

Unified model for full-stage shear thickening via surface chemistry and friction

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Shear thickening fluid exhibits complex properties in a wide range of external conditions, leading to the significance for probing its state-transition property at the molecular level. Here, we propose a constitutive model that unifies the three rheological stages of shear thinning, shear thickening, and secondary shear thinning by considering the short-range attractive forces governed by particle surface chemistry in shear thickening dense suspensions. The proposed model reproduces the secondary shear thinning phenomenon precisely and predicts the evolution of cluster number, size, and dispersion with a marked error reduction. Besides, based on the proposed model, the distribution of particles can be divided into isolated, uniform-aggregated, and overaggregated states according to the dissipative particle dynamics simulation results. This model provides a framework to design rheological behavior via particle surface chemistry, bridge the relationship between microstructure and macroscopic performance at various scales, and accelerate the understanding to the state-transition phenomenon in shear thickening dense suspension.

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I. INTRODUCTION

Shear thickening fluid (STF) is type of dense suspensions formed by dispersing solid particles in a low-viscosity liquid carrier [1–3]. Upon shear, STF exhibits a reversible mechanical property that rapidly switches from liquid state to quasi-solid-state owing to the interfacial interactions forces and frictional contact forces [4–7]. Once the stimulus is off, it will return to the initial state immediately. Besides, increasing $\dot{\gamma}$ leads to three successive non-Newtonian stages: shear thinning (Stage I), shear thickening (Stage II), and secondary shear thinning (Stage III), once $\dot{\gamma}$ exceeds a critical value [8–11]. Thus, developing the full-stage shear thickening model to predict the flow behavior precisely is crucial for understanding the natural phenomena and applying these materials under different conditions.

Several theoretical models have been proposed to explain its microscopic origins and macroscopic response, mainly

including the order-to-disorder transition, hydrodynamic lubrication, and frictional lubrication models [5,12]. These models commonly attribute secondary shear thinning at high $\dot{\gamma}$ to the breakdown of frictional contacts and a return to the lubrication-dominated regime [6,13]. The origin of Stage III in dense suspensions has been extensively studied with several proposed mechanisms. Mari *et al.* demonstrated through simulations that nonmonotonic flow curves arise naturally from the frictional-to-lubricated transition when hydrodynamic forces at high shear rates exceed the threshold for maintaining particle friction [8]. Ovarlez *et al.* observed spatiotemporal density heterogeneity in shear thickening suspensions, suggesting that flow instabilities and shear banding may also contribute to Stage III behavior [10]. Recent work on RIGIDITY percolation and shear jamming has provided additional insights into the emergence of force-bearing networks under shear and their subsequent breakdown [14,15]. However, none of these existing models explicitly account for the role of particle surface chemistry in determining the onset of Stage III, which represents a significant gap in our current understanding.

Nevertheless, our experimental results show that the shear thickening dense suspensions containing particles with higher hydroxyl density enter the secondary shear thinning regime earlier at high $\dot{\gamma}$ (Fig. 1). This observation is inconsistent with the consensus that a more compact particle cluster resulting from higher attractive forces is prone to be destroyed

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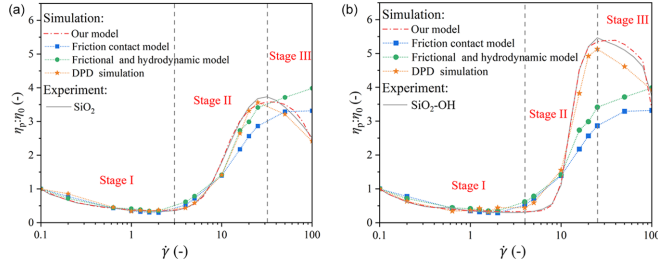


FIG. 1. Normalized viscosity ($\eta_p : \eta_0$) vs dimensionless shear rate ($\dot{\gamma}$) for STFs. (a) Comparison of experimental and theoretical data for STF containing SiO_2 particles. (b) Comparison of experimental and theoretical data for STF containing $\text{SiO}_2\text{-OH}$ particles. Experimental data (gray line) from Ref. [26] are compared with theoretical predictions: our proposed model [red dashed line, Eq. (7)], friction contact model [27] (blue square), and frictional and hydrodynamic model [28] (green circle). DPD simulation results (orange pentagram) validate the proposed model across all three rheological stages.

at a higher $\dot{\gamma}$ [16,17], entering the secondary shear thinning regime later. Under the conventional cluster-breakdown framework, stronger interparticle attractive forces due to hydrogen bonding should stabilize particle clusters and delay the transition to Stage III. The observation of the opposite behavior indicates that an additional mechanism must be operative. Therefore, considering that the rearrangement of particles, restoration of lubrication layer, and structural failure are crucial in determining whether the system enters the secondary shear thinning regime, the short-range attractive force is essential to be considered.

Here, we present a full-stage shear thickening model considering the short-range attractive force resulted from the particle surface chemistry. The proposed model fits well with the experimental data at full stage and is further verified by the dissipative particle dynamics (DPD) simulation results. Besides, according to the distinct particle microstructures and aggregation degree, the distribution of particles can be divided into isolated, uniform-aggregated, and overaggregated states based on the proposed model, which yields a full range constitutive relation. Within this unified framework, the model represents the competition and cooperation among short-range attractive forces driven by surface functional groups, contact friction force arising from surface roughness, and hydrodynamic lubrication. We propose that short-range attractive forces governed by surface chemistry play a dual role: At intermediate shear rates, they promote cluster formation and enhance frictional contacts leading to shear thickening, while at high shear rates, strong attractive forces cause overaggregation and phase separation, providing an alternative pathway to Stage III that is fundamentally different from simple cluster breakdown. Although prior experimental studies have established that surface chemistry, hydrogen bonding, and particle roughness control the frictional transition in dense suspensions [18–20], no existing constitutive framework parametrizes these effects. The contributions of our work include (1) a constitutive model that parametrizes surface chemistry through ε , simultaneously controlling the activation threshold $\dot{\gamma}_c$, the

high-shear attenuation $\dot{\gamma}_s$, and the dimensionless adhesion contribution χ_a ; (2) demonstration that Stage III can arise from overaggregation rather than cluster breakdown alone; (3) identification of three distinct microstructural states (isolated, uniform-aggregated, and overaggregated); and (4) significant quantitative improvement with peak-stress prediction error reduced from 26.07% to 2.86%.

II. THEORY AND MODEL

The governing equation of effective viscosity is written as

$$\eta(\dot{\gamma}) = \eta_{\text{hydro}}(\dot{\gamma}) + \eta_{\text{friction}}(\dot{\gamma}) S_{\text{sep}}(\dot{\gamma}), \quad (1)$$

where η is the effective viscosity, η_{hydro} is the hydrodynamic contribution to the viscosity, η_{friction} is the frictional contribution to the viscosity, and S_{sep} is a phase-separation factor accounting for high-shear attenuation.

