Lab and pore-scale study of low permeable soils diffusional tortuosity

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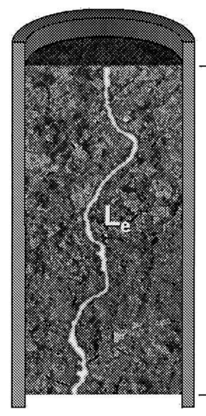
Problem and goal

Diffusion plays important role in subsurface contaminant spreading in low permeable units. The effective diffusion coefficient of saturated porous medium depends on this coefficient in water, porosity and structural parameter of porous space – tortuosity. Theoretical models of relationship between porosity and diffusional tortuosity are usually derived for conceptual granular models of medium filled by solid particles of simple geometry. These models usually do not represent soils with complex microstructure. The empirical models, like as Archie's law, based on the experimental electrical conductivity data are mostly useful for practical applications. Such models contain empirical parameters that should be defined experimentally for given soil type. In this work, we compared tortuosity values obtained in lab-scale diffusional experiments and pore scale diffusion simulation for the studied soil microstructure and exanimated relationship between tortuosity and porosity.

Theory



$$D = D_0 n \frac{L^2}{L_e^2}\delta = D_0 n \chi \delta = \varphi D_0$$

L – length of sample
L_e – minimum length of pore channel
χ – tortuosity (χ<1)
δ – constrictivity
φ – effective coefficient (D/D_0)
n – porosity

Using the analogy of Ohm's law, Fick's law and Archie empirical relationship for the electrical conductivity of the pore water

$$\rho = \rho_0 A n^{-m} \quad \text{Archie's law}$$

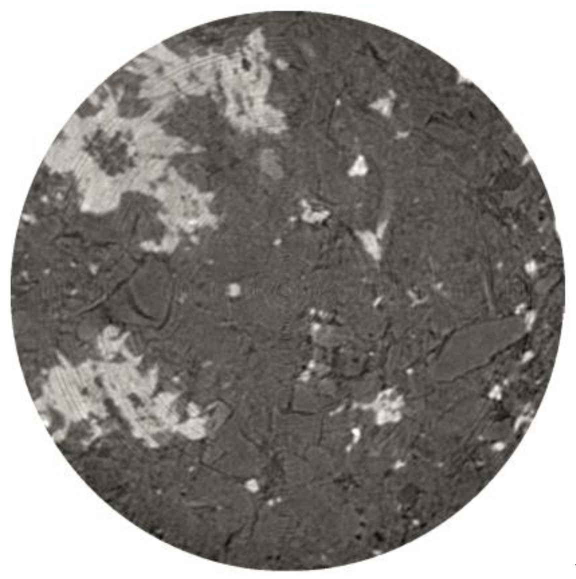
where ρ and ρ_0 is the electrical conductivities of the rock in pore water and the pore water, m is an empirical exponent, A is an empirical coefficient

Then the expression for the diffusion coefficient of efficiency can be written in the form

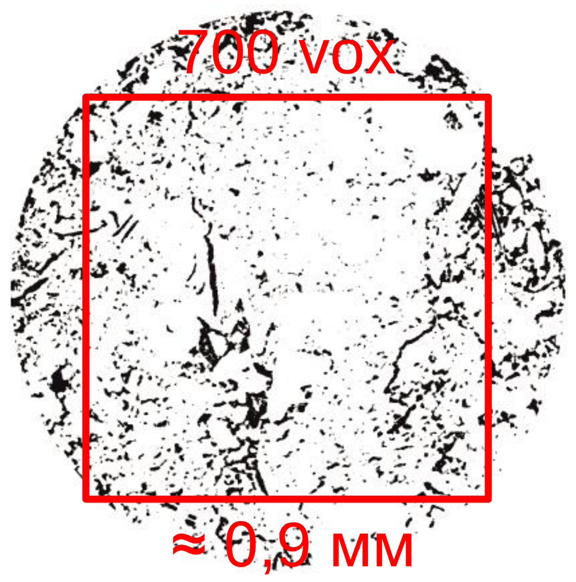
$$\varphi = A n^{m} \quad \text{Empirical correlation}$$

How do we got the tortuosity?

