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Detailed Simulation of Particle and Liquid Distribution in the Mixing Zone of a Twin-Screw Granulator

A. Kumar, S. Radl, J.G. Khinast, K.V. Gernaey, T. De Beer, I. Nopens

Wednesday, November 11, 2015: 9:38 AM

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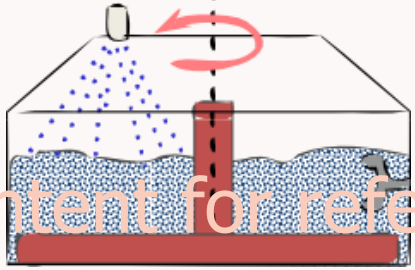
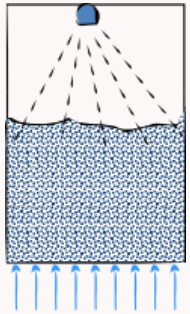
Traditional to new granulation method

High-shear mixer



Drum

Fluidised-bed

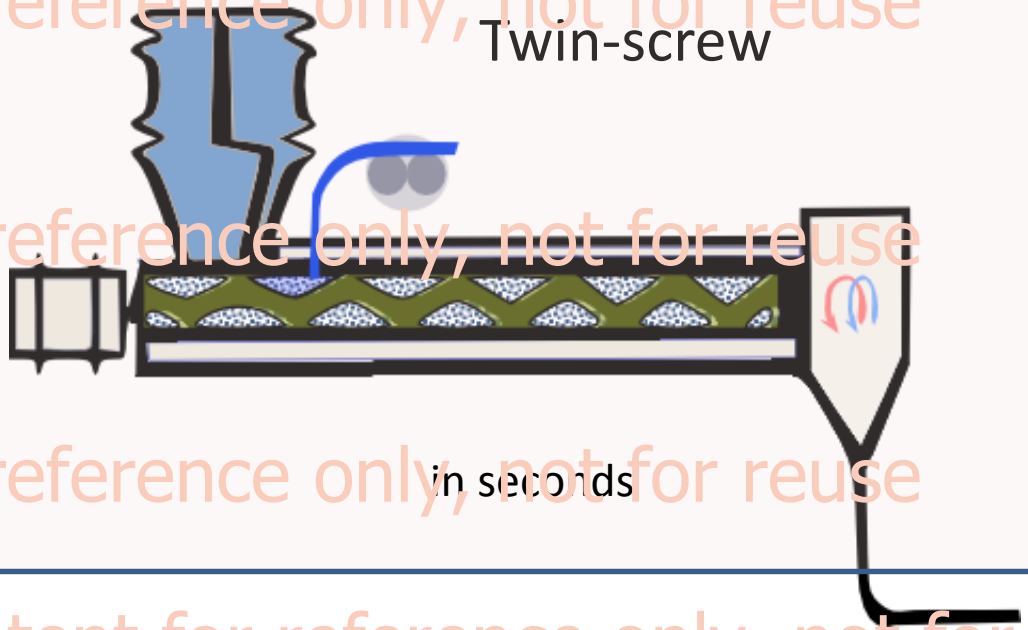


From minutes to hours

Batch

Continuous

Twin-screw



in seconds

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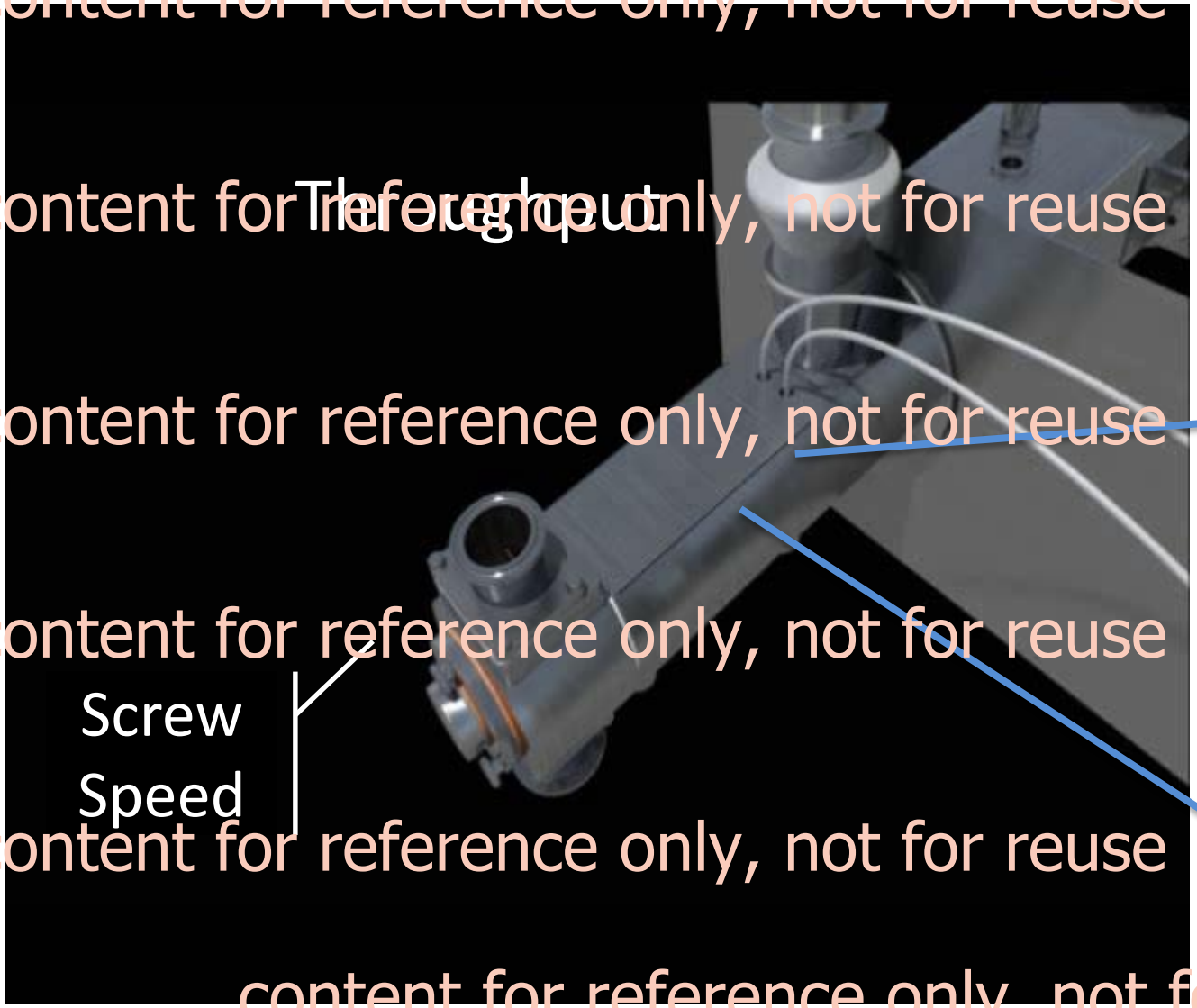
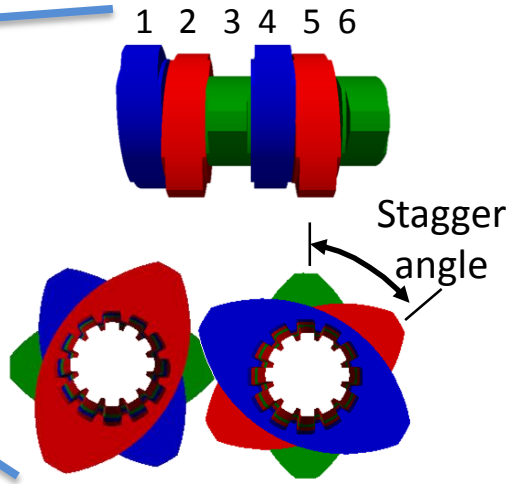
Design of granulator screw, screw speed, material feed rate control granulation



