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# Closure Relations of Non-Uniform Suspensions

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**Abstract** The mixture stress of non-uniform suspensions is expressed by the symmetric part and the anti-symmetric parts with the pseudo and the real vectors. The closure relations for the three components of the stress are derived from the basic criteria such as Galilean invariance and parity. By the numerical simulations of many particles under the Stokes approximation with the non-uniform ensemble averaging technique and the systematic parameterizations, the closure coefficients including the effective viscosity are determined in the large system limit. The resultant closure relations are valid not only for the specific problem but for force, torque, and shear problems, and, as a result, for arbitrary flows generated by the linear combination of the three problems, because of the linearity of the Stokes approximation.

## 1 Introduction

One of the most important problems of suspensions is to derive the governing equation from the detailed many-body dynamics. The present work takes into account non-uniformity systematically, and derives the constitutive relation of the mixture stress from detailed numerical simulations of particles [6, 4].

Using numerical simulations of many particles under the Stokes approximation [7], we solve three types of problems – force, torque, and shear problems – under the periodic boundary condition. From the simulations, we can evaluate any quantities, such as translational and angular velocities of particle, mixture velocity, and viscous stress [8].

It is found [3] that there are couplings among three problems for non-uniform suspensions, while they are independent for uniform suspensions. In fact, for uniform suspensions, the slip velocity between the particles and the mixture is non-zero only in the sedimentation problem, the slip angular velocity is non-zero only in the torque problem, and the strain of the mixture is non-zero only in the shear problem. Therefore, the non-uniformity is important to capture the *general* behavior for arbitrary situations, which can be formed by a linear combination of the three problems from the linearity of the Stokes approximation.

For this aim, we first formulate a non-uniform ensemble averaging technique [5, 3] in §2. To compile various components of the non-uniform average for various quantities in various problems, parameterizations for arbitrary vectors, pseudo vectors, and symmetric traceless tensors are introduced in §3. In terms of the results of the non-uniform averages shown in §4, we determine the closure relations for the mixture stress of non-uniform suspensions in §5.

## 2 Non-uniform ensemble

In this section, we demonstrate how to evaluate ensemble averages for a non-uniform suspension on the basis of a statistically uniform ensemble of random arrangements of particles inside the fundamental cell, thus avoiding the generation of an actual non-uniform ensemble. The problems are solved in the fundamental cell with periodicity boundary conditions.

### 2.1 Universal ensemble

For the non-uniform ensemble averaging, we prepare "*universal ensembles*" consisting of random hard-sphere configurations for the particle volume fraction $\phi$ between 1 and 50% and the number of particles $N_p$ between 10 and 160. The number of configurations $N_c$ in each ensemble are between 256 and 2048. The statistical errors in the ensemble averages decrease rather slowly as $1/\sqrt{N_c}$.

In principle, this ensemble contains all possible configurations, uniform as well as non-uniform. If an equal probability weight is assigned to each configuration, the resulting ensemble averages will correspond to a homogeneous system. However, by giving the configurations unequal weights, this same ensemble can generate a spatially non-uniform system. It is for this reason that we refer to the ensemble thus constructed as "*universal*."

### 2.2 Uniform and non-uniform averages

Each realization $\mathcal{C}_i$ of the ensemble consists of a set of vectors $\mathbf{x}_i^1, \mathbf{x}_i^2, \cdots, \mathbf{x}_i^{N_p}$ denoting the position of the center of particle $1, 2, \cdots, N_p$. Given a generic quantity $A(\mathcal{C}_i)$ pertaining to the $i$-th realization of an ensemble of $N_c$ configurations $\{\mathcal{C}_1, \ldots, \mathcal{C}_{N_c}\}$, we define its average by

$$\langle A \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} \mathcal{W}(\mathcal{C}_i)\; A(\mathcal{C}_i), \tag{1}$$

where the $\mathcal{W}(\mathcal{C}_i)$'s are suitable weights. Clearly, when all the weights are taken equal to 1, we have the uniform-ensemble average, denoted by the index 0:

$$\langle A \rangle_0 = \frac{1}{N_c} \sum_{i=1}^{N_c} A(\mathcal{C}_i). \tag{2}$$

To generate weights for the non-uniform ensemble, we introduce a function $w(\mathbf{x})$, and assign to the $i$-th realization $\mathcal{C}_i$ the weight $\mathcal{W}(\mathcal{C}_i)$ defined by

$$\mathcal{W}(\mathcal{C}_i) = \frac{1}{N_p} \sum_{\alpha=1}^{N_p} w(\mathbf{x}_i^\alpha) = \frac{1}{N_p} \int d\mathbf{x}\; w(\mathbf{x}) n_i(\mathbf{x}) = \frac{1}{n_0} \sum_{\mathbf{k}} \tilde{w}(\mathbf{k})\; \tilde{n}_i(-\mathbf{k}), \tag{3}$$

where $n_i(\mathbf{x})$ is the number density for the realization $\mathcal{C}_i$ defined by

$$n_i(\mathbf{x}) = \sum_{\alpha=1}^{N_p} \delta\left(\mathbf{x} - \mathbf{x}_i^\alpha\right), \tag{4}$$

$\tilde{n}_i(\mathbf{k})$ is the Fourier coefficient given by

$$\tilde{n}_i(\mathbf{k}) = \frac{1}{V} \int d\mathbf{x}\; e^{i\mathbf{k}\cdot\mathbf{x}} n_i(\mathbf{x}) = \frac{1}{V} \sum_{\alpha=1}^{N_p} e^{i\mathbf{k}\cdot\mathbf{x}_i^\alpha}, \tag{5}$$

$n_0 = N_p/V$, and $V = L^3$ is the volume of the fundamental cell. The relation between the function $w(\mathbf{x})$ and the spatial structure of the ensemble is readily found by calculating the average number density with the above-defined weights [3] as

$$\tilde{w}(\mathbf{k} = \mathbf{0}) = 1, \qquad \tilde{w}(\mathbf{k} \neq \mathbf{0}) = \frac{V}{S(\mathbf{k})} \tilde{n}(\mathbf{k}), \tag{6}$$

where $\tilde{n}(\mathbf{k})$ is the Fourier coefficient of the *prescribed* number density, and $S(\mathbf{k})$ is the structure factor.

