Optimization of granular flows for industrial applications

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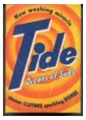


My Background:

- Ceramic Science and Engineering
- Started at P&G in 1993, focus on detergent.
  - Involved w/ IFPRI† while at P&G.

Ceramics…

- Aluminosilicate powder
- Add a little surfactant/ polymer as a process aid,
- Forming process…

Detergent…

- Surfactant active
- Add a little aluminosilicate as a process aid,
- Granulation process…

Industrial issue…

Products with high organic compositions may be softer, stickier and more susceptible to fouling in processes that require granular flow:

- Mixing,
- Milling,
- Agglomeration,
- Drying,
- Conveying…


Saint Gobain Ceramics

Procter & Gamble

Motivation – optimizing processes that handle particulates either as intermediates or end products

- We desire efficient processes:
  - Maximize production throughput ← Dense flows are of interest
  - Minimize the spent energy. ← Optimize the use of energy to achieve desired product transformation
- Two aspects in this optimization:
  1. Process equipment and its integration within a system; and
  2. Properties of the particulate material that are relevant to the processing conditions, specifically the material's response to flow and stress fields that are imposed by the process equipment.
- Industrially-relevant materials have a complex coupling among:
  - imposed flow field and boundary conditions,
  - constitutive properties of the material function of shear rate, packing density…

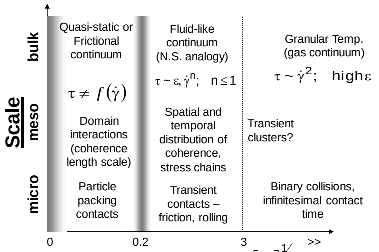
$$\int_{time} \frac{stress \cdot flow}{mass} = specific\,energy$$

  - resultant stress & energy consumption.
- Optimization requires understanding of flow and stress fields.

Multi-scale Approach to Particulate Flow

Is there an optimal particle flow operating regime?

- **Fluid-like;**
- **Dense flow;**
- **Efficient particle interactions:**
  - **Boundaries,**
  - **Particles,**
  - **added Liquid,**
  - **Gas.**
- **Low E/M.**



		0	0.2	3	>>	
Inertia / confinement,	$I = \frac{\dot{\gamma} \cdot d_p}{\sqrt{P \cdot \rho_0}}$	Dimensionless shear rate, $\dot{\gamma}^* = \dot{\gamma}\left[\frac{d_p}{g}\right]^{1/2}$				(Tardos, Savage) (GDR Midi)
Contact time	t_c / t_{bc}	high	~2	1		(Campbell)
Stiffness/shear	$\frac{k}{\dot{\gamma} \cdot \rho \cdot d^3}$	high		low		(Campbell)
Stokes #	$\frac{m\dot{\gamma}}{6\pi\eta d}$	0	~10	high		(Brady)

Coupling of particulate flow and stress fields – a multi-scale challenge

micro…

- Fundamental understanding of particulate flow and stress fields and their material coupling.
- Particle-particle and particle-boundary interaction:
  – particle characteristics such as size, size distribution, shape, surface characteristics, and properties such as complex modulus.
- Flow and stress in critical sections of the process, e.g., the gap between an impeller and a process boundary.
- Unit operation, its flow fields, residence time distributions and scale-up.
- System scale of ancillary process interactions:
  – feeders, intermediate storage, product and intermediate handling, recycle integration, etc.

…macro…

5) What can we infer about stress based on power and/or torque measures? Granular rheology

6) Implication of local stress fluctuations

1) Survey experiments and models of flow
2) Apply to mixing
3) Process optimization

4) Process control

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Survey of experiments and models of flow

– Optimize process using fluid-like flow; link regime map to operating strategy.

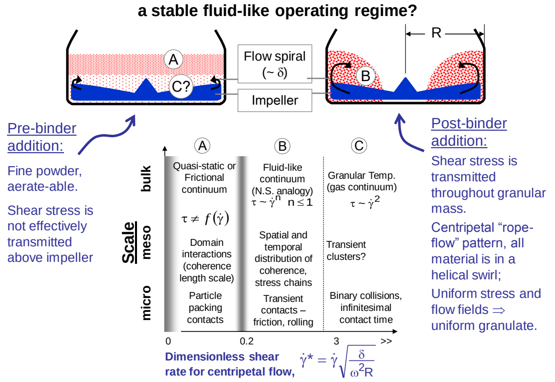
– Examples:
  - Centrifugal flow granulators.
  - Dual-axis mixers.