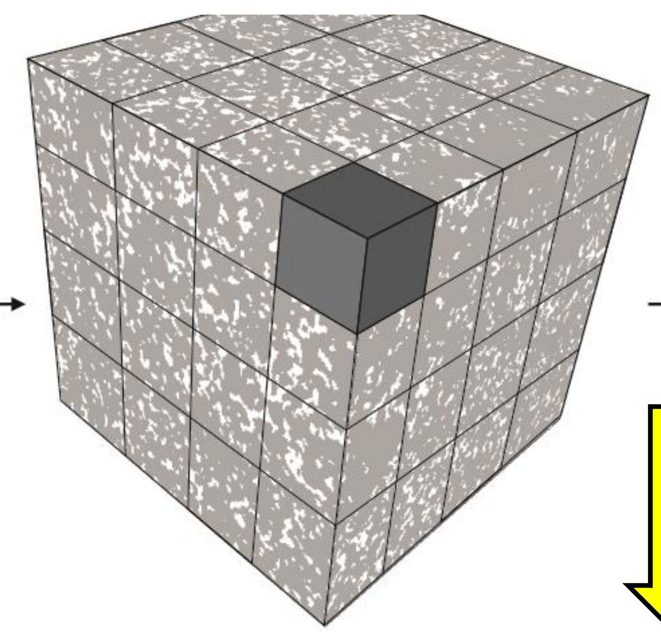
X-ray microtomography



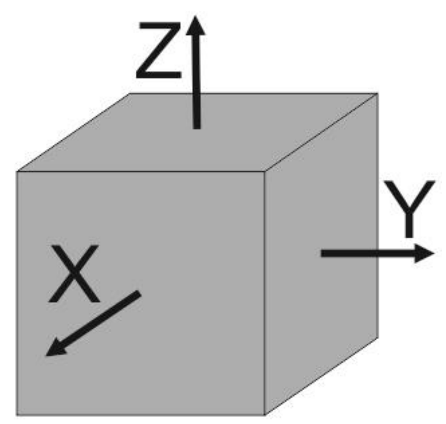
Pore – matrix binarization



Obtain the microstructure matrix and division



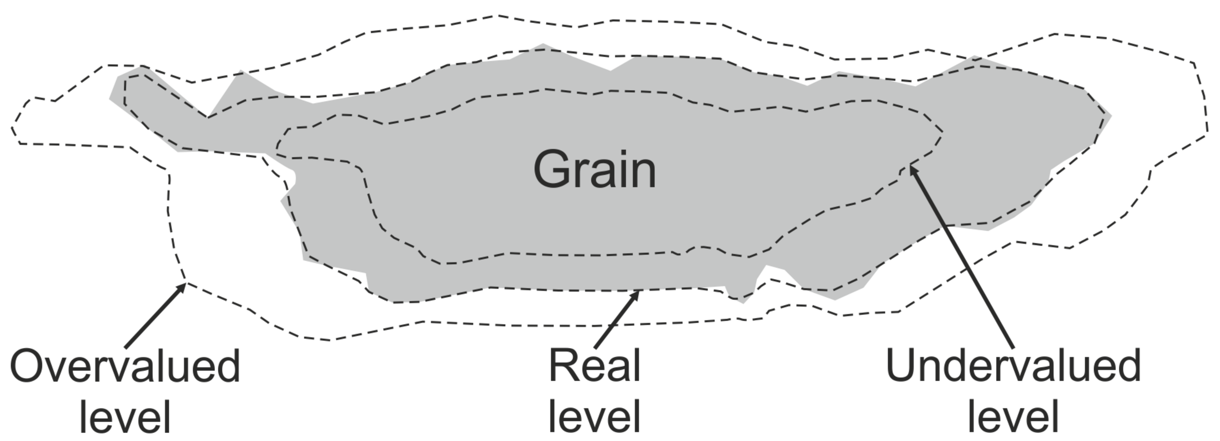
Diffusion simulation in X,Y and Z directions



Pore – matrix binarization

Using 6 low-permeable samples we studied the microstructure with X-ray microtomography. Shooting was performed on undisturbed microsamples of size 1^3 mm with a resolution ×300 (1024^3 vox).

