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MECHANISM OF ANOMALOUS STRAINING OF COLLOIDAL SIZE PARTICLES IN POROUS MEDIA

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MOTIVATION & OBJECTIVE

The presence and transport of colloids in the subsurface strongly affect ground water quality. Colloids are particles with effective diameters between 1 and 10 μm that are naturally present in the subsurface. Their nature can be organic (humic materials), inorganic (silicate clays and mineral precipitates), or biologic (viruses and bacteria). The colloids themselves can be contaminant (bacteria and viruses) or they can act as carriers of contaminants such as pesticides or heavy metals.

The classical retention theories consider filtration as the mechanism responsible for the retention of colloidal size particles, and grain surfaces as the locations where retention occurs. Several independent studies observed the retention of particles much smaller than the smallest pore throat under conditions that minimize retention by attachment. However, until now no mechanism for this anomaly has been proposed. Investigators concluded that **straining** must have contributed to retention. The objective of this work is to determine whether straining in small **gaps** between pairs of grains can account for the observed retention.

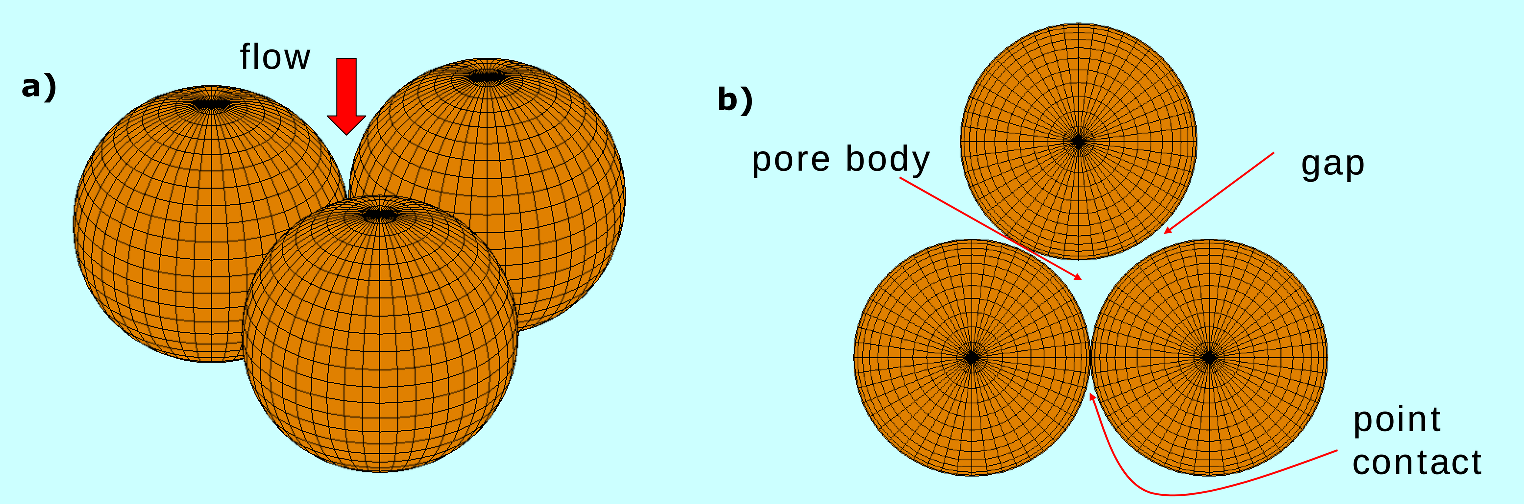
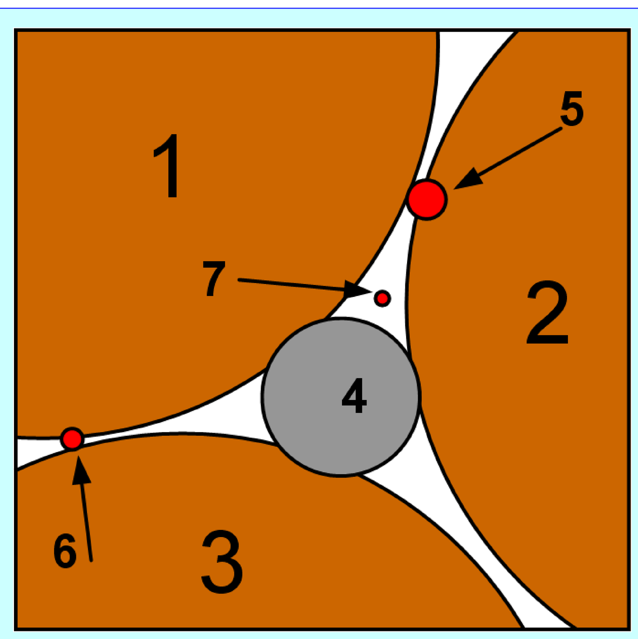