Flow Fields in Mixer-Granulators

- Stress-bounded flow, at least one free surface
- Dominant driving force:
  - Gravity / Centripetal force / Air fluidization

$Fr = \omega^2 r/g > 1$

Vertical axis mixer/granulators – a stable fluid-like operating regime?



$$\dot{\gamma}^* = \dot{\gamma}\sqrt{\frac{\delta}{\omega^2 R}}$$

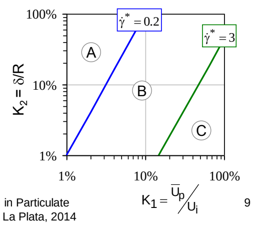
Centripetal flow-field analysis for scale-up

- At high Fr#, substitute $\omega^2 r$ for g.
- Let K_1 be the ratio of tangential particle velocity vs. impeller velocity, U_p/U_i
- Let K_2 be the ratio of axial shear transmission / mixer radius, δ/R
- Then the rotational speed drops out of the equation…
- …providing a fairly broad "intermediate regime" flow field.

$$\dot{\gamma}^* = \dot{\gamma}\sqrt{\frac{\delta}{\omega^2 R}}$$

$$\dot{\gamma} = \frac{\overline{U}_p}{\delta/2} = \frac{2K_1 U_i}{\delta} = \frac{4K_1 \omega R}{\delta}$$

$$\dot{\gamma}^* = \dot{\gamma}\sqrt{\frac{\delta}{\omega^2 R}} = \frac{2K_1}{\sqrt{K_2}}$$



What about scale-up of stress field?

Examples: Modeling and Characterization of Flow

Considerable work has been reported on characterization and modeling of powder flow behavior during mixing under various process conditions.

A partial list:

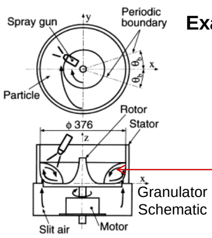
- M. Moakher, T. Shinbrot, F. Muzzio, "Experimentally validated computations of flow, mixing and segregation of non-cohesive grains in 3D tumbling blenders," (2000).
- Y. Muguruma, T. Tanaka, Y. Tsuji, "Numerical simulation of particulate flow with liquid bridge between particles simulation of centrifugal tumbling granulator," (2000).
- Motion in a Particle Bed Agitated by a Single Blade, AIChE Journal, Volume 46, 2000, B. F. C. Laurent, J. Bridgwater and D. J. Parker
- R. Yang, R. Zou, A.B. Yu, "Micro-dynamic analysis of particle flow in a horizontal rotating drum," (2003).
- S. Forrest et al, "Flow patterns in granulating systems," (2003).
- A. Hassanpour, HS Tan, et al, "Analysis of Particle Motion in a Paddle Mixer," (2009).

Experimental validation of flow fields vs. Discrete Element Method simulations provide reasonable agreement:

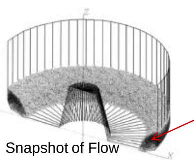
- DEM uses "ideal particles" and manipulated DEM model parameters (stiffness, damping, restitution, friction, simplified boundary conditions…)
- Experimental measures (PEPT, NMR, optical tracers…) include realistic particles in small-scale industrial mixers.

Example: Model and validation of a centrifugal-flow granulator

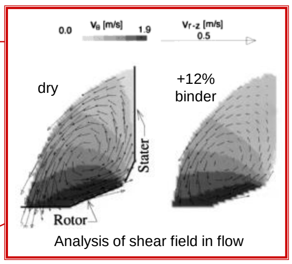
*Y. Muguruma, T. Tanaka and Y. Tsuji, "Numerical simulation of particulate flow with liquid bridge between particles," Powder Technology, 109 (2000).