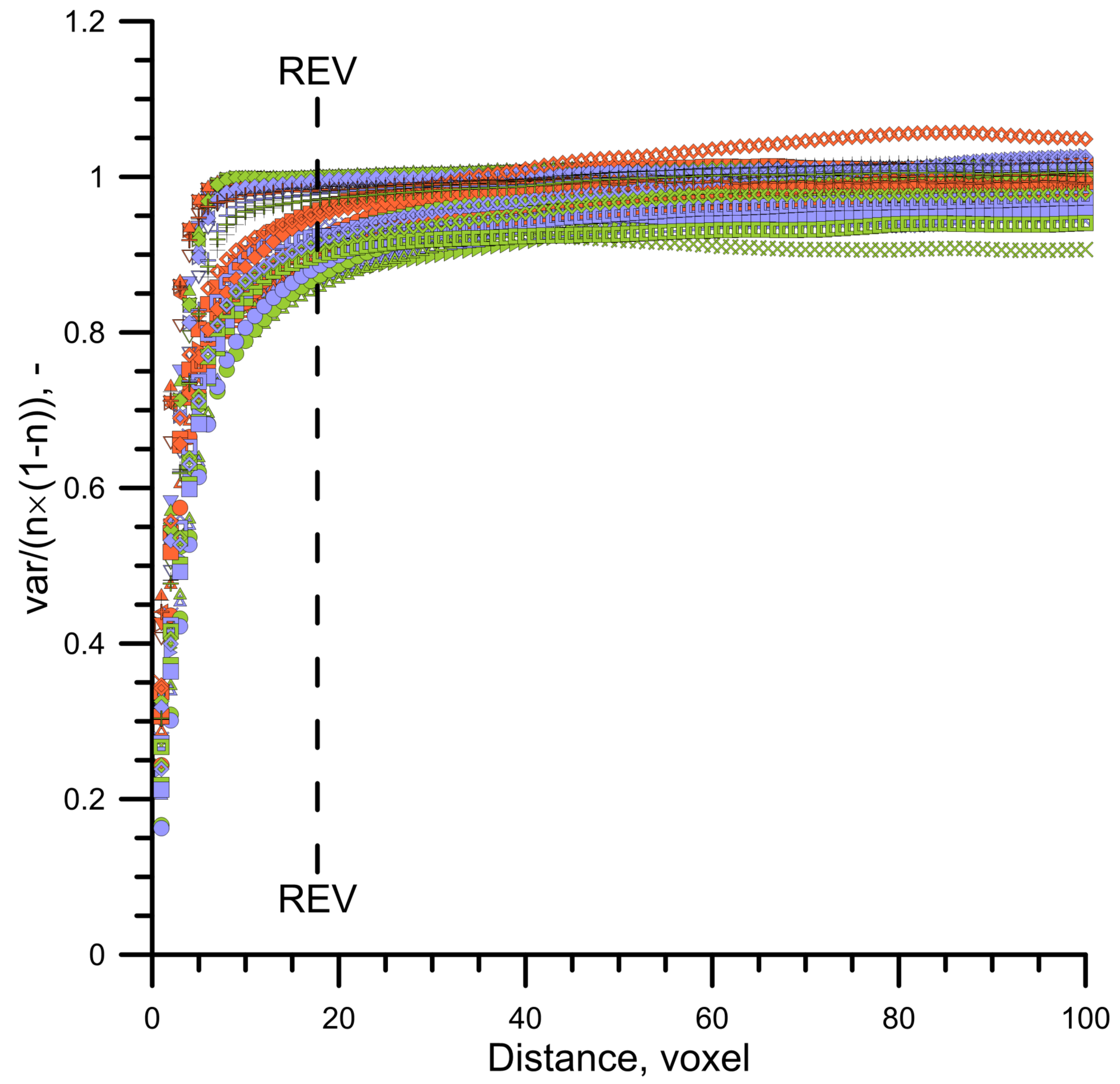
Pore space



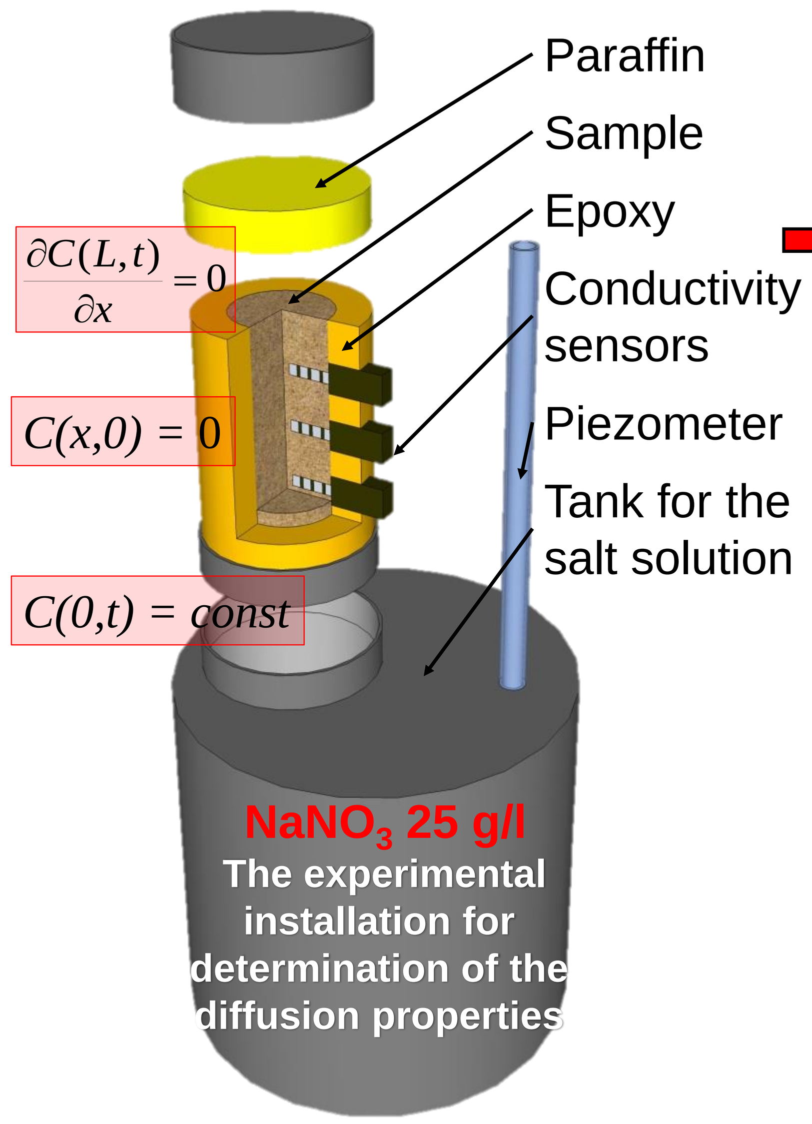
Sample	Porosity for different level of binarization		
	n_{under}, –	n_{real}, –	n_{over}, –
1	0.056	0.13	0.30
2	0.10	0.28	0.38
3	0.07	0.11	0.21
4	0.07	0.16	–
5	0.02	0.06	0.20
6	0.03	0.11	0.32

Spatial correlation analysis

After binarization of each 3-D structure was obtained and spatial correlation analysis was performed. This analysis