### 2.3 Field and particle quantities

In this method, formulations and calculations are done in the Fourier space. For a generic field quantity $A(\mathbf{x})$, we expand it in a Fourier series as

$$A(\mathbf{x}) = \tilde{A}(\mathbf{0}) + \sum_{\mathbf{k}>0} \left\{ \tilde{A}^c(\mathbf{k}) \cos(\mathbf{k}\cdot\mathbf{x}) + \tilde{A}^s(\mathbf{k}) \sin(\mathbf{k}\cdot\mathbf{x}) \right\}, \tag{7}$$

where the symbol $\mathbf{k} > 0$ appended to the summation restricts it to wave numbers all the components of which are positive, and $\tilde{A}^c(\mathbf{k})$ and $\tilde{A}^s(\mathbf{k})$ are defined by

$$\tilde{A}^c(\mathbf{k}) = \frac{2}{V}\int d\mathbf{x}\, A(\mathbf{x}) \cos(\mathbf{k}\cdot\mathbf{x}), \qquad \tilde{A}^s(\mathbf{k}) = \frac{2}{V}\int d\mathbf{x}\, A(\mathbf{x}) \sin(\mathbf{k}\cdot\mathbf{x}). \tag{8}$$

In addition to field variables, the averages of quantities $A^\alpha$ carried by each particle $\alpha$, such as the translational and angular velocity, are of interest. To calculate these averages, we first transform $A^\alpha$ to a field variable by writing

$$A(\mathbf{x}) = \sum_{\alpha=1}^{N_p} \delta(\mathbf{x} - \mathbf{x}^\alpha) A^\alpha, \tag{9}$$

and then, the Fourier coefficients are given by

$$\tilde{A}^c(\mathbf{k}) = \frac{2}{V}\sum_{\alpha=1}^{N_p} A^\alpha \cos(\mathbf{k}\cdot\mathbf{x}^\alpha), \qquad \tilde{A}^s(\mathbf{k}) = \frac{2}{V}\sum_{\alpha=1}^{N_p} A^\alpha \sin(\mathbf{k}\cdot\mathbf{x}^\alpha). \tag{10}$$

After this step, the particle average is calculated, in terms of the proper normalization, as

$$\langle A\rangle^P(\mathbf{x}) = \frac{\langle A\rangle(\mathbf{x})}{\langle n\rangle(\mathbf{x})}. \tag{11}$$

In the formulation, we can treat in a unified way both field and particle quantities through their Fourier coefficients $\tilde{A}(\mathbf{k})$.

### 2.4 Linear sinusoidal non-uniformity

In the present study, we limit ourselves to a non-uniform suspension with a weak spatial non-uniformity specified by the number density

$$n(\mathbf{x}) = n_0 (1 + \epsilon \sin(\mathbf{k}\cdot\mathbf{x})), \tag{12}$$

where $\epsilon$ is a small parameter denoting the degree of non-uniformity, and we present results valid to the first order in this quantity. We take $|\mathbf{k}|$ equal to the smallest wave number as

$$ka = \frac{2\pi a}{L} = \left(\frac{6\pi^2\phi}{N_p}\right)^{1/3}, \tag{13}$$

where $a$ is the particle radius. With this choice of $n(\mathbf{x})$, all the weight coefficients vanish except

$$\tilde{w}(\mathbf{0}) = 1, \quad \tilde{w}^s(\mathbf{k}) = \epsilon n_0 \frac{V}{S(\mathbf{k})}, \tag{14}$$

where $\tilde{w}^s$ is $\sin$ coefficient of $w(\mathbf{x})$. Therefore, the non-uniform ensemble average of a the Fourier coefficients $\tilde{A}$ becomes

$$\langle\tilde{A}\rangle = \langle\tilde{A}\rangle_0 + \epsilon\langle\tilde{A}\rangle_s, \tag{15}$$

where the non-uniform part $\langle \tilde{A} \rangle_s$ is given by

$$\langle \tilde{A} \rangle_s = \frac{1}{2} \frac{V}{S(k)} \langle \tilde{n}^s(\mathbf{k})\, \tilde{A} \rangle_0, \tag{16}$$

with, on the basis of (5),

$$\tilde{n}^s(\mathbf{k}) = \frac{2}{V} \sum_{\alpha=1}^{N_p} \sin\left(\mathbf{k} \cdot \mathbf{x}^\alpha\right). \tag{17}$$

The ensemble average of the Fourier expansion (7) therefore takes the form

$$\langle A \rangle(\mathbf{x}) = \langle \tilde{A}(\mathbf{0}) \rangle_0 + \epsilon \left[ \langle \tilde{A}^c(\mathbf{k}) \rangle_s \cos\left(\mathbf{k} \cdot \mathbf{x}\right) + \langle \tilde{A}^s(\mathbf{k}) \rangle_s \sin\left(\mathbf{k} \cdot \mathbf{x}\right) \right], \tag{18}$$

since all other coeffi cients vanish, and for particle averages, (11) gives, up to $O(\epsilon)$,

$$\langle A \rangle^P(\mathbf{x}) = \frac{1}{n_0} \left\{ \langle \tilde{A}(\mathbf{0}) \rangle_0 + \epsilon \left[ \langle \tilde{A}^c(\mathbf{k}) \rangle_s \cos\left(\mathbf{k} \cdot \mathbf{x}\right) + \left( \langle \tilde{A}^s(\mathbf{k}) \rangle_s - \langle \tilde{A}(\mathbf{0}) \rangle_0 \right) \sin\left(\mathbf{k} \cdot \mathbf{x}\right) \right] \right\}. \tag{19}$$

# 3 Parameterization

To study the general behavior of suspensions, it is useful to present the results using a suitable parameterization. We study three kinds of mobility problems for non-uniform suspensions – force, torque, and shear problems.

## 3.1 Force problem

For the force problem, i.e., sedimentation, we conduct numerical simulations where the same force $\mathbf{F}_0$ is applied to each particle. The uniform version of this problem is therefore characterized by a single fundamental vector

$$\mathbf{W}_F = \frac{\mathbf{F}_0}{6\pi\mu a} \tag{20}$$

with $\mu$ the fluid viscosity, and, therefore, any vectorial dependent variable $\mathbf{p}$, such as the mean settling velocity, must take the form

$$\langle \mathbf{p} \rangle = [p]_F^0\, \mathbf{W}_F, \tag{21}$$

where $[p]_F^0$ is a coeffi cient calculated numerically by taking the ensemble average of the values of $\mathbf{p}$.