Kneading discs at certain stagger angle



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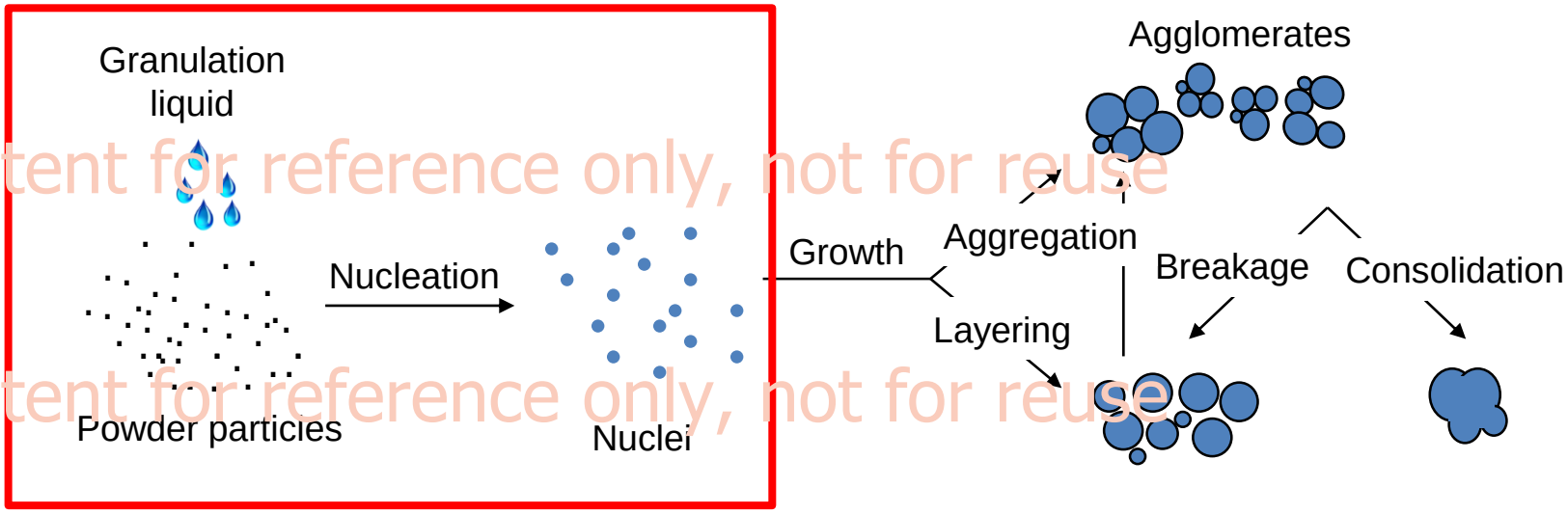
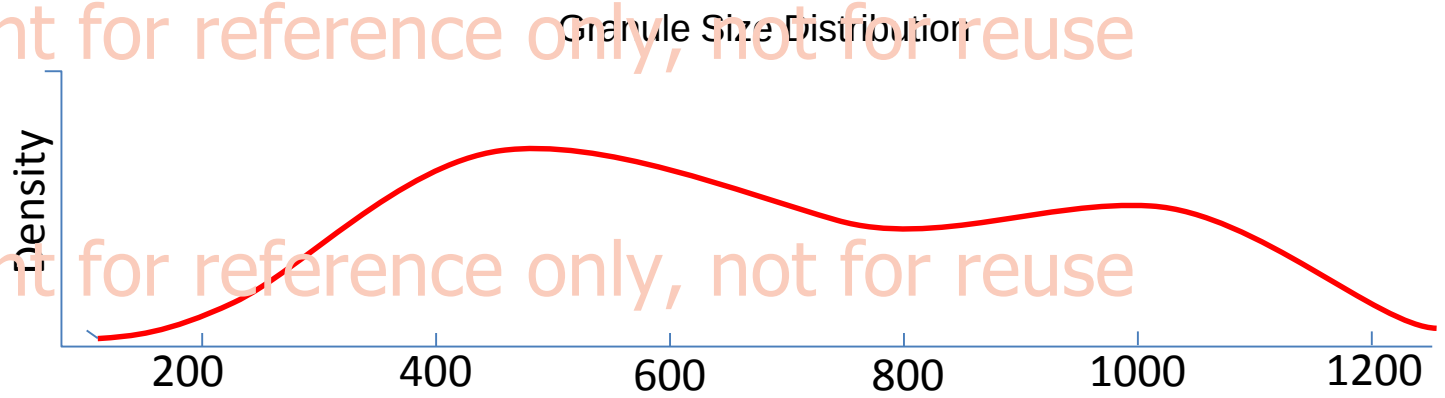
Wet Granulation involves different events which are *queueing*





