Supplementary Material (SM)

Simulation of bidisperse colloidal centrifugal sedimentation using a mixture viscosity model

Hangyu Chen (陈航宇)[a,b*], Thomas C. Sykes[c], Oguzhan Kivan[a], Xiaodong Jia (贾晓东)[a], Michael Fairweather[a], Timothy N. Hunter[a*]

[a]University of Leeds, School of Chemical and Process Engineering, Leeds LS2 9JT, U.K.
[b]School of Aerospace Engineering, Tsinghua University, Beijing 100084, P.R. China
[c]University of Oxford, Department of Engineering Science, Oxford OX1 3PJ, U.K.

Section S1: Calculation example of maximum volume fraction and relative viscosity for bidisperse sedimentation.

This example is based on a 1 vol% 500:800 nm dispersion and mixing ratio 1:1 as an illustration. Here, the standard ϕ_{rcp} = 0.639, k = 0.5/1.0, λ = 800/500. The ξ_k and ξ_λ can be calculated and the results are 0.131 and 0.990, respectively. Then, the $\phi_{\max,b}$ can be calculated, as per Eq S1,

$$\phi_{\max,b} = \phi_{rcp} + \xi_k \xi_\lambda \phi_{rcp}(1-\phi_{rcp}). \quad \text{S1}$$

This results in $\phi_{\max,b}$ = 0.669. The minimum separation distance $\bar{s}$ is obtained through the DLVO theory and the result for 500:800 silica suspension is 307 nm. Then, the volume fractions of small and large particles are used to calculate average spherical diameter of the particle mixtures, with Eq. S2.

$$d_{ave} = \frac{d_L d_S(\phi_L + \phi_S)}{d_L \phi_S + d_S \phi_L}, \quad \text{S2}$$

This results in d_{ave} = 615.38 nm. The effective maximum volume fraction can be calculated from Eq. S3, giving $\phi^{eff}_{\max,b}$ = 0.199.

$$\phi^{\mathrm{eff}}_{\max,\mathrm{b}} = \phi_{\max,b}\left(\frac{d_{ave}+\bar{s}}{d_{ave}}\right)^{-3}. \quad \text{S3}$$

Finally, the relative fluid viscosity of bidisperse suspension can be calculated using the calculated modified effective maximum volume fraction and bidipserse viscosity model of Qi and Tanner (2011)[1], Eqs. S4

$$\mu_r = [(1-\frac{\phi_L}{1-c_L\phi_L})(1-\frac{\phi_S}{1-c_S\phi_S})]^{-\frac{5}{2}},\ c_L = \frac{1-\phi_{rcp}}{\phi_{rcp}},\ c_S = \frac{1-(\phi^{eff}_{\max,b}-\phi_L)}{\phi^{eff}_{\max,b}-\phi_L}. \quad \text{S4}$$

For this example, the overall relative viscosity = 1.03. For 2 vol% and 3 vol%, the results are 1.05 and 1.08, respectively.

[1] F. Qi, and R. I. Tanner, "Relative viscosity of bimodal suspensions," Korea-Australia Rheology Journal 23, 105 (2011) (appears also in main paper)

Section S2: Supplementary figures

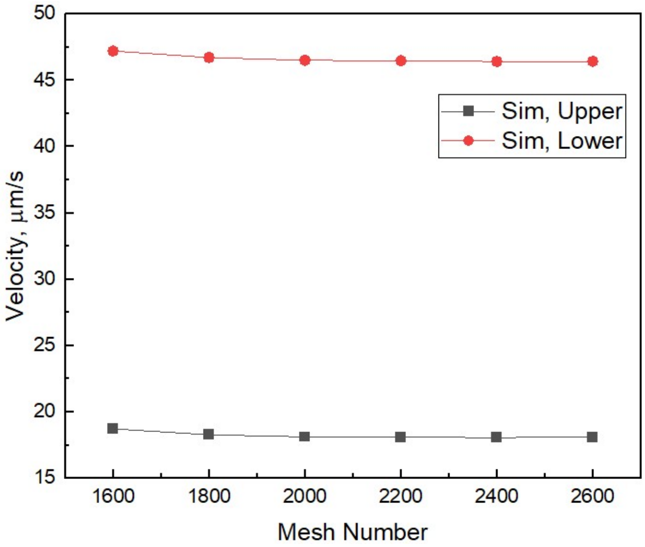

Fig. S1: Independence grid verification using 500 nm (Upper):800 nm (Lower) particles under 1000 rpm and a mixing ratio = 1:1.