When we turn to the non-uniform case, in addition to $\mathbf{W}_F$, also the wave vector $\mathbf{k}$ specifying the direction of the non-uniformity in (12) is introduced. Therefore, it must be possible to parameterize the non-uniform part of each vectorial dependent variable as

$$\langle \mathbf{p} \rangle = [p]_F^{\parallel}\, \mathbf{W}_F^{\parallel} + [p]_F^{\perp}\, \mathbf{W}_F^{\perp}, \tag{22}$$

where the superscripts $\parallel$ and $\perp$ are based on the direction of the unit wave vector $\hat{\mathbf{k}}$ and

$$\mathbf{W}_F^{\parallel} = \left( \hat{\mathbf{k}}\hat{\mathbf{k}} \right) \cdot \mathbf{W}_F, \qquad \mathbf{W}_F^{\perp} = \left( \mathsf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}} \right) \cdot \mathbf{W}_F. \tag{23}$$

Clearly, $\mathbf{W}_F = \mathbf{W}_F^{\parallel} + \mathbf{W}_F^{\perp}$. The only characteristic pseudo-vector is

$$a\omega_F^{\perp} \;=\; \hat{\mathbf{k}} \times \mathbf{W}_F, \tag{24}$$

which is perpendicular to $\mathbf{k}$; the factor $a$ is included so that $\omega_F^{\perp}$ has the dimensions of an angular velocity. Therefore, any pseudo vector $\mathbf{q}$ must be parameterized as

$$\langle \mathbf{q} \rangle = [q]_F^{\perp}\, \omega_F^{\perp}. \tag{25}$$

Note that $a\hat{\mathbf{k}} \times \omega_F^{\perp} = -\mathbf{W}_F^{\perp}$, and the parallel component $\omega_F^{\parallel}$ is zero.

### 3.2 Torque problem

In the second problem, we apply a constant torque $\mathbf{T}_0$ to each particle and use the subscript $T$ to denote the pertaining quantities. Here, for the uniform case, pseudo vectors must be parameterized as

$$\langle \mathbf{q} \rangle = [q]^0_T \, \omega_T, \tag{26}$$

with

$$\omega_T = \frac{\mathbf{T}_0}{8\pi\mu a^3}. \tag{27}$$

For the non-uniform case we have a single vector and two pseudo vectors:

$$\mathbf{W}^{\perp}_T = a\hat{\mathbf{k}} \times \omega_T, \qquad \omega^{\parallel}_T = \left(\hat{\mathbf{k}} \cdot \omega_T\right)\hat{\mathbf{k}}, \qquad \omega^{\perp}_T = \left(\mathsf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}}\right) \cdot \omega_T. \tag{28}$$

Note that $\hat{\mathbf{k}} \times \mathbf{W}^{\perp}_T = -a\omega^{\perp}_T$.

### 3.3 Shear problem

In the third problem, we apply a linear shear flow, so that, even in the uniform case, there is an imposed velocity field given by

$$\mathbf{u}^{\infty}(\mathbf{x}) \;\; = \;\; \mathsf{E}^{\infty} \cdot \mathbf{x}. \tag{29}$$

where $\mathsf{E}^{\infty}$ is the rate-of-strain tensor of the flow. The corresponding results will carry an index $E$. Because we cannot construct any vector or pseudo vector from $\mathsf{E}^{\infty}$ only, there cannot be any uniform contribution to vectors $\mathbf{a}$ or pseudo-vectors $\mathbf{b}$ for the shear problem. In the non-uniform case, one can construct two characteristic vectors and one characteristic pseudo vector:

$$\mathbf{W}^{\parallel}_E = a\left(\hat{\mathbf{k}}\hat{\mathbf{k}}\right) \cdot \left(\mathsf{E}^{\infty} \cdot \hat{\mathbf{k}}\right), \qquad \mathbf{W}^{\perp}_E = a\left(\mathsf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}}\right) \cdot \left(\mathsf{E}^{\infty} \cdot \hat{\mathbf{k}}\right), \qquad \omega^{\perp}_F = \hat{\mathbf{k}} \times \left(\mathsf{E}^{\infty} \cdot \hat{\mathbf{k}}\right). \tag{30}$$

Note that $a\hat{\mathbf{k}} \times \omega^{\perp}_E = -\mathbf{W}^{\perp}_E$.

### 3.4 Symmetric traceless tensor

For a quantity in the form of symmetric traceless tensor, such as deviatoric viscous stress, the similar parameterization is also expected. For uniform situations, we have only in the shear problem a symmetric traceless tensor $\mathsf{E}^{\infty}$, while for non-uniform situations, we also have two kinds of tensor for all problems:

$$\mathsf{G}^{\perp} = \mathbf{W}^{\perp}\hat{\mathbf{k}} + \hat{\mathbf{k}}\mathbf{W}^{\perp}, \qquad \mathsf{G}^{\parallel} = \frac{1}{2}\left(\mathbf{W}^{\parallel}\hat{\mathbf{k}} + \hat{\mathbf{k}}\mathbf{W}^{\parallel}\right) - \frac{1}{3}\left(\hat{\mathbf{k}} \cdot \mathbf{W}^{\parallel}\right)\mathsf{I}, \tag{31}$$

where each vector $\mathbf{W}$ carries the appropriate index $F, T$, or $E$.

### 3.5 Summary

Because of the linearity of the Stokes flow, the results for these three problems can be superposed. Therefore, vectors $\langle \mathbf{p} \rangle$, pseudo-vectors $\langle \mathbf{q} \rangle$, and symmetric traceless tensors $\langle \mathsf{s} \rangle$ are generally parameterized as

$$\begin{aligned}
\langle \mathbf{p} \rangle &= [p]^0_F \, \mathbf{W}_F + [p]^{\parallel}_F \, \mathbf{W}^{\parallel}_F + [p]^{\perp}_F \, \mathbf{W}^{\perp}_F + [p]^{\perp}_T \, \mathbf{W}^{\perp}_T + [p]^{\parallel}_E \, \mathbf{W}^{\parallel}_E + [p]^{\perp}_E \, \mathbf{W}^{\perp}_E, && (32)\\
\langle \mathbf{q} \rangle &= [q]^0_T \, \omega_T + [q]^{\parallel}_T \, \omega^{\parallel}_T + [q]^{\perp}_T \, \omega^{\perp}_T + [q]^{\perp}_F \, \omega^{\perp}_F + [q]^{\perp}_E \, \omega^{\perp}_E, && (33)\\
\langle \mathsf{s} \rangle &= [s]^0_E \, \mathsf{E}^{\infty} + [s]^E_E \, \mathsf{E}^{\infty} + [s]^{\parallel}_E \, \mathsf{G}^{\parallel}_E + [s]^{\perp}_E \, \mathsf{G}^{\perp}_E + [s]^{\parallel}_F \, \mathsf{G}^{\parallel}_F + [s]^{\perp}_F \, \mathsf{G}^{\perp}_F + [s]^{\perp}_T \, \mathsf{G}^{\perp}_T. && (34)
\end{aligned}$$

The coefficients in the averages denoted by [ ] in the above parameterizations are the building blocks of the present analysis of non-uniform suspensions.