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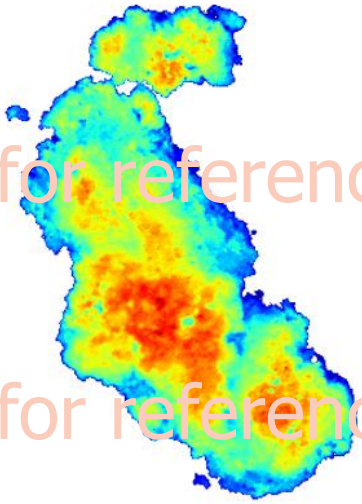
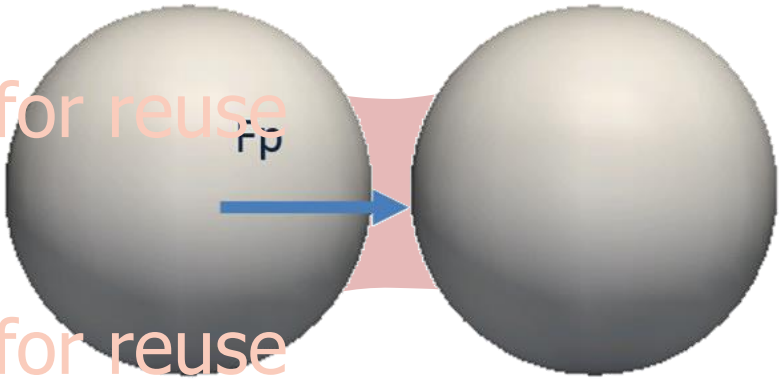
Characterizing liquid distribution in TSG is crucial both at micro and meso-scale

Experimental investigation (meso-scale)



Spectroscopy

Particle scale modelling (micro-scale)



Discrete element method

Abstract (572d), Presentation today at 4:25 PM Ballroom B (Salt Palace Convention Center)

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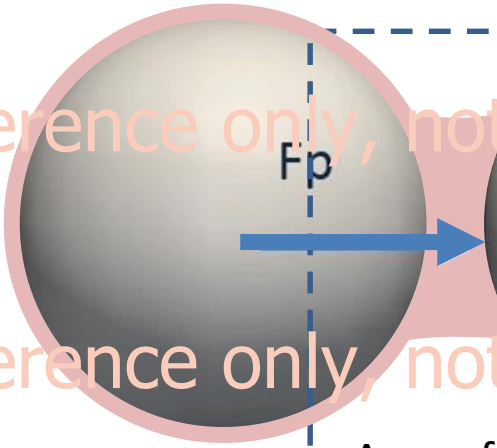
Particle scale for detailed investigation of liquid distribution

Discrete element method



Particles added per second

150,000,000

Area of detail

Viscous force

Contact force

Supplementary models for predicting liquid transfer[1] during collisions of wet particles and conductive liquid flux

Source: metro.co.uk

[1]Mohan et al., *Powder Technology* (2014)

