not entirely satisfactory as a predictor of permeability for  
94 the entire data set. Plotting the permeability data against the Kozeny predictor,  $nR^2$ ,  
95 reveals an obvious nonlinearity at large and small values of  $nR^2$  that is not captured by  
96 the linear (in the predictor) Kozeny model. Hence, scale-invariant power law alternatives  
97 depending upon porosity,  $n$ , the square of hydraulic radius,  $R$ , and the Kozeny predictor,  
98  $nR^2$ , that is their product, are derived and compared to the Kozeny equation. Focus is  
99 placed on the Kozeny equation and related power laws rather than the Kozeny-Carman  
100 equation because the tortuosity of the data is highly correlated with porosity and mean  
101 hydraulic radius.

102 The power law alternatives provide better fits to the physical and virtual data, although  
103 at the expense of adding an extra parameter, than does the Kozeny equation over the  
104 entire range of data. We attribute this to the ability of simple power laws to capture the  
105 nonlinear effects of pore space interconnectivity on permeability at extremes of porosity  
106 and mean hydraulic radius. This seems born out by a power law based on the Kozeny  
107 predictor,  $nR^2$ , which yields a sum of squared errors for the virtual data that is significantly  
108 smaller than the errors of power laws based on porosity or mean hydraulic radius alone.  
109 Goodness of fit and model performance for these data are evaluated using a standard  
110 statistical technique, the Analysis of Variance, to gauge the relative advantage conferred  
111 by the additional parameter. The overall fit of the models to both real and synthetic data  
112 is evaluated and compared using chi-squared tests.

113 Section 2 reviews previous studies to determine permeability computationally and places  
114 the present work within context of the previous studies. Section 3 describes simulations of  
115 pore networks and flow; computational methods for generating virtual porous media along  
116 with a characterization of the physical data (Section 3.1), numerical techniques for resolv-  
117 ing flow in the explicit pore networks (Section 3.2), and estimation of transfer function  
118 variables including porosity, hydraulic radius, tortuosity, and permeability (Section 3.3-  
119 3.4). A preliminary study to determine a proper grid resolution for the study is performed  
120 prior to derivations of the power law alternatives to the Kozeny equation (Section 3.5).  
121 Next the empirical pedotransfer functions are derived and evaluated (Section 4.1), and  
122 their ranges of applicability are discussed (Section 4.2). We finish with a summary of the  
123 experiment and offer a few remarks about the generality of the results in Section 5.

## 2. Background

124 Pedotransfer functions are mathematical or computational models used to estimate  
 125 hydraulic soil properties, e.g. saturated hydraulic conductivity, on the basis of pedological  
 126 data [Wösten *et al.*, 2001; Schaap *et al.*, 2001], and are commonly derived empirically using  
 127 soil samples in continuum scale laboratory experiments where  $k$ ,  $n$ ,  $R$ , and  $\tau$  are measured  
 128 in bulk. Computational experiments with flow at the pore-scale allow these quantities to  
 129 be observed in detail and generalized pedotransfer functions to be empirically derived at  
 130 scales similar to those Kozeny and Carman considered but in more complicated networks.

131 The Kozeny (1) and and Kozeny-Carman (2) equations are generalized pedotransfer  
 132 functions for predicting permeability, a macroscopic soil property, derived analytically via  
 133 considerations of microscopic pore scale dynamics (they are general in the sense that the  
 134 predictors are not specific to a particular type of soil); Lebron *et al.* [1999] and Rawls  
 135 *et al.* [2005] provide comparisons between (1), (2) and other pedotransfer functions.

### 2.1. Permeability Based on Pore-scale Simulations

136 Computational solutions for the flow of a viscous fluid through an explicit pore space go  
 137 back at least to *Hasimoto* [1959] who solved for flow in a periodic array (cubic) of spheres  
 138 by deriving the fundamental solution to the Stokes equations using Fourier transforms.  
 139 He also obtained an expression for drag by expanding the velocity profile in terms of the  
 140 fundamental solution and its derivatives. *Launier and Massey* [1978] numerically solved  
 141 the Navier-Stokes equations for flow through a periodic array of long cylinders with known  
 142 geometric configurations. *Sangani and Acrivos* [1982a, b] and *Zick and Homsy* [1982]  
 143 computed Stokes drag on slow flows in porous media composed of simple elements like  
 144 spheres. Permeability has been estimated by simulating flow through more realistic pore

145 networks by *Lemaitre and Adler* [1990], *Fourie et al.* [2007], [SW10], and *Mostaghimi et al.*  
146 [2013] to name a few. *Fourie et al.* [2007] found good agreement between their numerical  
147 estimates and measured permeabilities for a small volume of coarse sand (0.81 mm on a  
148 side). *Matyka et al.* [2008] and [HSW12] found evidence for the existence of representative  
149 elementary volumes in simulated flows through realistic random pore networks. *Meakin*  
150 *and Tartakovsky* [2009] provide a current discussion of other methods for modeling flow  
151 in porous networks.

152 The behavior of the Kozeny equation has been investigated through computational  
153 experiments with flow in random or fractal pore networks. Scaling arguments indicate  
154 good agreement between the Kozeny coefficient,  $c_0$ , and data obtained from computational  
155 experiments with flow through networks based on Sierpinski carpets [*Adler and Jacquin,*  
156 1987]. On the other hand, *Adler et al.* [1990] found that the Kozeny coefficient is about  
157 half the standard value of  $1/5$  given by *Carman* [1939] when based on simulations of  
158 flow through random media with statistics like Fontainebleau sandstone. *Lemaitre and*  
159 *Adler* [1990] discovered that agreement between observed and theoretical values of the  
160 Kozeny coefficient varied according to the porosity of networks they simulated: the Kozeny  
161 equation did not hold for random media at relatively high or low porosities (in the latter  
162 case, close to the percolation threshold they used to generate random media), nor did it  
163 hold for media generated from regular fractals when the largest pores were held constant as  
164 resolution was increased. The simulations performed in this paper also indicate nonlinear  
165 behavior of permeability at high and low porosities, and also at extremes of mean hydraulic  
166 radii.

## 2.2. Physical Evidence for Kozeny Equation

167 The Kozeny and Kozeny-Carman equations have been validated and verified in experi-  
 168 ments with flow through physical media composed of arrays of glass beads, other shapes  
 169 like rods, and natural porous media [*Carman*, 1956; *Bear*, 1988]. Soil scientists have  
 170 shown that (1) and (2) provide estimates of permeability that are superior to some other  
 171 soil transfer functions [*Chapuis and Aubertin*, 2003; *Dvorkin*, 2009]. The estimate given  
 172 by *Carman* [1939] of  $c_0 = 1/5$  for the Kozeny coefficient seems adequate for media in  
 173 a middle range of porosity ( $0.2 < n < 0.7$ ) [*Xu and Yu*, 2008]. In some circumstances  
 174 high correlation between tortuosity and porosity makes the simpler Kozeny equation a  
 175 cost-effective alternative to the Kozeny-Carman equation [*Koponen et al.*, 1996].

176 The Kozeny and Kozeny-Carman equations have been found, however, to yield poor  
 177 estimates of permeability at the extremes of porous medium types: either when total fluid  
 178 discharge through a porous medium is negligible or at the other extreme where the effect  
 179 of the medium on the overall flow is local and small [*Kyan et al.*, 1970; *Xu and Yu*, 2008].  
 180 These results are consistent with the pore-scale computational experiments of *Lemaitre*  
 181 *and Adler* [1990] mentioned above and the experiments reported here. *Heijs and Lowe*  
 182 [1995] found that the Kozeny-Carman equation predicted the permeability of a particular  
 183 random array of spheres well (porosity  $n = 0.6$ ), but failed to do so in a soil sample that  
 184 had porosity near one. *Sullivan* [1942], *Kyan et al.* [1970], *Davies and Dollimore* [1980]  
 185 and *Xu and Yu* [2008] all note that the Kozeny coefficient varies nonlinearly with porosity  
 186 and most significantly at its extreme values.

