TRAPPING OF COLLOIDS IN SOILS BY STRAINING

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MOTIVATION

Modeling the retention of colloidal particles in soils provides a better understanding of the danger of water contamination from viruses, bacteria or contaminants adsorbed on the colloids. We investigate the trapping of colloids by **straining**, a simple geometric mechanism: colloids transported by fluid remain in the soil when they arrive at constrictions in pore space too small to admit them. Pore throats have been typically considered the place where colloids are trapped. However, several column experiments offer clear evidence of trapping of colloids that are smaller than the smallest pore throat in the column.

OBJECTIVE

Explain the mechanism of a long-standing anomaly in the **straining** of colloids: colloids too small too be trapped in the smallest **pore throat** in a granular medium are nevertheless retained.

HYPOTHESIS

Colloids are strained in **gaps** between pairs of grains besides throats between three grains.

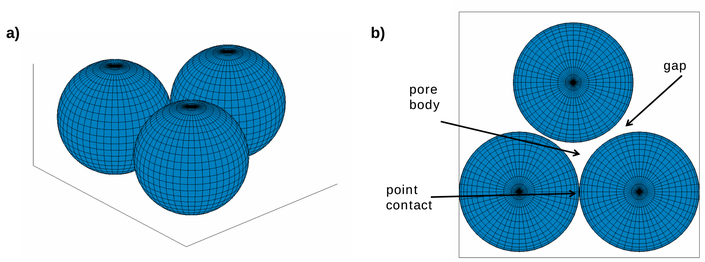

Figure 1: **a)** Three spheres simulating soil grains in space **b)** Cross section of a pore throat. A gap is defined as the void space between the centers of two neighboring grains

Based on experimental results

- Gap width of interest: **$0.03R<w_{gap}<0.1R$**
- Particle sizes investigated: **$0.02<d/D<0.05$**
- R= grain radius

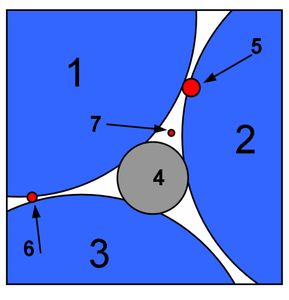

Figure 2: Trapping of particles in gaps and throats. Flow is perpendicular to the plane of the paper. Spheres 1, 2 and 3 have equal radius *R* and represent soil grains. Flow is assumed to be normal to the plane of the paper. The radius of sphere 4 is 0.2*R*, i.e., the 20% of the radius of soil grains and it is retained in the pore throat. The radius of sphere 5 is 0.05*R*, i.e., 5% of the grain radius and it is strained in a gap between grains 1 and 2 of size 0.03*R*. The radius of sphere 6 is 0.03*R* and it is trapped in a gap of size 0.02*R*. The radius of sphere 7 is 0.02R, i.e., 2% of the grain radius and is shown in the pore throat for size comparison. Spheres 5, 6 and 7 are too small to be trapped in the pore throat; nevertheless particles 5 and 6 are strained in gaps.

1st TEST

Examination of **Model Soils**: Computer Generated packs of random mono-disperse spheres

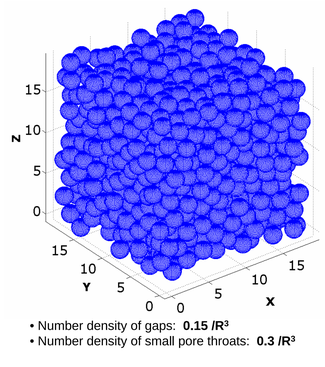

Figure 3: Example of a model soil (1000 spheres). The number density of gaps is comparable with the number density of small pore throats. The geometric analysis reveals that the occurrence of right sized gaps is enough to trap a significant number of colloids.