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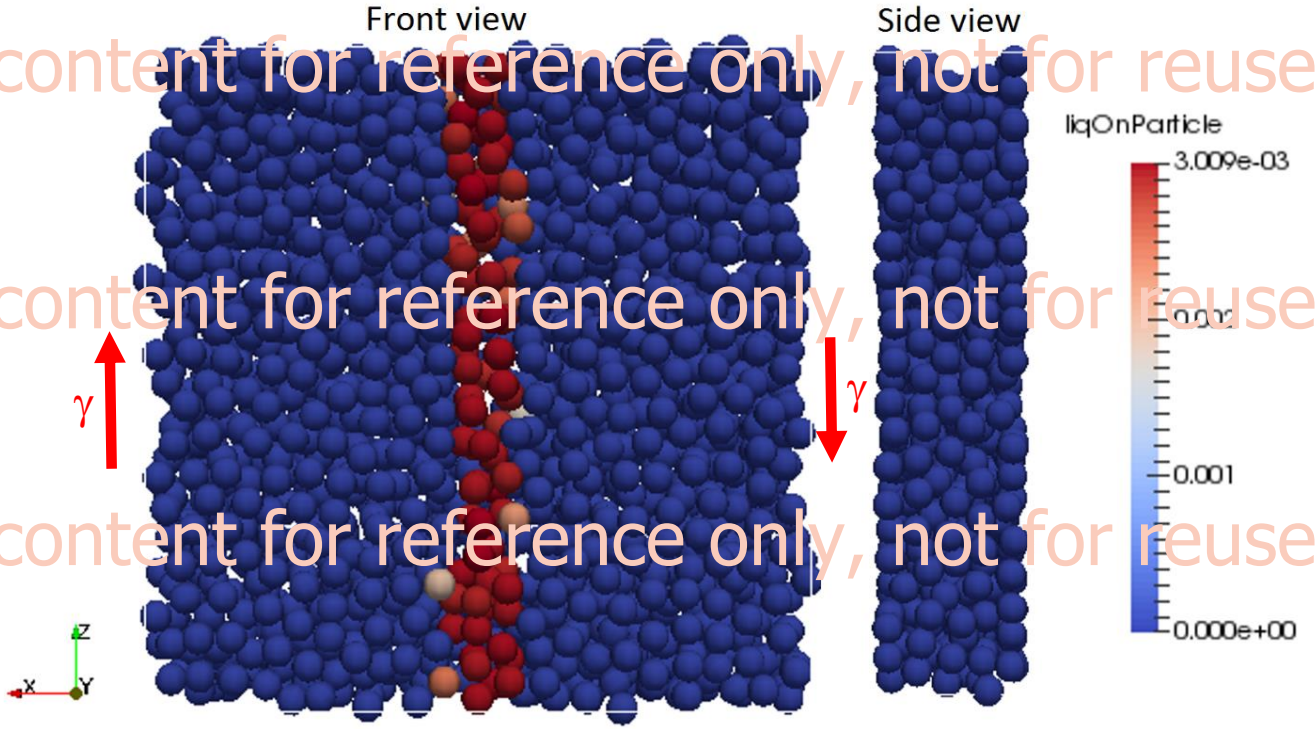
Setup for simple shear simulation



LIGGGHTS

$$\gamma^* = \gamma d_p^{3/2} \sqrt{k_n/\sigma_p}$$

- Approximately 1500 particles in a periodic box (S/D_p=15)
- Shear gradient in x-direction (Lees–Edwards boundary conditions)
- Stiffness based on dimensionless shear rate γ^*
- Particles in the center are wet (L_p^* = 1) other dry (L_p^*= 0)

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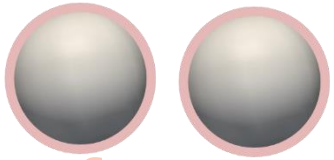
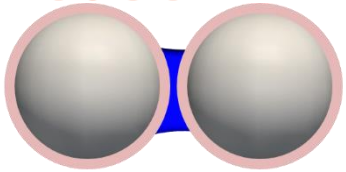
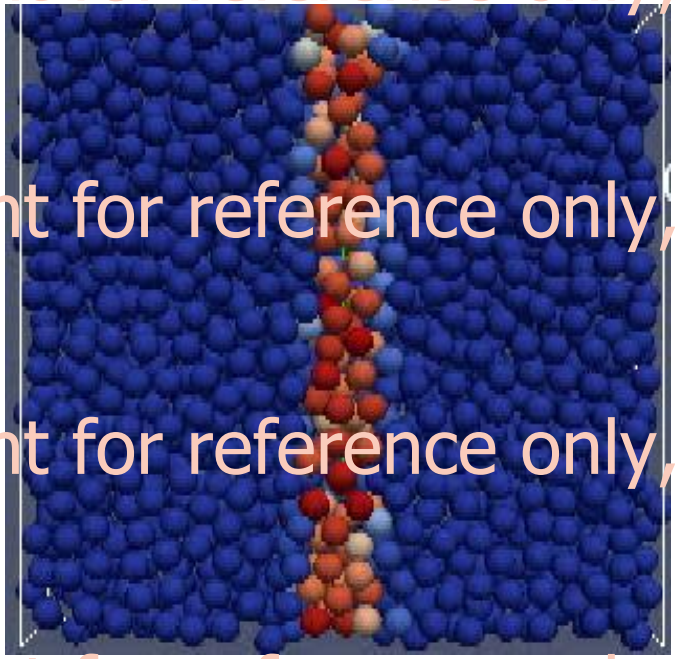
Liquid distribution was tracked applying simple shear to particles in a periodic box