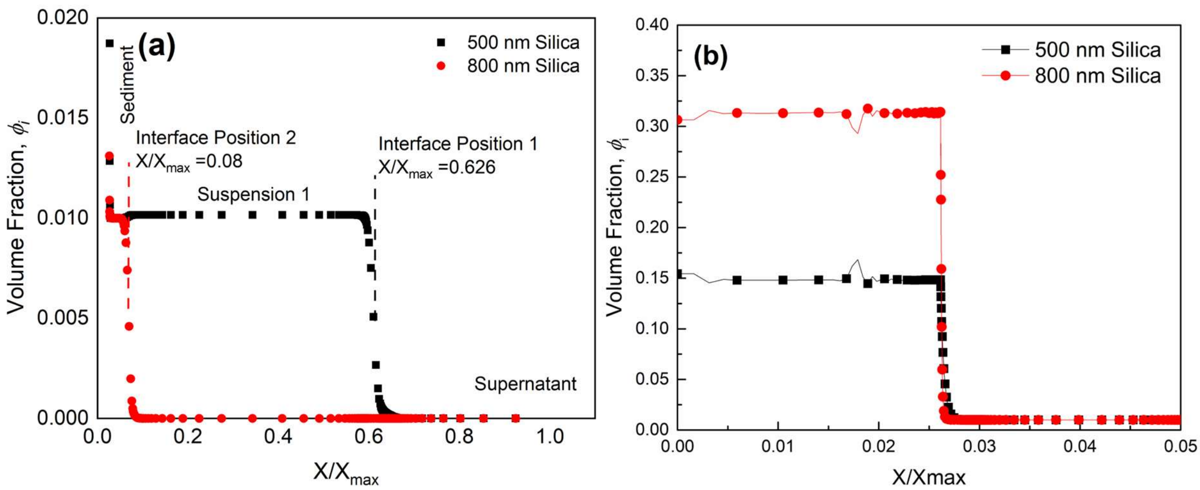

Fig. S2: (a), simulated concentration profile for a 500:800 nm suspension mixture in 1:1 mixing ratio with ϕ_0 =0.02 under earth gravity condition after 16 h. The general data are plotted at the spatial points where the solution is calculated according to the meshes. X/X_{max} is the relative position. (b) the near-bed zone in detail, which changes to the bidisperse effective maximum volume fraction.