At low to moderate $\dot{\gamma}$, the suspension exhibits shear thinning behavior captured by the Cross model [21]:

$$\eta_{\text{hydro}}(\dot{\gamma}) = \eta_{\infty} + \frac{\eta_0 - \eta_{\infty}}{1 + (\dot{\gamma}/\dot{\gamma}_p)^{m_r}}, \quad (2)$$

where η_0 and η_{∞} are the zero- and infinite-shear viscosities, $\dot{\gamma}_p$ is a characteristic thinning rate, and m_r is an empirical exponent [22–24]. The rheology of dense suspensions involves a complex interplay between hydrodynamic interactions and direct particle contacts [25].

Shear thickening is governed by stress-activated frictional contact networks [5,7,29]. We close the frictional viscosity by the scaling form

$$\eta_{\text{friction}}(\dot{\gamma}) = C \mu Z(\phi) \left[\dot{\gamma}^{m_n-1} + \frac{\chi_a(\varepsilon)}{\dot{\gamma}} \right] f(\dot{\gamma}), \quad (3)$$

where $C = O(1)$ is a geometric prefactor, μ is the particle friction coefficient, m_n reflects the dominant kinematics, and the contact coordination is $Z(\phi) = Z_0 \phi / (1 - \phi/\phi_m)$, with $Z_0 \simeq 6$ and $\phi_m \simeq 0.64$ [30,31]. The fraction of frictional contacts is $f(\dot{\gamma}) = (\dot{\gamma}/\dot{\gamma}_c)^\beta / [1 + (\dot{\gamma}/\dot{\gamma}_c)^\beta]$, with β controlling the sharpness of the transition. The dimensionless adhesion contribution explicitly incorporates surface chemistry effects:

$$\chi_a(\varepsilon) = \frac{U^*(\varepsilon)}{\eta_s a^3 h_c}, \quad U^*(\varepsilon) = U_0 \left(1 + \alpha \frac{\varepsilon}{\varepsilon_{\text{ref}}} \right), \quad (4)$$

where a is particle radius, h_c is a nanometric contact length [32], η_s is the solvent viscosity, and ε is a measure of surface functionality (e.g., hydroxyl density). Experiments show that hydrogen bonding, adhesion, and roughness promote frictional contacts and lower activation thresholds [18–20]. To incorporate chemistry into the trigger rate, we adopt a phenomenological Arrhenius dependence:

$$\dot{\gamma}_c(\varepsilon) = \dot{\gamma}_c^0 \exp \left(-\frac{U^*(\varepsilon)}{k_B T_{\text{eff}}} \right), \quad T_{\text{eff}} = T + \frac{\eta_s \dot{\gamma}^2 a^3}{k_B}, \quad (5)$$

which is consistent with a stress-driven crossover from lubrication to frictional states [18,29]. The thermal energy $k_B T$ entering T_{eff} accounts for the Brownian contribution to the activation barrier, so that the Wyart-Cates structure adopted here remains applicable to Brownian suspensions, with thermal fluctuations effectively shifting the stress-dependent jamming

point as shown by Mari *et al.* [28] and by Kawasaki and Berthier [33].

At sufficiently high $\dot{\gamma}$, dense suspensions commonly develop spatiotemporal heterogeneity [10,34], which weakens sustained frictional networks. We describe its mean effect by

$$S_{\text{sep}}(\dot{\gamma}) = \frac{1}{1 + (\dot{\gamma}/\dot{\gamma}_s(\varepsilon))^q}, \quad \dot{\gamma}_s(\varepsilon) = \dot{\gamma}_s^0 \left[\frac{k_B T}{U^*(\varepsilon) Z(\phi)} \right]^{1/2}, \quad (6)$$

where q is an empirical exponent that embeds a dimensional balance between aggregation and breakage. The scaling $\dot{\gamma}_s \propto [k_B T / (U^*(\varepsilon) Z(\phi))]^{1/2}$ encodes the competition between thermal agitation and surface-chemistry-modulated aggregation, so that stronger attraction or denser packing both lower $\dot{\gamma}_s$, in agreement with the experimental observation that hydroxyl-rich particles enter Stage III at lower shear rates.

Combining Eqs. (2)–(6), we obtain the complete constitutive relation:

$$\begin{aligned} \eta(\dot{\gamma}) = & \left[\eta_\infty + \frac{\eta_0 - \eta_\infty}{1 + (\dot{\gamma}/\dot{\gamma}_p)^{m_r}} \right] \\ & + C \mu Z(\phi) \left[\dot{\gamma}^{m_n-1} + \frac{\chi_a(\varepsilon)}{\dot{\gamma}} \right] \\ & \times \frac{(\dot{\gamma}/\dot{\gamma}_c)^\beta}{1 + (\dot{\gamma}/\dot{\gamma}_c)^\beta} \frac{1}{1 + (\dot{\gamma}/\dot{\gamma}_s)^q}, \end{aligned} \quad (7)$$

which recovers classic theory limits under specific conditions: (1) as $\dot{\gamma} \ll \dot{\gamma}_c$, Eq. (7) reduces to the volume-fraction-controlled low-shear limit [35]; (2) for $U^* \rightarrow 0$ and $S_{\text{sep}} \rightarrow 1$, it reduces to the Wyart-Cates frictional framework [29]; (3) in the strong thickening window $\dot{\gamma}_c < \dot{\gamma} < \dot{\gamma}_s$, it is consistent with friction-dominated power-law scaling [5,28]; and (4) choosing $m_n = 2$ and $\beta = q = 2$ renders a structure equivalent to the unified three-term fit of Ref. [36]. With the chemistry parameter ε explicitly embedded in χ_a , $\dot{\gamma}_c$, and $\dot{\gamma}_s$, Eq. (7) provides a unified description of the three rheological stages, while remaining consistent with friction-triggered thickening theory. Using a single parameter set per formulation, the model achieves an average error of 7.96% across the entire $\dot{\gamma}$ range from 0.01 to 100 s⁻¹, with particular success in capturing the secondary shear thinning behavior [Figs. 1(a) and 1(b)]. At higher volume fractions approaching ϕ_m , Eq. (7) inherits from the Wyart-Cates structure the capability to produce discontinuous shear thickening and shear jamming, whose quantitative experimental validation, including S-shaped and reentrant flow curves, is left for future work.