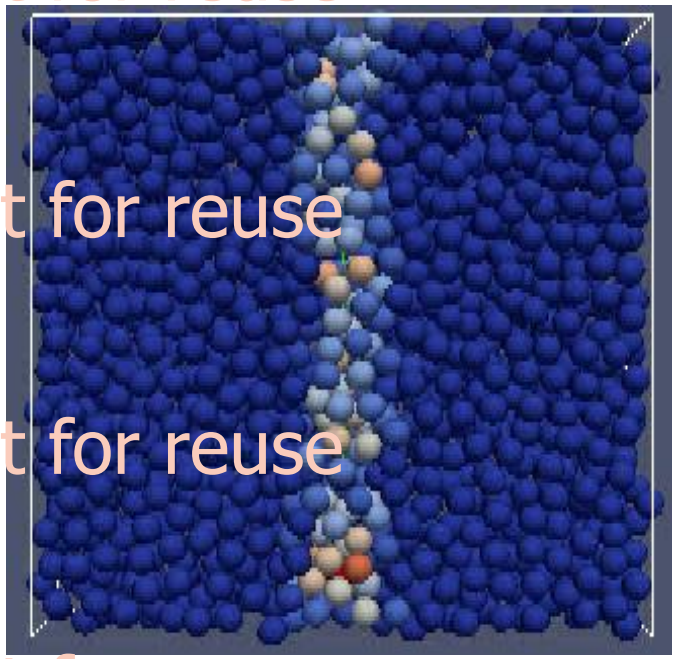


Liquid on Particle surface



Liquid in Bridges

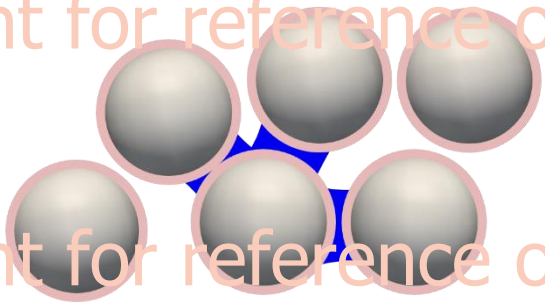


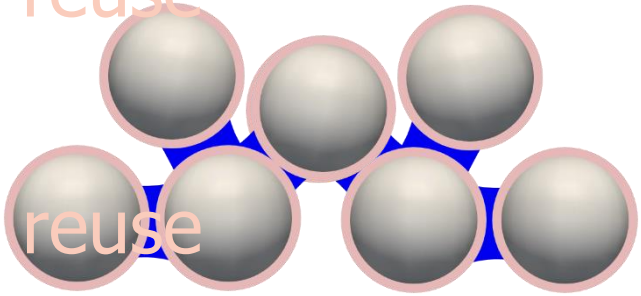


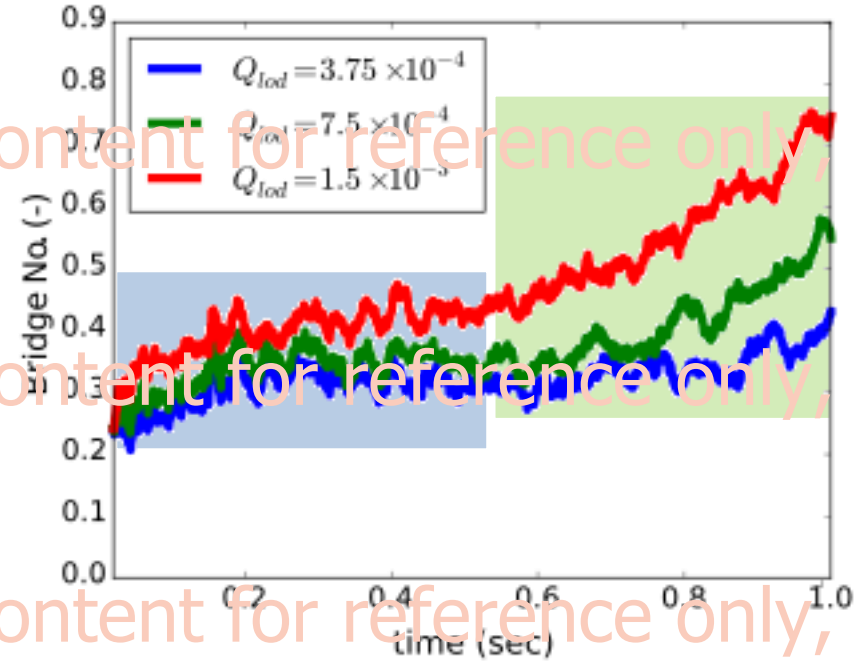
0 0.025