showed that the spatial correlation scale of the indicator variogram is considerably smaller than microsample length.



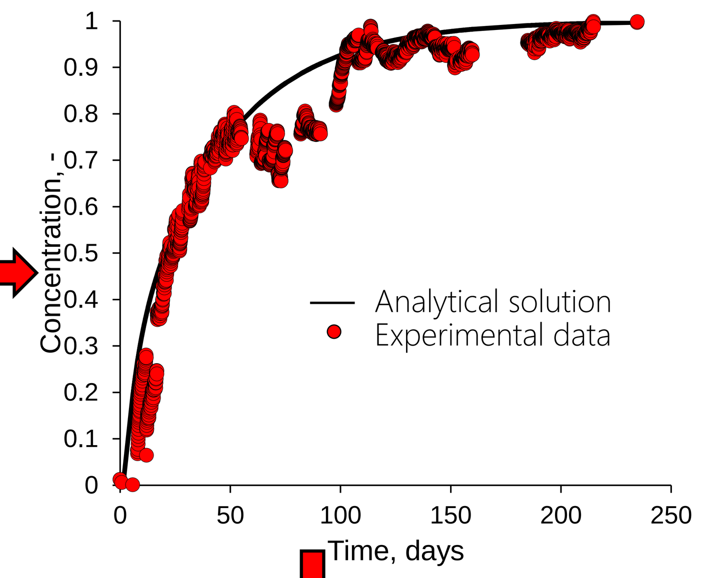
Lab study of diffusion coefficient



The differential equation of diffusion mass transfer

$$D\frac{\partial^2 C}{\partial x^2} = n_e \frac{\partial C}{\partial t}$$

where D is diffusion coefficient, n_e is effective porosity
C is concentration, x is coordinate, t is time.