Figure 1: a) Three spheres simulating soil grains in space **b)** Cross section of a pore throat. A gap is defined as the void space between the centers of two neighboring grains



Based on experimental results

- Gap width of interest: **$0.03R<w_{gap}<0.1R$**
- Particle sizes investigated: **$0.02<d/D<0.05$**
- $R=D/2$ = 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 3 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 the 0.02R, i.e., 2% of the grain radius and it 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.

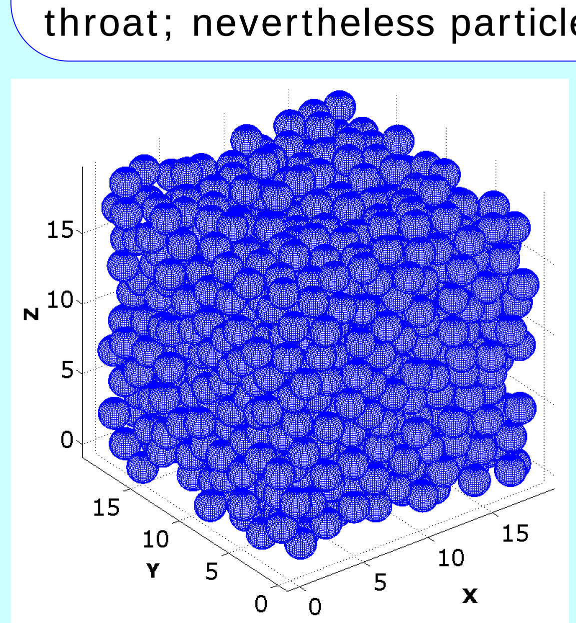


Figure 3: Example of a model soil (1000 spheres). The number density of gaps is comparable with the number density of small pore throats. The geometric analysis reveals that the occurrence of right sized gaps is enough to trap a significant number of colloidal size particles.

- Number density of gaps: **$0.15/R^3$**
- Number density of small pore throats: **$0.3/R^3$**

Straining rate (k_{str}) is related with **particle size (d/D)**[1]

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

1. 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.

HYPOTHESIS 1: In a given gap the rate of retention, and therefore the rate constant for straining, is proportional to the flow that passes through the gap.