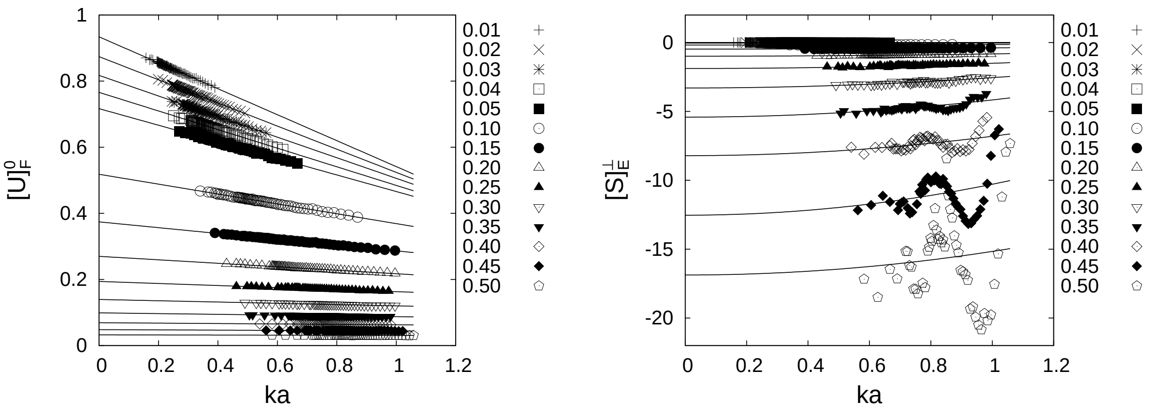



Figure 1: $(ka, \phi)$-dependence of the averages $[U]_F^0$ and $[S]_E^\perp$. The points are the numerically calculated ensemble averages and the lines least-squares fits.

# 4 Averages

## 4.1 Particle translational and angular velocities

The particle velocity $\mathbf{U}$ is a vector, and parameterized as

$$\begin{aligned} \langle \mathbf{U} - \mathbf{U}^\infty \rangle^P(\mathbf{x}) &= [U]_F^0 \, \mathbf{W}_F + \epsilon \sin(\mathbf{k}\cdot\mathbf{x}) \left( [U]_F^\parallel \, \mathbf{W}_F^\parallel + [U]_F^\perp \, \mathbf{W}_F^\perp \right) \\ &+ \epsilon \cos(\mathbf{k}\cdot\mathbf{x}) \, [U]_T^\perp \, \mathbf{W}_T^\perp + \epsilon \cos(\mathbf{k}\cdot\mathbf{x}) \left( [U]_E^\parallel \, \mathbf{W}_E^\parallel + [U]_E^\perp \, \mathbf{W}_E^\perp \right). \end{aligned} \tag{35}$$

The components of the non-uniform average $[U]$'s depend on the number of particles and the size of the fundamental cell $(N_p, L)$, or equivalently, the wave number and the volume fraction $(ka, \phi)$. Because the $k$-dependence partially has the effect of the system size, our interest is rather in the $\phi$-dependence. Therefore, we first fit the averages by the simple combination of powers of $ka$, and obtain the fitting coefficients depending on $\phi$. For $[U]_F^0$, we have the $k$-fitting

$$[U]_F^0 \, (ka, \phi) = A^{[U]_F^0} + (ka) B^{[U]_F^0}, \tag{36}$$

where $A$ and $B$ are obtained by the least square method (See Fig. 1). The constant term $A^{[U]_F^0}$ is the hindrance function for sedimentation, $U(\phi)$:

$$A^{[U]_F^0} = \lim_{k\to 0} [U]_F^0 = U(\phi). \tag{37}$$

Therefore, $A^{[U]_F^0}$ is the sedimentation velocity extrapolated to infinite cell size. Figure 2 shows $U(\phi)$. Note that our numerical results are the solutions of the many-body problems including multipoles only up to the fifth order.

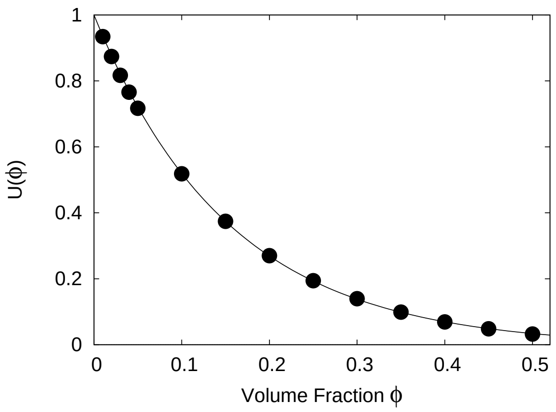
Similarly, for the particle angular velocity $\mathbf{\Omega}$, we have

$$\begin{aligned} \langle \mathbf{\Omega} - \mathbf{\Omega}^\infty \rangle^P(\mathbf{x}) &= [\Omega]_T^0 \, \mathbf{W}_T + \epsilon \cos(\mathbf{k}\cdot\mathbf{x}) \, [\Omega]_F^\perp \, \omega_F^\perp \\ &+ \epsilon \sin(\mathbf{k}\cdot\mathbf{x}) \left( [\Omega]_T^\parallel \, \omega_T^\parallel + [\Omega]_T^\perp \, \omega_T^\perp \right) + \epsilon \sin(\mathbf{k}\cdot\mathbf{x}) \, [\Omega]_E^\perp \, \omega_E^\perp. \end{aligned} \tag{38}$$

For fixed $\phi$, the uniform part of the particle angular velocity has essentially no $k$ dependence and is well fitted by a constant:

$$[\Omega]_T^0 \, (k, \phi) = A^{[\Omega]_T^0} = \Omega(\phi), \tag{39}$$

where $\Omega(\phi)$ is the hindrance function for the torque problem (See Fig. 2).



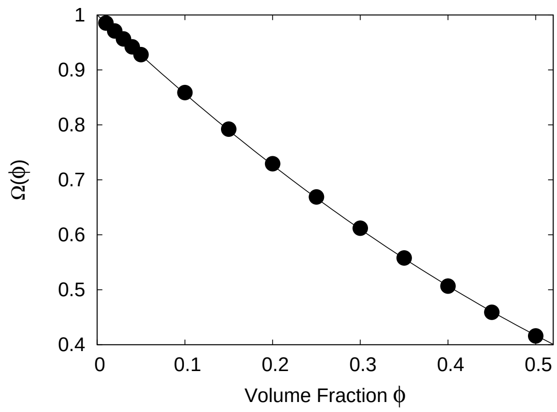




Figure 2: Hindrance functions for sedimentation $U(\phi)$ and rotation $\Omega(\phi)$.