### 2.3. Alternatives to Kozeny Equation

187 Efforts have been made to compensate for these weaknesses by modifying the Kozeny  
 188 and Kozeny-Carman equations. The Kozeny-Carman equation has been expanded to  
 189 include effective porosity [*Koponen et al.*, 1997], percolation threshold and geometric  
 190 properties of the pore network [*Nabovati et al.*, 2009], and fractal geometry [*Xu and Yu*,  
 191 2008]. However *Schaap and Lebron* [2001] found that modifications do not always improve  
 192 on estimates given by (1) and (2). *Revil and Cathles* [1999] derive a power-law relation,

$$193 \quad k \propto d^2 n^{3m}, \quad (3)$$

194 between permeability of a clay-free sand,  $k$ , and grain diameter,  $d$ , and porosity,  $n$ , based  
 195 on an electrical cementation exponent,  $m$ , that reflects the connectivity of the pore space.  
 196 Their method depends on the Archie relationship [*Archie*, 1942],

$$197 \quad n = \mathcal{F}^m, \quad (4)$$

198 that expresses porosity as a power of an electrical formation factor,  $\mathcal{F}$ , whose reciprocal  
 199 quantifies the effective interconnected porosity of a porous medium. Values of  $m$  vary  
 200 between 1 and 4 according to *Sen et al.* [1981]. *Revil and Cathles* [1999] derive power  
 201 laws for permeability of a pure shale and sand-shale mixtures in a similar way with the  
 202 specific value of  $m$  depending on the porous material. *Jacquin* [1964] quoted in [*Adler*  
 203 *et al.*, 1990] found evidence for

$$204 \quad k \propto n^{4.15} \quad (5)$$

205 for samples of Fontainebleau sandstone. *Lemaitre and Adler* [1990] indicate that perme-  
 206 ability behaves like a power of porosity near the percolation limit (the value of porosity  
 207 below which there are no continuous pore channels through one of their realizations) of

208 the random porous media they construct. Other variants of the Kozeny equation that  
209 depend solely on porosity have been proposed by *Nielsen et al.* [1984] and *Ahuja et al.*  
210 [1989].

211 In sum, estimates of permeability based on the Kozeny and Kozeny-Carman equations  
212 are reasonably accurate when applied to an intermediate range of porosities. This is true  
213 for simulations based on pore-scale flows and physical experiments at laboratory scales.  
214 For low porosity porous media like the Fontainebleau sandstone, shales, or sand-shale mix-  
215 tures, however, estimates of permeability based on the Kozeny equation are frequently  
216 inaccurate, probably because linear dependence on porosity and the square of mean hy-  
217 draulic radius ( $R^2$ ) does not completely capture the detailed effects of interconnectivity  
218 within a pore network. When interconnectivity is accounted for by means of a formation  
219 factor, permeability is fairly well captured by a power law based on porosity. The effect  
220 that (squared) mean hydraulic radius has on permeability is not as well-established in the  
221 literature as the effect of porosity. *Revil and Cathles* [1999] include it as a linear factor in  
222 the porosity-based power law that they propose.

### 3. Simulation of Pore Network Flow and Permeability

223 First we provide the methods used to generate the virtual porous media and describe  
224 the physical data samples. Next, the procedure used to numerically integrate the Navier-  
225 Stokes equations within the explicit pore spaces is sketched, (see [SW10] for a complete  
226 description). Last, we detail the methods for observing and estimating variables of the  
227 pedotransfer functions.

#### 3.1. Porous Media

228 The seventy-eight three dimensional porous media used as data sets for this study  
 229 are comprised of a volcanic tuff, a column of glass beads, thirteen unique sandpacks,  
 230 sandstones, and carbonates provided in Table 2 of *Mostaghimi et al.* [2013], and sixty-  
 231 three realizations drawn from ensembles of virtual porous media with specified expected  
 232 geometry and topology.

### 233 3.1.1. Virtual Porous Media

234 Each virtual porous medium is a three-dimensional pore space with sides of length  
 235  $L_x = L_y = 1.27$  cm, height  $L_z = 2.55$  cm, and volume  $V = 4.11\text{cm}^3$  with individual pore  
 236 areas typically 1-10  $\mu\text{m}^2$  at a horizontal cross section. Level-set percolation [*Alexander*  
 237 *and Molchanov*, 1994; *Alexander*, 1995] is used to generate realizations of porous media  
 238 from underlying random topographies.

239 To generate each virtual pore space realization, independent identically distributed ran-  
 240 dom values are sampled uniformly on the interval  $[0, 1]$  and one value,  $f_{\mathbf{i}}$ , is assigned to  
 241 each node,  $\mathbf{i}$ , on a three-dimensional grid. Correlated random topographies are gener-  
 242 ated from  $f_{\mathbf{i}}$  using three different methods. In the first method,  $f_{\mathbf{i}}$  is convolved with  
 243 a symmetric Gaussian kernel to generate an isotropic correlated random topography by  
 244 transforming  $f_{\mathbf{i}}$  into frequency space, multiplying it by a Gaussian function, and then  
 245 transforming it back into real space. The correlation length of this random topography is  
 246 determined by the standard deviation of the Gaussian function which is fixed at  $\sigma = 0.01$ ;  
 247 see [*HSW12*] for details of this method. In the second method, a uniform kernel is ap-  
 248 plied by uniformly weighting every point in a cube centered on  $\mathbf{x}$  with sides of length  
 249  $l = 4$ . In the third method the random field  $f_{\mathbf{i}}$  is low-pass filtered using  $m$  consecutive  
 250 applications of the tensor product  $f^{flt} = f^{flt_x} \otimes f^{flt_y} \otimes f^{flt_z}$ ; see [*SW10*] for details of

251 this method. Here, the symmetric weighting operator sweeps over  $f_i$  four times,  $m = 4$ .  
252 Values of  $\sigma = 0.01$ ,  $l = 4$ , and  $m = 4$  are chosen so the correlation lengths of realizations  
253 are approximately the same,  $\sim 0.05$  cm. Since the convolution kernels have unit  $\mathcal{L}^2$  norm  
254 the convolutions do not change the expected value or range of the topographies. More-  
255 over, the central limit theorem implies that all three methods yield topographies whose  
256 elements are approximately Gaussian.

257 A pore space realization is derived by applying a level threshold,  $\gamma \in [0, 1]$ , to each  
258 node value in the topography. If the value at the node is greater than  $\gamma$ , then the node  
259 is placed in the solid matrix, otherwise it is in the void space. For physical intuition,  $\gamma$   
260 can be thought of as a control parameter which determines the expected porosity of a  
261 pore space realization (Fig. 1), the exact linear relationship between the two is given in  
262 Section II. A of [HSW12]. As  $\gamma$  increases, porosity and hydraulic radius also increase, while  
263 tortuosity decreases (Table 1). The result of applying this level set percolation method is  
264 a statistically stationary pore volume in the sense that the finite-dimensional probability  
265 distributions of pore space membership are invariant with respect to translation in space.

266 The level threshold determines the flow volume, the geometric properties of porosity and  
267 mean hydraulic radius, and topological properties such as the number of connected pore  
268 channels and number of connected solid components. Another topological effect of the  
269 level threshold is revealed by the existence of a percolation limit for topographies generated  
270 by a given kernel, a threshold below which no amount of pressure will drive significant  
271 flows through a pore space realization. At high values of the threshold parameter the flow  
272 regime resembles slow flow around disconnected bodies with Reynolds numbers ranging  
273 between 1 and 2.