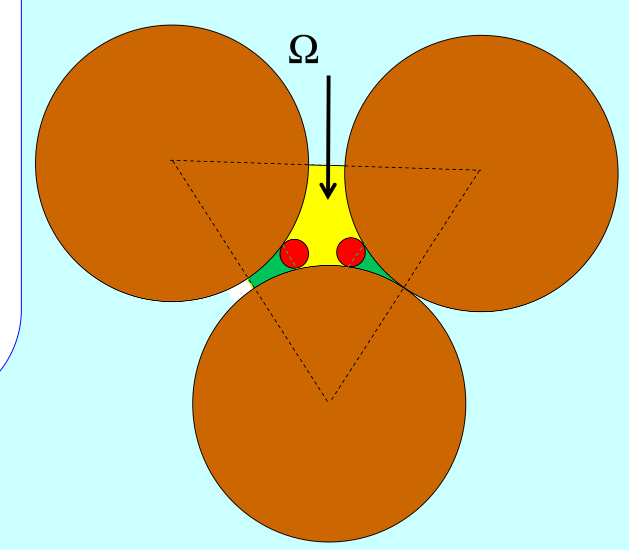
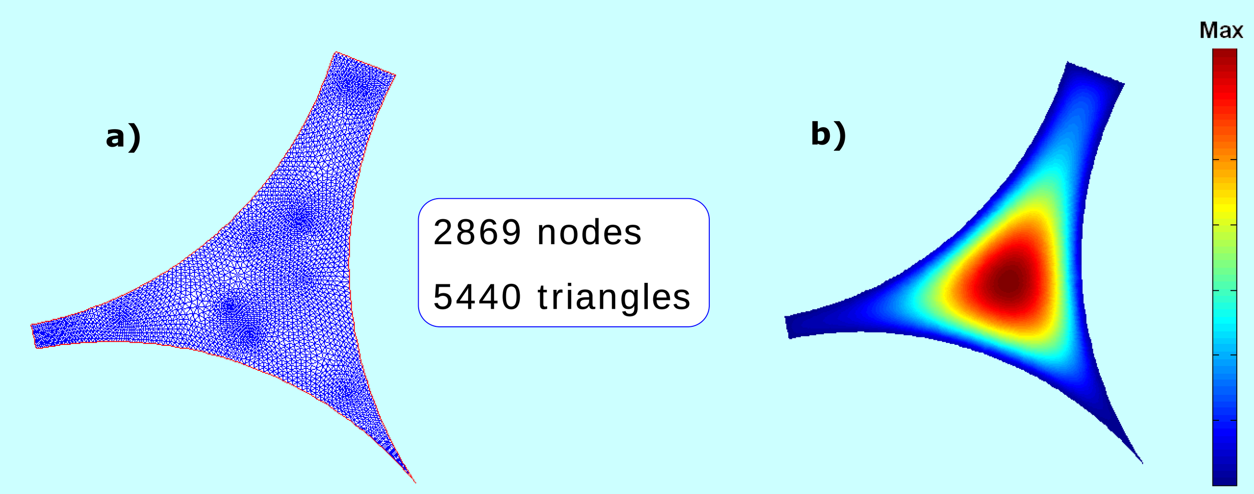


Figure 4: Particle (red) being trapped in a gap and a constriction associated with a pore throat. The constant for straining will be calculated as the ratio of flow through the regions of the throat that would trap the particle (in green) and the total flow through the throat (green + yellow + red).

