Supporting Information for:

Extending Applicability of Correlation Equations to Predict Colloidal Retention in Porous Media at Low Fluid Velocity

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Porosity-Dependent Sherwood Number at No Fluid Flow Limit

Following the analysis for the isolated sphere model by Sherwood et al. (p215),[1] the Sherwood number for the Happel sphere-in-cell model is derived below for the limiting case of no fluid flow. Under no fluid flow conditions, the mass transfer of small size colloids occurs only by molecular diffusion (when the small effect of gravity is neglected). Suppose a steady-state will be established within the Happel model; the molal flux (N) through the spherical shell at radius r ($r > a_c$) is then given by

$$N(4\pi a_c^2) = -D(4\pi r^2)\frac{dC}{dr}, \qquad \text{(S1)}$$

where a_c is the collector radius, D is the molecular diffusion coefficient, and C is the colloid concentration. Re-arranging eq S1 and integration between the limits $C = C_i$ at $r = a_c$ and $C = C_0$ at $r = b$ (b is the radius of the Happel outer fluid shell) yields,

$$N a_c^2 \int_{a_c}^{b} \frac{1}{r^2} dr = \int_{C_i}^{C_0} (-D) dC$$

$$N a_c^2 \left(\frac{1}{a_c} - \frac{1}{b}\right) = D(C_i - C_0) = \Delta C$$

$$\frac{2Na_c}{D\Delta C} = \frac{2}{1-\frac{a_c}{b}}. \qquad \text{(S2)}$$

Note that the left-hand-side of eq S2 defines the Sherwood number, and for the Happel model, $a_c/b = \gamma = (1-\varepsilon)^{1/3}$, where ε is the porosity, so one obtains for the limiting case of no fluid flow

$$N_{sh} = \frac{2}{1-\frac{a_c}{b}} = \frac{2}{1-\gamma} = \frac{2}{1-(1-\varepsilon)^{1/3}}. \qquad \text{(S3)}$$

Derivation for η_D in eq 5 in the Main Text

At low fluid velocity conditions and for diffusion-dominated regime, and neglecting the gravity, the particle flux for introduced colloids includes two contributions: convection and diffusion. Following the analysis of Tien (p124-125),[2] we now derive the expression for collector efficiency due to diffusion (η_D) when both convective and diffusive fluxes are taken into account. First let us consider the case when surface interaction forces are absent so that the deposition of Brownian particles onto collector surfaces may be treated as a mass transfer process. Let I denote the particle mass flux over a collector grain. The Sherwood number (N_{sh}) for mass transfer is given by

$$N_{sh} = \frac{d_c}{D}\frac{I}{(\Delta c)S} = \frac{d_c}{D}\frac{I}{\Delta c(4\pi a_c^2)}, \qquad \text{(S4)}$$

where D is the diffusion coefficient, ΔC is the concentration difference that drives mass transfer process, and d_c and S are the diameter and surface area of the collector grain, respectively. The second equal sign in eq S4 holds if the grains are spherical. The driving force for mass transfer may be taken as the difference between the bulk concentration (C_0) and the colloid concentration at the fluid-grain interface. For particle deposition without surface interaction forces, the interface concentration vanishes, so that $\Delta C \approx C_0$.

For the Happel model, the convective particle flux is given by $\pi b^2 U C_0$, where b is the radius of the outer fluid envelope, U is the approach fluid velocity and C_0 represents the bulk colloid concentration. Let N_D denote the molal flux through a spherical shell due only to molecular diffusion, the collector efficiency due to diffusion (η_D) is then given by

$$\eta_D = \frac{I}{\pi b^2 U C_0 + N_D(4\pi a_c^2)}. \qquad \text{(S5)}$$

Equating the term *I* from eqs S4 and S5 yields

$$\eta_D = \frac{N_{sh} D \Delta C \left(4\pi a_c^2\right)/d_c}{\pi b^2 U C_0 + N_D\left(4\pi a_c^2\right)} = \frac{N_{sh}}{\frac{1}{4}\left(\frac{b}{a_c}\right)^2 \frac{U d_c}{D} + \frac{N_D d_c}{D \Delta C}}. \qquad \text{(S6)}$$

Note that $N_{Pe} = Ud_c/D$; and the term $N_D d_c/(D\Delta C)$ in the denominator of eq S6 represents the Sherwood number due solely to molecular diffusion, which may be approximated by the Sherwood number for the limiting case of no fluid motion as derived in eq S3. Since expressions for the Sherwood number are only available for the limiting case of no fluid flow (only natural molecular diffusion, eq S3) or convective flow when $N_{Pe} > 70$ (eq 2 in the main text), here we superimpose these expressions of limiting cases to approximate the general Sherwood number in the numerator of eq S6, which leads to

$$\eta_D \approx \frac{\frac{2}{1-(1-\varepsilon)^{1/3}} + A_s^{1/3} N_{Pe}^{1/3}}{\frac{1}{4}\left(\frac{b}{a_c}\right)^2 N_{Pe} + \frac{2}{1-(1-\varepsilon)^{1/3}}} = \frac{\frac{2}{1-\gamma} + A_s^{1/3} N_{Pe}^{1/3}}{\frac{1}{4}\frac{1}{\gamma^2} N_{Pe} + \frac{2}{1-\gamma}} = \gamma^2 \frac{8 + 4(1-\gamma) A_s^{1/3} N_{Pe}^{1/3}}{(1-\gamma) N_{Pe} + 8\gamma^2}$$