The simulations model spherical silica nanoparticles with diameter $\sigma = 300$ nm dispersed in a Newtonian solvent with viscosity $\eta_s = 0.001$ Pa s. This particle size directly corresponds to the silica nanoparticles used in the experiments by Liu *et al.* [26] that we compare against. Each nanoparticle is represented as a RIGID aggregate of 30 DPD beads, with each bead having a diameter of approximately 80 nm, ensuring low fluid permeability and accurate contact mechanics. The shear rate range $\dot{\gamma} = 0.01$ –100 in simulation units is mapped to match the experimental range of 0.01–100 s⁻¹. At the intermediate shear rate $\dot{\gamma} = 10$ s⁻¹, the Péclet number $\text{Pe} \approx 0.15$, while at $\dot{\gamma} = 100$ s⁻¹, $\text{Pe} \approx 1.5$, indicating that the system spans the transition from Brownian-dominated to hydrodynamically dominated behavior within the experimental shear

rate range. Shear thickening in submicron colloidal particles is well documented experimentally [23,37] and arises from stress-activated frictional contacts when hydrodynamic forces begin to dominate. Our choice of DPD is motivated by its ability to capture both thermal fluctuations important at this length scale and the contact mechanics essential for shear thickening.

To validate the proposed constitutive equation, we employ the DPD model shown in Fig. 2(a). Our simulation approach builds on established techniques for modeling dense suspension dynamics [38], extended here to incorporate short-range attractive forces governed by surface chemistry. The diameter of the 30 beads is equal to that of the solid SiO₂ particle to ensure the accurate representation of low permeability. Liquid bead cores occupy only 2% of the bead radius, simulating interpenetrability and microscopic interactions during shear [39]. The system contains 81 000 beads at solid volume fraction $\phi = 0.45$, within a cubic domain measuring $30 \times 30 \times 30$ Lennard-Jones (LJ) units.

Seven forces act on beads [Fig. 2(b)]. All beads (both solid and liquid) experience three fundamental DPD forces [40,41]: the conservative force providing interparticle repulsion, the random force introducing thermal fluctuations, and the dissipative force ensuring proper thermalization. Solid particles additionally experience four forces compared to liquid beads: (1) a short-range repulsive force acting normal to the surface [5]; (2) hydrodynamic lubrication force [42]; (3) contact force based on Hertzian collision with sliding friction [43,44]; and (4) short-range attractive force described by a soft LJ potential [45,46] [Fig. 2(c)]. Liquid beads follow standard DPD dynamics, while solid particles obey coupled translational and rotational equations of motion. This formulation ensures accurate representation of particle rotation during shear thickening. All results are reported in reduced LJ units unless specified otherwise. Detailed force expressions, equations of motion, and all parameter values are provided in Appendix A. The robustness of our results to parameter variations is demonstrated through sensitivity analyses in Appendix B. The mapping between simulation units and physical units is provided in Appendix C, and computational details including code availability are described in Appendix D.

Liu *et al.* [26] proposed a method to vary surface hydroxyl density without changing particle morphology. The experimental details, including materials, suspension preparation, particle characterization, and rheological measurement protocols, are provided in Appendix E. Using their experimental data, we validate our model through the normalized viscosity $\eta^* = \eta_t/\eta_0$. With particle morphology fixed, the friction coefficients (k_n , k_t , μ_s) remain constant, whereas the short-range attractive potential depth ϵ reflects the binding strength of surface groups. The particle radius a , volume fraction ϕ , solvent viscosity η_s , and temperature T are obtained directly from experimental measurements, $\mu_s = 0.3$ is referenced from established silica values [5,7], ϵ is estimated from the surface modification data of Liu *et al.* [26], and the exponents m_n , β , and q are fixed to 2 in line with Ref. [36], so that only $\dot{\gamma}_c^0$ and $\dot{\gamma}_s^0$ are fitted per formulation. Our model reproduces all three shear thickening stages with an average relative error $E_{\text{avg}} = (1/N) \sum_i |\eta_{\text{pred},i}^* - \eta_{\text{exp},i}^*|/\eta_{\text{exp},i}^* = 7.96\%$, where N is the

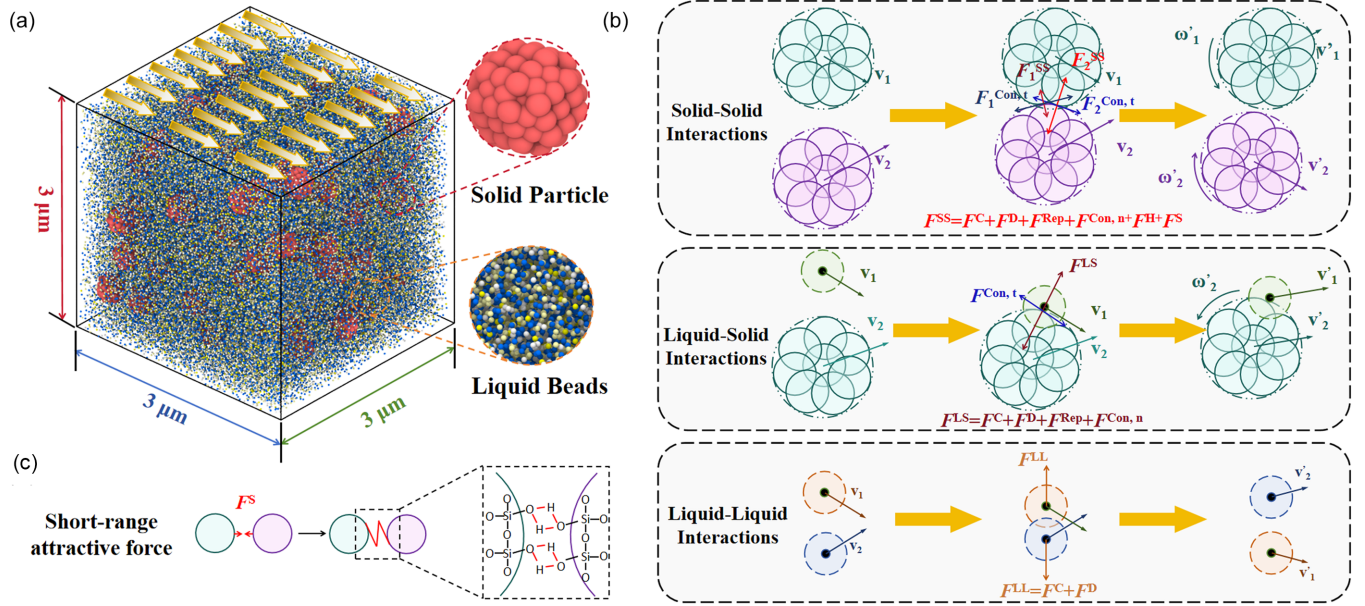


FIG. 2. Coarse-grained DPD model for shear thickening dense suspensions. (a) Schematic of the coarse-grained model; each silica particle is represented as an aggregate of 30 beads. (b) Force analysis between two beads. (c) Short-range attractive force (simplified schematic).

number of data points. In contrast, traditional models without chemical interactions fit only SiO_2 conditions ($E_{\text{avg}} = 17.10\%$ and 15.85% for friction contact model and frictional and hydrodynamic model, respectively), fail to represent $\text{SiO}_2\text{-OH}$ systems ($E_{\text{avg}} = 29.92\%$ and 32.09%), and omit the viscosity decrease in Stage III [Figs. 1(a) and 1(b)]. The relative error at maximum stress $E_{\text{max}} = |\sigma_{\text{pred, max}} - \sigma_{\text{exp, max}}|/\sigma_{\text{exp, max}}$ decreases by 89.03% (from 26.07% to 2.86%) when surface chemical interactions are included. These quantitative comparisons demonstrate the model's enhanced capability in describing the rheological behavior and capturing the secondary shear thinning precisely.

