Kinetic theory of shear thickening

Hisao Hayakawa[1], Satoshi Takada[2]

[1] Yukawa Institute for Theoretical Physics, Kyoto University, [2] Department of Physics, Kyoto University

概要

定常のレオロジー曲線を熱浴とカップルした非弾性ボルツマン方程式に基づき理論的に導出し、シアシックニングがあることを導いた。

Abstract

The steady flow curve between the shear viscosity and the shear rate is theoretically obtained based on the inelastic Boltzmann equation under the influence of drag friction from background and a thermal activation. This flow curve exhibits a S-shape which suggests the existence of a discontinuous shear thickening in this setup.

1 Introduction

Rheology of granular fluids is important in both science and technology to control the flow of granular materials. The central concern of the rheology is the constitutive equation between the shear stress or the viscosity and the shear rate. The most fundamental rheological constitutive equation for many fluids is Newtonian in which the viscosity is independent of the shear rate. On the other hand, an assembly of dry granular particles obeys Bagnold's scaling in which the shear viscosity is proportional to the shear rate $\dot{\gamma}$. There are, however, many situations in which the viscosity has the rate dependence. In particular, the shear thickening process in which the viscosity increases as the shear rate increases attract much interest among researchers. This process is commonly observed in dense suspensions such as corn starch [1], but this can be observed even in granular flows.

One of interesting recent trends is that the mutual frictions between grains play important roles in the discontinuous shear thickening (DST) [2, 3, 4, 5, 6, 7, 8, 9]. Seto *et al.*[4, 5] have performed simulation for suspensions which have frictional contact force based on the Stokesian dynamics and found that there exists the DST even for such a system. There are some similar papers which also report important roles of frictional force between grains [6, 7, 8]. We stress that the interstitial fluid is no longer important for such systems to exhibit DSTs. Therefore, DST can be studied as an interesting subject of granular physics.

There are some phenomenologies to discuss the DST [10, 11, 12, 13] in which they introduction of the order parameter to reproduce a S-shape in a plane of stress-strain rate (flow curve). The most important question, however, on the origin of the S-shape has not been answered by them. Later, Grob *et al.* have examined the validity of the order parameter model for the DST of dry frictional granular particles [14]. Therefore, one of key remaining problems for the DST is to clarify the physical origin of the S-shape in the flow curve.

There are few theoretical papers on shear thickening. One of remarkable achievements is that by

Santos *et al.*[15] in which they demonstrate the existence of a continuous shear thickening in moderately dense hard-core gases by using the revised Enskog theory. Recently, the present authors have proposed a new theory of DST based on BGK equation [16].

The purpose of this paper is to demonstrate the existence of S-shape in the flow curve, which suggests the occurrence of the DST in a dilute granular gases associated with a drag and a thermal agitation under a plane shear within the framework of the inelastic Boltzmann equation. This model is a simple physical model to describe a model of granular gases under vertical vibration or mixture of granular gases in which smaller grains can be regarded as environmental fluid [17, 18].

2 Kinetic theory

Let us consider a collection of mono-disperse spherical grains (the diameter σ, the mass m and the restitution coefficient e) distributed in $d-$dimensional space influenced by the background fluid under a uniform shear flow characterized by the macroscopic velocity field $\boldsymbol{u}=(u_x,\boldsymbol{u}_\perp)$ under the shear rate $\dot\gamma$ as

$$u_x=\dot\gamma y,\quad \boldsymbol{u}_\perp=\boldsymbol{0}. \tag{1}$$

Introducing the peculiar velocity $\boldsymbol{V}\equiv(v_x-\dot\gamma y)\boldsymbol{e}_x+\boldsymbol{v}_\perp$ with the unit vector $\boldsymbol{e}_x$ parallel to $x-$direction (shear direction) and the velocity $\boldsymbol{v}_\perp$ perpendicular to $x-$direction as well as the microscopic velocity $\boldsymbol{v}$, we assume that the one-body distribution function $f(\boldsymbol{V},t)$ under the plane shear satisfies [17]

$$\begin{aligned}&\left(\frac{\partial}{\partial t}+\dot\gamma V_y\frac{\partial}{\partial V_x}\right)f(\boldsymbol{V},t)\\&=\zeta\frac{\partial}{\partial \boldsymbol{V}}\cdot\left(\left\{\boldsymbol{V}+\frac{T_{\rm ex}}{m}\frac{\partial}{\partial\boldsymbol{V}}\right\}f(\boldsymbol{V},t)\right)+J,\end{aligned}\tag{2}$$