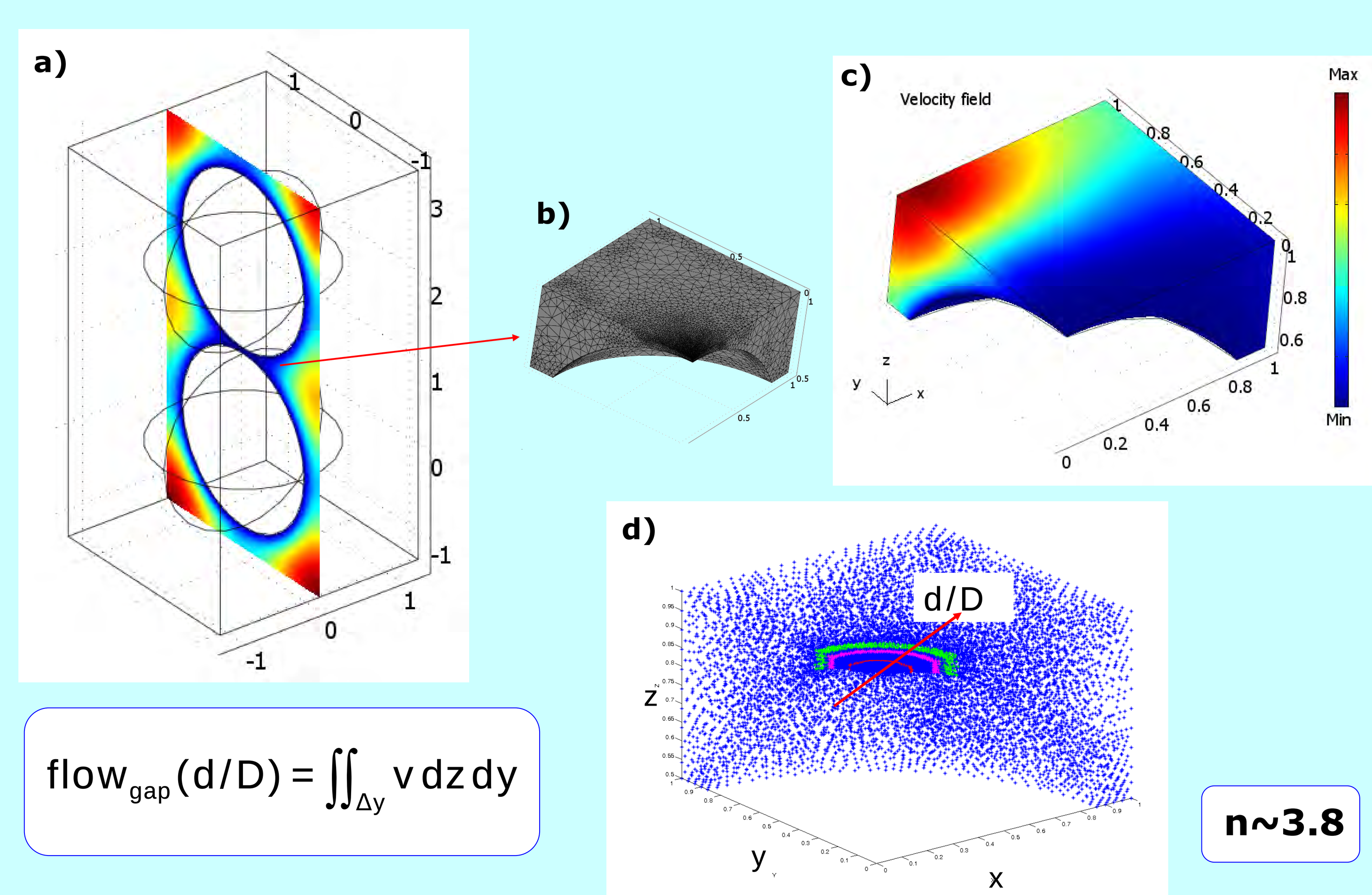
$$k_{str} = \frac{flow_{gap}(d/D)}{flow_{\Omega}(d/D)}$$



2869 nodes
5440 triangles

n~3.8

Figure 5: Detailed 2D flow distributions within throats, within gaps, and near the point contacts were computed using Matlab PDE tool to test this hypothesis. The figure represent the void space between three grains. Part a) shows the mesh and part b) shows the velocity contour. The calculated straining exponent is larger than the experimental, so Hypothesis 1 is invalid.



$$flow_{gap}(d/D) = \iint_{\Delta y} v\,dz\,dy$$

n~3.8

Figure 6: a) Slice of the velocity field around two spheres having a gap of width 0.01*D*. COMSOL was used for the velocity calculations. b) Part of the system used in the calculations in order to get a more detailed velocity field in the gap. A pressure difference was imposed through the gap. The surface of the sphere has a no-slip boundary condition and the rest of the walls have a symmetry boundary conditions. c) Detailed velocity flow in the vicinity of a gap situated at (0, 0, 0). d) The region where a particle can be trapped is now an annulus, which radius increases with particle size. The large scaling exponent found with this 3D flow field confirms that Hypothesis 1 is not valid.

Key Insight: Flow into a gap does not guarantee retention in the gap!

