water

Supporting Information

The Comparison of Seven Models to Simulate the Transport and Deposition of Polydisperse Particles under Favorable Conditions in a Saturated Medium

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Table S1: Summary of dimensionless parameters present in the existing models.

Parameter	Definition [a]	Value Range	Physical Interpretation
Advection	U	0-10^{-7} m/s	fluid approach velocity
Diffusion	$D = \frac{AT}{6\pi\mu a_p}$	10^{-9}-10^{-6} m^2/s	bulk diffusion
London group	$N_{Lo} = \frac{H}{9\pi\mu U a_p^2}$	10^{-7}-10^{-3}	attraction number
Attraction number	$N_A = \frac{H}{12\pi\mu U a_p^2}$	10^{-8}-10^{-3}	attraction number; represents combined influence of van der Waals attraction forces and fluid velocity on particle deposition rate due to interception
Gravity	$V = \frac{2}{9}\frac{a_p^2(\rho_p-\rho)}{\mu}g$	0-10^{-5} m/s	gravity number; ratio of Stokes particle settling velocity to approach velocity of the fluid
Van der Waals number	$N_{vdW} = \frac{H}{AT}$	10^{-1}-10^{1}	van der Waals number characterizing ratio of van der Waals interaction energy to the particle's thermal energy
Peclet number	$N_{Pe} = \frac{2a_c U}{D}$	10^{-1} -2.37×10^{5}	Peclet number characterizing ratio of convective transport to diffusive transport
Gravity number	$N_G = \frac{V}{U}$	0-10^{2}	Gravity number
	$N_{Gi} = \frac{N_G}{1+N_G}$	10^{-4}	Modified gravity number
Aspect ratio	$N_R = \frac{a_p}{a_c}$	0-10^{-3}	aspect ratio
A_s	$A_s = \frac{1(1-\gamma^5)}{2-3\gamma+3\gamma^5-2\gamma^6}$	2-7.15	Porosity dependant variable
γ	$\gamma = (1-\varepsilon)^{1/3}$	0.60-0.80	Porosity dependant variable

[a] The parameters in the various dimensionless groups are as follows: d_p is the particle diameter, 2.932×10^{-6} m, a_p is particle radius, 1.466×10^{-6} m, d_c is the collector diameter, 5.03×10^{-4} m, a_c is collector radius, 2.51×10^{-4} m, U is the fluid approach velocity, 3.51×10^{-5} m/s, D is the bulk diffusion coefficient, 2.31×10^{-6} m^2/s, H is the Hamaker constant, 10^{-20}J, A is the Boltzmann constant, 1.38×10^{-23}, T is fluid absolute temperature, 298K, ε is the porosity, 0.378, ρ_p is the particle density, 2.53×10^{3} kg/m^3, ρ is the fluid density, 1000 kg/m^3, μ is the absolute fluid viscosity, 9.8×10^{-4} Pa·s, and g is the gravitational acceleration, 9.806 m/(s*s).

Table S2: List of the existing equations for comparison. See Table S1 for the parameter's definition.

Acronym	Authors	Equation
Yao	Yao et al. 1971	$\eta_0 = 4.04N_{Pe}^{-2/3} + \frac{3}{2}N_R^2 + N_G$
RT	Rajagopalan and Tien 1976 Corrected by Logan **Error! Reference source not found.**	$\eta_{0,\gamma} = \gamma^2[4.04N_{Pe}^{-\frac{2}{3}}A_S^{\frac{1}{3}} + A_S N_R^{\frac{15}{8}}N_{Lo}^{\frac{1}{8}} + 0.00338A_S N_G^{1.2}N_R^{-0.4}]$
TE	Tufenkji and Elimelech 2004 **Error! Reference source not found.**	$\eta_0 = 2.4N_R^{-0.081}N_{Pe}^{-0.715}A_S^{\frac{1}{3}}N_{vdW}^{0.052} + 0.55A_S N_R^{1.675}N_A^{0.125} + 0.22A_S N_G^{1.11}N_R^{-0.24}N_{vdW}^{0.053}$
MPFJ	Ma et al. 2009	$\eta_{0,\gamma} = \gamma^2[2.3N_{Pe}^{-0.65}A_S^{\frac{1}{3}}N_R^{-0.08}N_A^{0.052} + 0.55A_S N_R^{1.8}N_A^{0.15} + 0.2N_G^{1.1}N_R^{-0.1}N_A^{0.053}N_{Pe}^{0.053}]$
NG	Nelson and Ginn 2011	$\eta_{0,\gamma} = \gamma^2[2.4N_{Pe}^{-0.68}A_S^{\frac{1}{3}}N_{Gi}^{0.8}N_{Lo}^{0.015}(\frac{N_{Pe}}{N_{Pe}+16})^{0.75} + A_S N_R^{\frac{15}{8}}N_{Lo}^{\frac{1}{8}} + 0.7N_G N_R^{-0.05}(\frac{N_{Gi}}{N_{Gi}+0.9})]$
MHJ	Ma et al. 2013	$\eta_{0,\gamma} = \gamma^2[N_R^{0.028}N_{Gi}^{0.8}N_{Lo}^{0.015}(\frac{8+4(1-\gamma)A_S^{1/3}N_{Pe}^{1/3}}{8+(1-\gamma)N_{Pe}^{0.97}}) + A_S N_R^{\frac{1}{8}}N_{Lo}^{\frac{15}{8}} + 0.7N_G N_R^{-0.05}(\frac{N_{Gi}}{N_{Gi}+0.9})]$
MMS	Messina et al. 2015	$\eta_0 = \frac{(\eta_{0,a_c})^b}{(I)^c}$

b: $\eta_{0,a_c} = [1.5062A_S N_R^{1.9834} + N_G(1 + 6.0187N_R^2) + N_{Pe}^{-1}\frac{7.5609+4.9534N_R^1}{2-2\gamma} + A_S^{0.1259}N_G^{0.8741}(0.0442 + 0.122N_R^{0.421}) + A_S^{0.3662}N_{Pe}^{-0.6338}(2.9352 + 2.748N_R^{0.3737}) + N_G^{0.8741}N_{Pe}^{-0.345}(0.9461+1.1626N_R^{0.6012}) + A_S^{0.1562}N_G^{0.5873}N_{Pe}^{-0.2565}(-0.674 - 0.7119N_R^{0.5438})$

c: $I = [(1 + A_S^{6.0098}N_R^{1.9834}) + N_G(1 + 6.0187N_R^2) + (1 - \sqrt{1-\gamma^2})N_{Pe}^{-1}\frac{7.5609+4.9534N_R^1}{2-2\gamma} + A_S^{0.1259}N_G^{0.8741}(0.0442 + 0.122N_R^{0.421}) + A_S^{0.3662}N_{Pe}^{-0.6338}(2.9352 + 2.748N_R^{0.3737}) + N_G^{0.6550}N_{Pe}^{-0.345}(2.7972+3.4372N_R^{0.6012}) + A_S^{0.1562}N_G^{0.5873}N_{Pe}^{-0.2565}(-1.1945 - 1.2616N_R^{0.5438})$