### 4.2 Mixture velocity

The mixture velocity $\mathbf{u}_m$, in other words, the volumetric flux is also important quantity. Since the mixture is incompressible as a whole,

$$\nabla \cdot \mathbf{u}_m = 0. \tag{40}$$

Therefore, all parallel components vanish and it is parameterized as

$$\langle \mathbf{u}_m - \mathbf{u}^\infty \rangle(\mathbf{x}) = \epsilon \sin(\mathbf{k}\cdot\mathbf{x})\,[u_m]_F^\perp\,\mathbf{W}_F^\perp + \epsilon\cos(\mathbf{k}\cdot\mathbf{x})\,[u_m]_T^\perp\,\mathbf{W}_T^\perp + \epsilon\cos(\mathbf{k}\cdot\mathbf{x})\,[u_m]_E^\perp\,\mathbf{W}_E^\perp. \tag{41}$$

The angular velocity of the mixture, $\mathbf{\Omega}_m$, is given by

$$\mathbf{\Omega}_m = \frac{1}{2}\nabla \times \mathbf{u}_m. \tag{42}$$

Therefore, all components in the parameterization are obtained by those of the mixture velocity $\mathbf{u}_m$.

### 4.3 Slip velocities

The translational slip velocity $\langle \mathbf{u}_\Delta \rangle$ is defined by

$$\langle \mathbf{u}_\Delta \rangle = \langle \mathbf{U} - \mathbf{U}^\infty \rangle^P - \langle \mathbf{u}_m - \mathbf{u}^\infty \rangle. \tag{43}$$

From the parameterizations (35) and (41), we have

$$\begin{aligned} \langle \mathbf{u}_\Delta \rangle(\mathbf{x}) &= [u_\Delta]_F^0\,\mathbf{W}_F + \epsilon\sin(\mathbf{k}\cdot\mathbf{x})\left([u_\Delta]_F^\parallel\,\mathbf{W}_F^\parallel + [u_\Delta]_F^\perp\,\mathbf{W}_F^\perp\right) \\ &+ \epsilon\cos(\mathbf{k}\cdot\mathbf{x})\,[u_\Delta]_T^\perp\,\mathbf{W}_T^\perp + \epsilon\cos(\mathbf{k}\cdot\mathbf{x})\left([u_\Delta]_E^\parallel\,\mathbf{W}_E^\parallel + [u_\Delta]_E^\perp\,\mathbf{W}_E^\perp\right). \end{aligned} \tag{44}$$

For the force problem, the slip velocity is characterized by the hindrance function $U(\phi)$ as

$$[u_\Delta]_F^0 = U(\phi), \qquad [u_\Delta]_F^\parallel = \phi\frac{\mathrm{d}U}{\mathrm{d}\phi}, \qquad [u_\Delta]_F^\perp + C(\phi)\,(ka)^2[u_m]_F^\perp = \phi\frac{\mathrm{d}U}{\mathrm{d}\phi}, \tag{45}$$

where $C$ is defined by

$$C(\phi) = \lim_{k\to 0}\frac{1}{(ka)^2\,[u_m]_F^\perp}\left([u_\Delta]_F^\parallel - [u_\Delta]_F^\perp\right). \tag{46}$$

Figure 3 shows $[u_\Delta]_F^\parallel$, $[u_\Delta]_F^\perp$, and $\phi\,(\mathrm{d}U/\mathrm{d}\phi)$, where the derivative of the hindrance function is evaluated by numerical differentiation of the results for $[u_\Delta]_F^0$. Difference between $[u_\Delta]_F^\parallel$ and $[u_\Delta]_F^\perp$ shows the existence of $C(\phi)$. Equation (45) suggests the Faxén-like relation

$$U(\phi)\frac{\mathbf{F}_0}{6\pi\mu a} = \langle \mathbf{u}_\Delta \rangle - C(\phi)\,a^2\nabla^2\langle \mathbf{u}_m \rangle. \tag{47}$$

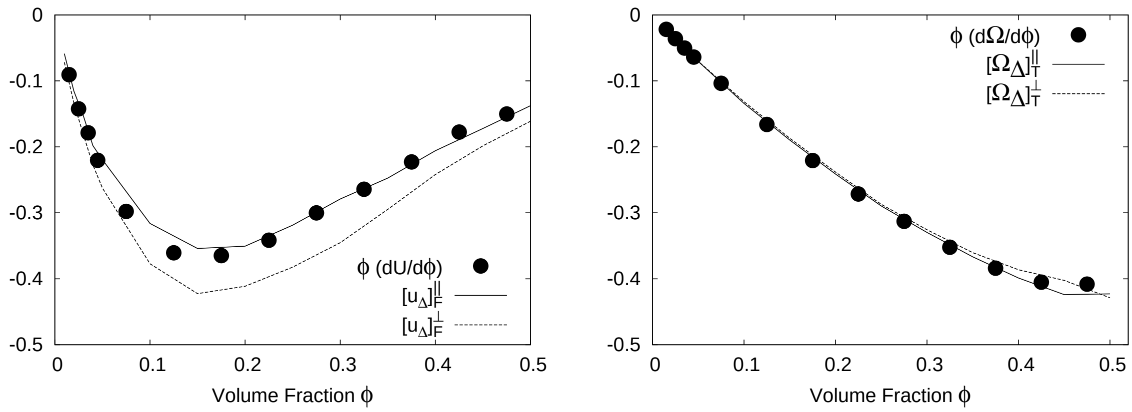



Figure 3: Comparison among $\phi\,(\mathrm{d}U/\mathrm{d}\phi)$, $[u_\Delta]_F^\parallel$, and $[u_\Delta]_F^\perp$, and that among $\phi\,(\mathrm{d}\Omega/\mathrm{d}\phi)$, $[\Omega_\Delta]_T^\parallel$, and $[\Omega_\Delta]_T^\perp$.