2nd TEST

Explain the dependence of **straining rate (k_{str})** upon **particle size (d/D)***

$$k_{str} \propto \left(\frac{d}{D}\right)^n \quad 1.2 < n < 1.5$$

Calculate flow in gaps

↓

Slit model for gaps

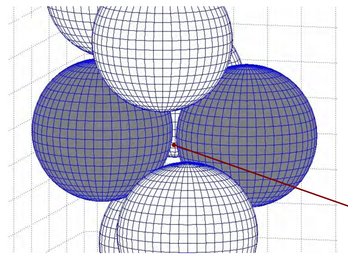

Figure 4: Detail of a gap between two spheres

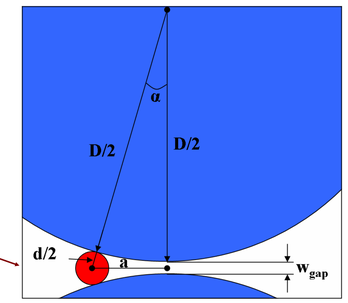

Figure 5: Scheme of the range of capture. The particle of diameter "d" is moving perpendicular to the plane of the paper. It will be trapped if it enters the gap, which has width wgap, within a lateral distance "a" of the center of the gap.

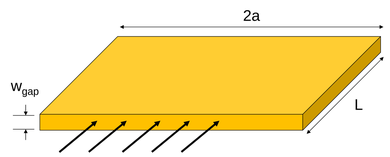

Figure 6: The gap is modeled as a slit of width equal to the gap width w_{gap} and length equal to twice the range of capture (2a). The arrows represent the direction of the flow.

Velocity $u_{gap} = -\frac{w_{gap}^2}{12\mu}\nabla P$

Flow $q_{gap} = 2aw_{gap}u_{gap}$

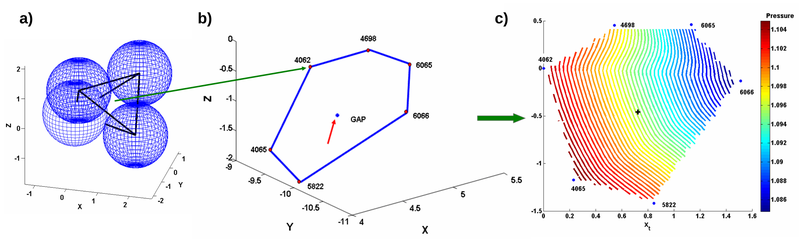

Figure 7: ∇P in gaps is calculated from a steady state calculation of the flow in throats. **a)** Delaunay cells are tetrahedra whose faces correspond to pore throats. **b)** The center of the Delaunay cells that contain the two spheres having a gap and the center of the gap are in the same plane. **c)** Contours of Pressure in the plane defined by the centers of the Delaunay cells and the center of the gap. The gradient of pressure is nearly constant and this is found to be true nearly for all gaps in the reference porous medium.

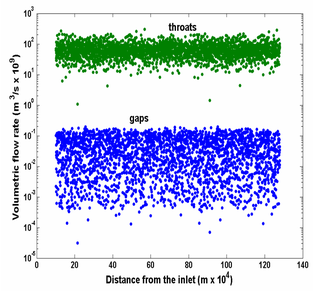

Figure 8: Volumetric flow rate through gaps and volumetric flow through pore throats *vs.* distance from the inlet for particles of size d/D=0.05. The flow in gaps is about 3 orders of magnitude smaller than the flow in throats

PREDICTION OF STRAINING RATE: Sharma and Yortsos Theory

$$k_{str} \propto \frac{I(d/D)}{I(\infty)}$$

I is a cumulative distribution function

Flow rate $I(r) = \int_0^r q_R f_p dr_p \qquad k_{str} \propto \left(\frac{d}{D}\right)^{4.03}$

Geometry $I_c(r) = \int_0^r f_p dr_p \qquad k_{str} \propto \left(\frac{d}{D}\right)^{0.88}$

Range of capture $I_a(r) = \int_0^r a(r_p) f_p dr_p \qquad k_{str} \propto \left(\frac{d}{D}\right)^{1.55}$

Retention in Gaps is not guaranteed

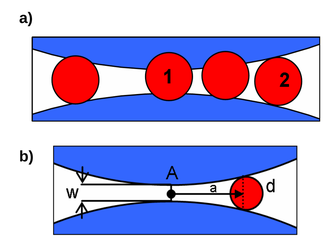

Figure 9: **a)** Front view of a gap showing the range of capture *a* for a particle of size d>w. The point A indicates the middle of the gap. **b)** Front view of a gap showing possible locations where a particle of size d>w can be trapped. Particle 2 is trapped at the maximum range of capture. Particle 1 is trapped in the middle of the gap.

