

Supporting Information

Single collector attachment efficiency of colloid capture by a cylindrical collector in laminar overland flow

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S1. DLVO interaction energy profiles.

DLVO theory^{1, 2} was used to calculate the total interaction energy (sum of London-van der Waals attraction and electrostatic double-layer repulsion) between colloid and glass cylinder surfaces under different conditions.

The Lifshitz - van der Waals attraction energy (ΔG_{LW}) for a sphere-plate system can be written as ³:

$$\Delta G_{LW} = -\frac{A}{6} \left[\frac{r}{h} + \frac{r}{h+2r} + \ln \left(\frac{h}{h+2r} \right) \right] \quad (1.1)$$

where A (1×10^{-20} J) is the Hamaker constant for the polystyrene-water-glass system ^{4, 5}, h is the separation distance, and r is the radius of the particle. The EDL repulsion energy (ΔG_{EDL}) for a sphere-plate system can be written as ³:

$$\Delta G_{EDL} = 64\pi r \varepsilon \varepsilon_0 \left[\frac{kT}{ze} \right]^2 \tanh \left[\frac{ze\psi_1}{4kT} \right] \tanh \left[\frac{ze\psi_2}{4kT} \right] \exp(-\kappa h) \quad (1.2)$$

where ε is the dielectric constant of the medium (78.4 for water), ε_0 is the vacuum permittivity (8.854×10^{-12} C² N⁻¹ m⁻²), k is the Boltzmann's constant (1.381×10^{-23} C² J K⁻¹), T is the temperature, z is the valence of electrolyte, e is the electron charge (1.602×10^{-19} C), ψ_1 and ψ_2 are the surface potential of the colloid and the collector surface, and κ is the reciprocal of the Debye length. The surface potential of colloids and collector can be determined following van Oss et al. ⁶:

$$\psi = \xi \left(1 + \frac{d}{r} \right) \exp(\kappa d) \quad (1.3)$$

where d is the distance between the surface of the charged particle and the slipping plane and usually taken as 5 angstroms (10^{-10} m).

S2. Existing models of estimating attachment efficiency

I. Maxwell model

Detailed description of the Maxwell model can be found in the literature^{7,8}. The model assumes that velocity distribution of a colloid in the secondary minimum follows the Maxwell function:

$$f_{Max}(v) = 4\pi \left(\frac{m}{2\pi kT} \right)^{3/2} v^2 \exp\left(\frac{-\frac{1}{2}mv^2}{kT} \right) \quad (2.1)$$

$$\int_0^\infty f_{Max}(v) dv = 1 \quad (2.2)$$

where m is mass of the colloid and v is the velocity.

The fraction of successful collision resulting in the colloid deposition in the secondary minimum, α_{sec} can be written as:

$$\alpha_{sec} = \int_0^{\sqrt{\Phi_{sec}}} \frac{4}{\pi^{1/2}} x^2 \exp(-x^2) dx \quad (2.3)$$

$$x^2 = \frac{mv^2}{2kT} \quad (2.4)$$

Similarly, the fraction of successful collision resulting in the colloid deposition in the primary minimum, α_{pri} can be written as:

$$\alpha_{pri} = \int_{\sqrt{\Delta\Phi}}^\infty \frac{4}{\pi^{1/2}} x^2 \exp(-x^2) dx \quad (2.5)$$

The single collector attachment efficiency, α , can be written as:

$$\alpha = \int_{\sqrt{\Delta\Phi}}^\infty \frac{4}{\pi^{1/2}} x^2 \exp(-x^2) dx + \int_0^{\sqrt{\Phi_{sec}}} \frac{4}{\pi^{1/2}} x^2 \exp(-x^2) dx \quad (2.6)$$

II. Modified Maxwell model

To account for the influence of fluid hydrodynamic drag on the attachment efficiency, two hydrodynamic factors, f_{pri} and f_{sec} , are introduced to modify the Maxwell model ⁹:

$$\alpha = f_{pri}\alpha_{pri} + f_{sec}\alpha_{sec} \quad (2.7)$$

where f_{pri} and f_{sec} , are the fractions of single collector surface area over which the adhesive torques acting on the colloids retained in the primary and secondary minimum are greater than the fluid hydrodynamic drags, respectively.

The values of adhesive force (F_A) are estimated as the sum of $\frac{\Phi_{pri}}{h}$ and $\frac{\Phi_{sec}}{h}$ for colloids retained in the energy wells⁹:

$$F_A = \frac{\Phi_{pri}}{h} + \frac{\Phi_{sec}}{h} \quad (2.8)$$

where Φ_{pri} and Φ_{sec} are primary and secondary minimum, respectively; and h is separation distance. The value of lever arm (l_x) of the adhesive torque can be estimated with: ⁹

$$l_x = \left(\frac{F_A a_p}{K} \right)^{1/3} \quad (3.9)$$

where a_p is colloid radius, and K is the composite Young's modulus ($4.014 \times 10^9 \text{ Nm}^{-2}$).