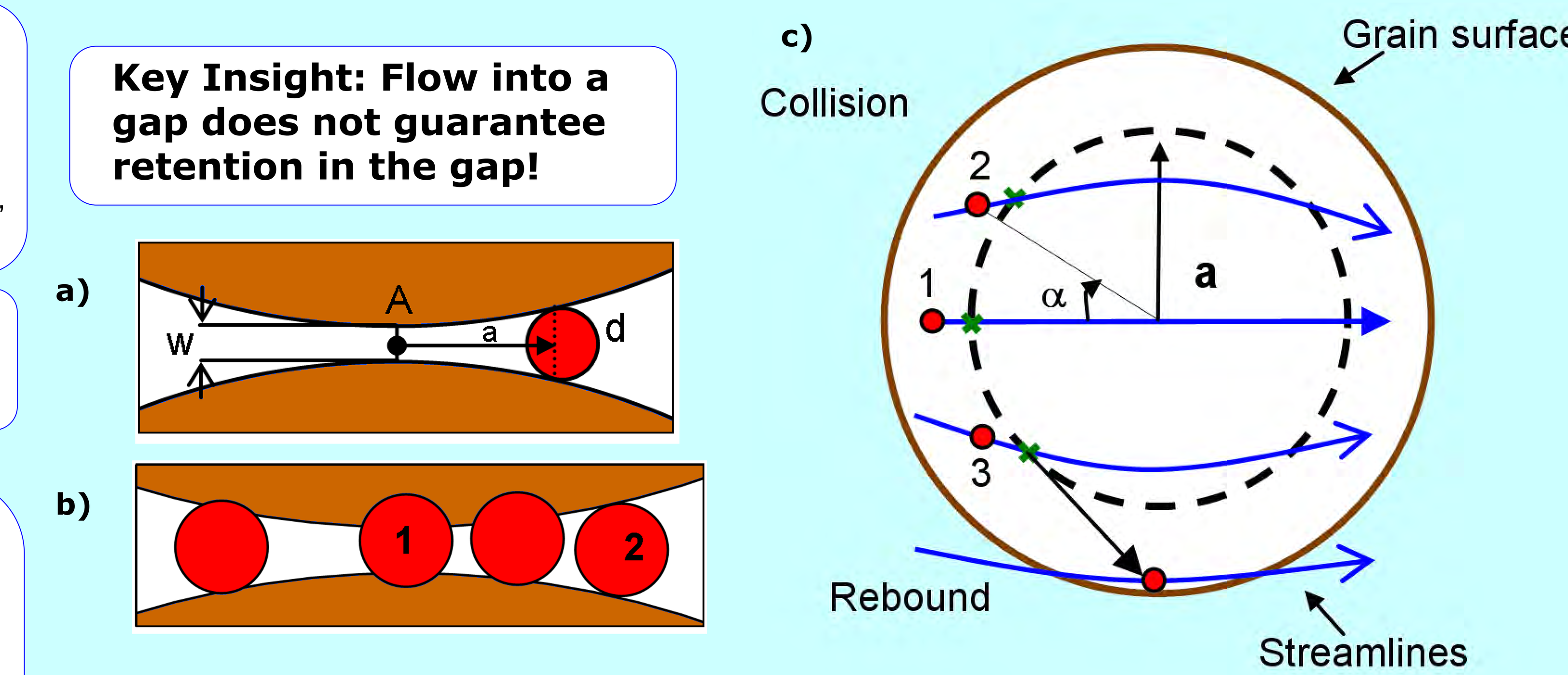


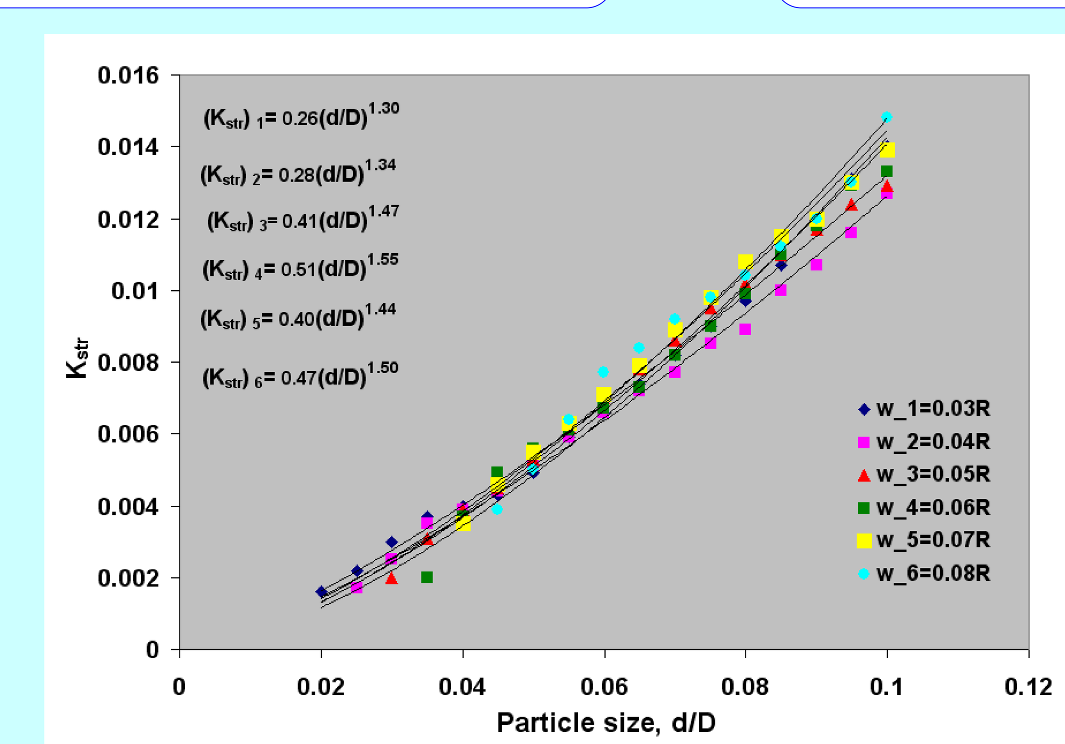
Figure 7: a) Front view of a gap showing the range of capture ***a*** for a particle of size d>w. The point A indicates the middle of the gap. b)Front view of a gap showing possible locations where a particle of size d>w can be trapped. Particle 2 is trapped at the maximum range of capture. Particle 1 is trapped in the middle of the gap. c) Top view of a gap. The effective range of capture maybe smaller than **a**. The trapping probability is **1** in point 1. The cross (**x**) indicate the points where particles of size d>w touch both grains. Particle 3 can collide with the grain and escape from the gap instead of being trapped.

HYPOTHESIS 2: There is a nonzero probability of colloid escape, even if the colloid enters the gap.

The possibility of collision and rebound of colloids when approaching constrictions will be considered by assuming that the probability of trapping is correlated with the angle of incidence of the colloids (α) and with the average flow velocity $\langle v \rangle$.

$$flow_{gap}(d/D) = \iint_{\Delta y} v \cdot \cos(\alpha)\,dz\,dy$$

$$k_{str} \propto \frac{flow_{gap}(d/D)/\langle v \rangle_{annulus}}{flow_{\Omega}(d/D)/\langle v \rangle_{\Omega}}$$



n~1.3 to 1.55

Figure 8: Straining rate constant (k_{str}) for different gap sizes (w), evaluated using the formulas shown above. The exponent of the power law dependence between k_{str} and d/D ranges between 1.3 and 1.55, closely matching experimental observations.

CONCLUSIONS

- This model confirmed a reported empirical relationship between the straining rate constant and the ratio of colloid to grain size, thereby identifying the role of the small gaps between grains in the mechanism behind the anomalous observations of straining.
- The assumption that the straining rate is fully dependent of flow rate overestimated the straining exponent.
- Our model found that the straining rate is directly proportional to the flow through the gap and the angle of incidence of the colloid and inversely proportional to the momentum (velocity) of the colloid in the gap.