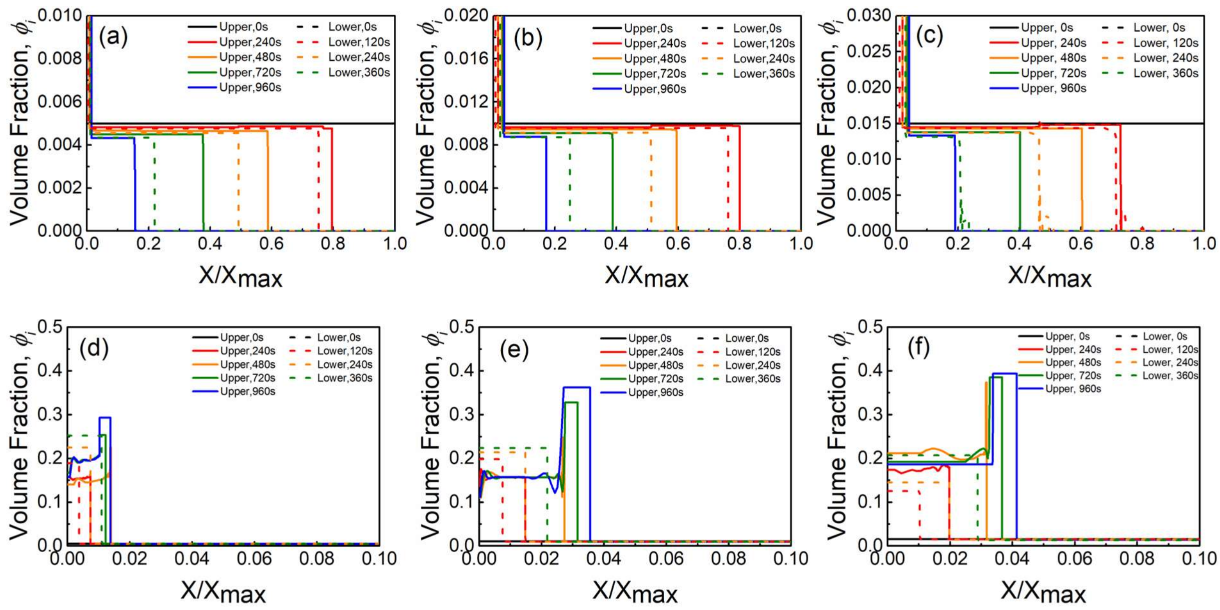

Fig. S3: (a), simulated concentration profiles of 500 nm (Upper) and 800 nm (Lower) particles under 1000 rpm, at a mixing ratio = 1:1, using 1-D bidisperse model. (a) ϕ_0 = 0.01, (b) ϕ_0 = 0.02, (c) ϕ_0 = 0.03. (d)–(f), concentration changes in the near-bed region, which changes to the bidisperse effective maximum volume fraction.

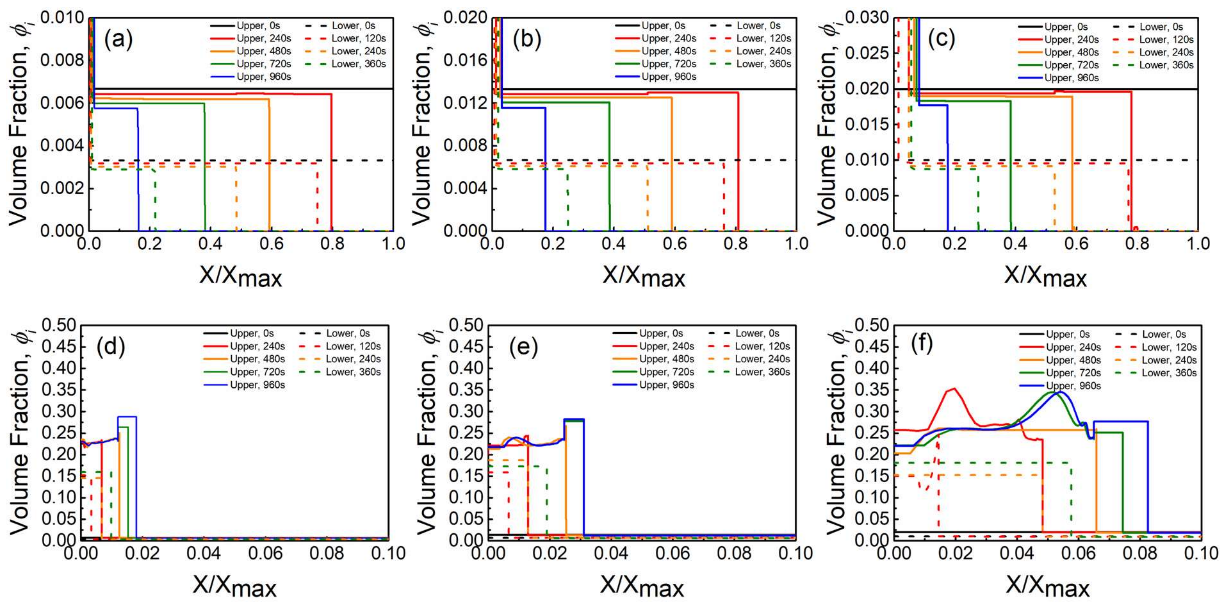

Fig. S4: Simulated concentration profiles of 500 nm (Upper) and 800 nm (Lower) particles under 1000 rpm, at a mixing ratio = 2:1, using 1-D bidisperse model. (a) ϕ_0 = 0.01, (b) ϕ_0 = 0.02, (c) ϕ_0 = 0.03. 03. (d)–(f), concentration changes in the near-bed region, which changes to the bidisperse effective maximum volume fraction.