The slip angular velocity $\mathbf{\Omega}_\Delta$ is defined similarly by

$$\langle \mathbf{\Omega}_\Delta \rangle = \langle \mathbf{\Omega} - \mathbf{\Omega}^\infty \rangle^P - \langle \mathbf{\Omega}_m - \frac{1}{2}\nabla \times \mathbf{u}^\infty \rangle, \tag{48}$$

and parameterized as

$$\begin{aligned} \langle \mathbf{\Omega}_\Delta \rangle(\mathbf{x}) &= [\Omega_\Delta]_T^0\, \mathbf{W}_T + \epsilon \cos(\mathbf{k}\cdot\mathbf{x})\, [\Omega_\Delta]_F^\perp\, \omega_F^\perp \\ &+ \epsilon \sin(\mathbf{k}\cdot\mathbf{x}) \left( [\Omega_\Delta]_T^\parallel\, \omega_T^\parallel + [\Omega_\Delta]_T^\perp\, \omega_T^\perp \right) + \epsilon \sin(\mathbf{k}\cdot\mathbf{x})\, [\Omega_\Delta]_E^\perp\, \omega_E^\perp. \end{aligned} \tag{49}$$

For the torque problem, the slip angular velocity is characterized by $\Omega(\phi)$ as

$$[\Omega_\Delta]_T^0 = \Omega(\phi), \qquad [\Omega_\Delta]_T^\parallel = [\Omega_\Delta]_T^\perp = \phi \frac{\mathrm{d}\Omega}{\mathrm{d}\phi}, \tag{50}$$

as shown in Fig. 3. This implies that the local slip angular velocity is only dependent on the local value of the rotational hindrance function:

$$\Omega(\phi) \frac{\mathbf{T}_0}{8\pi\mu a^3} = \langle \mathbf{\Omega}_\Delta \rangle. \tag{51}$$

# 5 Closure relations

We will use as our starting point an expression for the particle stress $\mathbf{\Sigma}$ developed in Ref. [8], where the divergence of the stress can be written as

$$\nabla \cdot \mathbf{\Sigma} = \mu \left[ \nabla^2 \mathbf{u}_m + \nabla \cdot \mathsf{S} + \nabla \times (\mathbf{R} - \nabla \times \mathbf{V}) \right]. \tag{52}$$

Here $\mathsf{S}$ is a traceless symmetric two-tensor, $\mathbf{R}$ an axial vector, and $\mathbf{V}$ a polar vector. As shown in Ref. [8], the exact expressions of $\mathsf{S}$, $\mathbf{R}$, and $\mathbf{V}$ involve an infinite series of multipole coefficients. In this paper, we will limit our consideration up to the fifth order of the multipoles. We may also note that, in the dilute limit, it is possible to show that

$$\mathsf{S} = 5\phi \mathsf{E}_m, \tag{53}$$

$$\mathbf{R} = 3\phi \mathbf{\Omega}_\Delta, \tag{54}$$

$$\mathbf{V} = \frac{3}{10}\phi\, \mathbf{u}_\Delta + \frac{1}{7} a^2 \mathsf{E}_m \cdot \nabla\phi - \frac{11}{140}\phi a^2 \nabla^2 \mathbf{u}_m, \tag{55}$$

where $\mathsf{E}_m$ is the rate-of-strain tensor of the mixture defined by

$$\mathsf{E}_m = \frac{1}{2}\left[\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^\dagger\right]. \tag{56}$$

Equation (53) is the well-known Einstein viscosity correction.

### 5.1 The symmetric part of the stress

We assume that the contributions to the stress can be expressed in terms of the local particle volume fraction $\phi$, mixture velocity $\mathbf{u}_m$, the slip velocity $\mathbf{u}_\Delta$, and the slip angular velocity $\mathbf{\Omega}_\Delta$. Since $\mathsf{S}$ is a symmetric traceless tensor, if such a representation is possible, it must have the form

$$\mathsf{S} = 2\left(\mu_e - 1\right)\mathsf{E}_m + 2\mu_\Delta \mathsf{E}_\Delta + 2\mu_\nabla \mathsf{E}_\nabla + 2\mu_\Omega \mathsf{E}_\Omega + \cdots, \tag{57}$$

where $\mathsf{E}_\Delta$, $\mathsf{E}_\nabla$ and $\mathsf{E}_\Omega$ are defined respectively by

$$\begin{aligned}
\mathsf{E}_\Delta &= \frac{1}{2}\left[\nabla \mathbf{u}_\Delta + (\nabla \mathbf{u}_\Delta)^\dagger\right] - \frac{1}{3}\left(\nabla\cdot\mathbf{u}_\Delta\right)\mathsf{I}, && (58)\\
\mathsf{E}_\nabla &= \frac{1}{2}\left[\mathbf{u}_\Delta \nabla\phi + (\mathbf{u}_\Delta \nabla\phi)^\dagger\right] - \frac{1}{3}\left(\mathbf{u}_\Delta\cdot\nabla\phi\right)\mathsf{I}, && (59)\\
\mathsf{E}_\Omega &= \frac{1}{2}\left\{\left[\nabla\left(\nabla\times\mathbf{\Omega}_\Delta\right)\right] + \left[\nabla\left(\nabla\times\mathbf{\Omega}_\Delta\right)\right]^\dagger\right\}. && (60)
\end{aligned}$$

In (57), $\mu_e$ is the usual effective viscosity (normalized by the viscosity of the suspending fluid), while the other $\mu$'s are additional viscosity parameters.

The symmetric stress $\mathsf{S}$ can also be calculated from the results of the numerical simulations and the ensemble average is parameterized as

$$\begin{aligned}
\langle \mathsf{S}\rangle &= [S]_E^0 \mathsf{E}^\infty + \epsilon\sin\left(\mathbf{k}\cdot\mathbf{x}\right)\left([S]_E^E \mathsf{E}^\infty + [S]_E^\perp \mathsf{G}_E^\perp + [S]_E^\parallel \mathsf{G}_E^\parallel + [S]_T^\perp \mathsf{G}_T^\perp\right)\\
&+ \epsilon\cos\left(\mathbf{k}\cdot\mathbf{x}\right)\left([S]_F^\perp \mathsf{G}_F^\perp + [S]_F^\parallel \mathsf{G}_F^\parallel\right). && (61)
\end{aligned}$$

At this point, both sides of the closure relation (57) have the form of a linear combination of the tensors $\mathsf{E}^\infty$, $\mathsf{G}^\perp$, and $\mathsf{G}^\parallel$. Taking into account the $k$-dependences of averages, we only have the first term in (57) with the effective viscosity $\mu_e$, in the limit $k\to 0$, as

$$\mathsf{S} = 2\left(\mu_e - 1\right)\mathsf{E}_m, \tag{62}$$

and we find several expressions for the effective viscosity:

$$\begin{aligned}
\mu_e - 1 &= \lim_{k\to 0}\frac{[S]_E^0}{2}, && (63)\\
\frac{\mathrm{d}\mu_e}{\mathrm{d}\phi} &= \lim_{k\to 0}\frac{[S]_E^E}{2\phi}, && (64)\\
\mu_e - 1 &= -\lim_{k\to 0}\frac{[S]_E^\perp}{(ka)[u_m]_E^\perp},\quad -\lim_{k\to 0}\frac{[S]_T^\perp}{(ka)[u_m]_T^\perp},\ \text{and}\ \lim_{k\to 0}\frac{[S]_F^\perp}{(ka)[u_m]_F^\perp}. && (65)
\end{aligned}$$

In the dilute region $\phi \le 0.05$, $\mu_e$ is well fitted by

$$\mu_e = 1 + \frac{5}{2}\phi + 5.07\phi^2, \tag{66}$$

which is consistent with the existing theoretical results [1, 2].