Granulator Schematic

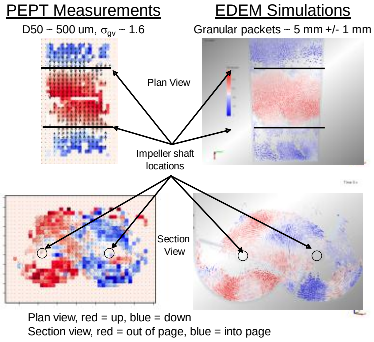


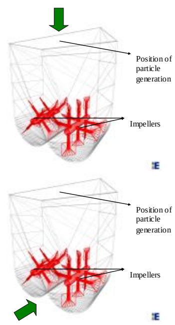
Snapshot of Flow



Analysis of shear field in flow

Example: Comparison of Time-Averaged Particle Flow





A Hassanpour et al, "Analysis of Particle Motion in a Paddle Mixer," Sheffield Granulation Conference (2009).

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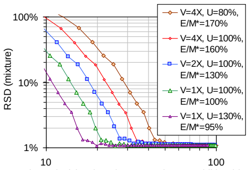
Apply flow model to mixing process

- Markov Chain model
  - adapted from Freireich & Wassgren, Purdue Univ.

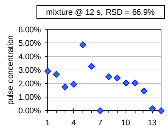
Batch mixing analysis – Markov Chain approach

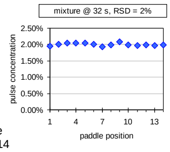
	Channel A			Channel B			
paddle	type	forward	cross	cross	forward	type	paddle
1	fwd	70%	30%	100%	0%	rev	14
2	fwd	70%	30%	30%	70%	fwd	13
3	fwd	70%	30%	30%	70%	fwd	12
4	fwd	70%	30%	30%	70%	fwd	11
5	fwd	70%	30%	30%	70%	fwd	10
6	fwd	70%	30%	30%	70%	fwd	9
7	rev	0%	100%	30%	70%	fwd	8

- Add “pulse” tracer over a paddle position.
- Model dispersion over time.
- Asymptote at about 13-14 revolutions.
  - Blend # (B) scales with revolutions.



- Mixer volume (V)
- Tip speed (U)
- E/M* is specific energy (kJ/kg) required to mix to <2% RSD





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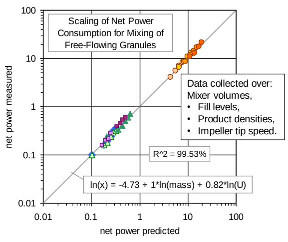
Process optimization

- Mixer example (using Markov model)

Process optimization

Empirical model for free-flowing granular materials:

- Power (P) scales with mass (M) and dimensionless impeller speed (υ):
  $P / M = k \cdot \upsilon^m$
- Specific Energy (E/M) calculated over residence time (τ):
  $E / M = (P/M) \cdot \tau = k \cdot B \cdot 2\pi R \cdot (\upsilon)^{m-1}$
  Blend # (B)
  Mixer radius (R)



Production efficiency model:

$M' / V = (\phi \cdot \rho) / [(2\pi R \cdot B / u) + \beta]$

- Paddle tip speed (u)
- Product density (ρ)
- Fill level (φ)
- Batch transition idle time, →0 for continuous (β)
- Mass throughput / mixer volume (M' / V)

Process optimization…

Integrate rate and energy models. Consider:

- achievable production efficiency (M'/V)
- specific energy input (E/M)

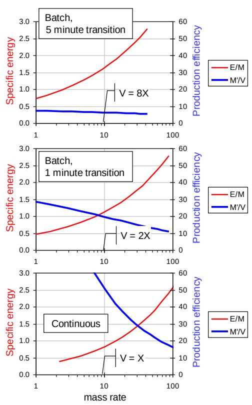
as a function of mixer size and operating strategy:

- batch or continuous,
- batch transition time;

all other parameters held equal (tip speed, Blend #, density, fill level).

Continuous operation can improve efficiency & simplify scale-up.

Continuous operation requires achievable steady-state operation.



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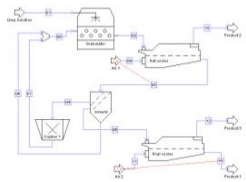
Process control

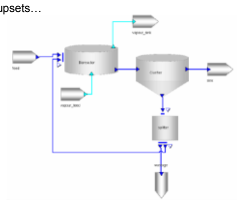
- System flowsheets
- Agglomerator example
  - Doyle group, UCSB, IFPRI project

Particulate process control – achievable steady state?

