SIMULATION MODEL OF DRYING COLLOIDAL SUSPENSION ON SUBSTRATE

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OUTLINE

- Continuous coating of colloidal suspension on substrate
- Direct simulation model for drying colloidal suspension
- Demonstration of present simulation model
CONTINUOUS COATING ON SUBSTRATE

- Suspension
- Flow
- Drying
- Film
- Structure formation

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PECLÉT NUMBERS

coating Peclét number  
\[ \text{Pe}_c = \frac{cd^2}{Dh} \]

drying Peclét number  
\[ \text{Pe}_d = \frac{eh}{D} \]

Peclét numbers ratio  
\[ \frac{\text{Pe}_c}{\text{Pe}_d} = \frac{c}{e} \left( \frac{d}{h} \right)^2 \]

\[ \frac{\text{Pe}_c}{\text{Pe}_d} \sim 1 \]

Both flow and drying influence structure formation
OBJECTIVES OF THIS STUDY

- Develop direct simulation model for drying colloidal suspension
- Perform flow simulations of colloidal suspension on sliding substrate with drying of solvent
- Quantify coating-drying dynamics
  - structure of particles
  - variable drying rate
DIRECT SIMULATION MODEL

- Solves gas-liquid two phase flow on lattice using VOF (volume of fluid) method
- Solves translational/rotational motion of particles subject to contact, DLVO, capillary interactions
- Couples motion of particles with flow of solvent using immersed boundary method

Interparticle hydrodynamic interaction is included without analytical model
EQUATIONS OF FLUID MOTION

\[ \rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p - \frac{2}{3} \nabla \cdot \left\{ \mu (\nabla \cdot \mathbf{v}) \mathbf{I} \right\} + \nabla \cdot \mu \left\{ \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right\} + \nabla \cdot \mathbf{S} + \Phi \alpha \]

fluctuating stress

acceleration

\[ \alpha = \rho \frac{\mathbf{v}^p - \mathbf{v}}{\Delta t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p + \frac{2}{3} \nabla \cdot \left\{ \mu (\nabla \cdot \mathbf{v}) \mathbf{I} \right\} - \nabla \cdot \mu \left\{ \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right\} - \nabla \cdot \mathbf{S} \]

\[ \rho = f \rho_1 + (1 - f) \rho_g, \quad \mu = f \mu_1 + (1 - f) \mu_g \]

\[ \frac{\partial f}{\partial t} + (\mathbf{v} + \mathbf{v}_e) \cdot \nabla f = 0 \]

local drying velocity

\[ \nabla \cdot \mathbf{v} = \frac{\rho_1 - \rho_g}{\rho} \mathbf{v}_e \cdot \nabla f \]
EQUATIONS OF PARTICLE MOTION

\[ m \frac{dv}{dt} = F^{co} + F^D + F^{ca} + F^h \]

\[ I \frac{d\omega}{dt} = T^{co} + T^h \]

\[ F^h = - \int_{V_p} \rho \Phi \alpha dr \]

\[ T^{h} = - \int_{V_p} (r \times \rho \Phi \alpha) dr \]

acceleration
SIMULATION CONDITION

- drying
- sliding substrate

$d = 0.1 \mu m, \phi_0 = 20 \text{ vol}\%, \zeta = -50/0 \text{ mV}$
$c = 13 \text{ cm/s}, e = 1.4 \text{ cm/s} \quad \Rightarrow \quad \text{Pe}_c / \text{Pe}_d = 1$
QUANTIFICATION OF STRUCTURE

Non-dimensional Boundary Area (NBA)

\[ \text{NBA} = \frac{\text{surface area of aggregates}}{\text{total surface area of particles}} = \frac{1}{12N} \sum_{k=0}^{12} \left( (12 - k) n(k) \right) \]

- \( k \) : coordinate number
- \( n(k) \) : number of particles with coordinate number of \( k \)
- \( N \) : total number of particles

- NBA=0 : 3D hexagonal close-packed
- NBA=0.5 : 2D hexagonal close-packed
- NBA=1 : complete-dispersed
STRUCTURE OF PARTICLES

\[ \zeta = -50 \text{ mV} \]

NBA vs interface height

potential induced aggregation

drying induced aggregation

\[ \zeta = 0 \text{ mV} \]
\[ \zeta = -50 \text{ mV} \]
VARIABLE DRYING RATE

drying rate vs interface height

$drying rate \text{ vs interface height}$

$\dfrac{m'}{[g/cm^2s]}$

$\dfrac{h}{d}$

--- pure solvent
--- calculated ($\zeta=-50mV$)
--- smoothed
CONCLUSION

- Developed direct simulation model for drying colloidal suspension
- Quantify structure formation of particles using NBA
- Quantify variable drying rate in which constant rate of drying changes to decreasing rate of drying.