### 274 3.1.2. Physical Porous Media

275 The tuff data comes from a  $0.34\text{cm}^3$  sample volume with porosity 0.37 [*Wildenschild*  
 276 *et al.*, 2004], and the glass beads are from a sample volume of  $0.032\text{cm}^3$  with porosity  
 277 0.31 [*Culligan et al.*, 2004]. Horizontal cross sections of these physical media are shown  
 278 in Fig. 2. *Mostaghimi et al.* [2013] obtain binarized three dimensional rock images of six  
 279 sandpacks, five sandstones, and two carbonates using micro CT imaging, and determine  
 280 the permeability of the thirteen samples by numerically solving the Stokes equations in  
 281 the void space to attain steady state flow and pressure fields and then inverting Darcy's  
 282 law. The samples' porosity, specific surface, and permeability are provided in Table 2  
 283 of *Mostaghimi et al.* [2013].

### 3.2. Computational Fluid Dynamics

284 Flow in the virtual media is simulated by numerically solving the incompressible Navier-  
 285 Stokes equations on a Cartesian domain with dimensions  $L_x = L_y = 1.27$  cm and  $L_z =$   
 286  $2.55$  cm, and volume  $V = 4.11\text{cm}^3$ . The grids have 128 nodes in the horizontal directions  
 287 and 256 in the vertical direction. Computational limitations require that sub-volumes  
 288 of the beads and tuff be extracted from the center of the entire sample. Each medium,  
 289 whether virtual or physical, is periodic in the vertical direction with no flow allowed  
 290 across lateral boundaries. The real media are reflected across a horizontal plane to create  
 291 periodic boundaries in the vertical; *Siena et al.* [2012] demonstrated that this reflection  
 292 does not affect results.

293 The multi-scale computational fluid dynamics modeling system EULAG [*Prusa et al.*,  
 294 2008] is used to solve the governing Navier-Stokes equations for water flow, as in [*SW10*]  
 295 and [*HSW12*], and the three components of velocity and pressure gradient are computed

296 at every point within each porous medium. The EULAG system accommodates a broad  
297 class of flows and underlying fluid equations in a variety of domains on scales ranging from  
298 wind tunnel and laboratory [*Wedi and Smolarkiewicz, 2006; Smolarkiewicz et al., 2007;*  
299 *Waite and Smolarkiewicz, 2008*] through terrestrial environments and climate [*Grabowski*  
300 *and Smolarkiewicz, 2002; Abiodun et al., 2008a, b; Ortiz and Smolarkiewicz, 2009*], to  
301 stellar [*Ghizaru et al., 2010*].

### 302 **3.2.1. Immersed Boundary Method**

303 The crux of our computational approach for simulating flows in porous media is an  
304 immersed-boundary method [*Peskin, 1972; Mittal and Iaccarino, 2005*] that inserts ficti-  
305 tious body forces into the equations of motion to mimic the presence of solid structures  
306 and internal boundaries. The resulting dynamics are such that velocity is negligible and  
307 pressure irrelevant within the solid matrix where the body forces are high. The particular  
308 technique employed is a variant of feedback forcing [*Goldstein et al., 1993*], with implicit  
309 time discretization admitting rapid attenuation of the flow to stagnation within the solid  
310 matrix in  $\mathcal{O}(\delta t)$  time comparable to the time step  $\delta t = 5 \times 10^{-5}$  seconds of the fluid  
311 model. The flow simulations are run for  $5 \times 10^{-2}$  seconds with steady state conditions  
312 reached in  $2 - 3 \times 10^{-2}$  seconds. The complete description of this methodology for re-  
313 solving flow in explicit pore networks along with comparisons to other available methods  
314 are in [*SW10*], [*HSW12*], and *Siena et al. [2012]*. Nonetheless, the concept behind this  
315 method is provided for the reader's convenience.

316 Since we focus on gravity-driven flows of a homogeneous incompressible fluid (e.g. wa-  
 317 ter) through a porous medium, the Navier-Stokes equations are,

$$318 \quad \nabla \cdot \mathbf{v} = 0, \tag{6}$$

$$319 \quad \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla \pi' + \mathbf{g}' + \mu \Delta \mathbf{v} - \alpha \mathbf{v}.$$

320 The primes refer to perturbations with respect to static ambient atmospheric conditions  
 321 characterized by a constant density,  $\rho_0$ , and pressure,  $p_0 = p_0(z)$ , so  $\pi' = (p - p_0)/\rho$  and  
 322  $\mathbf{g}' = (0, 0, -g\rho'/\rho)$  where  $\rho = \text{const} \gg \rho_0$  denotes the density of fluid and  $g$  is gravitational  
 323 acceleration,  $g = 9.81 \text{ m/s}^2$ . The kinematic viscosity of water,  $\mu$ , is  $10^{-6} \text{ ms}^{-2}$ .

324 The last term on the right hand side of the momentum equation is the fictitious re-  
 325 pelling body force of the immersed-boundary method, with a non-negative time scale  
 326  $\alpha^{-1}(\mathbf{x}) = 0.5\delta t$  and the corresponding inverse time scale  $\alpha(\mathbf{x}) = 0$  within the solid and  
 327 fluid, respectively. Intuitively, setting  $\alpha(\mathbf{x}) = 0$  within the fluid admits Navier-Stokes  
 328 flows away from the solid boundaries, while requiring  $\alpha(\mathbf{x}) \rightarrow \infty$  within the solid assures  
 329  $\mathbf{v} \rightarrow 0$  there.

330 Unlike other immersed boundary methods, the pore space boundaries are aligned with  
 331 grid nodes and the resulting media are simulated only with first-order accuracy in space.  
 332 However, the macroscopic uncertainty of microscopic pore structure greatly exceeds nu-  
 333 merical inaccuracies in the detailed representation of internal boundaries. Therefore, the  
 334 first order approximation of a porous medium is adequate, at least for determining sta-  
 335 tistical bulk properties of the media and flow.

### 3.3. Variables for Transfer Functions

336 Porosity,

$$337 \quad n = V_P/V, \quad (7)$$

338 is the ratio of void volume,  $V_p$ , over bulk volume,  $V$ , and measures the relative capacity  
339 of a porous medium to hold water. Mean hydraulic radius,

$$340 \quad R = V_P/A_i, \quad (8)$$

341 is the ratio the void volume over the total interstitial area between the pore space and  
342 the solid matrix,  $A_i$ , and indicates the average level of connectivity in the network.

343 The tortuosity,

$$344 \quad \tau(a, b) = l_S/l, \quad (9)$$

345 of a fluid particle trajectory connecting two points  $a$  and  $b$  is the ratio of the trajectory  
346 length,  $l_S$ , over the Euclidean distance between its end points,  $l = \|a - b\|$ , hence  $1 \leq$   
347  $\tau(a, b) < \infty$ . A number of alternate definitions are in use including  $\tau^2$ ,  $\tau^{-1}$ , and  $\tau^{-2}$   
348 [Bear, 1988]. The average tortuosity,

$$349 \quad \bar{\tau} = \frac{1}{N} \sum_{i=1}^N \tau(a_i, b_i), \quad (10)$$

350 is taken over a sample of  $i = 1, \dots, N$  tortuosities,  $\tau(a_i, b_i)$ , each of which is derived  
351 from a particle trajectory that percolates through the entire medium. To determine the  
352 trajectory of a fluid particle, we follow [HSW12], and use every node in the void space  
353 at the top horizontal cross section as an initial position for a particle. To minimize the  
354 underestimation of tortuosity, only particles that percolate through the entire domain  
355 are included in the calculation of average tortuosity. The trajectory length,  $l_S$ , for every  
356 particle that percolates through the entire domain is used to compute tortuosity (9) and

357 the average tortuosity for a pore space realization (10), cf., Section III. B of [HSW12] for  
 358 a complete discussion.