An excellent consistency can indeed be observed in Fig. 4, which shows $\mu_e$ calculated from the uniform part of the shear problem (open squares), and from the non-uniform parts of the shear problem (open circles), of the torque problem (up-triangles), and of the force problem (down-triangles). A further consistency test is offered by comparing Eq. (64) for $d\mu_e/d\phi$ with the derivative calculated from the fitting. The observed consistencies imply that, $\mu_e$ is a robust quantity which has the same value in three very different physical situations, and for weak spatial non-uniformity as measured by $\epsilon$ in Eq.(12), the effective viscosity only depends on the local value of the volume fraction.

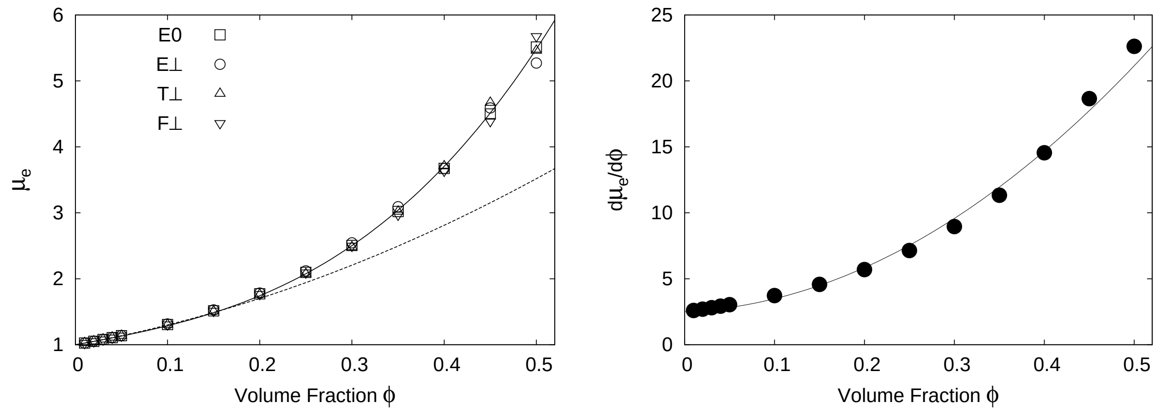



Figure 4: $\mu_e$ and $\mathrm{d}\mu_e/\mathrm{d}\phi$.

## 5.2 The axial vector of the antisymmetric stress

As in the case of the symmetric stress, the closure relation for the axial vector of the antisymmetric stress $\mathbf{R}$ is given by

$$\mathbf{R} \quad = \quad R_1 \boldsymbol{\Omega}_\Delta, \tag{67}$$

in the limit of $k \to 0$. From the parameterizations of $\mathbf{R}$ and $\boldsymbol{\Omega}_\Delta$, we have

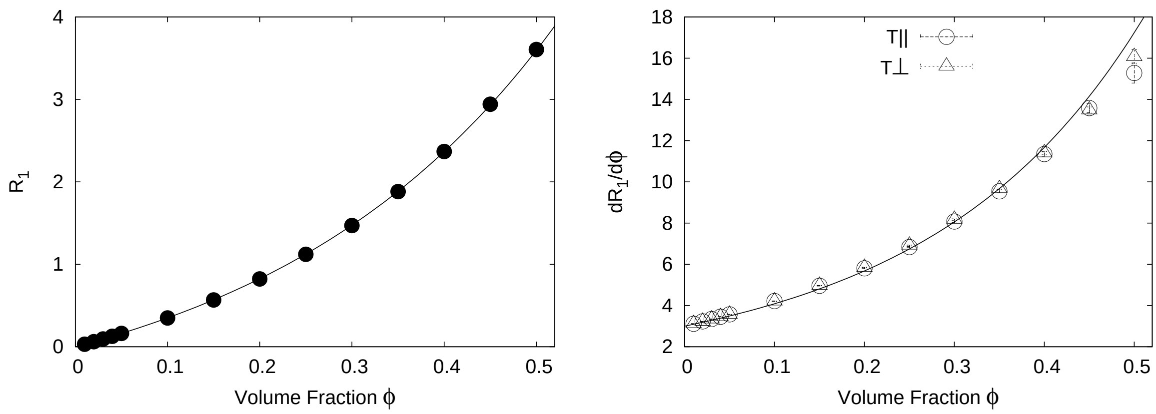



Figure 5: The coefficient $R_1$ and its derivative $\mathrm{d}R_1/\mathrm{d}\phi$.

$$R_1(\phi) \quad = \quad \lim_{k\to 0} \frac{[R]_T^0}{[\Omega_\Delta]_T^0} = \frac{3\phi}{\Omega(\phi)}, \tag{68}$$

$$\phi \frac{\mathrm{d}R_1}{\mathrm{d}\phi} \quad = \quad \lim_{k\to 0} \frac{1}{[\Omega_\Delta]_T^0} \left( [R]_T^{\parallel} - R_1 [\Omega_\Delta]_T^{\parallel} \right), \tag{69}$$

$$\phi \frac{\mathrm{d}R_1}{\mathrm{d}\phi} \quad = \quad \lim_{k\to 0} \frac{1}{[\Omega_\Delta]_T^0} \left( [R]_T^{\perp} - R_1 [\Omega_\Delta]_T^{\perp} \right). \tag{70}$$

Figure 5 shows $R_1$ from (68) and $\mathrm{d}R_1/\mathrm{d}\phi$ calculated from (69) and (70) with $R_1$ of (68). The results are consistent with themselves and with the dilute limit result (54).