III. RHEOLOGY RESULTS

To clarify the evolution of rheological responses and potential energy fields during shear thickening, three particle systems with distinct potential well depths ($\epsilon = 0, 0.1, 5.0$) were established to represent nonbonded, weakly bonded, and strongly bonded interactions. In Stage I, the viscosity η exhibits a consistent trend for all ϵ values [Fig. 3(a)]. The total potential energy U_{total} also follows a similar pattern for $\epsilon = 0$ and 0.1 , with differences resulting from initial configuration variations [Fig. 3(b)]. The analysis of interparticle potential energy indicates that the low shear rate $\dot{\gamma}$ in Stage I does not provide sufficient kinetic energy to overcome the potential barrier located at a particle spacing of approximately 1.1 [Fig. 3(c)]. This is supported by the radial distribution function (RDF), which shows d_{peak} of solid-solid is 0.69 relative to a particle diameter of 0.62 [Fig. 3(d)]. Consequently, conservative forces predominate in Stage I and the system energy varies primarily with particle separation, exhibiting a near-quadratic dependency.

As $\dot{\gamma}$ increases, U_{total} undergoes an abrupt decrease at $\dot{\gamma} = 0.7$ followed by a subsequent increase [Fig. 3(b)]. This

decrease arises from the rapid reduction in interparticle potential energy E_{inter} , caused by the increased kinetic energy that enables particles to cross the potential barrier and form more frequent contacts [Fig. 3(c)]. The d_{peak} of solid-solid confirms the transition to Stage II [Fig. 3(d)]. In this stage, ϵ affects the magnitude of the viscosity peak η^* , although the relationship is nonlinear. The change in η^* between $\epsilon = 0$ and

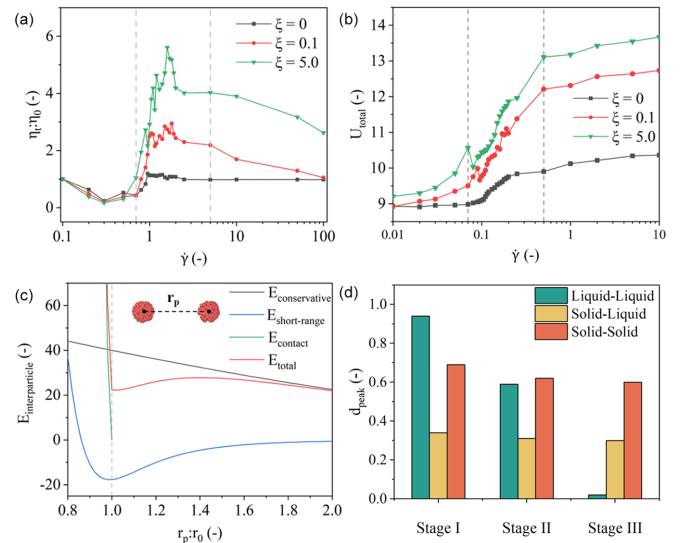


FIG. 3. Rheological response and potential energy evolution across three shear rate regimes for systems with varying short-range attractive force strength ($\epsilon = 0, 0.1$, and 5.0 kT). (a) Variation of potential energy with $\dot{\gamma}$. (b) Variation of relative viscosity with $\dot{\gamma}$. (c) Variation of interparticle interaction potential energy with distance between particles. (d) The corresponding radial positions (d_{peak}) of peak values of the RDF at different stages. The detailed RDF profiles are provided in Fig. 6.