359 [HSW12] and *Matyka et al.* [2008] both demonstrated that average tortuosity (10) is  
 360 underestimated if the extent of the observation domain through which particles are tracked  
 361 is not sufficiently large. Furthermore, as the extent of the observation domain increases the  
 362 dependence on the extent of the domain decays exponentially, fluctuations in the computed  
 363 values diminish, and a representative elementary volume with respect to tortuosity is  
 364 observed for random virtual media.

365 Linear correlations among porosity, hydraulic radius, and tortuosity are significant  
 366 across the entire data set (Table 2). The porosities of the glass beads and tuff are com-  
 367 parable to porosities for virtual media generated using the lowest value of the threshold  
 368 parameter. Tortuosities and hydraulic radii of the beads and tuff are also comparable to  
 369 those observed in the least permeable realizations of virtual media. The permeabilities  
 370 and hydraulic radii of the data provided in *Mostaghimi et al.* [2013] are two to four orders  
 371 of magnitude smaller than the stochastically generated pore networks used to derive the  
 372 power laws, but have porosities comparable to the lower end of the synthetic media.

### 3.4. Permeability Estimates

373 Experimental estimates of permeability are obtained by applying Darcy’s Law to the  
 374 results of computational experiments with saturated pore spaces at steady state. By  
 375 observing the pressure drop,  $\Delta p$ , and discharge of water,  $Q$ , from a column of sand of  
 376 length  $L$  and cross-sectional area  $A$ , Darcy, [*Darcy*, 1856], established that discharge per  
 377 unit area,  $Q/A$ , is proportional to the average pressure gradient,  $\Delta p/L$ , once steady-state

378 is reached,

$$379 \quad \frac{Q}{A} = -\frac{k}{\mu\rho} \frac{\Delta p}{L}. \quad (11)$$

380 The constant combines fluid density,  $\rho$ , and kinematic viscosity,  $\mu$ , with permeability,  
381  $k$ , a material characteristic of a porous medium; the ratio  $K = k/(\mu\rho)$  is the saturated  
382 hydraulic conductivity of water according to Darcy.

383 Here, the permeability of each column of porous material bounded by solid walls on the  
384 lateral sides is estimated using the steady state velocity field,  $\mathbf{v} = (u, v, w)$ , and associated  
385 pressure field,  $p$ , of a fluid moving predominantly in the vertical direction. The total flux  
386 at a cross section of height  $z$  is estimated by

$$387 \quad Q(z) = \int_A w(x, y, z)\chi(x, y, z)dxdy, \quad (12)$$

388 where  $\chi$  is the characteristic (indicator) function within the porous material,  $\chi(x, y, z) = 1$   
389 in the void space and  $\chi(x, y, z) = 0$  in the solid matrix. The total pressure is converted to  
390 hydraulic head,  $h = (p - p_o)/(\rho g) + z - z_o$ , where  $p_o$  is a reference pressure at the datum  
391  $z_o$  and  $g$  is gravitational acceleration, and then the average hydraulic head at each cross  
392 section is estimated as

$$393 \quad H(z) = \frac{1}{n(z)A} \int_A h(x, y, z)\chi(x, y, z)dxdy, \quad (13)$$

394 where  $n(z)$  is the porosity of the cross section at the level  $z$ . Expressing (11) in terms of  
395 (12) and (13) and rearranging terms, the permeability at each cross section is estimated

$$396 \quad k(z) = -\frac{\mu}{g \Delta \{ [n(z)]^{-1} \int_A h(x, y, z)\chi(x, y, z)dxdy \}} \frac{\int_A w(x, y, z)\chi(x, y, z)dxdy}{L}. \quad (14)$$

397 Because the dominant direction of flow is perpendicular to the cross sections, the average  
398 equivalent permeability for the entire sample is the harmonic average of the cross section

399 permeabilities

$$400 \quad k_e = L_z \left( \int_{L_z} \frac{1}{k(\zeta)} d\zeta \right)^{-1}. \quad (15)$$

401 In practice, the support volume of this procedure is the horizontal cross section of each  
 402 column with a vertical extent of three vertical grid levels. This volume is used to compute  
 403 a second order accurate centered difference approximation of the hydraulic gradient in the  
 404 vertical direction and the total flux (12) at each horizontal cross section.

### 3.5. Grid Resolution

405 In order to select a practical resolution for large numbers of flow simulations, a prelim-  
 406 inary investigation is performed to determine how variations in grid resolution influence  
 407 the observed Darcy flux,  $q = Q/A$  (11), and estimated permeability,  $k_e$  (15). Because the  
 408 generation procedure of virtual media depends on the grid, a physical sample with fixed  
 409 resolution is used to assess the grid resolution effects. Using a sub-volume of the column  
 410 of glass beads, whose physical characteristics are discussed in Section 3.1.2, the grid is  
 411 refined and coarsened to four different levels. Linear interpolation is used to map the data  
 412 set between varying grid resolutions. Table 3 displays grid dimensions, discretization step  
 413 size,  $\delta x$ , mean Darcy flux,

$$414 \quad \bar{q} \equiv \frac{1}{L_z} \int_{L_z} q(\zeta) d\zeta, \quad (16)$$

415 average relative deviation from mean Darcy flux, Dev q, estimated permeability,  $k_e$ , aver-  
 416 age relative deviation from estimated permeability, Dev  $k_e$ , average tortuosity (10), and  
 417 the variance of tortuosities for all four resolutions. Dev q and Dev  $k_e$  are defined as

$$418 \quad \text{Dev } q \equiv \overline{|\bar{q} - q(z)|/|\bar{q}|} \quad \text{and} \quad \text{Dev } k_e \equiv \overline{|k_e - k(z)|/|k_e|}, \quad (17)$$

419 respectively, where the over-bar on the right hand side denotes vertical average as in (16).

420 Since the flow system is at steady-state, conservation of mass dictates that Dev  $q$  should  
 421 be zero. On the other hand, Dev  $k_e$  is not similarly constrained and finer resolutions should  
 422 yield better estimates of variations in permeability. The mean Darcy flux and estimated  
 423 permeability are about the same for all grid resolutions; whereas the values of Dev  $q$  are  
 424 relatively low, showing that conservation of mass is approximately satisfied, and improves  
 425 with grid resolution, approaching first order asymptotic convergence as pointed out in the  
 426 last paragraph of Section 3.2. The decreasing differences in average tortuosity and the  
 427 convergence of the variance of tortuosity at finer grid resolution also indicate that the  
 428 local flow field is better resolved with the finer mesh.

429 We supplement our convergence study for the integral characteristics of the Darcy flows  
 430 with a local convergence study for three randomly selected and substantially separated  
 431 locations in the vertical. Table 4 displays grid discretization size and the  $\mathcal{L}^2$  difference  
 432 between the probability distribution functions (pdf) generated by each component in the  
 433 velocity vector,  $(u, v, w)$ , and the pdfs generated by velocity components at the finest  
 434 resolution. For each of the velocity components at all three levels the relative error from  
 435 the finest mesh resolution solution exhibits the aforementioned first order convergence.  
 436 Moreover, the error between finest and second finest resolution is small. Therefore, we  
 437 select the second most refined grid,  $\delta x = 1.e^{-4}\text{m}$ , for computational affordability.

#### 4. Generalized Pedotransfer Functions

438 The data consist of triples  $(k_i, n_i, R_i)$  for each of the  $i = 1, \dots, 63$  virtual pore spaces.  
 439 Models, whose parameters are fitted through least squares, produce an estimate,  $\hat{k}_i =$   
 440  $\hat{k}(\eta_i)$ , of permeability with  $\eta$  referring to  $n$ ,  $R^2$ , or  $nR^2$ . To evaluate the performance of

441 the models the independent real media data are withheld from the fitting and used to  
 442 evaluate the goodness-of-fit through plots and overall chi-squared tests.

