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STOCHASTIC FLUCTUATION ANALYSIS OF DYNAMIC YIELD OF MAGNETORHEOLOGICAL FLUID USING CHAINS-FRACTURE MODEL

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Abstract. Magneto-rheological fluid, due to its perfect controllability behaviors adaptive to operation conditions, serves as a promising materials building a family of intelligent control devices usually applied in performance control and risk reduction of engineering structures. While the complex dynamics of the fluid result in essential challenges on the accurate operation of control devices, of which the quantification of randomness inherent in this suspension system is a critical issue. In the present paper, a meso-scale model for dynamic yield analysis of magnetorheological fluids (MRFs) is developed. This model originates from the fracture mechanism of chains involved in the suspension system and accounts the fact that the particle chains go through the rotation, translation and fracture under steady magnetic fields and homogenous shear fields. The benefit of the chains-fracture model is that its critical parameter just hinges upon the rotation angle. The structured behavior of particle chains of magnetorheological fluids under magnetic and shear fields is simulated using a perspective software for large-scale atomic/molecular massively parallel simulation (LAMMPS). The applicability of the developed meso-scale model in the analysis of stochastic fluctuation of dynamic yield of MRFs is investigated based on the data of molecular dynamics simulation.

1 INTRODUCTION

It is understood that the particle dynamics simulation of micro-scale level of materials is viewed as the most efficient means revealing the suspensions-structured performance and dynamic yield behavior of magnetorheological fluids. Klingenberg et al made a prior investigation on the response of electricrheological fluids under the small shear-rate field using the molecular dynamics simulation [1]. Bonnecase and Brady built up the 2D non-thermal model in virtue of Stokesian dynamics, whereby the static and dynamic yield of electricrheological fluids were analyzed [2]. Ekwebelam et al explored the size and ingredient of magnetorheological suspensions and their effect upon the yield behavior using the particle dynamics simulation [3]. While the previous investigations mostly limited in the small-scale simulation (tens of particles) where the aggregate performance of suspension chains cannot be exposed pertinently. The few large-scale simulation exclusively ignored the effect of Brownian motion of suspensions upon the micro-structured performance. In recent years, we carried out the large-scale simulations of magnetorheological fluids and micro-structured analysis of suspensions, which reveals the physical mechanism of dynamic yield behavior of magnetorheological fluids [4,5].

As regards the analysis of dynamic yield of rheological fluids, using the micro-scale method such as the molecular dynamics simulation usually involves the loop-calculation upon inter-action of particles, which needs much computational cost. While the non-particle simulation method such as the finite element method could derive the approximate solution but not to mention the stochastic fluctuation analysis. It is well recognized that the macro-scale behavior of materials depends upon the structured motion and evolution of the materials at micro and meso scales. For this understanding, the present paper proposes a meso-scale analytical model of dynamic yield of magnetorheological fluids, which includes the fracture mechanism of particle chains under shear fields from their rotations and translations. On this basis, the analysis of stochastic fluctuation of dynamic yield of MRFs is investigated.

2 CRITERION OF PARTICLE CHAINS FRACTURE

Due to the behavior of magnetorheological fluids, the suspensions subjected to magnetic fields would form into chain-cluster structures along with the direction of magnetic field [4]. In case of steady status of these structures, the chains, when subjected to the shear field, would go through the evolution steps; see Fig.1 as follows:

- (i) Chains along with the direction of magnetic field before the loading of shear field.
- (ii) Rotation and translation of chains subjected to the shear field.
- (iii) Reaching to a critical value of rotation or translation, the chain would jump into fracture somewhere and becomes to shorter chains.

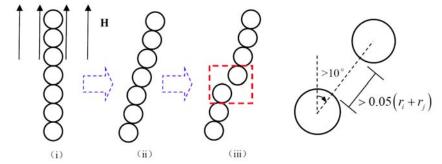


Figure 1: Schematic diagram of chain fracture under shear fields.