The adhesive torque can then be expressed as:

$$T_A = F_A \times l_x \quad (2.10)$$

The drag force (F_H) that acts on a colloid attached on the collector interface at a separation distance (h) can be written as ^{10, 11}:

$$F_H = 6\pi\mu\tau a_p(a_p + h)C_h \quad (2.11)$$

where μ is fluid viscosity and τ is hydrodynamic shear, C_h is a constant defined as ^{10, 11}:

$$C_h = \frac{1.7007337 + 1.0221616\left(\frac{h}{a_p}\right)}{1 + 1.0458291\left(\frac{h}{a_p}\right) - 0.0014884708\left(\frac{h}{a_p}\right)^2} \quad (2.12)$$

On a smooth surface the value of the applied hydrodynamic torque that acts on the colloid at h is given as ^{10, 11}:

$$T_H = a_p F_H + 4\pi\mu\tau a_p^3 C_{2h} \quad (2.13)$$

In this case, C_{2h} is a second dimensionless function that depends on h is given as ^{10, 11}:

$$C_{2h} = 0.054651334 \left\{ 18.276952 - \exp \left[-1.422943 \left(\frac{h}{a_p} \right) \right] \right\} \quad (2.14)$$

Where a_p is much greater than h , the value of T_H is more simply given as ^{9, 12}:

$$T_H = 14.287\pi\mu\tau a_p^3 \quad (2.15)$$

III. Bai-Tien model.

An empirical correlation equation developed by Bai and Tien ¹³ was also used in this work. The equation of the Bai-Tien model can be written as:

$$\alpha = 2.57 \times 10^{-3} (N_{LO})^{0.7031} (N_{E1})^{-0.3121} (N_{E2})^{3.5111} (N_{DL})^{1.352} \quad (2.16)$$

Definitions of the dimensionless parameters are listed in Table S1.

Table S1. Definition of Dimensionless parameters.

Parameter	Definition	
N_{LO}	$\frac{4A}{9\pi\mu d_p^2 u}$	London number
N_{E1}	$\frac{\varepsilon\varepsilon_0(\xi_p^2 + \xi_c^2)}{3\pi\mu u d_p}$	First electrokinetic parameter
N_{E2}	$\frac{2\xi_p\xi_c}{(\xi_p^2 + \xi_c^2)}$	Second electrokinetic parameter
N_{E3}	$N_A I d_c^3$	Third electrokinetic parameter
N_{DL}	κd_p	Double-layer force parameter
N_{Re}	$\frac{u d_c}{\nu}$	Reynolds number
N_R	$\frac{d_p}{d_c}$	Aspect ratio
N_{Pe}	$\frac{u d_c}{D_\infty}$	Peclet number

* A is the Hamaker constant, μ is the fluid viscosity, d_p is the colloidal particle diameter, u is the flow velocity, ε is the relative permittivity of the fluid, ε_0 is the permittivity in a vacuum, ξ_p and ξ_c are the surface potential of the colloidal particles and collectors respectively, κ is the reciprocal of double layer thickness, N_A is Avogadro's constant, I is the ionic strength, ν is kinetic viscosity, D_∞ is the bulk diffusion coefficient (described by Stokes-Einstein equation).

Table S2. Summary of stepwise-least square regression results.

Step 1 - Entering variable: log(NE2)**Summary measures**

Multiple R	0.7046
R-Square	0.4964
Adj R-Square	0.4850
StErr of Est	0.4167

ANOVA Table

Source	df	SS	MS	F	p-value
Explained	1	7.5325	7.5325	43.3739	0.0000
Unexplained	44	7.6412	0.1737		

Regression coefficients

	Coefficient	Std Err	t-value	p-value	Lower limit	Upper limit
Constant	-2.0256	0.0875	-23.1621	0.0000	-2.2019	-1.8494
log(NE2)	-9.2662	1.4070	-6.5859	0.0000	-12.1018	-6.4306

Step 2 - Entering variable: log(NE1)**Summary measures**

		Change	% Change
Multiple R	0.7683	0.0638	9.0%
R-Square	0.5903	0.0939	18.9%
Adj R-Square	0.5713	0.0863	17.8%
StErr of Est	0.3802	-0.0365	-8.8%

ANOVA Table

Source	df	SS	MS	F	p-value
Explained	2	8.9575	4.4787	30.9813	0.0000
Unexplained	43	6.2162	0.1446		

Regression coefficients

	Coefficient	Std Err	t-value	p-value	Lower limit	Upper limit
Constant	-2.2197	0.1009	-21.9934	0.0000	-2.4232	-2.0161
log(NE2)	-10.0772	1.3094	-7.6959	0.0000	-12.7179	-7.4365
log(NE1)	0.1588	0.0506	3.1396	0.0031	0.0568	0.2608

Step 3 - Entering variable: log(NDL)

