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Supplemental material for: Flow-induced segregation in confined multicomponent suspensions: Effects of particle size and rigidity

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This document contains results and discussion of segregation of elastic capsules in binary suspensions when both size and rigidity of the capsules are varied.

1. Effect of particle size and capillary number

In simulations presented in the main paper, we investigated the effect of particle size or capillary number in isolation. We saw that in simulations with equal sized particles, the stiffer particles in the mixture marginate when they are the dilute component, while the floppier particles in the mixture antimarginate when they are the dilute component. Further, in simulations with unequal sized particles, but with equal capillary numbers, the smaller particles undergo margination when they are the dilute component, while the bigger particles undergo antimargination when they are the dilute component. A natural question that arises at this point is what will happen when both the particle size as well

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Table 1. Parameter specification in various simulations.

Simulation	Ca_l	Ca_b	S	X_b	ϕ_b^0	a/h	N_p
1	0.5	0.1	0.8	$0-1$	0.08	0.197	40
2	0.5	0.2	0.8	$0-1$	0.08	0.197	40
3	0.5	0.5	0.8	$0-1$	0.08	0.197	40
4	0.2	0.5	0.8	$0-1$	0.08	0.197	40

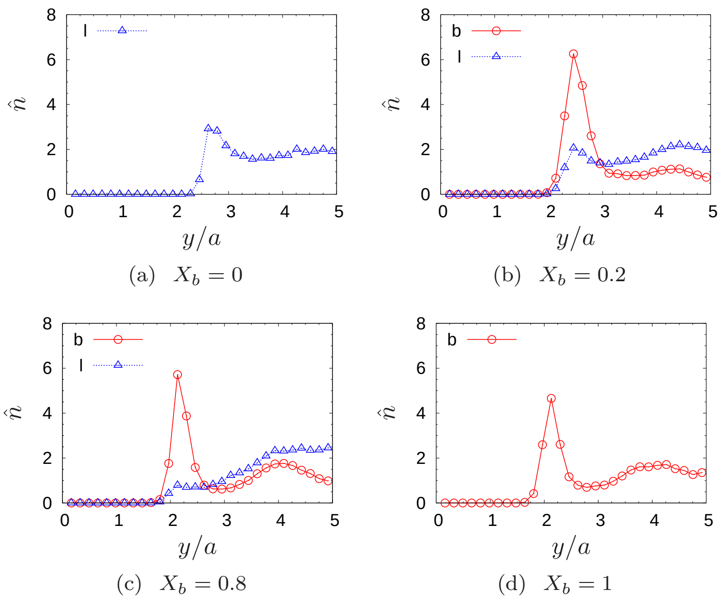
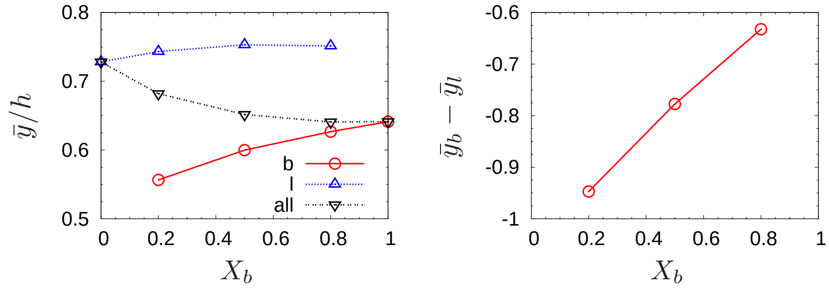


Figure 1. Normalized number density profile $\hat{n}$ for both the big and the small particles at several X_b. Other simulation parameters are: $\mathrm{Ca}_l = 0.5$, $\mathrm{Ca}_b = 0.1$, $S = 0.8$, $\phi_b^0 = 0.08$, and $a/h = 0.197$ (simulation 1 in Tb. 1).

as the capillary number are varied simultaneously. In particular, is it possible to make the bigger particle marginate corresponding to the leukocyte margination problem in blood flow? We address these questions in detail below – briefly, the results indicate that a bigger particle will marginate if it is made sufficiently stiffer than the smaller particle.



(a) $\bar{y}$ (b) $\Delta\bar{y} = \bar{y}_b - \bar{y}_l$

FIGURE 2. (a) Mean distance from the wall $\bar{y}$ of both the big and the small particles as a function of X_b, and (b) degree of segregation $\Delta\bar{y} = \bar{y}_b - \bar{y}_l$ as a function of X_b. Other simulation parameters are: $\mathrm{Ca}_l = 0.5$, $\mathrm{Ca}_b = 0.1$, $S = 0.8$, $\phi_b^0 = 0.08$, and $a/h = 0.197$ (simulation 1 in Tb. 1).