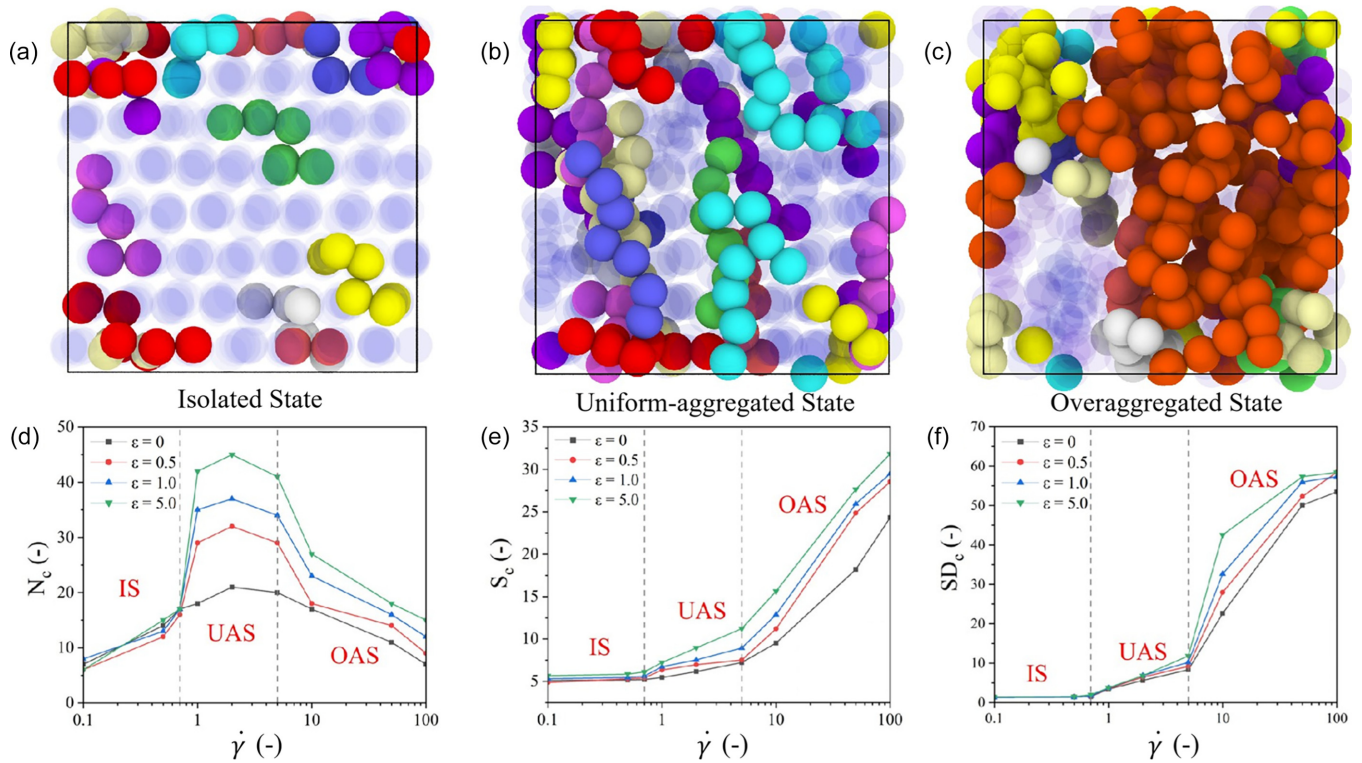


FIG. 4. Microstructural evolution and cluster statistics during shear-induced state transitions. (a) Microstructure of the isolated state. (b) Microstructure of the uniform-aggregated state. (c) Microstructure of the overaggregated state. (d) Variation of cluster number with $\dot{\gamma}$. (e) Variation of cluster size with $\dot{\gamma}$. (f) Variation of cluster-size standard deviation with $\dot{\gamma}$. In Figs. 4(a)–4(c), semitransparent particles denote dispersed silica particles, whereas opaque particles of the same color indicate silica particles belonging to the same cluster.

$\epsilon = 0.1$ is 17.92, which is substantially larger than the value of 0.54 observed when ϵ increases from 0.1 to 5.0. This finding indicates the presence of a threshold ϵ beyond which particle clusters remain sufficiently stable, such that further increases in ϵ do not significantly modify the particle distribution.

The duration of Stage II decreases as ϵ increases, indicating that stronger short-range attractions accelerate the transition to subsequent stages. For $\epsilon = 5.0$, Stage II spans the interval from $\dot{\gamma} = 0.06$ to 0.19, whereas for $\epsilon = 0.1$ it spans the interval from $\dot{\gamma} = 0.06$ to 0.50. Under $\epsilon = 0$, Stage III is barely detectable. Excessive aggregation at $\epsilon = 5.0$ and $\dot{\gamma} \approx 0.19$ likely induces phase separation, reducing the duration of the shear thickening regime. Stage II is thus characterized by enhanced particle contacts, a sharp decrease in potential energy, and a gradual recovery driven by short-range attractive interactions. The transition between microstructural states can be understood through the lens of rigidity percolation [14], where the connectivity of frictional contacts determines the mechanical response.

With further increases in $\dot{\gamma}$, the system enters secondary shear thinning. The rate of increase in U_{total} becomes slower [Fig. 3(b)]. The d_{peak} of liquid-liquid shifts to 0.03, and d_{peak} of solid-solid shows minimal movement [Fig. 3(d)]. These results indicate that the rise in U_{total} results primarily from reduced bead spacing rather than structural reorganization. The change in η^* during this stage is positively correlated with ϵ . For $\epsilon = 5.0$, η^* increases by 4.01 from $\dot{\gamma} = 0.19$ to 10. For $\epsilon = 0.1$, the corresponding increase is 1.59 from $\dot{\gamma} = 1.5$ to 10. Strong short-range attractions therefore

intensify particle aggregation and stratification under high shear rates. Stage III is governed by dynamic bead interactions, gradual potential energy growth, and the progressive formation of aggregates. The emergence of force-bearing net-

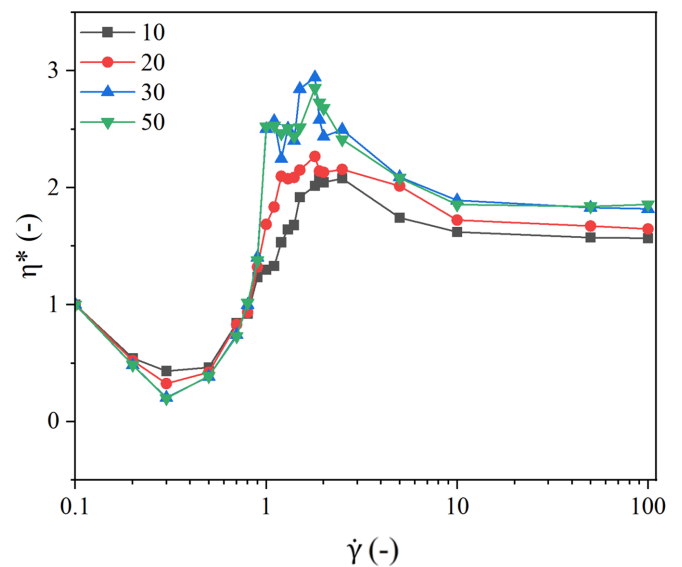


FIG. 5. Relative viscosity η^* as a function of shear rate $\dot{\gamma}$ for SiO_2 nanoparticle suspensions modeled with different numbers of DPD beads per particle ($N = 10, 20, 30$, and 50) at $\epsilon = 0.1$ and $\phi = 0.45$.

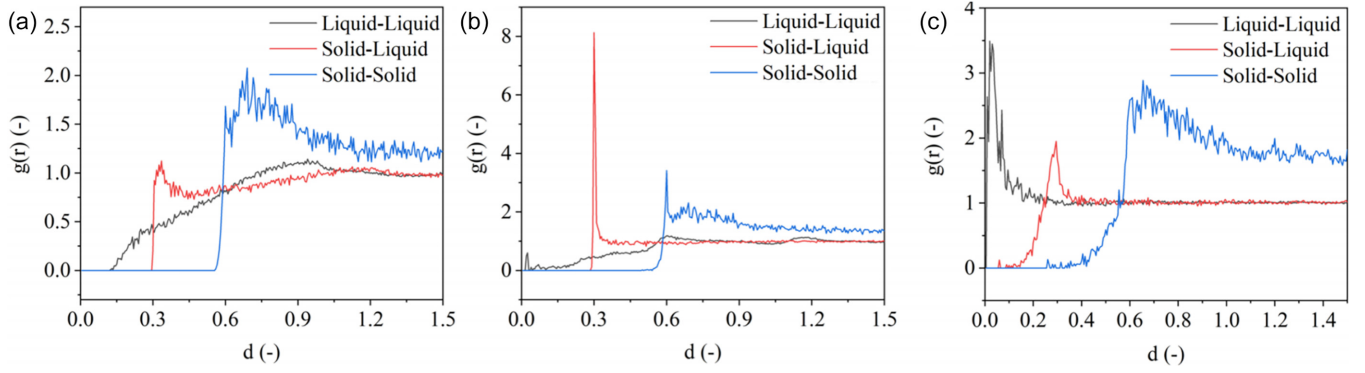


FIG. 6. The detailed RDF profiles of (a) Stage I, (b) Stage II, and (c) Stage III.

works under shear [15] underlies the transition from isolated to aggregated states observed in our simulations. The shift of the solid-solid d_{peak} to a value smaller than the particle diameter [Figs. 3(d) and 6(c)] indicates that particles are forced into closer contact than in Stage II, which is incompatible with simple cluster breakdown and is the structural hallmark of overconsolidation. The strongly saturating dependence of η^* on ϵ , with the change of 17.92 between $\epsilon = 0$ and $\epsilon = 0.1$ contrasted by only 0.54 between $\epsilon = 0.1$ and $\epsilon = 5.0$, further supports this picture, since a monotonic cluster-breakdown mechanism would predict a viscosity that grows continuously with attractive strength. Stage II is therefore a physical inevitability rather than a mathematical prerequisite of Eq. (7), since overaggregation in Stage III can only develop after the dense frictional contact network of Stage II has been established.