#### 4.1. Empirical Pedotransfer Functions

443 When the data are fitted to the Kozeny equation (1), the Kozeny coefficient is  $c_0 = 0.19$ ,  
 444 which is essentially the same as Carman's original value of  $1/5$  [Carman, 1939] and falls  
 445 within the range  $[1/6, 1/2]$  that he gave later [Carman, 1956]. However, the relationship  
 446 between permeability and the Kozeny predictor is nonlinear over the ranges of sample data  
 447 (Fig. 3). The Kozeny equation captures the basic rising trend of permeability with the  
 448 Kozeny predictor,  $nR^2$ , but the requirement that the model goes through the origin, which  
 449 is a necessary condition for a physically consistent law, constrains the performance of the  
 450 Kozeny equation. The best fit linear model to these data, which is not shown, has a linear  
 451 correlation of 0.9, but it does not go through the origin. The nominal 95% confidence  
 452 intervals for the Kozeny equation are so wide that they easily include the independent  
 453 real data. Confidence intervals are nominal in the sense that classic statistical formulae  
 454 are used to calculate them, but the data do not meet independence and distributional  
 455 criteria for statistical hypothesis testing. Nonetheless, the confidence intervals are useful  
 456 for comparisons. For these purposes, a useful confidence interval is narrow, yet includes  
 457 nearly all the data.

458 A better fit to the data can be attained using nonlinear models based on porosity  $n$ ,  
 459 hydraulic radius  $R^2$ , and their product  $nR^2$ . Three power law models to predict perme-  
 460 ability,  $\hat{k}(\eta) = a(\eta)^b$ , are derived and compared to the linear Kozeny equation. The free  
 461 parameters  $a$  and  $b$  are fitted using the nonlinear fit module in MATHEMATICA [Wol-  
 462 fram, 1999]. Due to the high correlation of tortuosity  $\tau$  with  $n$  and  $R^2$ ,  $\tau$  is not used as

463 a predictor variable in the power laws. All three power laws capture the nonlinear trend  
 464 of the data and their confidence intervals are fairly tight including the independent real  
 465 data (Fig. 4-6).

466 The sum of squared departures of the simulated data,  $\hat{k}$ , from the model estimates,

$$467 \quad s_d^2 = \sum_{i=1}^{N_s} (\hat{k}_i - k_i)^2, \quad (18)$$

468 is the total variability in the data that is not accounted for by the models where  $N_s$  is  
 469 the number of samples ( $N_s = 63$  for this data set). The sum of squared departures of the  
 470 Kozeny equation is an order of magnitude greater than those of the power laws (Table 5).

471 The additional parameter is one reason the power laws perform better than the Kozeny  
 472 equation. A statistical method, the Analysis of Variance [*Mood et al.*, 1963], takes this into  
 473 account by weighting the sum of squared departures with  $P$ , the number of parameters  
 474 in the model, and comparing it to the model sum of squares,

$$475 \quad s_M^2 = \sum_{i=1}^{N_s} (\hat{k}_i - \langle k \rangle)^2, \quad (19)$$

476 weighted by  $N_s - P$ , the degrees of freedom remaining in the sample after accounting for  
 477 the parameters. The model sum of squares reflects the ability of the model to capture the  
 478 structure of the data as departures from the sample mean,  $\langle k \rangle$ . The ratio,

$$479 \quad F = \frac{s_M^2/P}{s_d^2/(N_s - P)}, \quad (20)$$

480 can be used to compare models: the larger is  $F$ , the better is the fit of the model. The  
 481  $F$  ratios of the predictor power law is about four times greater than that of the Kozeny  
 482 equation despite the additional parameter (Table 6). The  $F$  ratios for the power laws  
 483 based solely on  $n$  or  $R^2$  are triple and double that of the Kozeny equation.

## 4.2. Range of Applicability

484 Porous media may fall into three classes. The first class consists of ordinary porous  
 485 media with porosities in the approximate range  $0.2 < n < 0.7$ . In these cases, porosity  
 486 is primary in the sense that it arises from voids in the material of the medium. In the  
 487 second class there are barely permeable media with low porosities,  $n < 0.2$ . Often such  
 488 media are composed of nearly solid rock with secondary channels arising from external  
 489 mechanical or thermal stresses [Davis, 1988]. In these cases flow often corresponds to flow  
 490 through a collection of discrete, sparsely connected pipes. Finally, the third class consists  
 491 of highly permeable media where flow is similar to slow flows with obstructions that are  
 492 relatively widely spaced, for instance fluidized beds. The porous media investigated here  
 493 fall into either the first or third class.

494 When restricted to media of the first class, porosities  $0.2 < n < 0.7$ , a version of the  
 495 Kozeny equation

$$496 \quad k = 0.35nR^2, \quad (21)$$

497 provides reasonable estimates of permeability in agreement with the conclusions of Xu  
 498 and Yu [2008]. In this range, the model (21) also provides a close fit to the real data  
 499 (Fig. 7). Moreover, the computed Kozeny coefficient,  $c_0 = 0.35$ , is within the range  
 500  $1/6 < c_0 < 1/2$  given by Carman [1956]. Within this normal range of porosity, the  
 501 Kozeny-Carman equation (2) is

$$502 \quad k = 0.45nR^2/\tau^2. \quad (22)$$

503 Carman [1956] mentions  $c'_0 = 0.40$  is plausible for non-circular sections.

504 The  $F$  ratio (20) for model (21) is  $F = 1770.55$ , which is greater than the  $F$  ratio  
 505 obtained for the power laws based upon  $n$  or  $R^2$  and thrice as large as that for the Kozeny

506 equation fitted to the entire data set. However, the  $F$  ratio of model (22),  $F = 551.09$ , is  
 507 less than half of that of (21).

508 The Kozeny equation does not account for variability over the full range of data as well  
 509 as the power laws, having a sum of squared errors that is an order of magnitude greater  
 510 than the power law models (Table 5). This is true even when the model sums of squares  
 511 are adjusted for the number of parameters (Table 6).

512 Of the four models considered here, the power law based on the Kozeny predictor,

$$513 \quad \hat{k} = 1.68 \cdot 10^{-4} (nR^2)^{0.58}, \quad (23)$$

514 fits the entire virtual data set best having an  $F$  ratio of 1866.17, which is nearly four times  
 515 that of the Kozeny equation over the entire set and roughly double that of (21). Power  
 516 laws based on porosity and hydraulic radius, the components of the Kozeny predictor,  
 517 also give good fits to all the data. The exponent appears to account for nonlinear effects  
 518 at the extremes of pore space interconnectivity consistent with observations of Jacquin  
 519 [1964] quoted in [Adler *et al.*, 1990], *Lemaitre and Adler* [1990] and *Revil and Cathles*  
 520 [1999].

521 Figures (3-6) indicate that the power-law models and the Kozeny equation fit the inde-  
 522 pendent observed data well. However, the power-law based on porosity alone does not fit  
 523 the low permeability samples obtained from *Mostaghimi et al.* [2013] as well as the other  
 524 models. Nonetheless, the power laws are clearly superior to the Kozeny equation when  
 525 the goodness of model fits is evaluated by chi-squared tests applied to both observed and  
 526 virtual data (Table 7). Chi-squared tests are based on distances between model estimates  
 527 and data weighted by the estimates [Mood *et al.*, 1963], and are used here qualitatively  
 528 in the same spirit as the Analysis of Variance results reported earlier (Table 6). Small

529 values of the chi-squared statistic indicate good fits, and the chi-squared values for the  
530 power laws are about five-six times smaller than the corresponding value for the Kozeny  
531 equation.