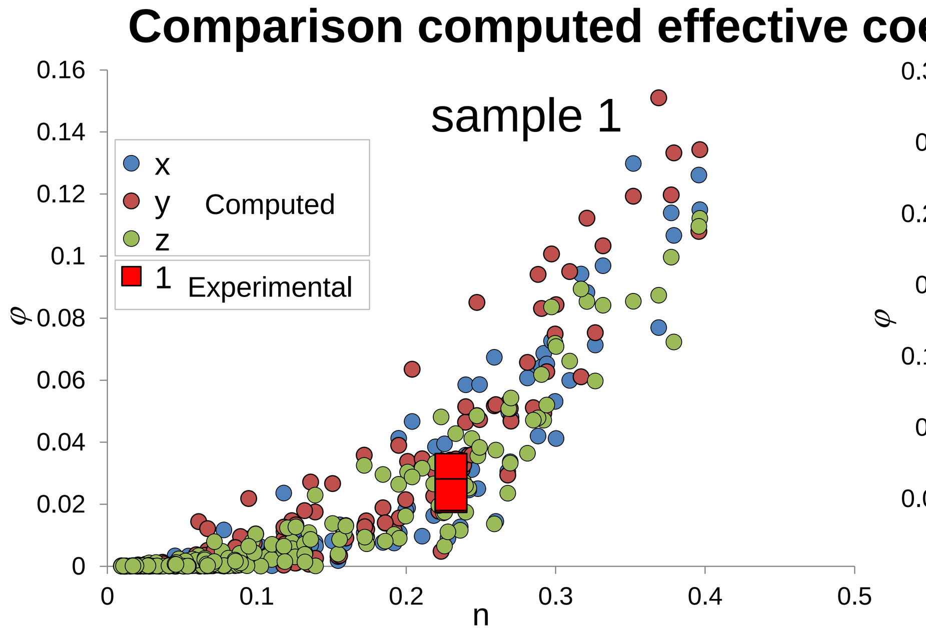


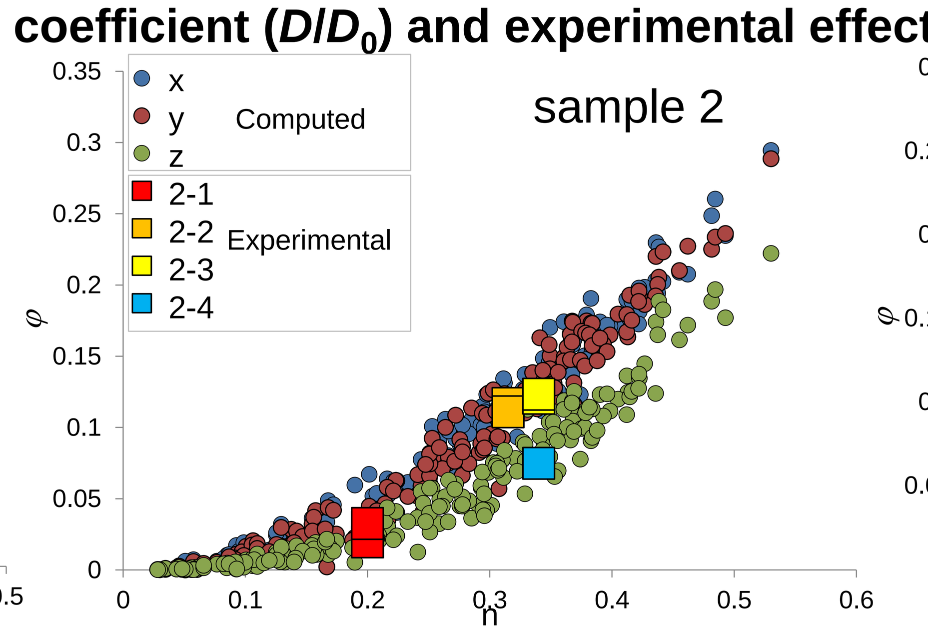
Sample	Time, days	n_a, -	D, m²/day
1	119	0.23	3.55×10^{-6}
2–1	77	0.2	3.72×10^{-6}
2–2	247	0.13	1.66×10^{-6}
2–3	175	0.315	1.41×10^{-5}
2–4	247	0.34	1.51×10^{-5}
3	89	0.18	2.07×10^{-6}
4	247	0.4	7.60×10^{-7}
5–1	247	0.35	4.11×10^{-6}
5–2	247	0.35	8.75×10^{-6}
6–1	247	0.16	6.77×10^{-6}
6–2	247	0.26	5.72×10^{-6}
6–3	247	0.21	7.25×10^{-6}