Across the three stages, the system exhibits a clear progression in particle distribution as $\dot{\gamma}$ increases. Stage I is dominated by conservative forces and dispersed particle configurations. Stage II involves a sharp decline in potential energy, the formation of particle clusters, and shear thickening promoted by short-range attractions. Stage III is characterized by secondary shear thinning arising from aggregation and stratification, which eventually results in phase separation. These findings demonstrate the intricate coupling among shear rate, particle interactions, and potential energy in determining non-Newtonian behavior.

IV. MICROSTRUCTURAL MECHANISM

To further validate the particle distributions characteristic of the three states, we examined the microstructures at three shear rates ($\dot{\gamma}$) [Figs. 4(a)–4(c)], focusing on cluster number, size, and heterogeneity. Here, a cluster is defined as an aggregate of at least four connected nanoparticles. In Figs. 4(a)–4(c), particles sharing the same color belong to the same cluster, and each sphere represents an individual solid nanoparticle; isolated particles are shown as semitransparent blue for clarity. These clusters are transient structures that continuously separate and recombine under shear.

At low $\dot{\gamma}$ [Fig. 4(a)], clusters are mostly small, with the maximum size S_c only 6.12 at $\dot{\gamma} = 0.7$ ($\epsilon = 5.0$), and their number remains limited (maximum $N_c = 17$ at $\dot{\gamma} = 0.7$, $\epsilon = 0, 0.5, 5.0$) [Figs. 4(d) and 4(e)]. Cluster-size variability is also minimal (maximum $SD_c = 1.98$ at $\dot{\gamma} = 0.7$, $\epsilon = 5.0$)

[Fig. 4(f)], while isolated particles dominate, with ω_c reaching 77.69%. These features characterize an isolated state in which most particles remain dispersed, and only a few small, widely separated clusters form, leading to a low probability of interparticle collisions and frictions and, consequently, no appreciable increase in viscosity.

As $\dot{\gamma}$ increases, the system enters Stage II [Fig. 4(b)]. Both the number and size of clusters rise markedly (for $\epsilon = 5.0$, from $\dot{\gamma} = 0.7$ to 2, $\Delta N_c = 28$, and $\Delta S_c = 2.84$), while ω_c drops from 77.69% to 21.25% [Fig. 4(d)]. Cluster-size variation also becomes more pronounced (for $\epsilon = 5.0$, at $\dot{\gamma} = 2$, $SD_c = 6.82$) [Fig. 4(e)]. These trends indicate a transition to the uniform-aggregated state, in which more than half of the particles join clusters that remain relatively uniform in size [Fig. 4(d)]. The frequent friction and reorganization among clusters impede the free motion of liquid beads under shear, marking the onset of shear thickening.

Once $\dot{\gamma}$ exceeds a critical value, the cluster size increases sharply (for $\epsilon = 5.0$, from $\dot{\gamma} = 2$ to 50, $\Delta S_c = 18.68$), while the cluster number decreases ($\Delta N_c = -27$) [Figs. 4(d) and 4(e)]. Meanwhile, the fraction of isolated particles ω_c rises slightly (from 21.25% to 25.79%), and cluster-size variability becomes substantial ($SD_c = 57.32$) [Fig. 4(f)]. The system thus transitions into the overaggregated state, where the largest cluster reaches 184 particles, accounting for 35.94% of the total. This reflects the formation of a dominant, massive aggregate that divides the system into a solidlike region controlled by the large cluster and a liquidlike region of dispersed particles. Such phase separation signifies the loss of a stable dispersed microstructure and is a primary cause of the reduced viscosity in the suspension. The Stage III viscosity reported here should therefore be interpreted as an effective bulk-averaged response of a microscopically heterogeneous suspension, with $S_{\text{sep}}(\dot{\gamma})$ in Eq. (6) acting as a mean-field representation that becomes increasingly approximate as macroscopic shear banding or density waves [10] develop.

V. CONCLUSIONS

The proposed model integrates hydrodynamic lubrication, frictional contact, and short-range surface-chemistry-driven attractions to formulate a comprehensive constitutive relation for shear thickening in dense suspensions. Its validity is confirmed through DPD simulations, which capture the shear-rate-dependent evolution of phase aggregation and

dispersion. The model reproduces shear thinning, shear thickening, and secondary shear thinning with substantially reduced prediction error relative to traditional models; notably, the peak-stress error decreases from 26.07% to 2.86%. It further identifies three microstructural regimes: the isolated state, uniform aggregation, and overaggregation. Overall, the model provides a unified framework for describing the non-Newtonian behavior of shear thickening dense suspensions and offers deeper insight for designing materials with tailored shear-responsive properties. Extending the experimental validation to higher volume fractions where discontinuous shear thickening, shear jamming, and S-shaped or reentrant flow curves are expected, together with spatially resolved measurements that probe the limits of the mean-field description in Stage III, is a natural direction for future work.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: COMPUTATIONAL DETAILS

In our model, seven forces act on beads. All beads (both solid and liquid) experience three fundamental DPD forces [41]. The conservative force is $\mathbf{F}_{ij}^C = a_{ij}(1 - r_{ij}/r_c)\hat{\mathbf{r}}_{ij}$, where $a_{ij} = 25kT/r_c$ is the maximum repulsion between particles i and j , r_{ij} is the interparticle distance, $r_c = 1.0\sigma$ is the cutoff radius, and $\hat{\mathbf{r}}_{ij}$ is the unit vector from particle i to j . The random force is $\mathbf{F}_{ij}^R = \xi\omega^R(r_{ij})\theta_{ij}\Delta t^{-1/2}\hat{\mathbf{r}}_{ij}$, where $\xi = 3.0$ is the noise amplitude, $\omega^R(r_{ij}) = (1 - r_{ij}/r_c)^{1/2}$ is the weight function, θ_{ij} is a Gaussian random number with zero mean and unit variance, and $\Delta t = 0.01\tau$ is the time step, with $\tau = \sigma(m/kT)^{1/2}$ being the LJ time unit. The dissipative force is $\mathbf{F}_{ij}^D = -\gamma\omega^D(r_{ij})(\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij})\hat{\mathbf{r}}_{ij}$, where $\gamma = \xi^2/(2kT) = 1.5$ is the dissipation coefficient ensuring proper thermalization, $\omega^D(r_{ij}) = [\omega^R(r_{ij})]^2$ is the weight function, and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity.

