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Understanding Transport of Soft Units through Porous Media by Correlating Pore-scale Dynamics and Macroscale Properties

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The goal of the project supported by this ACS PRF DNI grant is to understand the pore-scale dynamics of the transport of soft units, such as microgel particles and drops, through porous media and to correlate this pore-scale information with changes in macroscale permeability that result from the presence of soft units in the media. We proposed multi-scale experiments and mechanistic analysis to address our research objectives.

Transport dynamics of soft, spherical particles through confining channels or pores

The transport of soft particles through narrow channels or pores is ubiquitous in biological and industrial systems, including many enhanced oil recovery processes such as the gel treatment and emulsion flooding. On many occasions, the particles deform and temporarily block the channel, inducing a built-up pressure. This pressure buildup may have a profound effect on the behavior of the respective system, yet it is difficult to be characterized. In this project, we study the transport of an elastic, spherical particle in a constrictive or straight confining channel with a circular cross-section to quantitatively correlate the channel-blockage induced pressure with the radius ratio of the sphere to the channel, the elastic modulus of the particle, and the friction and adhesion properties between the particle and channel wall.

<u>*Experiments*</u>: We fabricate microgels with controlled diameter and properties by microfluidics. We then inject the microgels into circular constrictive or straight confining channels and monitor the built-up pressure. The motion of a microgel in a constrictive channel can be divided into three stages: (i) before contacting the constriction, (ii) being confined by the constriction, and (iii) after passing the constriction throat, as shown in Figure 1(a-b). Since many biological processes involve the passage of soft bodies in narrow, straight channels, we also injected microgels through a circular straight channel, as shown in Figure 1(c-d). We measured and compared the maximum pressure in straight and constricted channels as a function of the radius ratio Φ of the microgel to the channel. For constrictive channels, the maximum pressure is the pressure at point (a-2) in Figure 1. The variation of pass-through pressure (maximum pressure) P_0 as a function of Φ is plotted in Figure 2 (a). At the same Φ, the pressure in the constrictive channels is slightly smaller than but very close to that in the straight channels.

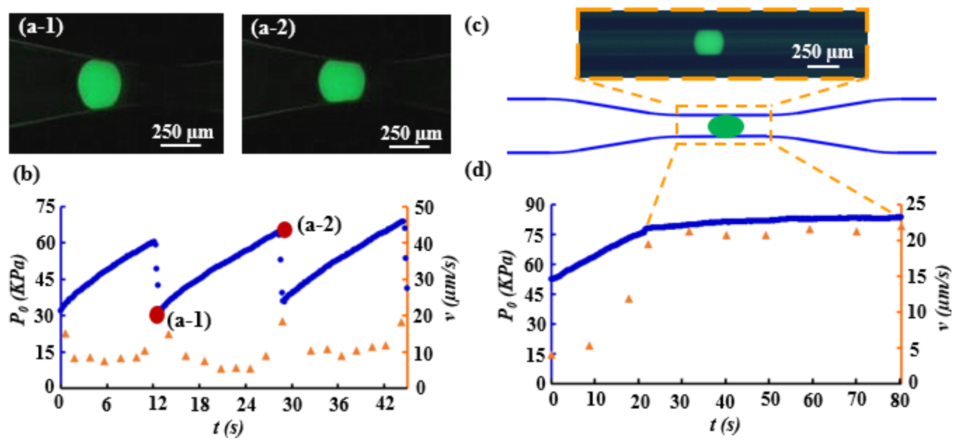

Figure 1. (a) Fluorescence micrograph of a deformed microgel in a constrictive channel; (b) variation of pressure (P) and microgel velocity *(v)* with time *(t)* as three microgels pass through a constrictive channel; (c) fluorescence micrograph of a deformed microgel in a circular straight channel; and (d) variation of pressure (P) and velocity *(v)* with time *(t)*.

<u>*Theoretical analysis:*</u> To gain quantitative understanding of the pass-through pressure, we establish a differential equation for the axial normal stress by balancing axial forces on an infinitesimal deformed disk element in the circular channel. Neo-Hookean material law is adopted for elastic deformation, which is applicable to a variety of elastomers, including highly stretchable hydrogels. We then find the relation among the driving pressure, material properties, and geometrical parameters by solving the differential equation. After some

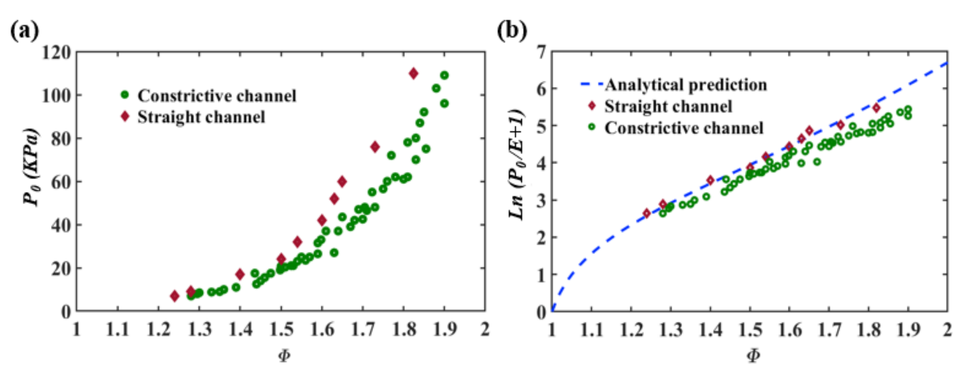

Figure 2. (a) Pressure variation with radius ratio Φ in constrictive channels (red diamonds) and straight channels (green circles); (b) comparison between analytical prediction and experimental data.