Summary measures		Change	% Change
Multiple R	0.8894	0.1211	15.8%
R-Square	0.7911	0.2007	34.0%
Adj R-Square	0.7761	0.2049	35.9%
StErr of Est	0.2747	-0.1055	-27.7%

ANOVA Table

Source	df	SS	MS	F	p-value
Explained	3	12.0034	4.0011	53.0086	0.0000
Unexplained	42	3.1702	0.0755		

Regression coefficients

	Coefficient	Std Err	t-value	p-value	Lower limit	Upper limit
Constant	-3.3878	0.1978	-17.1261	0.0000	-3.7870	-2.9886
log(NE2)	-6.4480	1.1053	-5.8339	0.0000	-8.6786	-4.2175
log(NE1)	0.2592	0.0398	6.5100	0.0000	0.1788	0.3396
log(NDL)	0.5649	0.0889	6.3525	0.0000	0.3855	0.7444

Step 4 - Entering variable: log(NLO)

Summary measures		Change	% Change
Multiple R	0.9233	0.0338	3.8%
R-Square	0.8524	0.0613	7.8%
Adj R-Square	0.8380	0.0619	8.0%
StErr of Est	0.2337	-0.0410	-14.9%

ANOVA Table

Source	df	SS	MS	F	p-value
Explained	4	12.9342	3.2335	59.2001	0.0000
Unexplained	41	2.2394	0.0546		

Regression coefficients

	Coefficient	Std Err	t-value	p-value	Lower limit	Upper limit
Constant	-3.2475	0.1717	-18.9171	0.0000	-3.5942	-2.9008
log(NE2)	-1.1545	1.5901	-0.7260	0.4719	-4.3658	2.0568
log(NE1)	-0.2072	0.1179	-1.7564	0.0865	-0.4453	0.0310
log(NDL)	0.9858	0.1270	7.7647	0.0000	0.7294	1.2422
log(NLO)	0.4453	0.1079	4.1280	0.0002	0.2274	0.6631

Step 5 - Leaving variable: log(NE2)

<i>Summary measures</i>		Change	% Change
Multiple R	0.9222	-0.0010	-0.1%
R-Square	0.8505	-0.0019	-0.2%
Adj R-Square	0.8398	0.0018	0.2%
StErr of Est	0.2324	-0.0013	-0.6%

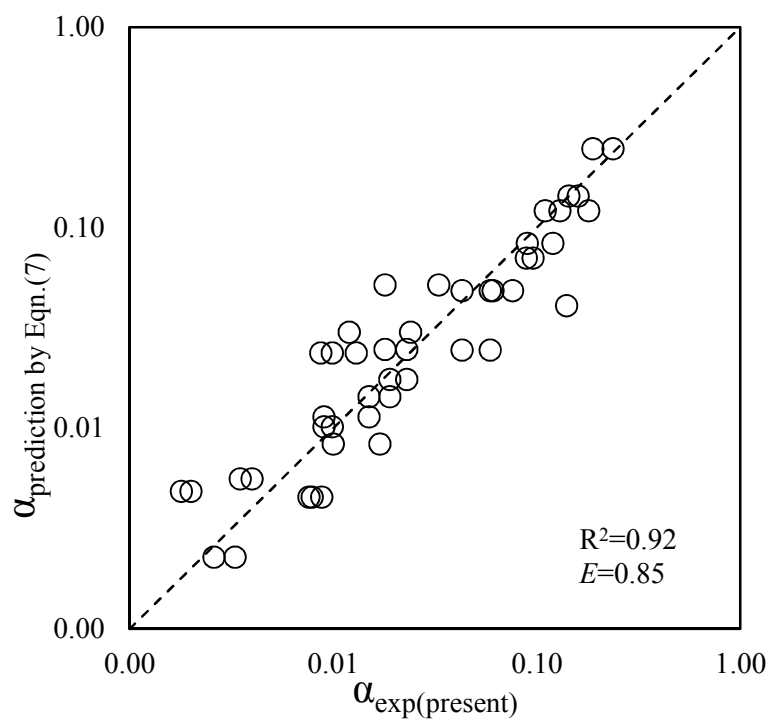
ANOVA Table

Source	df	SS	MS	F	p-value
Explained	3	12.9054	4.3018	79.6545	0.0000
Unexplained	42	2.2682	0.0540		

Regression coefficients

	Coefficient	Std Err	t-value	p-value	Lower limit	Upper limit
Constant	-3.2470	0.1707	-19.0216	0.0000	-3.5915	-2.9025
log(NE1)	-0.2726	0.0757	-3.6019	0.0008	-0.4253	-0.1199
log(NDL)	1.0623	0.0705	15.0774	0.0000	0.9201	1.2045
log(NLO)	0.5084	0.0634	8.0168	0.0000	0.3804	0.6364

Figure S1. Comparison of experimental attachment efficiency with predictions of the new correlation equation for development dataset.



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