It is seen that at the moment of chain fracture, two particles somewhere in the chain have a small relative movement which results in the chain becoming to upper and lower shorter

chains. There is an assumption in the present investigation that the relative distance of the two shorter chains is s, and the relative movement is translation; see Fig.2. According to the identification criterion of chains [4]: the distance between particle surfaces is less than the 0.05 times of summation of two particle radius, and the angle of line connecting two particle centers and the direction of magnetic field is less than 10 deg.; the minimum number of involved particles in a chain is set to 2. It is understood that if a chain happens to be broken, it should beyond one of the two restraints at least. The discussion relevant to the two cases is provided as follows:

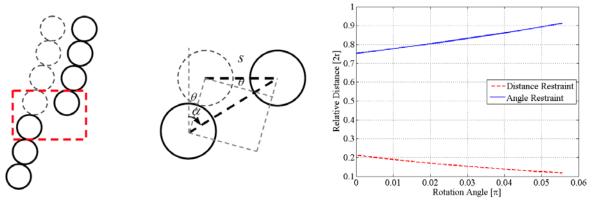


Figure 2: Schematic diagram of relative movement of chains. Figure 3: Relationship of distance and angle restraints upon the critical value of relative distance of particle surfaces.

(1) Distance Restraint

Since the distance between particle surfaces is less than the 0.05 times of summation of two particle radius, we have

$$\sqrt{\left(s \cdot \sin \theta + r_i + r_j\right)^2 + \left(s \cdot \cos \theta\right)^2} - (r_i + r_j) \le 0.05 \cdot (r_i + r_j) \tag{1}$$

The critical value of relative distance is then given by

$$s = \sqrt{(r_i + r_j)^2 \sin^2 \theta + 0.08(r_i + r_j)^2} - (r_i + r_j) \cdot \sin \theta$$
 (2)

(2) Angle Restraint

Since the angle of line connecting two particle centers and the direction of magnetic field is less than 10 deg., we have

$$\cos \alpha = \frac{s \cdot \sin \theta + r_i + r_j}{s} \le \cos 10^{\circ}$$
 (3)

The critical value of relative distance is then given by

$$s = \frac{r_i + r_j}{\cos 10^\circ - \sin \theta} \tag{4}$$

Fig.3 shows the relationship of distance and angle restraints upon the critical value of relative distance of particle surfaces ($r_i = r_j = r$). It is seen that the distance restraint acts more seriously than the angle restraint. Therefore, the fracture criterion of particle chains is that the distance between particle surfaces is more than the 0.05 times of summation of two particle radius.

3 FRACTURE MODEL OF MESO SCALE

The present fracture model describes the physical process of particle chains subjected to shear fields which starts from the rotation and translation to the fracture. Since the key moment of this process is the instant of the chain broken, so the critical value of distance restraint is the point. Fig. 4 shows the force diagram of the two parts of broken chains, where the particle number of the chain is n; the rotation angle and relative distance at the moment of fracture are θ and s, respectively.

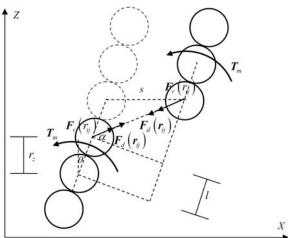


Figure 4: Force diagram at the moment of chain broken.

The magnetic moment could be denoted by

$$T_m = mH\sin\theta = \mu_0 MV_c H\sin\theta \tag{5}$$

where m denotes the magnetized intensity of particles; H denotes the magnitude of magnetic strength; μ_0 denotes the vacuum permeability; M denotes the unit magnetized intensity; V_c denotes the total volume of particles in the chain.

Since the unit magnetized intensity M is a function of the magnitude of magnetic strength H and the magnetisability β :

$$M = \beta H \tag{6}$$

Since

$$\beta = \frac{\mu_p(H) - \mu_c}{\mu_p(H) + 2\mu_c} \tag{7}$$

we then have

$$T_{m} = \frac{\mu_{p}(H) - \mu_{c}}{\mu_{p}(H) + 2\mu_{c}} \mu_{0} V_{c} H^{2} \sin \theta$$
 (8)

where $\mu_p(H)$ denotes the relative permeability of particles; μ_c denotes the relative permeability of fluids.

