Nondimentionalization

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Force balance equation

The following force balance equation is considered here;

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{R}} = 0. \tag{1}$$

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

$$\boldsymbol{F}_{\mathrm{H}} = -\boldsymbol{R} \cdot \boldsymbol{U}. \tag{2}$$

Representative quantities

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

From shear rate

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

$$U_{\mathrm{H}}^* = L^* \dot{\gamma}. \tag{3}$$

The typical hydrodynamic force is given by the typical velocity U_{H}^* and Stokes-drag form;

$$F_{\mathrm{H}}^* = 6\pi\eta_0 a U_{\mathrm{H}}^*. \tag{4}$$

Here, we indicate nondimensionalized variables in the hydrodynamic unit by using 'tilde', i.e., $\tilde{\boldsymbol{F}} = \boldsymbol{F}/F_{\mathrm{H}}^*$, etc.

[note] Since F_{H}^* is a function of shear rate $\dot{\gamma}$, it is not constant in stress controlled simulations and zero if system is not sheared.

From repulsive force

The repulsive force $\boldsymbol{F}_{\mathrm{R}}$ is a function of particle-to-particle distance. We take the amplitude F_{R}^* to represent its typical strength:

$$\boldsymbol{F}_{\mathrm{R}} = F_{\mathrm{R}}^* \hat{\boldsymbol{F}}_{\mathrm{R}}, \tag{5}$$

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

$$U_{\mathrm{R}}^* \equiv \frac{F_{\mathrm{R}}^*}{6\pi\eta_0 a}. \tag{6}$$

Hydrodynamic (or shear-rate) unit

In the hydrodynamic unit, the nondimensionalized force balance equation is

$$\frac{\boldsymbol{F}_{\mathrm{H}}}{F_{\mathrm{H}}^*} + \frac{\boldsymbol{F}_{\mathrm{R}}}{F_{\mathrm{H}}^*} = 0 \quad \Longrightarrow \quad -\boldsymbol{R}' \cdot \tilde{\boldsymbol{U}} + \tilde{\boldsymbol{F}}_{\mathrm{R}} = 0, \tag{7}$$

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

The origin of shear-rate dependence becomes clear if the repulsive force is expressed with the typical value F_{R}^*;

$$-\tilde{\boldsymbol{R}} \cdot \tilde{\boldsymbol{U}} + \frac{1}{\alpha}\hat{\boldsymbol{F}}_{\mathrm{R}} = 0. \tag{8}$$

This α indicates the competition between two representative forces:

$$\alpha \equiv \frac{\boldsymbol{F}_{\mathrm{H}}^*}{\boldsymbol{F}_{\mathrm{R}}^*} = \frac{\dot{\gamma}}{F_{\mathrm{R}}^*/6\pi\eta_0 a^2}. \tag{9}$$

The unit of time is

$$t_{\mathrm{H}}^* \equiv \frac{L^*}{U_{\mathrm{H}}^*} = \frac{1}{\dot{\gamma}}. \tag{10}$$

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

$$\tilde{t} \equiv \frac{t}{t_{\mathrm{H}}^*} = t\dot{\gamma} = \gamma. \tag{11}$$

The nondimensionalized shear rate is

$$\tilde{\dot{\gamma}} = \frac{\dot{\gamma}}{1/t_{\mathrm{H}}^*} = 1. \tag{12}$$

[note] We call this unit system "hydrodynamic". But, the essential origin for this unit system is the way to give typical velocity, i.e., $U^* = a\dot{\gamma}$. "Shear-rate" unit might be proper name.

Repulsive force unit

In the repulsive unit, the nondimensionalized force balance equation is

$$\frac{\boldsymbol{F}_{\mathrm{H}}}{F_{\mathrm{R}}^*} + \frac{\boldsymbol{F}_{\mathrm{R}}}{F_{\mathrm{R}}^*} = 0 \quad \Longrightarrow \quad -\boldsymbol{R}' \cdot \hat{\boldsymbol{U}} + \hat{\boldsymbol{F}}_{\mathrm{R}} = 0. \tag{13}$$

The time unit is

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

The nondimensionalized shear rate is

$$\hat{\dot{\gamma}} = \dot{\gamma} t_R^* = \alpha. \tag{15}$$

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

$$\gamma \equiv \dot{\gamma} t = \dot{\gamma} t_R^* \hat{t} = \frac{F_H^*}{F_R^*}\hat{t} = \alpha\hat{t}, \tag{16}$$

where α is defined in (9).

In stress controlled simulations, the strain is simply given by

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

Simulation data

In both ways of nondimensionalization, we can unify the output data with ones nondimensionalized by repulsive force.

	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	$\hat{t}$	$\tilde{t}/\alpha$	$\tilde{t}$	$\hat{t}$	$\hat{t}$
shear rate	$\hat{\dot{\gamma}}$	α	$\tilde{\dot{\gamma}} = 1$	$\hat{\dot{\gamma}}$	$\hat{\dot{\gamma}}$
shear stress	$\hat{\sigma}$	$\alpha\tilde{\sigma}$	$\tilde{\sigma}$	$\hat{\sigma}$	$\hat{\sigma}$