1.1. *Simulation results*

In the simulations conducted here, we keep $\phi_b^0 = 0.08$, $S = 0.8$, and $a/h = 0.197$ fixed, while several sets of $(\mathrm{Ca}_l, \mathrm{Ca}_b)$ were considered, namely, $(0.5, 0.1)$, $(0.5, 0.2)$, $(0.5, 0.5)$ and $(0.2, 0.5)$. A summary of these parameters is also provided in Tb. 1. The rigidity ratios $R_{lb} = \mathrm{Ca}_b/\mathrm{Ca}_l$ for these four systems are 0.2, 0.4, 1.0 and 2.5, respectively. A limited set of simulations with $\phi_b^0 = 0.12$ (not shown) shows essentially the same behavior. We first focus on the case $\mathrm{Ca}_l = 0.5$, $\mathrm{Ca}_b = 0.1$, which translates to $R_{lb} = 0.2$ (i.e., the bigger particle is stiffer). Figure (1) shows $\hat{n}$ for both the species as a function of X_b. In pure suspensions (Figs. 1a, 1d), the near wall peak for bigger particles is stronger than for smaller particles. Additionally, the cell-free-layer thickness for bigger particles is smaller than the same for smaller particles. Turning to mixtures, we find that in suspensions with big particles as the dilute component ($X_b = 0.2$), the big particles marginate (Fig. 1b). In contrast, in suspensions with small particles as the dilute component ($X_b = 0.8$), the small particles antimarginate (Fig. 1c).

We further characterize the particle distribution in the wall normal direction with the values of $\bar{y}$ for both species (Fig. 2). For the big particles this decreases as they

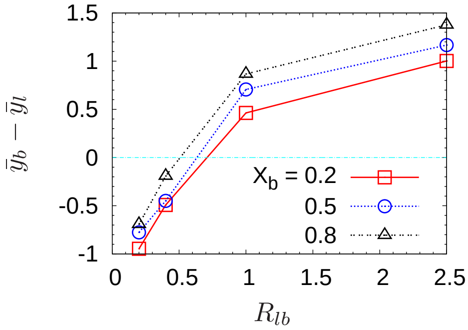


FIGURE 3. Degree of segregation $\Delta\bar{y} = \bar{y}_b - \bar{y}_l$ as a function of R_{lb} at several values of X_b. The common parameters in these simulations are $\phi_b^0 = 0.08$, $S = 0.8$ and $a/h = 0.197$. The four data points are for (Ca_l, Ca_b) of (0.5, 0.1), (0.5, 0.2), (0.5, 0.5) and (0.2, 0.5) corresponding to the rigidity ratio $R_{lb} = \mathrm{Ca}_b/\mathrm{Ca}_l$ of 0.2, 0.4, 1.0 and 2.5, respectively. See simulations 1–4 in Tb. (1) for a summary of all parameters.

become dilute in the suspension, i.e., with decreasing X_b, while for the small particles, it increases slightly with increasing X_b. The degree of segregation between the two species is characterized as usual by $\Delta\bar{y} = \bar{y}_b - \bar{y}_l$ (Fig. 2b). In contrast to the results presented in the main paper, $\Delta\bar{y}$ is negative here, implying that the small particles preferentially segregate near the centerline at the expense of the big particles. Additionally, the degree of segregation increases with decreasing X_b – this is consistent with observations in the main paper that the degree of segregation is typically larger when the marginating component is present in dilute amounts (except at smaller values of S).

The results from all sets of $(\mathrm{Ca}_l, \mathrm{Ca}_b)$ runs are summarized in Fig. 3, which shows $\Delta\bar{y}$ as a function of R_{lb} at several values of X_b. The values of R_{lb} in various runs conducted here have been noted above. In all cases we observe that $\Delta\bar{y}$ is positive at $R_{lb} = 1$, indicating at equal capillary numbers, the smaller particles have a tendency to marginate, or alternatively, the big particles have a tendency to antimarginate. With increasing R_{lb} the degree of segregation is found to increase as indicated by the increase in $\Delta\bar{y}$. Additionally, the sense of the segregation is the same as at $R_{lb} = 1$, namely the small particles