where we have introduced ζ and $T_{\rm ex}$ to characterize the friction from the back ground fluid and the environmental temperature. For simplicity, we have ignored hydrodynamic interactions such as lubrication force and long-range force between particles. Here, the collisional integral $J\equiv J(\boldsymbol{V}|f)$ is assumed to be the inelastic Boltzmann operator:

$$\begin{aligned}J(\boldsymbol{V}_1|f)&=\sigma^{d-1}\int d\boldsymbol{v}_2\int d\hat{\boldsymbol{\sigma}}\Theta(-\boldsymbol{v}_{12}\cdot\hat{\boldsymbol{\sigma}})|\boldsymbol{v}_{12}\cdot\hat{\boldsymbol{\sigma}}|\\&\left\{\frac{f(\boldsymbol{V}_1^{**})f(\boldsymbol{V}_2^{**})}{e^2}-f(\boldsymbol{V}_1)f(\boldsymbol{V}_2)\right\},\end{aligned}\tag{3}$$

where $\Theta(x)=1$ for $x\ge 0$ and $\Theta(x)=0$ otherwise and $\boldsymbol{V}_i^{**}=\boldsymbol{v}_i^{**}-\boldsymbol{u}$ for $i=1,2$ is the pre-collisional velocity of $\boldsymbol{V}_i$ defined by

$$\boldsymbol{v}_1^{**}=\boldsymbol{v}_1-\frac{1+e}{2}(\boldsymbol{v}_{12}^{**}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}},\quad \boldsymbol{v}_2^{**}=\boldsymbol{v}_2+\frac{1+e}{2}(\boldsymbol{v}_{12}^{**}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\tag{4}$$

with $\boldsymbol{v}_{12}=\boldsymbol{v}_1-\boldsymbol{v}_2$. One of the most important quantities is the pressure tensor

$$P_{\alpha\beta}=m\int d\boldsymbol{v}V_\alpha V_\beta f(\boldsymbol{V},t).\tag{5}$$

This is related to the pressure as $P=P_{\alpha\alpha}/d=nT$ with the number density $n=\int d\boldsymbol{V}f(\boldsymbol{V},t)$, where the last equation is valid for the inelastic Boltzmann equation in the dilute limit.

Now let us assume the Grad's approximation [19, 20, 21]

$$f(\boldsymbol{V})=f_{\rm eq}(\boldsymbol{V})\left[1+\frac{m}{2T}\left(\frac{P_{\alpha\beta}}{nT}-\delta_{\alpha\beta}\right)V_\alpha V_\beta\right]\tag{6}$$

with

$$f_{\rm eq}(\boldsymbol{V})=n\left(\frac{m}{2nT}\right)^{d/2}\exp\left(-\frac{mV^2}{2T}\right),\tag{7}$$

where we have introduced the kinetic temperature T defined by $T=\int d\boldsymbol{v}m(\boldsymbol{v}-\boldsymbol{V})^2/(dn)$ and used Einstein's notation for the sum rule in which duplicated Greek indices take summation from $\alpha=1$ to $\alpha=d$. Substituting Eq. (6) into Eq. (2) with multiplying $mV_\alpha V_\beta$ and integrate it over $\boldsymbol{v}$, we obtain

$$\frac{\partial}{\partial t}P_{\alpha\beta}+\dot\gamma(\delta_{\alpha x}P_{y\beta}+\delta_{\beta x}P_{y\alpha})=-\Lambda_{\alpha\beta}+2\zeta(nT_{\rm ex}\delta_{\alpha\beta}-P_{\alpha\beta}),\tag{8}$$

where we have introduced

$$\Lambda_{\alpha\beta}\equiv -m\int d\boldsymbol{v}V_\alpha V_\beta J(\boldsymbol{V}|f)\tag{9}$$

When we adopt Eq. (6) it is straightforward to show the relation

$$\Lambda_{\alpha\beta}=\nu(P_{\alpha\beta}-nT\delta_{\alpha\beta})+\gamma nT\delta_{\alpha\beta},\tag{10}$$

where ν and γ are, respectively, given by [21]

$$\nu = \frac{\sqrt{2}\pi^{(d-1)/2} n\sigma^{d-1} v_T A}{d(d+2)\Gamma(\frac{d}{2})} \quad (11)$$

$$\gamma = \frac{\sqrt{2}\pi^{(d-1)/2} n\sigma^{d-1} v_T (1-e^2)}{d\Gamma(\frac{d}{2})}, \quad (12)$$

where we have introduced $A = 2d + 3 + 2de - 3e^2$, $v_T = \sqrt{2T/m}$ and $\ell = (n\sigma^{d-1})^{-1}$ with the Gamma function $\Gamma(x) = \int_0^\infty dt t^{x-1} e^{-t}$. From Eq. (10) with Eqs. (11) and (12), Eq. (8) can be rewritten as three coupled equations:

