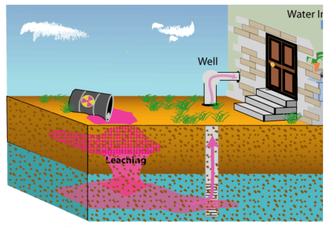
High performance computational study of colloid transport in saturated porous media

Q. Qiu[1], H. Gao[1], L.P. Wang[1], J. Yan[2]
[1]Department of Mechanical Engineering, University of Delaware, Newark, DE 19716, USA
[2]Department of Plant and soil science, University of Delaware, Newark, DE 19716, USA

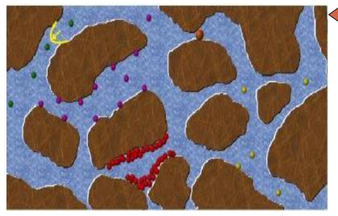
Research objective

Investigate colloid concentration distribution in soil porous media, colloid retention ratio, etc, to help design sand filters for waste water treatment, bio-remediation etc.



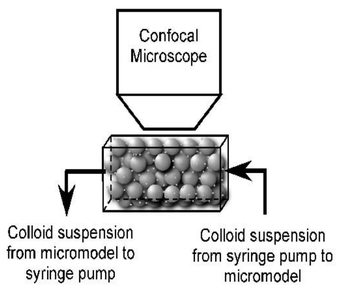
Field scale(>1m)

Column scale(~10cm)

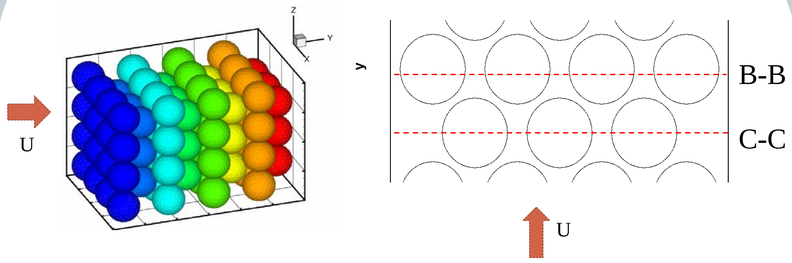


Pore scale(<1mm)

Column experiment setup (J. Yan's Group)

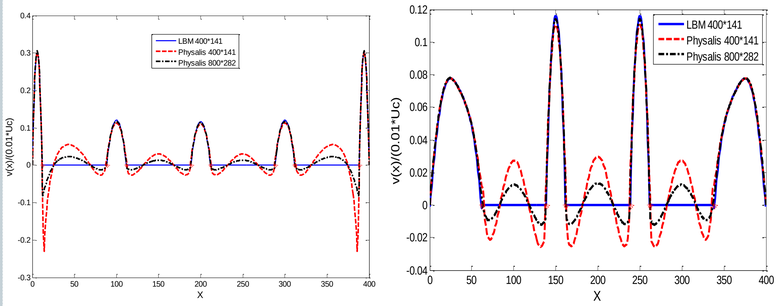


2D & 3D porous media in simulation



(a) (b)

Glass beads packed in channel used as the model porous media to simulate colloid transport: (a) 3D domain, (b) 2D domain.

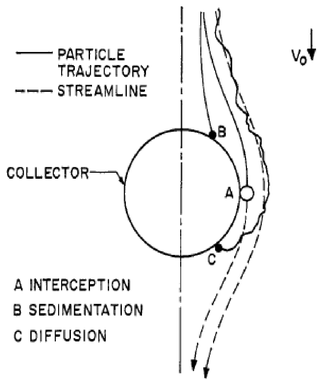


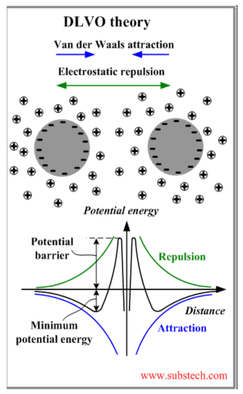
(a) (b)

Comparison of steady-state, transverse velocity profiles from Lattice Boltzmann Method and Physalis at the same locations shown in the 2D model: (a) B-B cut, (b) C-C cut.

Colloid deposition mechanism

A colloid motion is governed by Brownian force, colloid-collector DLVO forces, drag force, gravitational force etc.