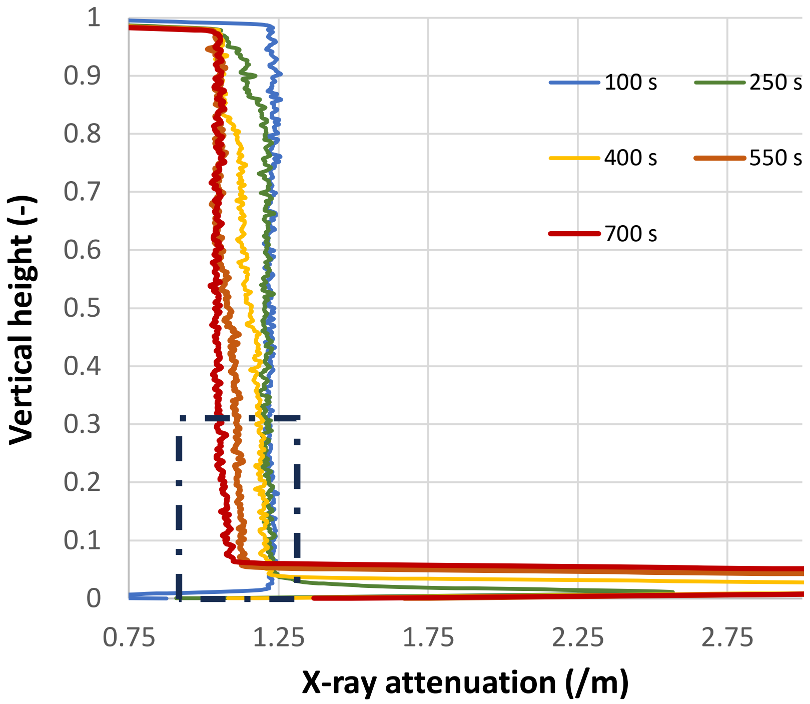

Fig. S5: Normalized X-ray sedimentation data, presenting total attenuation versus sample height for a 500:800 nm suspension at a mixing ratio 1:1 and total volume fraction, $\phi_0 = 0.03$. Full profile shown in the figure and expanded near-bed zone shown in Fig. 4 is the dashed box.

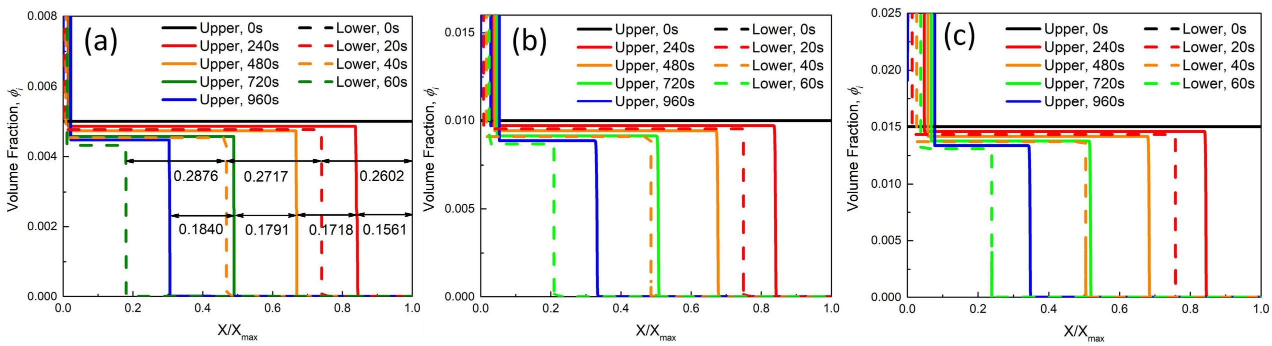

Fig. S6: Simulated concentration profiles of 100 nm (Upper) and 500 nm (Lower) particles under 4000 rpm and a mixing ratio = 1:1. Here, (a) $\phi_0 = 0.01$, (b) $\phi_0 = 0.02$, (c) $\phi_0 = 0.03$.