$$\frac{\partial}{\partial t} T = -\frac{2\dot{\gamma}}{dn} P_{xy} - \gamma T + 2\zeta(T_{\rm ex} - T), \quad (13)$$

$$\frac{\partial}{\partial t} \Delta T = -\frac{2}{n}\dot{\gamma} P_{xy} - (\nu + 2\zeta)\Delta T, \quad (14)$$

$$\frac{\partial}{\partial t} P_{xy} = \dot{\gamma} n \left(\frac{\Delta T}{d} - T\right) - (\nu + 2\zeta) P_{xy}, \quad (15)$$

where we have introduced $\Delta T \equiv (P_{xx} - P_{yy})/n$ and used $P_{yy} = P_{\perp\perp}$ with $P_{yy} = (P_{yy} - P_{xx})/d + P_{\alpha\alpha}/d$ with the notation of $P_{\perp\perp}(= P_{yy})$ for any perpendicular component to x, i. e. $\perp = y, z, \cdots$. It should be noted that the temperature T should be larger than $(1 + \gamma/(2\zeta))^{-1} T_{\rm ex}$ because of the viscous heating.

3 Rheology

Equations (13), (14) and (15) gives a rheological relation between the shear rate $\dot{\gamma}$ and the viscosity $\eta \equiv -P_{xy}/\dot{\gamma}$. For its explicit calculation we have to determine the form ζ. It is natural that we assume that ζ depends on $T_{\rm ex}$, because the drag coefficient should be larger if the temperature is higher.

Let us introduce the following dimensionless quantities:

$$\nu^* = \frac{\nu}{\sqrt{\theta}\zeta}, \quad \gamma^* = \frac{\gamma}{\sqrt{\theta}\zeta}, \quad \dot{\gamma}^* = \frac{\dot{\gamma}}{\zeta} \quad (16)$$

where we have introduced $\theta = T/T_{\rm ex}$.

In a steady state under this condition, Eqs. (13) and (14) are reduced to

$$\frac{\Delta T}{T} = \frac{d(\gamma^*\sqrt{\theta} + 2(1-\theta^{-1})}{\nu^*\sqrt{\theta} + 2}. \quad (17)$$

Substituting this into Eq. (14) we obtain the equation for $P_{xy}^* = P_{xy}/(nT_{\rm ex})$:

$$P_{xy}^* = -\frac{d\theta}{2\dot{\gamma}^*}\left\{\gamma^*\sqrt{\theta} + 2(1-\theta^{-1})\right\}. \quad (18)$$

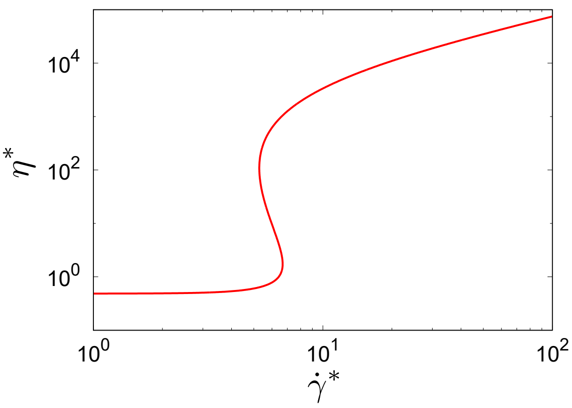

図 1: Plot of the dimensionless viscosity η^* against the shear rate $\dot{\gamma}^*$ for $e = 0.90$, where we adopt $d = 3$ and $n\sigma^3 = 0.01$.

Then, substituting Eqs. (17) and (18) into the steady equation of (15) we obtain

$$\dot{\gamma}^* = (\nu^*\sqrt{\theta} + 2)\sqrt{\frac{d[\gamma^*\sqrt{\theta} + 2(1-\theta^{-1})]}{2[(\nu^* - \gamma^*)\sqrt{\theta} + 2\theta^{-1}]}}. \quad (19)$$

Therefore, the dimensionless viscosity $\eta^* = P_{xy}^*/\dot{\gamma}^*$ is given by

$$\eta^* = \frac{\theta\{(\nu^* - \gamma^*)\sqrt{\theta} + 2\theta^{-1}\}}{(\nu^*\sqrt{\theta} + 2)^2}. \quad (20)$$

This model exhibits the crossover from Newtonian regime $\eta^* \to \theta_{\rm min}/(\nu^*\sqrt{\theta_{\rm min}} + 2)$ at $\theta = \theta_{\rm min}$, where $\theta_{\rm min}$ is a real solution of $\theta = (1 + \gamma^*\sqrt{\theta}/2)^{-1}$, to Bagnold's viscosity $\eta^* \to \sqrt{2/d}(\nu^* - \gamma^*)^{3/2}\dot{\gamma}^*/(\sqrt{\gamma^*}\nu^{*3})$ in the high shear rate limit $\theta \to 2(\nu^* - \gamma^*)\dot{\gamma}^{*2}/(d\nu^{*2}\gamma^*)$. Note that ν^* and γ^* depend on the restitution coefficient e as shown in Eqs. (11) and (12).

