

Nondimensionalization

seto

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Force balance equation

The following force balance equation is considered here;

$$\mathbf{F}_H + \mathbf{F}_R = 0. \quad (1)$$

The hydrodynamic interaction is assumed to be linear form of velocities.

$$\mathbf{F}_H = -\mathbf{R} \cdot \mathbf{U}. \quad (2)$$

Representative quantities

From shear rate

Particle radius is commonly considered as the representative length in our particle simulations:
 $L^* = a$.

One way to give the representative particle velocity in a sheared suspension is

$$U_H^* = a\dot{\gamma}. \quad (3)$$

The typical hydrodynamic force is given by the typical velocity U_H^* and Stokes-drag form;

$$F_H^* = 6\pi\eta_0 a U_H^*. \quad (4)$$

Here, we indicate nondimensionalized variables in the hydrodynamic unit by using ‘tilde’, i.e., $\tilde{\mathbf{F}}_H = F_H^* \mathbf{F}_H$, etc.

[note] F_H^* is a function of shear rate $\dot{\gamma}$. Thus, it is not constant in the stress controlled simulation, and zero if system is not sheared.

From repulsive force

The repulsive force \mathbf{F}_R is a function of particle-to-particle distance. We take the amplitude F_R^* to represent the typical strength:

$$\mathbf{F}_R = F_R^* \hat{\mathbf{F}}_R, \quad (5)$$

where ‘hat’ indicates nondimensionalized variables based on this repulsive force. The corresponding velocity can also be given via the Stokes-drag form;

$$U_R^* = \frac{F_R^*}{6\pi\eta_0 a}. \quad (6)$$

Hydrodynamic (or shear-rate) unit

In the hydrodynamic unit, the nondimensionalized force balance equation is

$$\frac{F_H}{F_H^*} + \frac{F_R}{F_R^*} = 0 \implies -\mathbf{R}' \cdot \tilde{\mathbf{U}} + \tilde{F}_R = 0 \quad (7)$$

where $\mathbf{R}' \equiv \mathbf{R}/6\pi\eta_0 a$.

In order to see the shear rate dependence, it is convenient to represent the typical repulsive force F_R^* .

$$-\tilde{\mathbf{R}} \cdot \tilde{\mathbf{U}} + \frac{1}{\alpha} \hat{F}_R = 0 \quad (8)$$

This α indicates the competition between two forces:

$$\alpha \equiv \frac{F_H^*}{F_R^*} = \frac{\dot{\gamma}}{F_R^*/6\pi\eta_0 a^2} \quad (9)$$

The unit of time is

$$t_H^* \equiv \frac{L^*}{U_H^*} = \frac{1}{\dot{\gamma}}. \quad (10)$$

Therefore, the nondimensional time \tilde{t} is shear strain (when shear rate is constant):

$$\tilde{t} \equiv \frac{t}{t_H^*} = t\dot{\gamma} = \gamma \quad (11)$$

The nondimensionalized shear rate is

$$\tilde{\dot{\gamma}} = \dot{\gamma} t_H^* = 1 \quad (12)$$

[note] We call this unit system “hydrodynamic”. But, the essential origin for this unit system is the way to give typical velocity, i.e., $U^* = a\dot{\gamma}$. “Simple shear” unit would be more proper name.

Repulsive force unit

In the repulsive unit, the nondimensionalized force balance equation is

$$\frac{F_H}{F_R^*} + \frac{F_R}{F_R^*} = 0 \implies -\mathbf{R}' \cdot \hat{\mathbf{U}} + \hat{F}_R = 0 \quad (13)$$

The time unit is

$$t_R^* \equiv \frac{L^*}{U_R^*} = \frac{6\pi\eta_0 a^2}{F_R^*}. \quad (14)$$

The nondimensionalized shear rate is

$$\hat{\gamma} = \dot{\gamma} t_R^* = \alpha. \quad (15)$$

In rate controlled simulations, the relation between the nondimensionalized time $\hat{t} \equiv t/t_R^*$ and shear strain is

$$\gamma \equiv \dot{\gamma} t = \dot{\gamma} t_R^* \hat{t} = \frac{F_H^*}{F_R^*} \hat{t} = \alpha \hat{t} \quad (16)$$

where α is defined in (9).

In stress controlled simulations, the strain is simply given by

$$\gamma = \int^t \dot{\gamma} dt = \int^{\hat{t}} \alpha d\hat{t}. \quad (17)$$

Simulation data

	Output	Output in H.U.	Calc in H.U.	Output in R.U.	Calc in R.U.
strain	γ	\tilde{t}		γ	
relative viscosity	η_r	$6\pi\tilde{\sigma}$		$6\pi\hat{\sigma}/\alpha$	
time	\hat{t}	\tilde{t}/α	\tilde{t}	\hat{t}	\hat{t}
shear rate	$\hat{\gamma}$	α	$\tilde{\gamma} = 1$	$\hat{\gamma}$	$\hat{\gamma}$
shear stress	$\hat{\sigma}$	$\alpha\tilde{\sigma}$	$\tilde{\sigma}$	$\hat{\sigma}$	$\hat{\sigma}$