Solid particles additionally experience four forces compared to liquid beads. (1) The repulsive force $\mathbf{F}_{ij}^{\text{Rep}} = F_0 \exp(-h/\lambda_\omega)\mathbf{n}_{ij}$ acts normal to the surface [5], where $h = r_{ij} - \sigma_i - \sigma_j$ is the interparticle surface separation distance, $F_0 = 1.5 \times 10^{-9}$ N is the characteristic repulsion magnitude, $\lambda_\omega = 0.1$ nm is the decay length, and $\mathbf{n}_{ij}$ is the surface normal unit vector. (2) The hydrodynamic lubrication force is $\mathbf{F}_{ij}^H = -6\pi\eta_0 r_{ij}^{\text{eff}2} h^{-1}(\mathbf{v}_n \cdot \mathbf{n}_{ij})\mathbf{n}_{ij}$ [42], where $\eta_0 = 0.001$ Pa s is the fluid viscosity, $r_{ij}^{\text{eff}} = r_i r_j / (r_i + r_j)$ is the effective radius, and $\mathbf{v}_n$ is the normal component of relative velocity.

TABLE I. Effect of friction coefficient μ_s on rheological parameters at $\epsilon = 0.1$ and $\phi = 0.45$.

μ_s	$\dot{\gamma}_c$ (Stage II onset)	η_{max}^*	$\dot{\gamma}_s$ (Stage III onset)
0.1	1.8	3.2	15.2
0.2	1.7	4.1	14.3
0.3	1.6	5.2	13.9
0.4	1.6	6.0	13.1
0.5	1.5	6.8	12.7

(3) The contact force $\mathbf{F}_{ij}^{\text{Con}} = \sqrt{hr_i r_j / (r_i + r_j)}[k_n \mathbf{h}_{ij} - k_t \Delta \mathbf{s}_t]$ is based on Hertzian collision with sliding friction [43], where $k_n = 10^4$ N m $^{-1}$ is the normal elastic spdfness, $k_t = 2 \times 10^3$ N m $^{-1}$ is the tangential spdfness, and $\Delta \mathbf{s}_t$ is the tangential displacement vector truncated by the Coulomb friction criterion $|\Delta \mathbf{s}_t| \leq \mu_s |k_n \mathbf{h}|$ with friction coefficient $\mu_s = 0.3$. (4) The short-range attractive force is $\mathbf{F}_{ij}^S = -\nabla E^S$, where the soft LJ potential is $E^S = \lambda^n 4\epsilon(1/L_s^2 - 1/L_s)$, with $L_s = \alpha_{\text{LJ}}(1 - \lambda)^2 + (r_{ij}/\sigma)^6$ [45,46]. Here, $\epsilon = 2.5kT$ at $T = 300$ K is the potential well depth, $\lambda = r_{ij}/r_{\text{cut}}$ is the normalized distance, $n = 1$ is the softness exponent, $\alpha_{\text{LJ}} = 0.5$ is the softness parameter controlling potential shape, $r_{\text{cut}} = 1.1\sigma$ is the cutoff distance beyond which $\mathbf{F}^S = 0$, and $\sigma = 300$ nm is the particle diameter, corresponding to the silica nanoparticle size used in the experiments by Liu *et al.* [26]. Each nanoparticle is represented by 30 DPD beads with individual bead diameter of approximately 80 nm.

Liquid beads follow standard DPD dynamics governed by $m_i d\mathbf{v}_i/dt = \sum_j (\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^R + \mathbf{F}_{ij}^D)$, where $m_i = \rho_l(4\pi/3)\sigma^3$ is the bead mass with liquid density $\rho_l = 1000$ kg m $^{-3}$, $\mathbf{v}_i$ is the velocity, and the summation is over all neighboring particles within r_c . Solid particles obey coupled translational and rotational equations. The translational motion is $m_i d\mathbf{v}_i/dt = \sum_j (\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^R + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^H + \mathbf{F}_{ij}^{\text{Con}} + \mathbf{F}_{ij}^S + \mathbf{F}_{ij}^{\text{Rep}})$, where $m_i = \rho_s(4\pi/3)\sigma^3$ with solid density $\rho_s = 2500$ kg m $^{-3}$. The rotational motion is $I_i d\boldsymbol{\omega}_i/dt = \sum_j \boldsymbol{\tau}_{ij}$, where $I_i = (2/5)m_i\sigma^2$ is the moment of inertia for spherical particles, $\boldsymbol{\omega}_i$ is the angular velocity, and $\boldsymbol{\tau}_{ij} = \mathbf{r}_{ij} \times (\mathbf{F}_{ij,t}^{\text{Con}} + \mathbf{F}_{ij,t}^H)$ is the torque with subscript t denoting tangential components. This formulation ensures accurate representation of particle rotation during shear thickening. All results are reported in reduced LJ units unless specified otherwise. Stress converts to pascals via $\sigma_{\text{physical}} = (\epsilon/\sigma^3)\sigma_{\text{LJ}}$.

APPENDIX B: PARAMETER SENSITIVITY ANALYSIS

To assess the robustness of our simulation results, we conducted systematic parameter sensitivity studies. The key findings are summarized below.

Simulations with friction coefficients μ_s ranging from 0.1 to 0.5 were performed at fixed $\epsilon = 0.1$ and $\phi = 0.45$. As shown in Table I, the three-stage rheological behavior is observed for all tested values of μ_s . Increasing μ_s enhances the peak viscosity η_{max}^* and shifts both the Stage II onset ($\dot{\gamma}_c$) and Stage III onset ($\dot{\gamma}_s$) to lower shear rates, consistent with friction-based shear thickening theories. Importantly, the qualitative effect of surface chemistry on the Stage III onset is

preserved across all tested friction coefficients: higher ε consistently leads to earlier Stage III, confirming the robustness of the proposed overaggregation mechanism. The relationship between ε and the Stage III onset shear rate $\dot{\gamma}_s$ follows the theoretical prediction in Eq. (B1),

$$\dot{\gamma}_s \propto \left[\frac{k_B T}{U^*(\varepsilon) Z(\phi)} \right]^{1/2}, \quad (\text{B1})$$

confirming that the model captures the correct underlying physics. The robustness of our conclusions stems from the fact that the three-stage behavior arises from the competition among three distinct physical mechanisms operating in different shear rate regimes—hydrodynamic lubrication, frictional contacts, and short-range attractions. This separation of scales makes the qualitative behavior relatively insensitive to exact parameter values. Furthermore, the model successfully reproduces experimental data with physically reasonable parameters, providing external validation, and recovers established theoretical limits (e.g., classical frictional thickening at $\varepsilon = 0$) under appropriate conditions.