### 5.3 The polar vector of the antisymmetric stress

We proceed in the same way for the polar vector of the antisymmetric stress, $\mathbf{V}$. By including all the terms with the correct parity and vectorial nature which contribute to leading order in $k$, we write

$$\mathbf{V} = V_1\mathbf{u}_\Delta + V_2 a^2 \mathsf{E}_m \cdot \nabla\phi + V_3 a^2 \nabla^2 \mathbf{u}_m + a^2 \nabla \times (V_\Omega \mathbf{\Omega}_\Delta) . \tag{71}$$

Solving the closure equation for the coeffi cients, we have

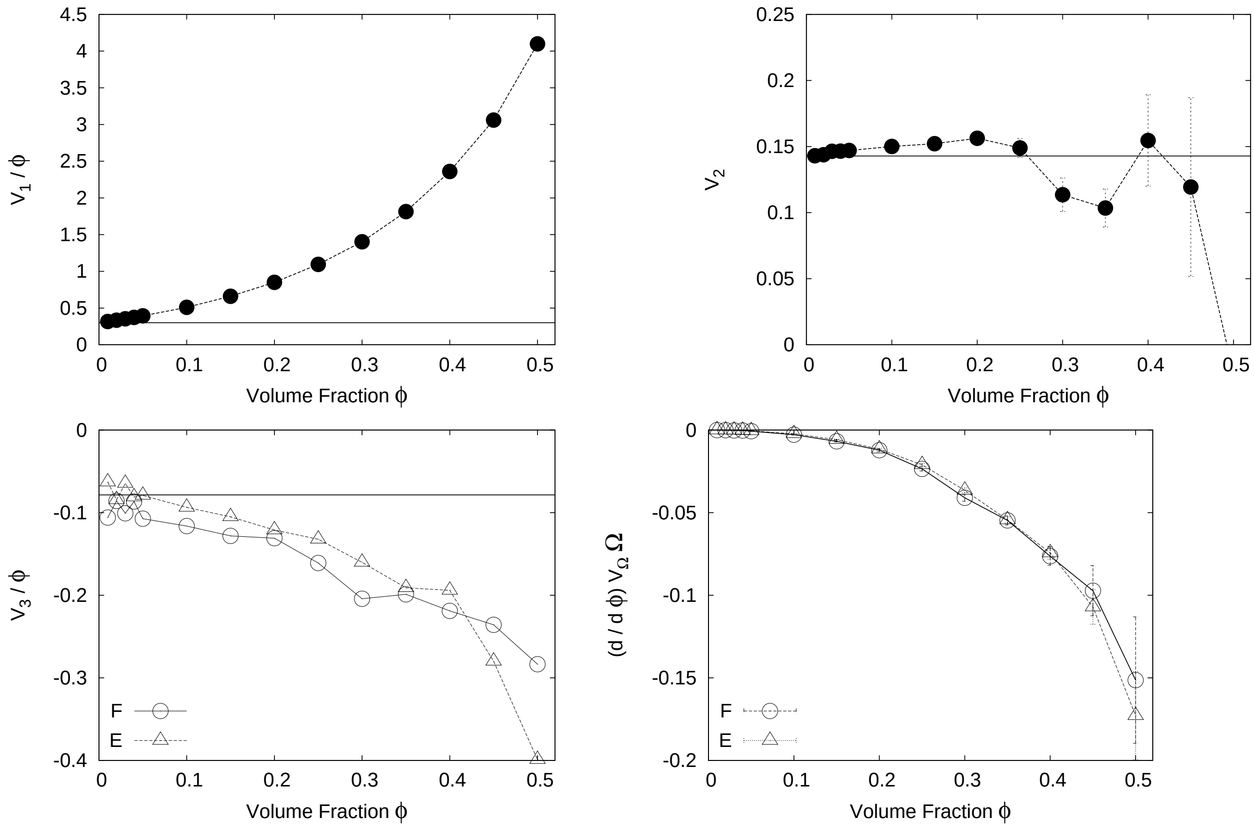



Figure 6: The closure coeffi cients of $\mathbf{V}$.

$$\begin{aligned}
V_1 &= \lim_{k\to 0} \frac{[V]_F^0}{[u_\Delta]_F^0}, & (72)\\
\phi\frac{\mathrm{d}V_1}{\mathrm{d}\phi} &= \lim_{k\to 0} \frac{1}{[u_\Delta]_F^0}\left([V]_F^{\parallel} - V_1[u_\Delta]_F^{\parallel}\right), & (73)\\
V_2(\phi) &= \lim_{k\to 0} \frac{1}{(ka)\phi}\left([V]_E^{\parallel} - V_1[u_\Delta]_E^{\parallel}\right), & (74)\\
V_3(\phi) &= -\lim_{k\to 0} \frac{1}{(ka)^2[u_m]_F^{\perp}}\left([V]_F^{\perp} - V_1[u_\Delta]_F^{\perp} - \phi\frac{\mathrm{d}V_1}{\mathrm{d}\phi}[u_\Delta]_F^0\right), & (75)\\
V_3(\phi) &= -\lim_{k\to 0} \frac{1}{(ka)^2[u_m]_E^{\perp}}\left([V]_E^{\perp} - V_1[u_\Delta]_E^{\perp} - V_2(ka)\phi\right), & (76)\\
\phi\frac{\mathrm{d}}{\mathrm{d}\phi}(V_\Omega\,\Omega) &= \lim_{k\to 0}\left([V]_T^{\perp} - V_1[u_\Delta]_T^{\perp} + V_3(ka)^2[u_m]_T^{\perp}\right). & (77)
\end{aligned}$$

The numerical results are shown in Fig. 6. We observe that the consistencies of $V_1$, $V_2$ and $V_3$ with the dilute limit result in (55), as well as the consistencies between two estimations for $V_3$ and $(\mathrm{d}/\mathrm{d}\phi)V_\Omega\,\Omega$.

# 6 Conclusions

We have developed a non-uniform ensemble averaging technique. Applying this technique for the linear sinusoidal non-uniformity in (12), the particle translational and rotational velocities $\mathbf{U}$ and $\mathbf{\Omega}$, the mixture velocity $\mathbf{u}_m$, the symmetric tensor and antisymmetric vectors of the mixture stress $\mathsf{S}$, $\mathbf{R}$, and $\mathbf{V}$ have been evaluated in the systematic parameterizations. Based on the general criteria, the closure relations of $\mathsf{S}$, $\mathbf{R}$, and $\mathbf{V}$ have been formed, and in the limit $k \to 0$, we have (62) for $\mathsf{S}$, (67) for $\mathbf{R}$, and (71) for $\mathbf{V}$. Using the non-uniform averages, the closure coefficients, such as the effective viscosity $\mu_e$, have been determined, and confirmed their consistency with the dilute limit results in (53), (54), and (55).

The results show that, in the limit $k \to 0$, the mixture stress $\mathbf{\Sigma}$ is written for arbitrary flows as

$$\frac{\mathbf{\Sigma}}{\mu} = 2\mu_e(\phi)\,\mathsf{E}_m + R_1(\phi)\,\varepsilon \cdot \mathbf{\Omega}_\Delta, \tag{78}$$

where $\varepsilon$ is the Levi-Civita (permutation) tensor.

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