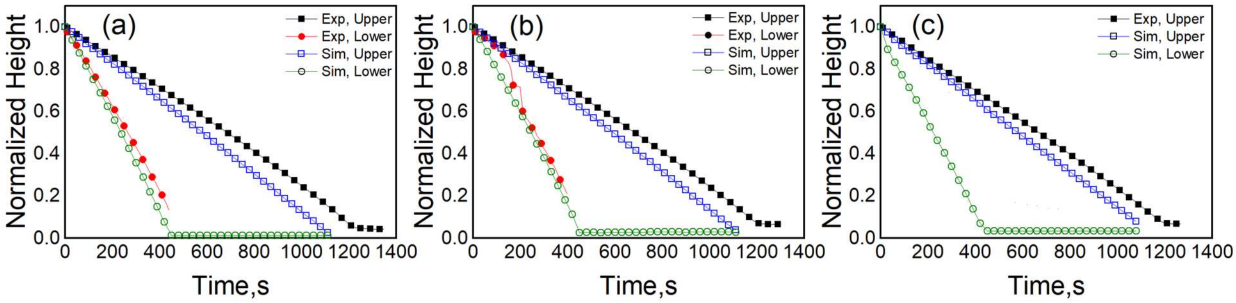

Fig. S7: Height vs Time profiles of 500 nm (Upper) and 800 nm (Lower) particles under 1000 rpm, at a mixing ratio = 1:1, comparing the 1-D model to experimental data. Here, (a) ϕ_0 = 0.01, (b) ϕ_0 = 0.02, (c) ϕ_0 = 0.03.

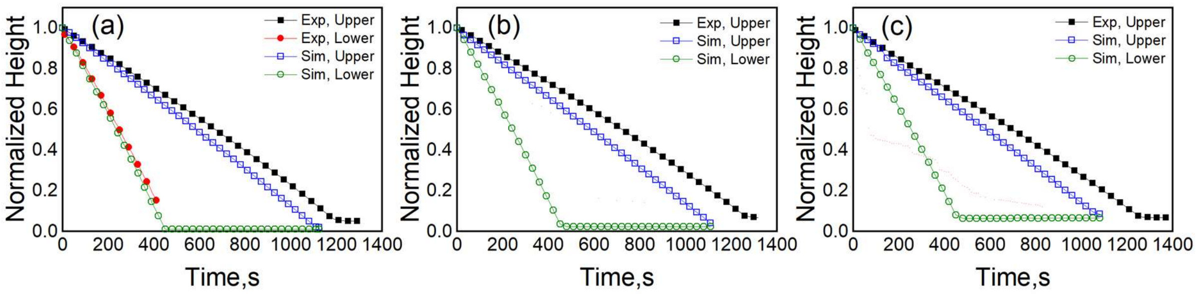

Fig. S8: Height vs Time profiles of 500 nm (Upper) and 800 nm (Lower) particles under 1000 rpm, at a mixing ratio = 2:1, comparing the 1-D model to experimental data. Here, (a) ϕ_0 = 0.01, (b) ϕ_0 = 0.02, (c) ϕ_0 = 0.03.

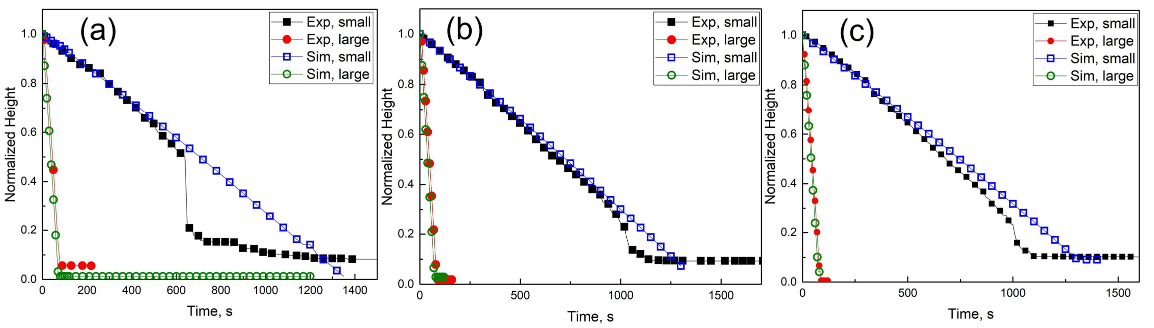

Fig. S9: Height vs Time profiles of 100 nm (Upper) and 500 nm (Lower) particles under 4000 rpm, at a mixing ratio = 1:1, comparing the 1-D model to experimental data. Here, (a) ϕ_0 = 0.01, (b) ϕ_0 = 0.02, (c) ϕ_0 = 0.03.