simplification, the result is given by Eq. (1)

$$\frac{P_0}{E} = \mu(\Phi^2 - 1)^{1.5} e^{(10.7\mu+3.6)(\Phi-1)+1} + \frac{\bar{\tau}}{\mu}[e^{\frac{4\mu}{3}\sqrt{\Phi^2-1}(2\Phi^2+1)} - 1] \qquad (1)$$

where E is the elastic modulus of the microgel, μ and $\bar{\tau}$ are two constants parameters in the friction constitutive law, relating to the friction and adhesion properties between the sphere and channel wall. The model prediction agrees very well with the pressure measurement conducted at moderate particle deformation (Figure 2), which shows an exponential dependence on the radius ratio. Moreover, the model recovers the classical theory of contact at small deformation, which reduces to $\frac{P_0}{E} = \mu(\sqrt{\Phi^2 - 1})^3 e + 4\bar{\tau}\sqrt{\Phi^2 - 1}$. Featuring a balance between simplicity and accuracy, the developed pressure-properties correlation could shed light on understanding many industrial and biological processes involving the passage of deformable particles through narrow channels or pores. A manuscript about our findings has been submitted to *Applied Physics Letters*. The manuscript is currently under review.

Correlate pore-scale dynamics and macroscale properties

To extend our understanding to flow of particle suspensions in porous media, we model a homogenous porous medium as parallel capillary channels (Figure 3(a)), while maintaining the key geometrical parameters, such as pore throat size and porosity, the same as the original porous medium. When multiple particles moving in a capillary channel, the total pressure drop consists of the pressure drop over the particles and the pressure drop due to fluid flow, which can be described by We adopt Eq. (1) for the pressure drop over one particle and Poiseuille's Law for the pressure drop caused by fluid flow. From Figure 3(b), $P_{d-d} = P_{up} + \Delta P_f$, P_{up} is the pressure drop over one particle, given by Eq. (1), and $\Delta P_f = 32\nu u \Delta L_f / D^2$, where ν is the dynamic viscosity of the fluid, u is the average fluid velocity and D is the diameter of the channel. If there are n particles in one channel, then the total pressure is $P_{total} = nP_{d-d}$. Therefore, the effective permeability of the porous medium is $k = \frac{\nu LQ}{nA(P_0 + \frac{32\nu u \Delta L_f}{D^2})}$ with Q the flow rate and A the cross section area of the porous media. ΔL_f and n can be determined from the concentration of the particles in the fluid.

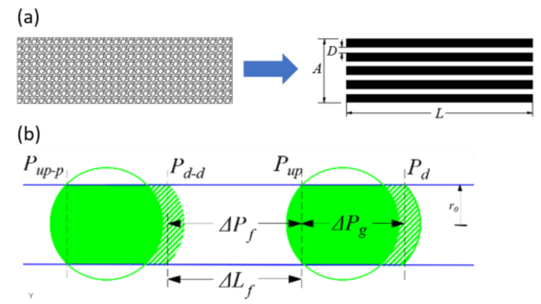

Figure 3. (a) Approximation of a homogeneous porous medium with parallel channels; (b) pressure distribution in a channel with multiple deformed particles.

We are working on the validation of this model by conducting 2D and 3D micromodel experiments. We have designed and fabricated by soft lithography a series of 2D micromodels consisting of pillar arrays with different pore throat sizes. We plan to inject microgel suspensions with various concentrations into the micromodels and measure the overall pressure drop, and then compare the results with the prediction of our 2D analytical model as described in the above paragraph. If the model and experiments agree well with each other, we will further extend the model to 3D and compare with experiments in 3D micromodels constructed by sintering glass beads.

Career and student training impacts

This grant has had substantial positive impact on the careers of the PI and participating students. Two PhD students, Shuaijun Li and Alimohammad Anbari, and one master student, Hung-Ta Chien, have been financially supported by this grant. Hung-Ta Chien graduated from CCNY in 2018 and is currently a PhD student at Texas A&M. Shuaijun Li has been focusing on this project since 2017. Alimohammad Anbari has been partially working on this project. In addition, 4 summer intern students, including 1 visiting student from Polytech Montpellier at France, have also contributed to the project, both in simulation and experiments, although they were supported by other funding sources. We have published a review article on micromodels in *Small* (2018,14, 1703575) and submitted a manuscript to *Applied Physics Letters. The* research findings have also been presented in various conferences, including the 91st ACS Colloid & Surface Science Symposium, 2018 IMECE International Mechanical Engineering Congress & Exhibition, 2019 APS March Meeting, Society of Engineering Science 56th Annual Technical Meeting (SES 2019), and 11th Northeastern Complex Fluids and Soft Matter Workshop. We expect to have at least 1 more manuscript to be submitted in the near future.

This project may have a profound impact to the career development of the participating students. For example, Shuaijun Li has developed significant interests on the oil industry because of this project, and actively attended some career development events organized by ASME and supported by some oil companies. Moreover, the PI is in the process of composing a grant application based on the findings from this project to seek for further financial support from NSF to continue the relevant research.