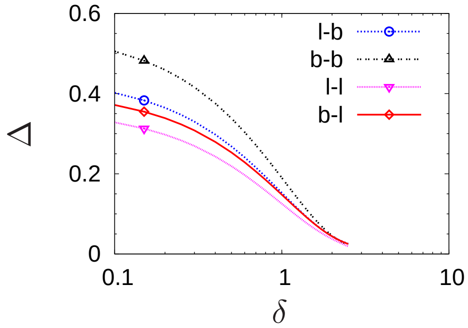


FIGURE 4. Cross-stream displacement Δ as a function of δ in a binary system with $S = 0.8$, $\mathrm{Ca}_l = 0.5$, and $\mathrm{Ca}_b = 0.1$.

marginate, while the big particles antimarginate. In all cases where $\Delta\bar{y}$ is positive, the degree of segregation increases with increasing X_b at any given value of R_{lb}, i.e. when the marginating component is present in dilute fractions. Lastly, Fig. 3 also illustrates that as R_{lb} is reduced sufficiently below one, $\Delta\bar{y}$ becomes negative implying that the big particles marginate, or, alternatively, the small particles antimarginate. The degree of segregation clearly increases with decreasing R_{lb} in this case. Moreover, the degree of segregation at any given R_{lb} increases as X_b is decreased, which again corresponds to an increase in segregation when the marginating component is present in dilute fractions in the suspension.

1.2. *Pair collision results*

In pair collision studies in the main paper, we focused on two specific types of systems. The first system illustrated the effect of rigidity on the cross-stream displacements in pair collisions, while the second illustrated the effect of size on the cross-stream displacements in pair collisions. In this section, we consider an additional case in which both of these effects are simultaneously present, i.e., a system in which $S \neq 1$ and $R_{lb} \neq 1$. Figure 4 summarizes $\Delta(\delta)$ in various types of pair collisions in a system with $S = 0.8$ and with $\mathrm{Ca}_l = 0.5$ and $\mathrm{Ca}_b = 0.1$. In this case, the bigger particle is stiffer than the smaller

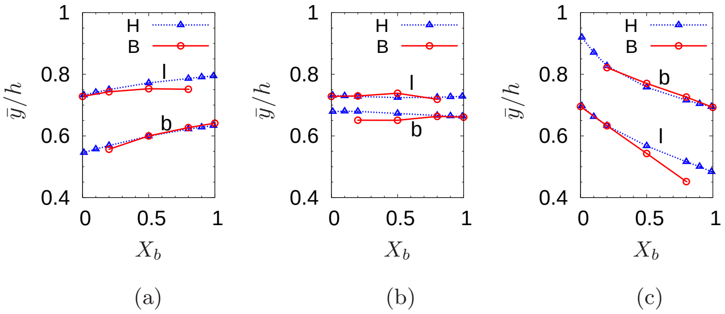
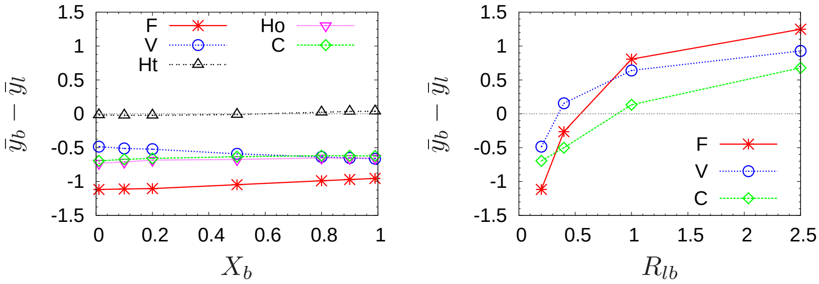


FIGURE 5. Mean normalized distance of a species $\bar{y}/h$ from the wall as function of X_b in HMC (H) and BI (B) methods in (a) $\mathrm{Ca}_l = 0.5$ and $\mathrm{Ca}_b = 0.1$ mixture (b) $\mathrm{Ca}_l = 0.5$ and $\mathrm{Ca}_b = 0.2$ mixture, and (c)$\mathrm{Ca}_l = 0.2$ and $\mathrm{Ca}_b = 0.5$ mixture. In all cases $S = 0.8$, ϕ_b^0 and $a/h = 0.197$.

particle, as a result of which the difference between Δ^{bl} and Δ^{lb} is expected to decrease due to the effect of rigidity on the cross-stream displacement in heterogeneous collisions. This is indeed confirmed by the data in Fig. 4, which shows that Δ^{bl} and Δ^{lb} are very close in this case. In fact, for $\delta \gtrsim 2a$, $\Delta^{lb} < \Delta^{bl}$. Thus, in the present case, the relative values of Δ in various types of pair collisions satisfies: $\Delta^{ll} < \Delta^{bl}, \Delta^{lb} < \Delta^{bb}$, i.e. the cross-stream displacement in heterogeneous collisions of both particle types lie in between the cross-stream displacements in the two types of homogeneous collisions.