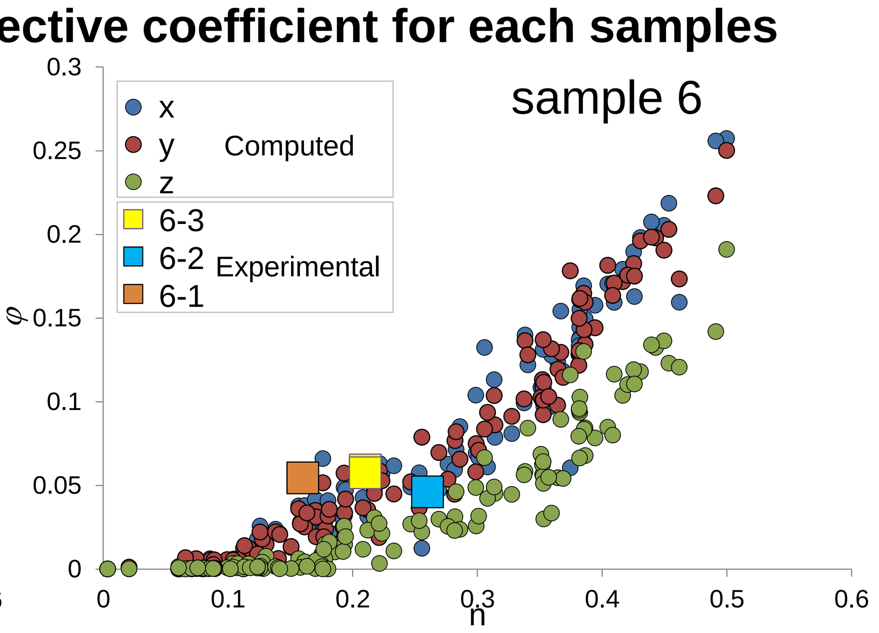
Diffusion steady-state simulation

Then there was the numerical simulation of the Laplace equation with binary coefficients (1 – pore, 0 – grain) for each microsamples. The total number of simulations at the finite-difference grid of 175^3 cells was 3500. As a result the effective diffusion coefficient and effective coefficient values were obtained for all studied microsamples. The results were analyzed in the form of graph of effective coefficient versus porosity.

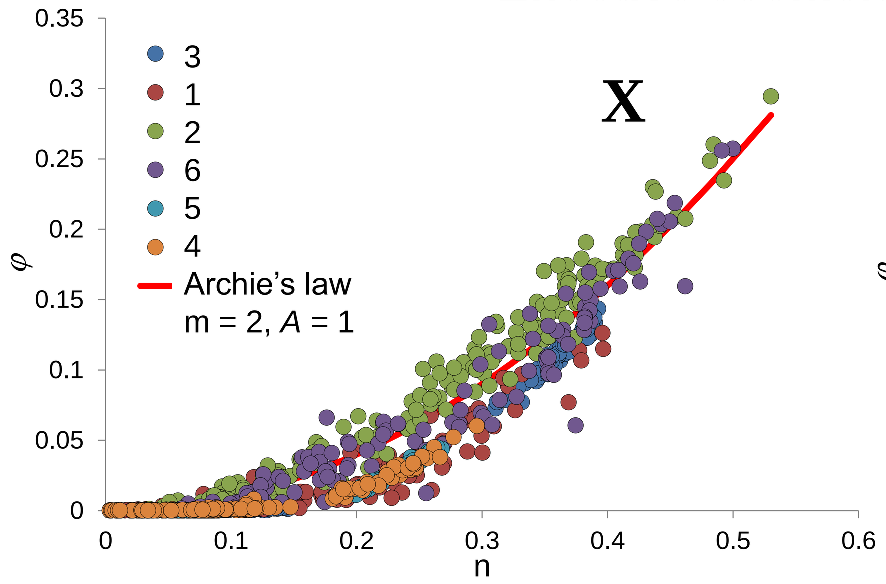
Comparison computed effective coefficient (D/D_0) and experimental effective coefficient for each samples

