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Sheng Chen

Microparticle Dynamics in Electrostatic and Flow Fields

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Dedicated to my family.

Supervisor's Foreword

Adhesive particle flow arises in many applications in industry, nature, and life sciences and has driven great research interests in areas of aerosol filtration, dust mitigation, nanoparticle deposition, ceramics manufacturing, fouling of MEMS devices, sediment transport, and production of fuel cells. An in-depth understanding of the relationship between microscopic interparticle interactions and the collective behavior of a large number of particles would be helpful to understand and further design large-scale devices. However, linking the microscopic properties of discrete particles to the macroscopic behaviors of particle flow systems is never a simple task. The difficulty lies in the complicated interacting modes between particles, namely the electrostatic interaction, the hydrodynamic interaction, and the contact interactions, across several orders of magnitude in time and length scales.

Within the past few decades, the discrete element method (DEM), in which the motion, collision, and adhesion of individual particles are resolved in time and space, has been developed to model particle collective dynamics from single-particle level. DEM coupled with computational fluid dynamics (i.e., CFD-DEM) has shown powerful capabilities in investigating particle-laden flows. Moreover, there has recently been rapid progress on understanding the physics related to the intermolecular and surface forces, which enable us to develop more rational adhesive contact models. Scalable and efficient computational frameworks have also been proposed for handling long-range many-body interactions and for collision resolution. It is recognized that merging the expertise across various disciplines of fluid and solid mechanics, condensed matter physics, materials science, and applied mathematics will significantly improve our understanding of particle dynamics in electrostatic and flow fields.

The objective of this thesis is to propose new approaches for modeling contacting interactions and electrostatic interactions between microparticles in the framework of discrete element methods and to present an insightful view on the agglomeration, migration, and deposition of microparticles in electrostatic and flow fields. The first chapter discusses various applications of adhesive particle flows. Chapter 2 starts with a simple case of binary collisions of adhesive particles to show how the discrete element method gives the information on the force, the displacement, and the energy conversion. A novel fast DEM based on the reduced particle Young's modulus is then proposed to accelerate the computation. In Chap. 3, the fast DEM is coupled with direct numerical simulation to investigate the agglomeration of particles in homogeneous isotropic turbulence. The structure and the size distribution of agglomerates are obtained. The agglomeration and collision-induced breakage rates are formulated based on the classic theory for particle collisions in turbulence. In Chap. 4, the evolution of spherical clouds of charged particles that migrate in a uniform external electrostatic field is then investigated by Oseen dynamics and a continuum approach, and the scaling laws for evolution of cloud radius and particle number density are derived. Finally, in Chaps. 5 and 6, an elaborate investigation of the deposition of charged particles on a flat plane and fibers is presented. The findings, together with previous results for neutral particles, form a more complete picture of filtration and deposition of microparticles.

I believe that the results in this book will substantially impact the field relevant to adhesive particle flows. Beyond that, the findings here may also have broader implications for granular fluidization, liquid–solid suspensions, and colloidal gels, where complicated particle–particle interactions exist.

Beijing, China Prof. Shuiqing Li
January 2021

Parts of this thesis have been published in the following journal articles

- **S. Chen**, S. Li. Collision-induced breakage of agglomerates in homogenous isotropic turbulence laden with adhesive particles, Journal of Fluid Mechanics, 2020, 902, A28.
- **S. Chen**, S. Li, J. S. Marshall. Exponential scaling in early-stage agglomeration of adhesive particles in turbulence, Physical Review Fluids, 2019, 4(2): 024304.
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- **S. Chen**, T. Bertrand, W. Jin, M. D. Shattuck, C. S. O'Hern, Stress anisotropy in shear-jammed packings of frictionless disks, Physical Review E, 2018, 98(4): 042906.
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- **S. Chen**, S. Li, W. Liu, H. A. Makse, Effect of long-range repulsive Coulomb interactions on packing structure of adhesive particles. Soft Matter, 2016, 12:1836–1846.
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Contents

Nomenclature

English Characters (Lowercase)

a	Radius of contact region between two colliding particles (m)
$\hat{b}$	Impact parameter
$\mathrm{d}t_F$	Fluid time step (s)
$\mathrm{d}t_P$	Particle convective time step (s)
$\mathrm{d}t_C$	Collision time step (s)
e	Coefficient of restitution
e_0	Elementary charge (1.6×10^{-19}C)
f	Friction factor for viscous drag
i	Particle ID
k	(i) Wave number; (ii) permeability (m^2)
k_N	Elastic coefficient in normal direction (N/m)
k_T	Elastic coefficient in tangential direction (N/m)
m	Mass (kg)
$\mathrm{g}(r)$	Radial distribution function
n	Particle number density (m^{-3})
$\dot{n}_c$	Collision rate of particles per unit volume ($\mathrm{s}^{-1}\mathrm{m}^{-3}$)
p	(i) Pressure (Pa); (ii) dipole strength (Cm)
q	(i) Turbulent kinetic energy ($\mathrm{m}^2/\mathrm{s}^2$); (ii) particle charge (C)
r	Position vector (m)
r_p	Particle radius (m)
r_f	Fiber radius (m)
t	Time (s)
u	Flow velocity, (m/s)
u'	Turbulent velocity fluctuations (m/s)
u_s	Slip velocity (m/s)
v	Particle velocity (m/s)
v_n	Normal component of the colliding velocity (m/s)

English Characters (Uppercase)

A	Agglomerate size
Ad	Adhesion parameter
El	Elasticity Parameter
D_f	Fractal dimension of particle agglomerate
E	Particle Young's modulus (Pa)
E	Electric field (V/m)
E_R	Reduced particle Young's modulus (Pa)
F	Force on particles (N)
F_C	Critical pull-off force (N)
F_l	Lubrication force (N)
I	Moment of inertia of particles (kgm^2)
M	Torque on particles (Nm)
N_C	Number of collision events
N_S	Number of sticking events
N_R	Number of rebound events
N_B	Number of breakage events
R_0	Radius of particle cloud (m)
R_{ij}	(i) Reduced particle radius (m); (ii) radius of collisional sphere (m)
Re	Reynolds number
Re_p	Particle-scale Reynolds number
Re_λ	Taylor-scale Reynolds number
R_g	Gyration radius of particle agglomerate (m)
S	Size ratio between a particle and a cloud
St	Stokes number
St_k	Kolmogorov-scale Stokes number
T_e	Large eddy turnover time (s)
V_{CN}	Normal component of critical sticking velocity (m/s)
V_{C0}	Critical sticking velocity for head-on collisions (m/s)
W_i	Volume of Voronoi cell
$\boldsymbol{W}_{ij}$	Kernel for particle–particle hydrodynamic interaction
Z	Coordination number

Greek Symbols

α	Damping coefficient for particle collisions
β	(i) Particle size ratio; (ii) parameter for the agglomerate size distribution
γ	Particle surface energy density (J/m^2)
Γ	Particle collision kernel (m^3/s)
Γ_a	Particle agglomeration kernel (m^3/s)
δ	Overlap between contact particles (m)