It is well recognized that the shear strength of magnetorheological fluids is contributed by the total energy of unit volume released by particle chains at the broken moment:

$$\tau = \frac{1}{V} \sum_{column\ contacts} \sum_{column\ contacts} r_z \cdot F_x \tag{9}$$

where τ denotes the shear stress of magnetorheological fluids at the simulation cell; V denotes the volume of simulation cell; the component of resultant force at projection of Z axis is given by

$$F_{x} = \left[F_{d} \left(\mathbf{r}_{ij} \right) + F_{r} \left(\mathbf{r}_{ij} \right) \right] \cdot \cos \theta \tag{10}$$

where $F_d(\mathbf{r}_{ij})$ denotes the dipole force between particles; $F_r(r_{ij})$ denotes the short-range force between particles.

In virtue of the principle of moment-equilibrium, the magnetic moment could also be expressed by

$$T_{m} = \left[F_{d} \left(\mathbf{r}_{ij} \right) + F_{r} \left(r_{ij} \right) \right] \cdot \cos \alpha \cdot l \tag{11}$$

We then have

$$F_{x} = \frac{T_{m} \cdot \cos \theta}{l \cdot \cos \alpha} \tag{12}$$

and

$$r_z = l \cdot \cos \theta \tag{13}$$

Assuming there is only one broken contact in a chain, then

$$\tau = \frac{1}{2} \cdot \frac{\mu_0 H^2 \left[\mu_p(H) - \mu_c\right]}{\mu_p(H) + 2\mu_c} \sum_{k=1}^N \frac{V_{c,k}}{V} \cdot \sin 2\theta_k \cdot \frac{\cos \theta_k}{\cos \alpha_k}$$
(14)

where

$$\alpha_{k} = \arccos\left(\frac{s_{k} \cdot \cos \theta_{k}}{\sqrt{\left(r_{k,i} + r_{k,j} + s \cdot \sin \theta_{k}\right)^{2} + \left(s_{k} \cdot \cos \theta_{k}\right)^{2}}}\right)$$
(15)

and k denotes the id number of the chain; $r_{k,i}$, $r_{k,j}$ denote radius of the two particles at the contact surface, respectively.

The rotation angles of all the chain at an instant of time are induced by a homogenous shear field. Their values exist small variation due to the randomness inherent in the initial condition of suspension particles and due to the effect of Brownian motion, which indicates that the mean of these angles features the population sufficiently. In this case, we have a simple model upon the shear stress of magnetorheological fluids:

$$\tau = \frac{1}{2} \cdot \frac{\mu_0 H^2 \left[\mu_p (H) - \mu_c \right]}{\mu_p (H) + 2\mu_c} \sum_{k=1}^{N} \frac{V_{c,k}}{V} \cdot \sin 2\overline{\theta} \cdot \frac{\cos \overline{\theta}}{\cos \overline{\alpha}}$$
 (16)

where

$$\overline{\theta} = \frac{1}{N} \sum_{k=1}^{N} \theta_k , \quad \overline{\alpha} = \frac{1}{N} \sum_{k=1}^{N} \alpha_k$$
 (17)

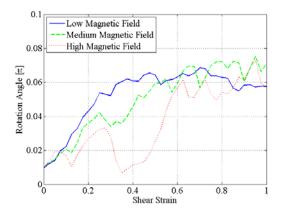
4 CASE STUDIES

A large-scale atomic/molecular massive parallel simulator (LAMMPS) [6] is employed, which provides an embedded routine for large-scale and 3D Brownian dynamics simulation. The initial topology and initial velocity of suspensions are generated as statistically independent with a uniform distribution and a Maxwell–Boltzmann distribution, respectively. The neighbor list algorithm with the strategy of radius cutoff is used to assess the interaction between particles. The boundaries at the 3D are represented by a sheared periodic boundary condition. The physical parameters of magnetorheological fluids for simulation are listed in Table 1.