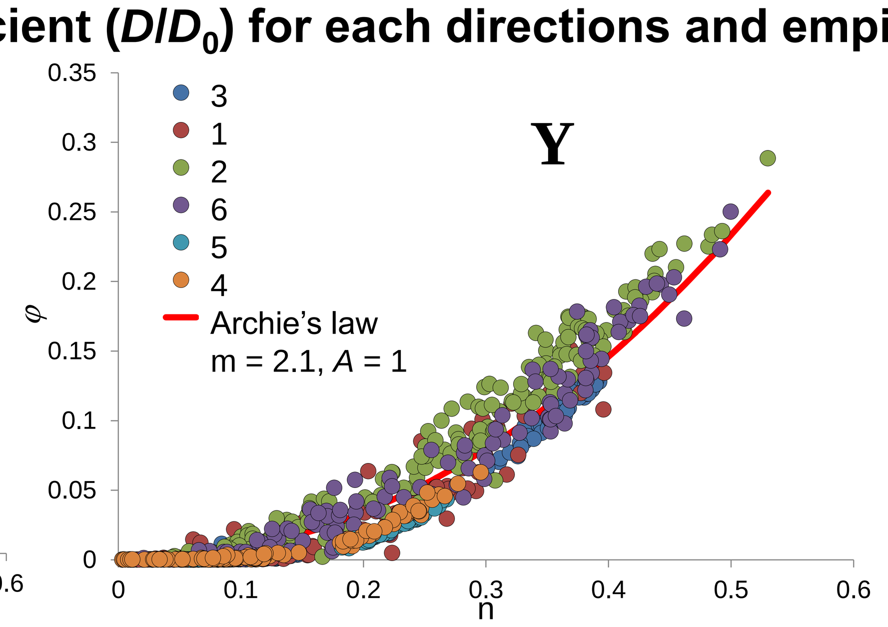


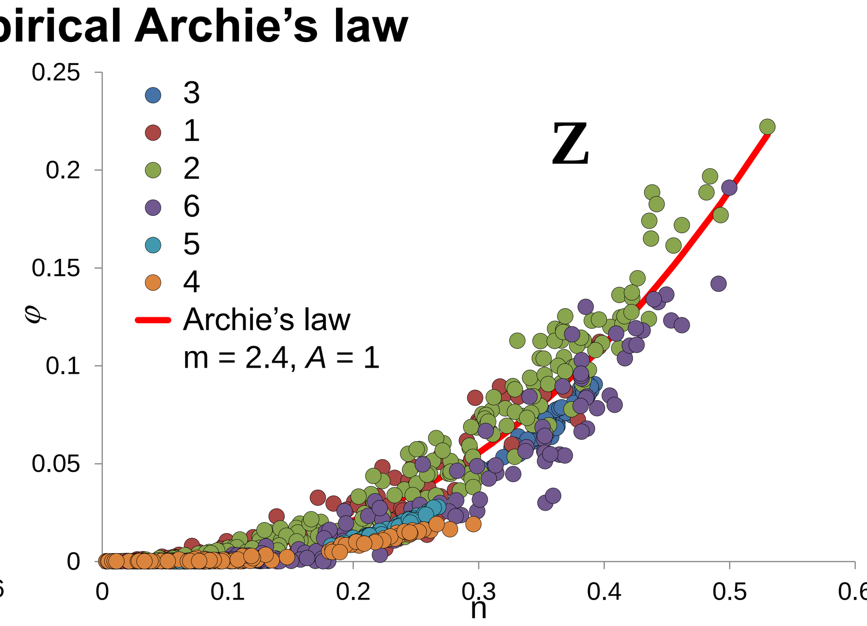




Effective coefficient (D/D_0) for each directions and empirical Archie's law







Conclusions

- Six experimental effective coefficient values well agree with pore-scale simulations matching with the general pattern that shows nonlinear decreasing of tortuosity with decreasing of porosity. Fitting Archie model to this function we found exponent value in the range between 2 and 2.4 and A=1.
- The samples are anisotropic in terms of tortuosity in the horizontal and vertical directions.

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