As shown in Fig. 1, the flow curve has S-shape at intermediate $\dot{\gamma}^*$. Then, if we gradually increases/decreases $\dot{\gamma}^*$, the viscosity η^* discontinuously increases/decreases at a certain value of the shear rate. Therefore, this S-shape flow curve strongly suggests the existence of the DST in this model [22].

4 Discussion and conclusion

Let us discuss our results. First, we need simulation to verify our theoretical results. This is one of our future problem [22].

Second, one can stress that our results are universal, though we have analyzed dilute granular gases. Indeed, we have already demonstrated the existence of DST behavior of a different model in which the collision term is replaced by a relaxation term. It is straightforward to extend the analysis presented here to a moderately dense granular gases by using Enskog equation [18]. Therefore, the extension of the analysis presented here will be important.

Because of the limitation of the length of this paper, we have not discussed the linear stability analysis of a steady state. This is not difficult. which would be the subject in a forthcoming paper.

In conclusion, we have demonstrated the existence of S-shape flow curve which strongly suggests the existence of the discontinuous shear thickening (DST) in granular fluid coupled with agitation characterized by $T_{\rm ex}$ and the drag force between granular particles and the background fluid within framework of inelastic Boltzmann equation. This model exhibits the crossover from Newtonian viscosity to Bagnold's viscosity in which the shear viscosity discontinuously changed as the shear rate increases.

参考文献

[1] E. Brown and H. M. Jeager, Rep. Prog. Phys. **77**, 040602 (2014).

[2] M. Otsuki and H. Hayakawa, Phys. Rev. E **83**, 051301 (2011).

[3] D. Bi, J. Zhang, B. Chakraborty, R. P. Behringer, Nature **480**, 355 (2011).

[4] R. Seto, R. Mari, J. F. Morris, and M. M. Denn, Phys. Rev. Lett. **111**, 218301 (2013).

[5] R. Mari, R. Seto, J. F. Morris, M. M. Denn, J. Rheol. **58**, 1693 (2014).

[6] M. Pica Ciamarra, R. Pastore, M. Nicodemi, and A. Coniglio, Phys. Rev. E **84**, 041308 (2011).

[7] C. Haussinger, Phys. Rev. E **88**, 050201(2013).

[8] M. Grob, C. Heussinger, and A. Zippelius, Phys. Rev. E **89**, 050201(2014).

[9] T. Kawasaki, A. Ikeda and L. Berthier, EPL **107**, 28009 (2014).

[10] M. Wyart and M. E. Cates, Phys. Rev. Lett. **112**, 098302 (2014).

[11] H. Nakanishi and N. Mitarai, J. Phys. Soc. Jpn. **80**, 033801 (2011).

[12] H. Nakanishi, S. Nagahiro, and N. Mitarai, Phys. Rev. E **85**, 011401 (2012).

[13] S. Nagahiro, H. Nakanishi, and N. Mitarai, EPL **104**, 28002 (2013).

[14] M. Grob, A. Zippelius and C. Heussinger, Phys. Rev. E **93**, 030901 (2016).

[15] A. Santos, J. M. Montanero, J. W. Dufty and J. J. Brey, Phys. Rev. E **57**, 1644 (1998).

[16] H. Hayakawa and S. Takada, arXiv:1610.06443v1.

[17] H. Hayakawa, Phys. Rev. E **68**, 031304 (2003).

[18] V. Garzó, M. G. Chamorro and F. Vega Reyers, Phys. Rev. E **87**, 032201 (2013).

[19] H. Grad, Commun. Pure Appl. Math. **2**, 331 (1949).

[20] V. Garzó, Phys. Rev. E **66**, 021308 (2002).

[21] A. Santos, V. Garzó and J. W. Dufty, Phys. Rev. E **69**, 061303 (2004).

[22] We have already obtained the perfect agreement between the theory and the simulation under SLLOD shear without introduction of any fitting parameter. We have also confirm the existence of DST in the simulation and no spatial instability of the uniformly sheared state.