Regarding the multibead representation (Fig. 5), each SiO_2 nanoparticle (diameter 300 nm) is represented as an aggregate of 30 DPD beads with an individual solid bead diameter of approximately 80 nm, while the liquid DPD beads have a diameter of 50 nm. The multibead representation serves two purposes: (1) A single large DPD bead would be too permeable to fluid, allowing unrealistic penetration, whereas the multibead representation creates an effectively impenetrable particle surface with low permeability; and (2) the multibead structure allows for realistic force transmission during particle collisions, including proper treatment of normal and tangential contact forces. Tests with 10, 20, 30, and 50 beads per particle (Fig. 5) show that 30 beads provide an optimal balance between computational efficiency and physical accuracy. Fewer beads (10–20) result in insufficient surface resolution and excessive fluid penetration through the particle interior, leading to artificially reduced viscosities. Moreover, the solid bead size increases substantially with fewer beads, creating an excessive volume mismatch between solid and liquid beads that distorts the lubrication forces and contact mechanics at the liquid-solid interface, thereby weakening the model's ability to capture shear thickening transitions. More beads (50) bring the solid bead size closer to that of the liquid beads but do not significantly improve the rheological results while substantially increasing computational cost. Therefore, the 30-bead representation maintains a reasonable solid-to-liquid bead size ratio (approximately 1.6:1) while ensuring particle impermeability, interfacial mechanical accuracy, and computational efficiency.

APPENDIX C: PHYSICAL UNIT MAPPING

The particle diameter in our simulations is $\sigma = 300$ nm, which directly corresponds to the silica nanoparticle size used in the experiments by Liu *et al.* [26]. Each nanoparticle is represented as a RIGID aggregate of 30 DPD beads, with each bead having a diameter of approximately 80 nm. The complete mapping between simulation units (LJ reduced form) and physical units is provided in Table II.

TABLE II. Mapping between simulation (LJ) units and physical units.

Quantity	LJ units	Physical units	Notes
Length (σ)	1	300 nm	Particle diameter
Bead diameter	—	80 nm	30 beads/particle
Energy (ϵ)	$2.5kT$	1.03×10^{-20} J	At $T = 300$ K
Mass (m)	1	3.5×10^{-17} kg	$\rho_s = 2500$ kg m $^{-3}$
Time (τ)	1	2.8×10^{-5} s	$\tau = \sigma(m/kT)^{1/2}$

The shear rate range in our simulations is mapped to match the experimental range of 0.01 to 100 s $^{-1}$ reported by Liu *et al.* [26]. At the intermediate shear rate $\dot{\gamma} = 10$ s $^{-1}$, the Péclet number $\text{Pe} = 6\pi\eta_s\dot{\gamma}a^3/(k_B T) \approx 0.15$, while at $\dot{\gamma} = 100$ s $^{-1}$, $\text{Pe} \approx 1.5$. This indicates that the system spans the transition from Brownian-dominated to hydrodynamically dominated behavior within the experimental shear rate range, which is precisely where shear thickening phenomena are most pronounced.

APPENDIX D: COMPUTATIONAL DETAILS AND CODE AVAILABILITY

All simulations were performed using LAMMPS (large-scale atomic/molecular massively parallel simulator), version 23 June 2022, which is a widely used open-source molecular dynamics package developed and maintained by Sandia National Laboratories. We utilized several standard packages included in the LAMMPS distribution: the DPD-BASIC package for standard DPD conservative, dissipative, and random forces; the GRANULAR package for Hertzian contact mechanics with sliding friction; and the RIGID package for treating multibead particles as RIGID bodies.

The short-range attractive force based on the soft Lennard-Jones potential was implemented as a custom pair style following the free energy perturbation formulation of Beutler *et al.* [45] and the shear thickening simulation approach of Pednekar *et al.* [46]. The hydrodynamic lubrication force was implemented as a pairwise correction following the formulation of Foss and Brady [42]. These custom implementations were written in C++ and compiled as shared libraries that interface with the main LAMMPS executable.

Simulations were performed on the High-Performance Computing Cluster. Typical production runs consisted of 10^7 time steps with $\Delta t = 0.01\tau$, requiring approximately 48–72 h on 64 CPU cores for each parameter set. All random number seeds are documented in the input scripts to ensure reproducibility, and we have verified that independent runs with the same parameters yield statistically consistent results within the expected thermal fluctuations.

APPENDIX E: EXPERIMENTAL DETAILS

1. Materials

Commercial SiO_2 nanoparticles were purchased from Andy Metal Materials Co., Ltd. (China). Polyethylene glycol with molecular weight of 200 (PEG200) was purchased from

Sinopharm Chemical Reagent Co., Ltd. (China). All materials were used as received without further purification.

2. Suspension preparation

Prior to use, commercial SiO₂ particles were dried in an oven at 100 °C for 10 h to remove surface-adsorbed moisture. According to the designated mass fractions, SiO₂ particles of different masses were weighed and placed into a ball mill tank, and the corresponding volume of PEG200 was measured and added. The mixture was ball milled for 24 h to obtain a homogeneous STF. The mass fraction of SiO₂ in the suspension was varied from 46 to 64 wt % to investigate concentration effects on shear thickening behavior.

3. Particle characterization

The microstructures of commercial SiO₂ particles were characterized using a scanning electron microscope (SEM, Gemini SEM 500) at an acceleration voltage of 3 kV. As shown in the SEM micrographs, SiO₂ exhibits uniform dispersion with an average diameter of 300 nm and a polydispersity of less than 5%, which is beneficial for forming a stable suspension. The particle size distribution was confirmed by

dynamic light scattering measurements, which yielded consistent results with the SEM observations.

4. Rheological measurements

The rheological properties of the prepared STF were tested using a rotational rheometer (Anton-Paar MCR 302) equipped with parallel plate geometry (25 mm in diameter). The experiments were conducted with a gap size of 1 mm at 25 °C under shear rates ranging from 0.1 to 1000 s⁻¹. In the test phase, a preshear at 0.1 s⁻¹ was applied for 20 s until the viscosity of the system was stable, and then the formal shear test began. This preshear protocol ensures reproducible initial conditions by eliminating any residual structure from sample loading.

To evaluate the stability of the prepared STF, steady-state shearing tests were performed at various constant shear rates (1, 10, 100, 200, and 500 s⁻¹) for 120 s each. The viscosity remained stable throughout these tests, confirming the stability of the suspension.

Temperature-dependent rheological measurements were also carried out at 15, 25, 35, 45, 55, and 65 °C. The STF exhibited shear thickening behavior over this entire temperature range, with the shear thickening effect becoming more pronounced at lower temperatures due to reduced Brownian motion of the dispersed phase particles.

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