- Continuous processes typically have recycle combined with raw material feeds.
  - Ratio of recycle / raw material affects the process;
    - An important parameter in a multivariate control problem.
- At steady state, recycle production must be balanced with its consumption.
  - Do we need a recycle surge to get to steady state?
- Flowsheet models integrate process models:
  - Useful to optimize *system performance*:
    - Achievable steady states
    - Dynamics, startup, shutdown, changeovers, upsets…



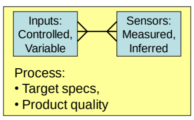
Urea granulator example, http://www.solidsim.com/www/examples-of-use

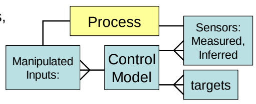


Bioreactor example, www.psenterprise.com/gproms/ …/biotreatment_white_paper.pdf

Multivariate process control

Particulate processes have many:many relations among sensors, actuators, and product attributes…





…use a control model to convert many:many relations into more tractable one:many relations.

For 1:1 relations (sensor:actuator), simple PI or PID controllers can be used.

- Note, a sensor may be inferred (soft) based on a model.

For multivariate relations, consider:

- Integrated mode control – may be empirical, e.g., based on a multivariate data regression.
- Model predictive control – predicts forward based on process simulation, compares predicted and measured outputs.

Example: Continuous Detergent Agglomeration

- High throughput production of Detergent Granules in continuous granulation.
- Integrated recycle systems.
- Variety of in-process sensors and actuators are used to meet product specifications, a multivariate problem.
- Agglomeration processes tend to be under-actuated – not easy to reverse coalescence…

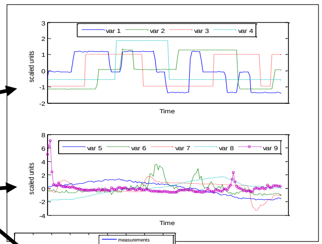
Normal production…

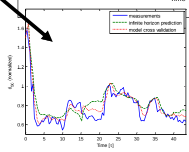
…is there a steady state in a binder-granulation process?

Material properties in coupling of flow & stress fields are critical to the answer!

Process control modeling and validation using "Persistent Excitation"

- Multiple handles are adjusted within relevant operational window (as per model prediction).
- Validate by statistical comparison of measured results and model prediction. Is there a bias?
- How do model biases compare to known operational biases in plants?





Frank Doyle group (UCSB), IFPRI project

5

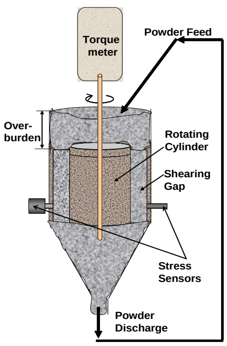
What can we infer about stress based on power and/or torque measures?

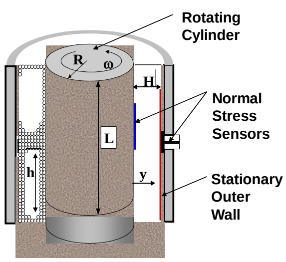
Granular rheology

- Instrumented axial Couette
  - Tardos & Kheiripour, CUNY
    - Constitutive characterization of dense flows in the intermediate regime (IFPRI)

Granular Rheology – stress analysis in Couette flow

- Tardos and Kheiripour, CCNY, IFPRI
- Interrogate stress field in a drained vertical couette flow





Experimental options:

- closed-bed (Batch, → close packed);
- open-bed (Continuous, → allow dilation)

Multi-scale Approach to Particulate Flow

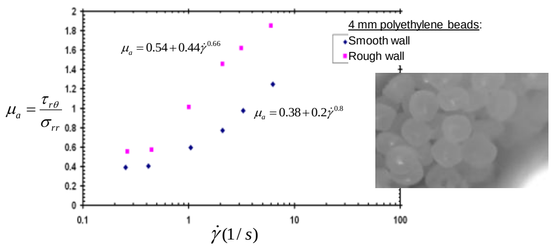
Is there an optimal particle flow operating regime?