## 5. Summary and Conclusions

532 Kozeny derived his equation by equating the velocity given by Poiseuille's law for flow  
533 through an idealized pore network to the specific discharge obtained via Darcy's law; he  
534 determined that the permeability of a porous medium,  $k$ , is linearly proportional to the  
535 product  $nR^2$  of its porosity,  $n$ , with the square of its mean hydraulic radius,  $R$ . This  
536 simplified model of a porous medium allowed him to attain an analytical solution to the  
537 governing equations of flow through porous media. However, topological alterations that  
538 make a pore network more realistic render analytical solutions nearly intractable. When  
539 applied over a wide range of porous media, computational experiments reveal a nonlinear  
540 relationship between permeability and its predictors, contrary to Kozeny's result. This  
541 nonlinearity is manifested by the wide range of values of the Kozeny coefficient observed  
542 at the extreme ends of porosity [*Sullivan*, 1942; *Kyan et al.*, 1970; *Davies and Dollimore*,  
543 1980; *Adler et al.*, 1990; *Xu and Yu*, 2008]. On one hand, Kozeny's linear (in the predictor  
544  $nR^2$ ) approximation appears satisfactory within a restricted range of porosities,  $0.2 < n <$   
545  $0.7$ . On the other hand, the nonlinearity cannot be adequately represented by a linear  
546 approximation when a wider range of porosity is considered.

547 We empirically derive three nonlinear generalized pedotransfer functions for permeabil-  
548 ity using computational experiments with flow through a set of stochastically generated  
549 pore networks with porosities ranging from 0.19 to 0.84 and varying degrees of connec-  
550 tivity. The transfer functions are power laws based on porosity  $n$ , mean hydraulic radius

551 squared  $R^2$ , and their product  $nR^2$ ; the same predictor which Kozeny used. The ex-  
552 perimental pore networks consist of sixty-three virtual networks whose permeabilities,  
553 porosities, and mean hydraulic radii are used to estimate the parameters of the transfer  
554 functions. Porosity and mean hydraulic radius are observed directly from images of the  
555 pore networks and Darcy's law is used to compute the permeability from steady-state flow  
556 fields within the porous media.

557 When fitting the Kozeny equation to the full range of data, the computed value of the  
558 Kozeny coefficient computed is  $c_0 = 0.19$ , essentially the value originally suggested by  
559 Carman,  $c_0 = 1/5$  [Carman, 1939]. However, the Kozeny equation does not provide good  
560 estimates of permeability over the full range of data, because of the nonlinear dependence  
561 of  $k$  on the Kozeny predictor,  $nR^2$ . On the other hand, the Kozeny equation is reasonably  
562 accurate within a limited range of porosities (Fig. 7), but not for the originally suggested  
563 value of the Kozeny coefficient. Nonetheless, the estimated value of  $c_0 = 0.35$  is within  
564 the wider range  $1/6 < c_0 < 1/2$  that Carman gave later [Carman, 1956].

565 All of the transfer functions include the fifteen independent real data samples within  
566 nominal 95% confidence intervals. The power laws fit the data in this study better than  
567 the Kozeny equation, even when they are penalized through an Analysis of Variance for  
568 including an additional model parameter (Table 5-6). The leading coefficient of each  
569 power law is an empirical fitting parameter and has dimensions of  $L^{2(1-b)}$ , where  $b$  is the  
570 power appearing in Table 5. Only in specialized cases, such as the Kozeny equation are  
571 the associated coefficients dimensionless. Similar functions to predict permeability having  
572 coefficients with dimensions are already present in the literature [Katz and Thompson,  
573 1986; Ahuja et al., 1989; Rodriguez et al., 2004; Costa, 2006].

574 The equation

$$575 \hat{k} = 1.68 \cdot 10^{-4} (nR^2)^{0.58} \quad (24)$$

576 provides the best fit to the full range of data. Additionally, its confidence intervals are  
577 tighter, its sum of squared departures is smaller, and its  $F$  (20) ratio is higher than any  
578 of the other models considered.

579 Even though Kozeny derived his equation through microscopic considerations, it has  
580 been applied on macroscopic scales as a generalized pedotransfer function. Commonly,  
581 pedotransfer functions are derived empirically using various soil samples in continuum  
582 scale laboratory experiments where the predictors, e.g., porosity and mean hydraulic  
583 radius, can be measured in bulk.

584 The virtual networks that are the basis for these transfer functions are homogeneous  
585 and isotropic with porosities and mean hydraulic radii spanning a wide range of repre-  
586 sentative values. Sample permeabilities are comparable to those found in well- sorted  
587 sands or sands and gravel. Since the networks are large enough to constitute represen-  
588 tative elementary volumes [HSW12], the physical basis and scale of these experiments  
589 is comparable to that which Kozeny used. Moreover, the derived pedotransfer functions  
590 are not formally limited to representations of explicit pore spaces or a particular soil type  
591 because porosity and hydraulic radius can be estimated in bulk using field observations  
592 or laboratory experiments and are general traits of porous media. As a result, it should  
593 be possible to test whether the proposed generalized pedotransfer functions apply in the  
594 field.

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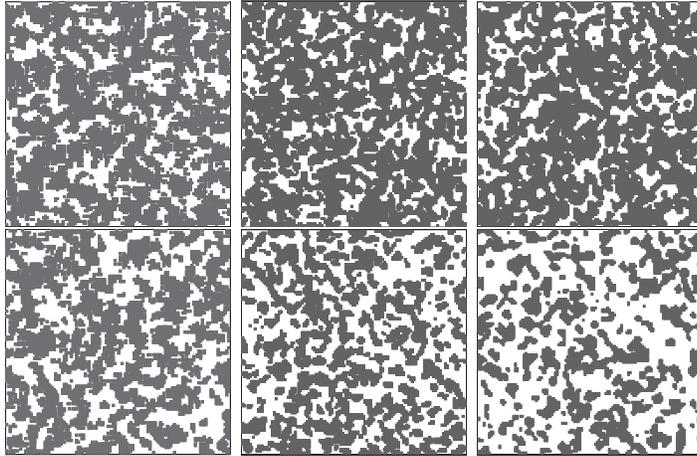
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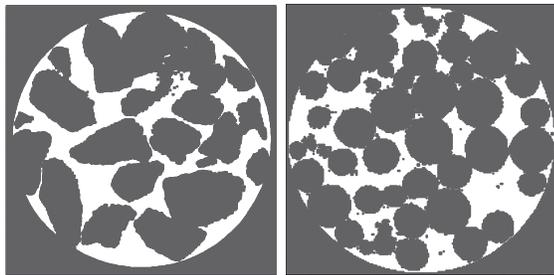
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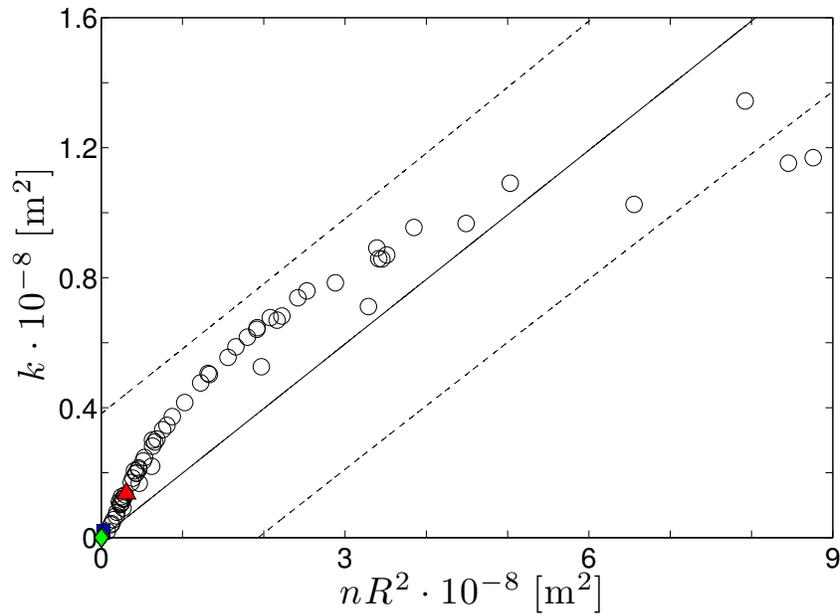
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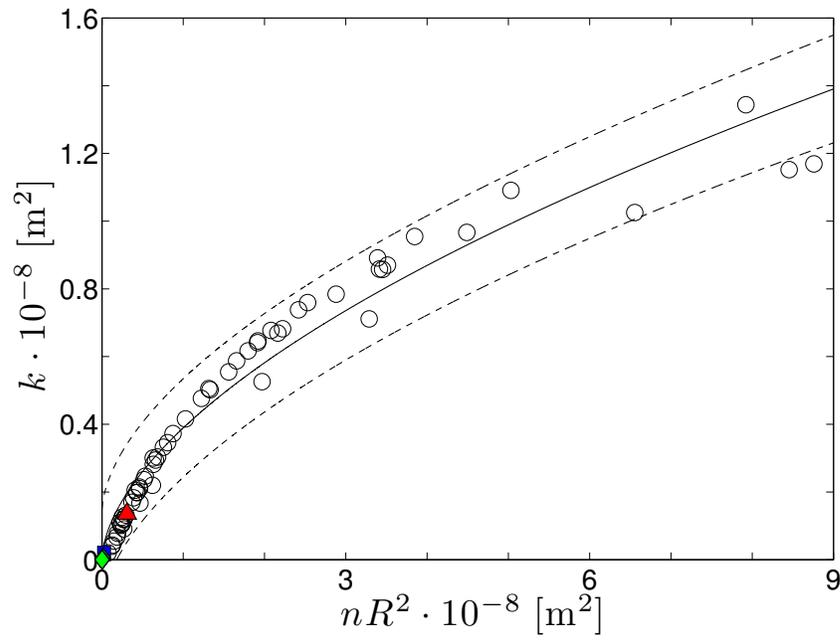
**Figure 1.** Porespace cross-sections in the x-y plane ( $1.27 \text{ cm} \times 1.27 \text{ cm}$ ). From left to right : uniform kernel, Gaussian kernel, and iterative method; top, Threshold Parameter 0.45 (Expected Porosity  $\approx 0.35$ ) ; bottom, Threshold Parameter 0.53 (Expected Porosity  $\approx 0.60$ ).