1.3. *Hydrodynamic Monte Carlo simulations*

For this section, we consider suspensions with $S = 0.8$, $a/h = 0.197$, and $\phi_b^0 = 0.08$. We examined this system in the main paper for $\mathrm{Ca}_l = 0.5$ and $\mathrm{Ca}_b = 0.5$, which yielded the following HMC parameters: $n_l^{0a} = 0.029a^{-2}$, $n_b^{0a} = 0.048a^{-2}$, and $\xi = 0.3$. With no further adjustment of these parameters, we predict $\bar{y}$ in suspensions with different $(\mathrm{Ca}_l, \mathrm{Ca}_b)$ of (0.5,0.1), (0.5,0.2) and (0.2,0.5) for a range of X_b in Figs. 5(a), 5(b), and 5(c), respectively. Good agreement is observed, though the discrepancy between the two results is generally greater here than was in cases where only one of S or R_{lb} differed from unity (see main paper).



(a) $\Delta\bar{y}$ vs. X_b (b) $\Delta\bar{y}$ vs. R_{lb}

FIGURE 6. (a) $\Delta\bar{y}$ as a function of X_b due to various sources of particle motion in mixtures with $\text{Ca}_l = 0.5$, $\text{Ca}_b = 0.1$, $S = 0.8$, $a/h = 0.197$, and $\phi_b^0 = 0.12$. See Tb. 2 in the main paper for specifics of various control simulations. (b) $\Delta\bar{y}$ as a function of R_{lb} for suspensions with $S = 0.8$, $a/h = 0.197$, $\phi_b^0 = 0.12$, and $X_b = 0.01$. The four data points from left to right respectively correspond to $(\text{Ca}_l, \text{Ca}_b)$ of (0.5,0.1), (0.5,0.2), (0.5,0.5) and (0.2,0.5).

2. Mechanisms of segregation at $S \neq 1$ and $R_{lb} \neq 1$

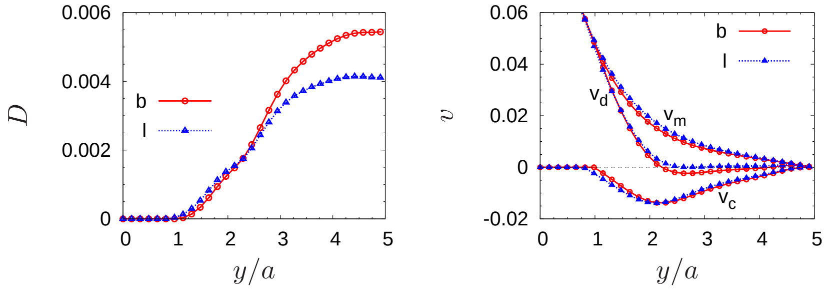
2.1. *Control HMC simulations*

We now turn to control HMC simulations as described in detail in the main article to disentangle the effects of wall-induced migration and pair collisions on the segregation behavior. The binary suspension considered here has the following parameters: $\phi_b^0 = 0.12$, $S = 0.8$, $\text{Ca}_l = 0.5$, and $\text{Ca}_b = 0.1$, such that $R_{lb} = 0.2$. Figure 6(a) shows $\Delta\bar{y} = \bar{y}_b - \bar{y}_l$ as a function of X_b for this suspension in various control HMC simulations. The contribution from heterogeneous collisions is very close to zero, while the contribution from homogeneous collisions is negative. The overall contribution from collisions is consequently negative, suggesting that differential particle displacement in collisions leads to the margination of big particles – this contribution is a significant fraction of the overall segregation from the full model. At equal rigidity ($R_{lb} = 1$), we showed that the collisions do not result in any significant segregation. Thus, the segregation due to collisions here is primarily due to the effect of rigidity differences between the species. In particular, in the present case, the big particles are also stiffer and due to the latter they displace more in heterogeneous collisions ($\Delta^{bl} > \Delta^{ll}$), which leads to their margination. The contribution from wall-induced migration is also negative and its magnitude is comparable to the contribution from collisions. Hence the margination of big particles here results both due to differential wall-induced migration of the species as well their differential displacements in various types of collisions.