- **Fluid-like;**
- **Dense flow;**
- **Efficient particle interactions:**
  - **Boundaries,**
  - **Particles,**
  - **added Liquid,**
  - **Gas.**
- **Low E/M.**

Scale	0 – 0.2	0.2 – 3	3 – >>
bulk	Quasi-static or Frictional continuum $\tau \neq f(\dot{\gamma})$	Fluid-like continuum (N.S. analogy) $\tau \sim \varepsilon, \dot{\gamma}^n;\ n \leq 1$	Granular Temp. (gas continuum) $\tau \sim \dot{\gamma}^2;$ high ε
meso	Domain interactions (coherence length scale)	Spatial and temporal distribution of coherence, stress chains	Transient clusters?
micro	Particle packing contacts	Transient contacts – friction, rolling	Binary collisions, infinitesimal contact time

		0	0.2	3	>>	
Inertia / confinement,	$I = \frac{\dot{\gamma} \cdot d_p}{\sqrt{P \cdot \rho_0}}$	Dimensionless shear rate, $\dot{\gamma}^* = \dot{\gamma}\left[\frac{d_p}{g}\right]^{1/2}$				(Tardos, Savage) (GDR Midi)
Contact time	t_c / t_{bc}	high	~2	1		(Campbell)
Stiffness/shear	$\frac{k}{\dot{\gamma} \cdot \rho \cdot d^3}$	high		low		
Stokes #	$\frac{m\dot{\gamma}}{6\pi\eta d}$	0	~10	high		(Brady)

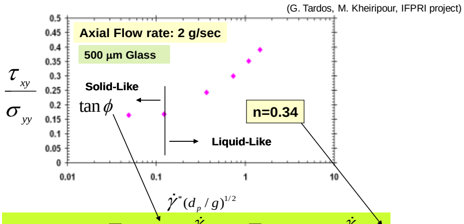
Shear / normal stress ratio as a function of boundary conditions



(G. Tardos, M. Kheiripour, IFPRI project)

Determine Constants in Constitutive Equation from Rheometer Experiments in Couette Device

(G. Tardos, M. Kheiripour, IFPRI project)



$$T_{ij} = p\delta_{ij} + \sqrt{2}p\sin(\phi)\frac{\dot{\gamma}_{ij}}{|\dot{\gamma}_{ij}|} + \sqrt{2}ap\cos(\phi)\frac{\dot{\gamma}_{ij}}{|\dot{\gamma}_{ij}|}\dot{\gamma}_{ij}^{n}$$

Schaeffer Equation (solid- like behavior) — Liquid-like behavior

Growing interest in applying intermediate regime rheology to <u>continuum</u> flow solvers

Effect of particle shape

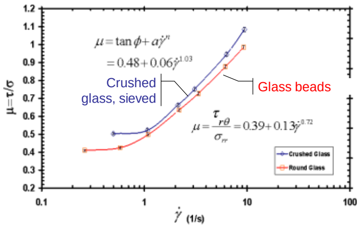


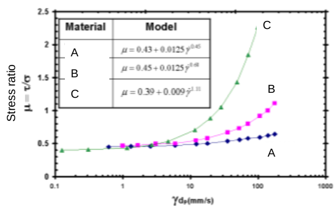
Figure 3: Measured ratio of shear to normal stresses (apparent friction coefficient) as a function of shearing rate; 1 mm in diameter, round and crushed (odd-shaped) glass. Fitted curve also shown in the figure.

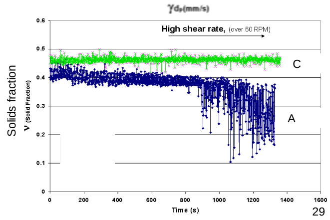
(G. Tardos, M. Kheiripour, IFPRI project)

Coupling of stress and dilation

Capacitance sensor measures solids fraction in Couette gap.

- Various elastomeric materials (A,B,C) show markedly different stress and packing profiles
- Power law rheology is stronger for materials that retain packing state with increasing shear.
  - Analogy w/ incompressible fluids?
- Materials that dilate with large fluctuations in packing can maintain relatively stable stress ratios at higher strain rates.
  - Average can be steady, local highly fluctuating.

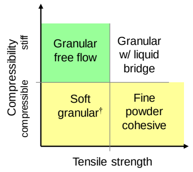




What about compressible powders?