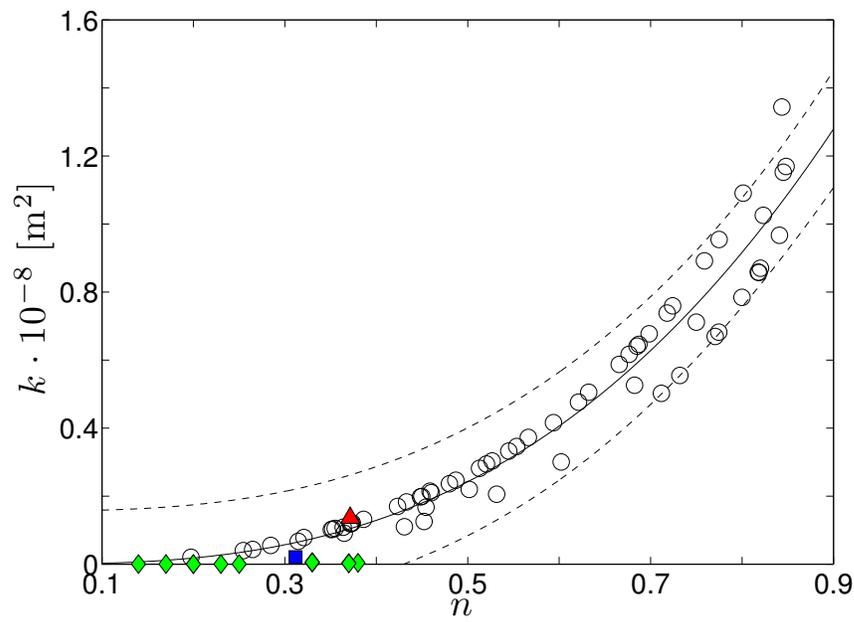
**Figure 2.** Physical porous media: tuff (left) and glass beads (right); corresponding values of  $(n, \tau, R)$  are  $(0.37, 1.23, 9.12 \cdot 10^{-5} \text{ m})$  and  $(0.31, 1.20, 2.89 \cdot 10^{-5} \text{ m.})$



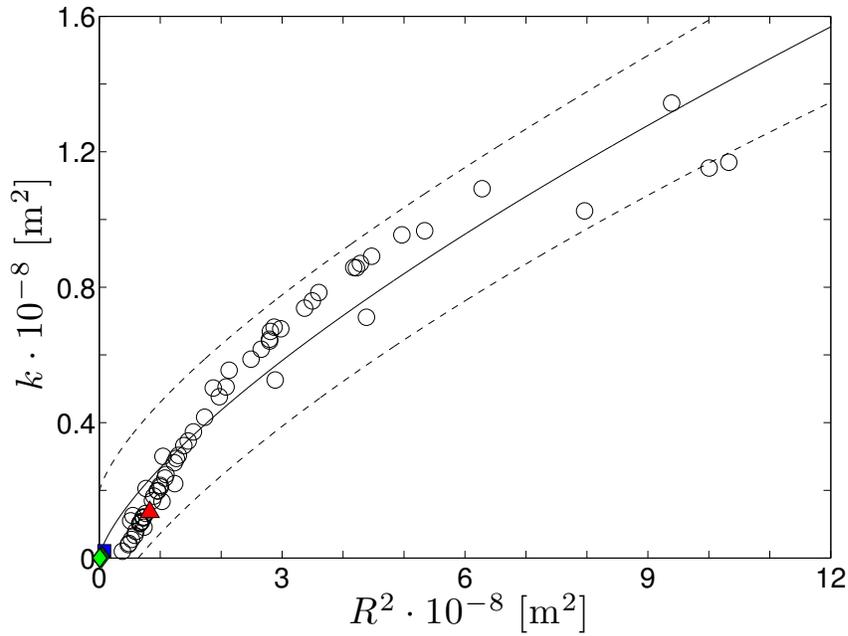
**Figure 3.** Kozeny equation  $k(nR^2) = c_0 nR^2$ . Points correspond to averaged amounts for each of the 63 stochastic realizations and fifteen sets of natural data. Circles, blue square, red triangle, and green diamonds denote synthetic data, glass beads, tuff, and the low permeability data of *Mostaghimi et al.* [2013] respectively. Least-squares models are solid lines, and nominal 95% confidence intervals are dashed lines.



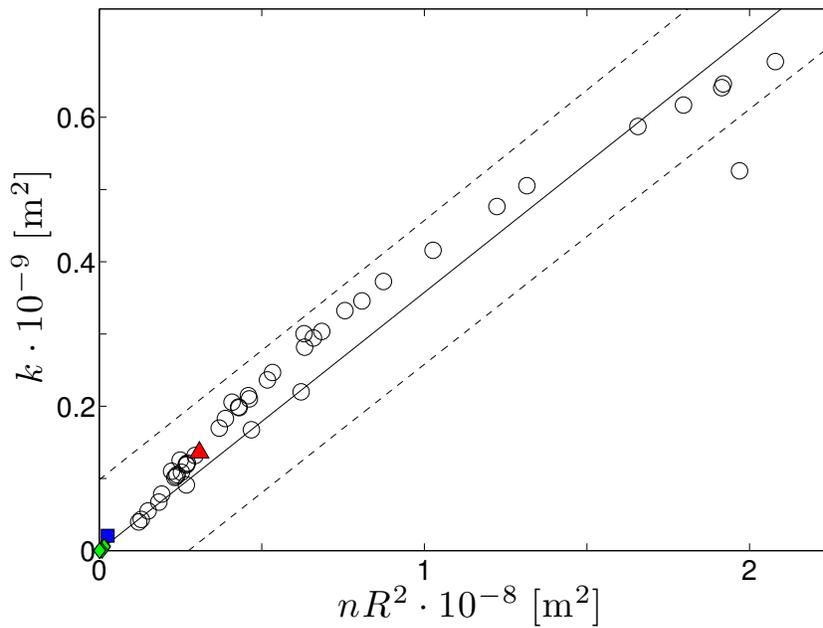
**Figure 4.** As in Fig. 3 but for power law  $k(R^2) = a(R^2)^b$ .