(S7)

where the relationships $\gamma = a_c/b = (1\text{-}\varepsilon)^{1/3}$ for the Happel model has been used. From eq S7, one can see that when $N_{Pe} = 0$ (no fluid flow), $\eta_D = 1$. However, eq S7 is not a monotonous function with respect to N_{Pe} (or particle size). To ensure that η_D will not be greater than unity after incorporation of the effects of surface interaction (e.g., van der Waals interactions) or gravity, and to also ensure that the overall collector efficiency (η) (which sums over the contributions due to diffusion, interception and gravitational settling) does not go above unity, the final form of eq S7 was slightly modified during the regression process of numerical simulation data, as shown in eq. 5 in the main text. For instance, the denominator of eq S7 after regression modification became $[8 + (1-\gamma)N_{Pe}^{0.97}]$, and this modification may slightly underestimate the predicted η_D values at high porosities when N_{Pe} approaches zero, as shown in Figure 4 in the main text; but this estimation of collector efficiency can be corrected from the asymptotes at the diffusion limit.

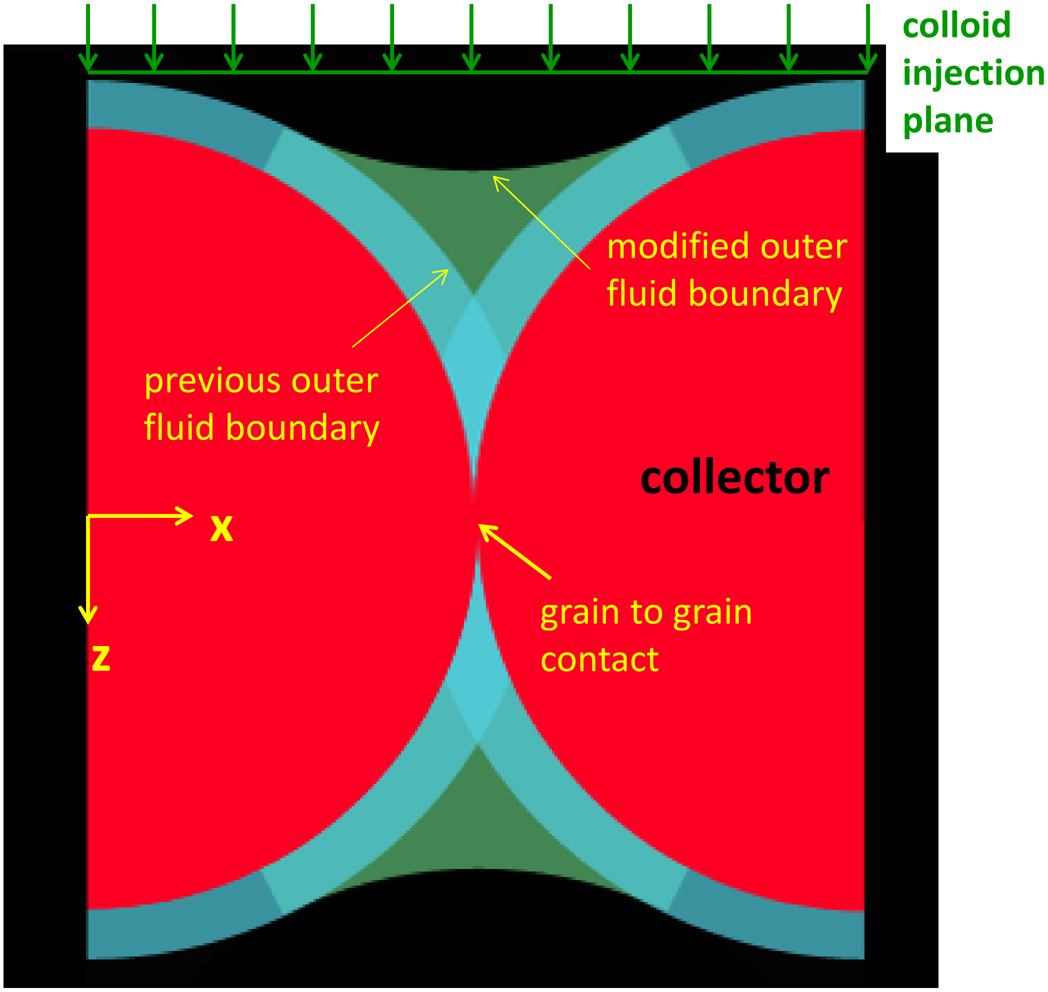

Figure S1. A two-dimensional representation of the hemispheres-in-cell model illustrating the differences in the outer fluid boundaries between our previous (blue) and current work (blue plus green). The green represents a greater porosity than the blue in this depiction. Two reasons for making this change: i) to obtain the convergence-divergence of flow streamlines around the grain-to-grain contact region (as demonstrated in Fig. 2 in the main text); and ii) to represent both saturated and unsaturated porous media, e.g., under unsaturated conditions a thin film exists on the grain surfaces distal to the grain to grain contact; whereas at the grain to grain contact exists a pendular ring of water. The outer fluid boundary condition in both contexts is very similar (non-tangential stress).

References Cited

1. Sherwood, T. K.; Pigford, R. L.; Wilke, C. R., *Mass transfer*. McGraw-Hill Kogakusha, Ltd.: Tokyo, 1975.
2. Tien, C., *Granular filtration of aerosols and hydrosols*. First edition ed.; Butterworth-Heinemann: Stoneham, MA, 1989.