Free-flowing granules tend to be stiff and elastic

- If particles are stiff and elastic, springback → dilation.
  - Note, "elastic-inertial" regime, C.S. Campbell / Powder Technol 162 (2006)
- If particles are soft (e.g., viscoplastic) and the local stress exceeds the particle's deformation yield stress (σ_y)…
- While average stress may be < σ_y, stress *fluctuations* may initiate fouling; once started, fouling may propagate.



… smearing and build-up on boundaries can happen (fouling).

† May become cohesive under higher consolidation stress, i.e., an upward curving flow fuction

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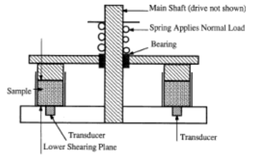
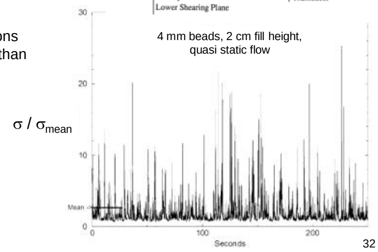
Local stress chains and stress fluctuations

- Stress chain visualization and measurement
  - Behringer group, Duke University
    - Dynamics and Rheology of Cohesive and Deformable Granular materials (IFPRI)

Stress fluctuations in volume-constrained flow

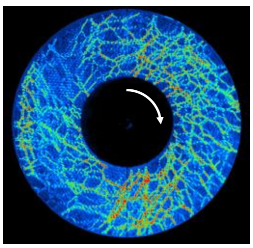


In a confined flow…
Local stress fluctuations may be much higher than the average stress.



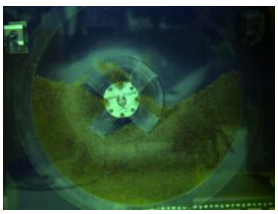
Behringer et al

Spatial distribution of stress chains



Iconic image of stress chains illuminated by photo-elastic particles in vertical axis 2-D Couette flow

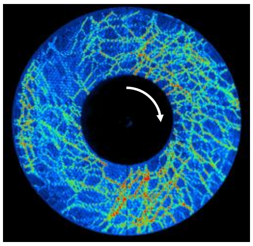
Behringer group, Duke University



Horizontal axis, modified impeller

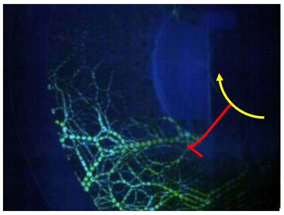
Behringer, Clark, IFPRI project

Spatial distribution of stress chains



Iconic image of stress chains illuminated by photo-elastic particles in vertical axis 2-D Couette flow

Behringer group, Duke University



Horizontal axis, modified impeller "paddle" edge highlighted in red.

Stress chains extend from paddle tip to wall of mixer – implies opportunity for jamming.

Summary 1: Constitutive relations in process optimization

- Take advantage of fluid-like granular rheology
  - "Intermediate" or "elastic-inertial" regime.
  - Innovation by analogy?
- Energy can be analyzed in terms of stress and flow fields. Stress and flow are coupled via granular constitutive properties.
  - Success or failure of particulate process scale-up and optimization depends on understanding of material-process interactions.
  - Much progress in DEM and continuum modeling; many challenges remain!

Summary 2: Apply granular rheology in process models

- Take advantage of continuum models in broader process context.
- Modeling can be used to drive process efficiency:
  - System scale, dynamic flowsheets
  - Macro scale (unit op), throughput and energy efficiency as a function of scale up and operating mode.
  - Model-based process control.
  - Multi-scale modeling continues to be an important opportunity.

Summary: Granular Flow Topics

- Flow fields in mixers – examples show growth of basic understanding and modeling capability.
  - DEM models show good predictive capability of macroscopic flow, even with "packet" particles up to 10X actual.
  - Growing interest and capability in continuum modeling using granular rheology.
- Stress fields (and energy dissipation) are coupled with flow via granular constitutive properties.
  - Granular flows can compress and dilate, rheology, $\sigma = f(\gamma', \varepsilon)$
  - Important considerations:
    - Boundary conditions,
    - Particle's material properties (e.g., elastic vs. visco-plastic),
    - Particle's shape, size distribution, frictional characteristics
- Understanding of fluctuations and jamming may be critical, especially in confined volume flows.
  - A statistical mechanics approach using stress chain characteristics?

Thank-you for your kind attention