**Figure 5.** As in Fig. 3 but for power law  $k(n) = an^b$ .



**Figure 6.** As in Fig. 3 but for power law  $k(n) = a(nR^2)^b$ .



**Figure 7.** Kozeny equation fitted to porous media with normal porosities,  $0.2 < n < 0.7$ ; Circles, square, triangle, and diamonds denote synthetic data, glass beads, tuff, and the low permeability data of *Mostaghimi et al.* [2013] respectively.

**Table 1.** Characteristics of virtual media in Fig. 1.

	Uniform	Gaussian	Iterative
$\gamma = 0.45$ (Expected Porosity $\approx 0.35$ ) :			
$k^a$	$1.10 \cdot 10^{-9}$	$1.32 \cdot 10^{-9}$	$9.10 \cdot 10^{-10}$
$n^b$	0.43	0.38	0.36
$R^2^c$	$5.16 \cdot 10^{-9}$	$7.63 \cdot 10^{-9}$	$7.33 \cdot 10^{-9}$
$nR^2^d$	$2.22 \cdot 10^{-9}$	$2.94 \cdot 10^{-9}$	$2.68 \cdot 10^{-9}$
$\tau^e$	1.25	1.23	1.33
$\gamma = 0.53$ (Expected Porosity $\approx 0.60$ ) :			
$k^a$	$3.00 \cdot 10^{-9}$	$4.76 \cdot 10^{-9}$	$5.26 \cdot 10^{-9}$
$n^b$	0.60	0.62	0.68
$R^2^c$	$1.05 \cdot 10^{-8}$	$1.97 \cdot 10^{-8}$	$2.88 \cdot 10^{-8}$
$nR^2^d$	$6.30 \cdot 10^{-9}$	$1.22 \cdot 10^{-8}$	$1.97 \cdot 10^{-8}$
$\tau^e$	1.16	1.12	1.14

<sup>a</sup> Permeability [m<sup>2</sup>]

<sup>b</sup> Porosity

<sup>c</sup> Hydraulic radius squared [m<sup>2</sup>]

<sup>d</sup> Kozeny predictor [m<sup>2</sup>]

<sup>e</sup> Tortuosity

**Table 2.** Correlations among predictor variables.

	$n$	$R$	$\tau$
$n$	1.00	0.90	-0.95
$R$	0.90	1.00	-0.84
$\tau$	-0.95	-0.84	1.00

**Table 3.** Grid Resolution Study

$n \times m \times l$ <sup>a</sup>	$\delta x$ <sup>b</sup>	$\bar{q}$ <sup>c</sup>	Dev $q$ [%] <sup>d</sup>	$k_e$ <sup>e</sup>	Dev $k_e$ [%] <sup>f</sup>	$\bar{\tau}$ <sup>g</sup>	$\sigma(\tau)$ <sup>h</sup>
$18 \times 18 \times 38$	4.e-04	-2.00e-02	1.16	2.04e-09	121.86	1.25	1.54e-02
$36 \times 36 \times 76$	2.e-04	-2.08e-02	0.86	2.12e-09	117.08	1.28	2.11e-02
$72 \times 72 \times 150$	1.e-04	-2.12e-02	0.39	2.16e-09	202.41	1.31	2.21e-02
$144 \times 144 \times 300$	5.e-05	-2.02e-02	0.22	2.06e-09	215.61	1.31	2.22e-02

<sup>a</sup> Grid dimensions<sup>b</sup> Grid discretization [m]<sup>c</sup> Mean Darcy flux [m/s]<sup>d</sup> Average relative deviation from the mean Darcy flux [%]<sup>e</sup> Estimated permeability [m<sup>2</sup>]<sup>f</sup> Average relative deviation from estimated permeability [%]<sup>g</sup> Average Tortuosity<sup>h</sup> Variance of Tortuosities**Table 4.** Local Grid Resolution Study

$\delta x$ <sup>a</sup>	Level 1			Level 2			Level 3		
	$L^2(u)$ <sup>b</sup>	$L^2(v)$ <sup>c</sup>	$L^2(w)$ <sup>d</sup>	$L^2(u)$ <sup>b</sup>	$L^2(v)$ <sup>c</sup>	$L^2(w)$ <sup>d</sup>	$L^2(u)$ <sup>b</sup>	$L^2(v)$ <sup>c</sup>	$L^2(w)$ <sup>d</sup>
4.e-04	1.73e-01	1.44e-01	1.15e-01	1.48e-01	1.14e-01	1.19e-01	1.46e-01	1.22e-01	1.04e-01
2.e-04	7.33e-02	7.01e-02	5.65e-02	6.41e-02	5.25e-02	5.20e-02	7.36e-02	6.93e-02	5.50e-02
1.e-04	3.39e-02	4.10e-02	3.25e-02	3.07e-02	2.75e-02	3.24e-02	3.20e-02	3.14e-02	2.98e-02

<sup>a</sup> Grid discretization [m]<sup>b</sup>  $L^2$  difference between pdf of  $u$  and pdf of  $u$  at finest resolution<sup>c</sup>  $L^2$  difference between pdf of  $v$  and pdf of  $v$  at finest resolution<sup>d</sup>  $L^2$  difference between pdf of  $w$  and pdf of  $w$  at finest resolution**Table 5.** Accuracy of the four fitted models.

Model Form	Fit	$s_d^2$
$k(nR^2) = c_0 n R^2$	$\hat{k} = 0.19 n R^2$	$2.26 \cdot 10^{-16}$
$k(nR^2) = a(nR^2)^b$	$\hat{k} = 1.68 \cdot 10^{-4} (nR^2)^{0.58}$	$3.15 \cdot 10^{-17}$
$k(n) = a n^b$	$\hat{k} = 1.72 \cdot 10^{-8} (n)^{2.83}$	$3.72 \cdot 10^{-17}$
$k(R^2) = a R^{2b}$	$\hat{k} = 1.37 \cdot 10^{-3} (R^2)^{0.71}$	$5.61 \cdot 10^{-17}$

**Table 6.** Analysis of Variance

Model	$P$	$s_M^2/P$	$N_s - P$	$s_d^2/(N_s - P)$	$F$
Kozeny eq.	1	$1.74 \cdot 10^{-15}$	62	$3.65 \cdot 10^{-18}$	475.77
power law $k(nR^2)$	2	$9.65 \cdot 10^{-16}$	61	$5.16 \cdot 10^{-19}$	1866.17
power law $k(n)$	2	$9.62 \cdot 10^{-16}$	61	$6.11 \cdot 10^{-19}$	1574.55
power law $k(R^2)$	2	$9.52 \cdot 10^{-16}$	61	$9.20 \cdot 10^{-19}$	1034.89

**Table 7.** Chi Squared Statistics

Model	$\chi^2$ Statistics
Kozeny eq.	$7.57 \cdot 10^{-08}$
power law $k(nR^2)$	$1.12 \cdot 10^{-08}$
power law $k(n)$	$1.19 \cdot 10^{-08}$
power law $k(R^2)$	$1.76 \cdot 10^{-08}$