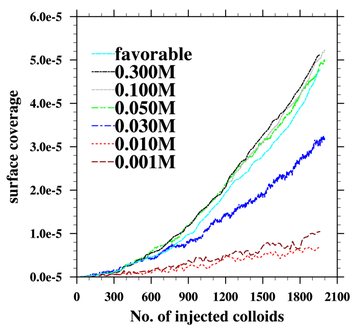


(Yao, et al. 1971)

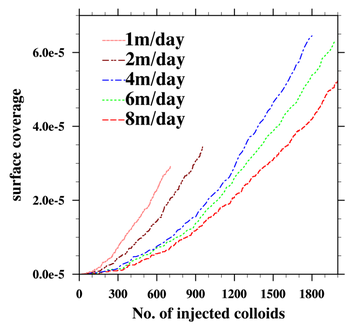
Colloid equations of motion in the Lagrangian tracking model:

Normal: $$m_c \frac{dV_{i,n}}{dt} = F_{i,n}^{drag} + F_{i,n}^{C} + F_{i,n}^{B}$$

Tangential: $$m_c \frac{dV_{i,t}}{dt} = F_{i,t}^{drag} + F_{i,t}^{other} + F_{i,t}^{B}$$



(a)

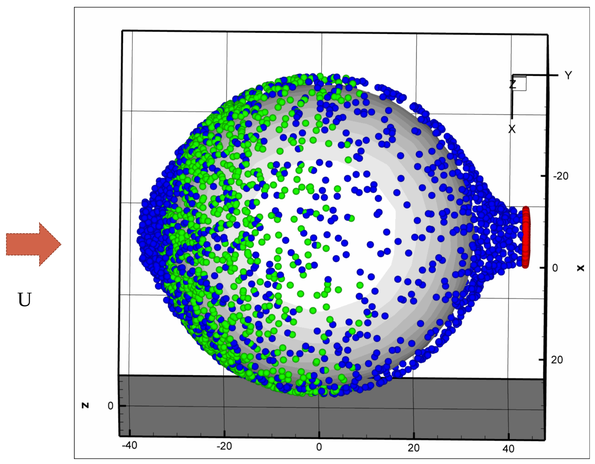


(b)

Predicted surface coverage of 1 ppm sulfate latex colloids:

(a) at different ionic strengths with a flow speed of 8m/day,

(b) at different flow speed with a ionic strength of 0.1M.

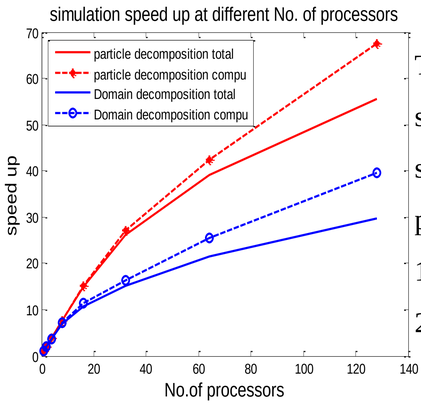


Colloid movement in a single sphere in shell model.

Green points: colloids retained on the grain surface.

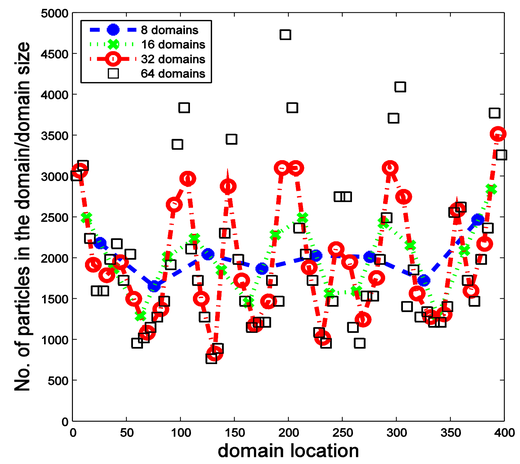
Blue points: moving colloids in bulk flow.

Simulation speed up by parallel computing



Two different parallel implementation schemes are used to speed up the simulation of colloid motion in porous media:

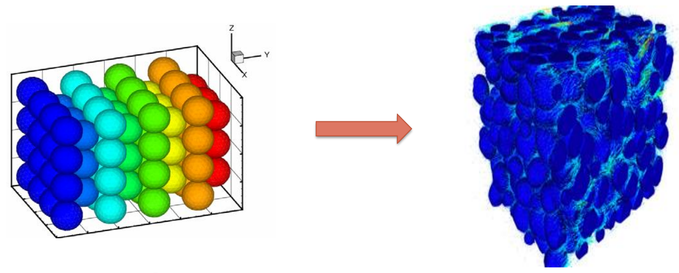
1. particle decomposition,
2. domain decomposition.



Colloid concentration fluctuation at different number of subdomains in the domain decomposition scheme.

Future work

1. Solve flow field and colloid transport in porous media with a larger domain size (pore scale → column scale).



Current domain Future domain

(http://vgest.net/applications/porous-media-flow)

2. Solve flow field and colloid transport around rough collector surface.

Summary

1. Flow fields in porous media solved by Lattice Boltzmann method and Physalis match well and makes good cross-validation.
2. A Lagrangian colloid tracking model is developed, colloid retention at different physical-chemical conditions is investigated.
3. MPI parallel computing improves computational efficiency of colloid tracking simulation by more than 50 times, providing the possibility of simulation in more complex geometries and larger domain size.