All the simulations are carried out with dimensionless units. The regulation of the basic dimensionless units and their relationship with SI units are rendered by the reference [4]. The simulation cell in the dimensionless units is $(L^*x, L^*y, L^*z) = (20^*, 10^*, 10^*)$. Magnetic field strengths are valued by 20 kA/m, 100 kA/m and 200 kA/m which denote low, medium and high magnetic fields, respectively. The shear rate of homogeneous shear field is 1000 sec⁻¹.

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Parameters	Values		
Radius of particles	5×10 ⁻⁶ m		
Mass of particles	1×10^{-13} kg		
Volume ratio between suspensions and matrix	0.3		
Relative permeability of matrix $\mu_{\rm c}$	1.0		
Relative permeability of particles μ_p	1000		
Viscosity of matrix	0.3Pa • s		
Density of matrix	$3.6 \times 10^3 \text{kg} \cdot \text{m}^{-3}$		
Temperature	298K		



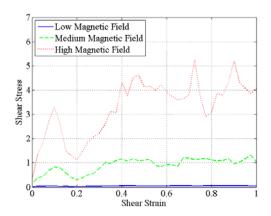


Figure 5: Mean of rotation angles of chains along with the loading of homogenous shear fields. Figure 6: Mean of shear stress of magnetorheological fluids in case of low, medium and high magnetic fields.

Fig. 5 shows the mean of rotation angles of chains, of one simulation sample (random sampling of initial condition of suspension particles), along with the loading of homogenous shear fields in case of low, medium and high magnetic fields, respectively. Using the simple model Eq.(16) and a collection of random sampling, we then have the mean of shear stress of magnetorheological fluids; see Fig.6. The mean and mean plus standard deviation of shear stress of magnetorheological fluids in case of medium magnetic field are shown in Fig.7. It is seen that there arises a significant stochastic fluctuation of dynamic yield of magnetorheological fluids: the maximum of coefficient of variation is up to 0.5.

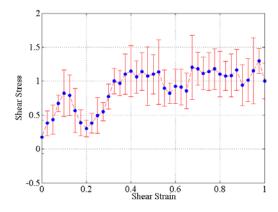


Figure 7: Mean and mean plus standard deviation of shear stress of magnetorheological fluids in case of medium magnetic field.

5 CONCLUSIONS

Using the large-scale atomic/molecular massive parallel simulator (LAMMPS), a meso-scale model of dynamic yield analysis of magnetorheological fluids is proposed. The model originates from the fracture mechanism of chains and accounts for the fact that the particle chains go through the translation, rotation and fracture under steady magnetic fields and homogeneous shear fields. The benefit of the chains-fracture model is that its critical parameter just hinges upon the rotation angle. Case studies indicate that the model is efficient for the dynamic yield analysis of magnetorheological fluids, and there exists a significant stochastic fluctuation of dynamic yield. The on-going work is the relationship analysis between rotation angles of particle chains and magnetic field strengths or shear rates of shear fields so as to derive an analytical meso-scale model of dynamic yield of magnetorheological fluids avoiding the high computational cost at the molecular dynamics simulations.

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REFERENCES

- [1] Klingenberg DJ, Van Swol F, Zukoski CF. The small shear rate response of electrorheological suspensions. I. Simulation in the point-dipole limit. The Journal of Chemical Physics. 1991; 94: 6160-6169.
- [2] Davis LC. Finite element analysis of particle-particle forces in electrorheological fluids. Applied Physics Letters. 2009; 60(3): 319-321.
- [3] Bonnecaze RT, Brady JF. Yield stresses in electrorheological fluids. Journal of Rheology, 1992; 36(1): 73-113.
- [4] Peng YB, Roger Ghanem, Li J. Investigations of microstructured behaviors of magnetorheological suspensions. Journal of Intelligent Material Systems and Structures, 2012; 23(12): 1349-1368.
- [5] Peng YB, Li J. Multiscale analysis for stochastic fluctuation of dynamic yield of magnetorheological fluids. International Journal for Multiscale Computational Engineering, 2011; 9(2): 175-191.
- [6] Plimpton SJ. LAMMPS web page. http://lammps.sandia.gov/, 2012.