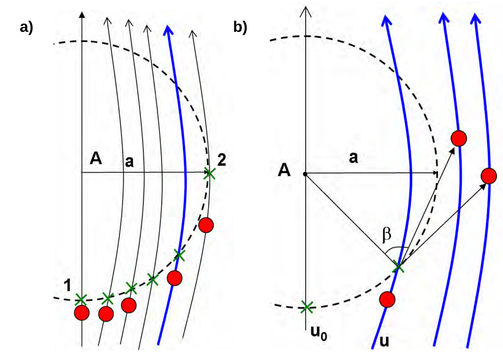

Figure 10: **a)** Top view of a gap. The effective range of capture may be smaller than **a**. The trapping probability is 1 in point 1 and 0 in point 2. The green **x's** indicate the points where particles of size d>w touch both grains. **b)** Top view of a gap showing collision and bouncing of the particles. A particle can collide with the grain and escape from the gap instead of being trapped.

Faster collisions (large u) and larger angles of incidence (β) are more likely to **rebound** the particle

Momentum: $P_{trapping} = \frac{\cos\beta}{|u|}$

Kinetic Energy: $P_{trapping} = \frac{\cos\beta}{|u|^2}$

Momentum $I_m(r) = \int_0^r \frac{q_R}{u_R} f_p dr_p \qquad k_{str} \propto \left(\frac{d}{D}\right)^{2.25}$

Kinetic Energy $I_k(r) = \int_0^r \frac{q_R}{u_R^2} f_p dr_p \qquad k_{str} \propto \left(\frac{d}{D}\right)^{1.11}$

Table 1: Scaling Exponents obtained after using different assumptions on the Sharma and Yortsos theory

Assumption	Exponent
Flow Weighted	4.03
Geometry	0.88
Range of Capture	1.55
Momentum	2.25
Kinetic	1.11

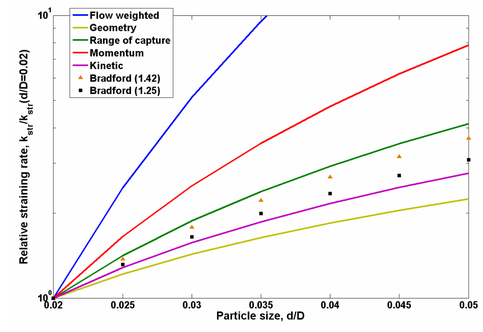

Figure 11: Straining rate constant (k_{str}) for different particle sizes (d/D), evaluated with the Sharma and Yortsos straining theory and the gap geometry and flow rates for a dense random packing of spheres. Five different assumptions have been considered in the theory. The results are shown together with the solutions from two of the experimental correlations having exponents 1.42 and 1.25.* The values of k_{str} have been normalized for easier comparison of the slopes.

CONCLUSIONS

- An existent theory of straining was extended to include gaps between pairs of grains as a potential locations for the trapping of colloids.
- The inclusion of gaps in the straining theory provided insight into the mechanisms that dominate straining: the scaling exponents for the "momentum-weighted" and "kinetic energy weighted" straining rate constants bracket the empirical scaling exponents reasonably well.
- A more detailed investigation into the dynamics of particle-grain collision is likely to improve the quantitative agreement.
- Applying the extended theory to void space near point contacts will be an important validation test.

*Bradford, S., Simunek, J., Bettahar, M., Van Genuchten, M.T., and Yates, S.: "Modeling colloid attachment, straining and exclusion in saturated porous media," *Environmental Sci. and Tech.*, 37, 2242-2250, 2003.

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