It will also be interesting to examine the variation of various contributions to $\Delta\bar{y}$ as a function of R_{lb}. This is shown in Fig. 6(b) for suspensions that are dilute in big particles ($X_b = 0.01$). Some other parameters in these set of runs are $\phi_b^0 = 0.12$, $S = 0.8$, while the specific choices of Ca_l and Ca_b are noted in the figure caption. For clarity, the figure only shows the effect of the full model, wall-induced migration and collisions. It is evident that $\Delta\bar{y}$ is an increasing function of R_{lb} in all three cases. Moreover, in all three cases, $\Delta\bar{y}$ intersects the x-axis (i.e. $\Delta\bar{y} = 0$). In the case of collisions, $\Delta\bar{y}$ is zero at $R_{lb} \approx 1$. This should be expected given the results at $R_{lb} = 1$ discussed in the main paper. The contribution from the wall-induced migration is zero at $R_{lb} \approx 0.4$, i.e., when the big particles become sufficiently stiffer than the small particles. The segregation from the full model is zero between the above two values of R_{lb} − in the present case it is $R_{lb} \approx 0.6$. Over the entire range of R_{lb} explored here, the contributions from the wall-induced migration and collisions are comparable in magnitude and are usually of the same sign. Thus, on the whole, it appears that the margination of big or the small particles (as the case may be) results both due to differential particle dynamics in pair collisions as well as due to differential wall-induced migration.

2.2. *Fokker-Planck model*

For this section, we consider the same system as in Sec. 2.1 with parameters $\phi_b^0 = 0.12$, $\mathrm{Ca}_l = 0.5$, $\mathrm{Ca}_b = 0.1$, and $S = 0.8$. Further, we focus on a suspension that is dilute in big particles with $X_b = 0.01$. The self-diffusivities for both species in this case are



(a) self-diffusion (b) drift

FIGURE 7. (a) Self-diffusivity and (b) drift due to various sources for both the big and small particles. The system parameters are $\mathrm{Ca}_l = 0.5$, $\mathrm{Ca}_b = 0.1$, $\phi_b^0 = 0.12$, $X_b = 0.01$, $S = 0.8$ and $a/h = 0.197$.

shown in Fig. 7(a). It is larger for the big particles than for the smaller ones in the region around the centerline, though they are nearly equal in the region closer to the wall. This is a reversal from the trends at $R_{lb} = 1$ where the small particles had the higher self-diffusivity. This reversal arises here because the small value of R_{lb} here corresponds to large stiff particles, which displace substantially in heterogeneous collisions due to their high rigidity.

The overall drift velocity as well as the contributions from various sources are shown in Fig. 7(b) for both species. The contribution from the wall-induced migration v_m is higher for the smaller particle. The contribution from collisions v_c is approximately the same for both species (v_c was more negative for smaller particles at $R_{lb} = 1$). As a result, the overall drift velocity v_d of the bigger particles is smaller than that of the smaller particles. Additionally, the drift velocity of the big particles is negative over a range of the channel height, while the drift velocity of the small particles is positive throughout the channel, though it is close to zero over a part of the channel.

Finally, Fig. 8 shows the particle distribution functions P_1 and P_2, which are defined in the main paper, for both the small and the big particles in the above suspension. In this case, the effect of both P_1 and P_2 is identical as they both lead to the margination

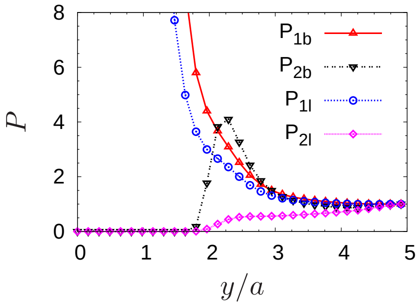


FIGURE 8. The particle distributions P_1 and P_2 in the Fokker-Planck model for both the big (b) and the small (l) particles. The system parameters are $\mathrm{Ca}_l = 0.5$, $\mathrm{Ca}_b = 0.1$, $\phi_b^0 = 0.12$, $X_b = 0.01$, $S = 0.8$, and $a/h = 0.197$.

of the big particles. In particular the peak in P_2 for the big particles in the near wall region is apparent, and occurs due to the negative drift velocity of the big particles in this region.