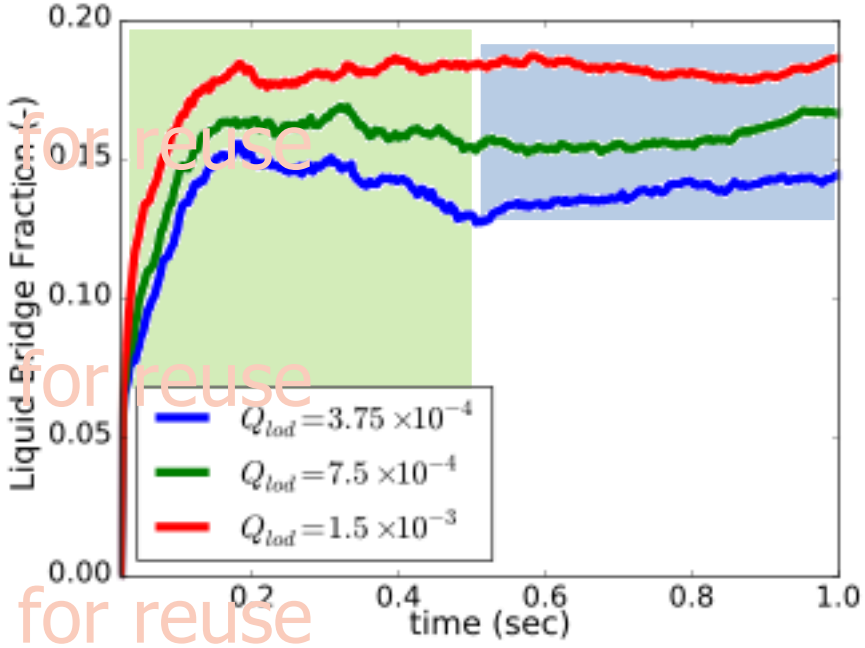
0 0.005

Overfilled-liquid bridges formed quickly which formed more liquid bridges later









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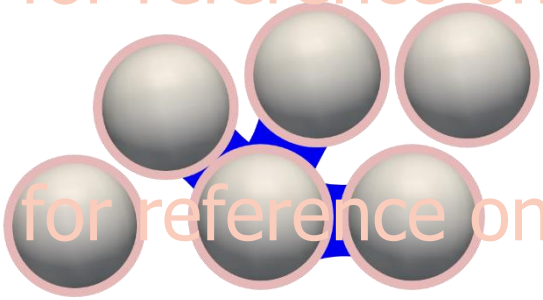
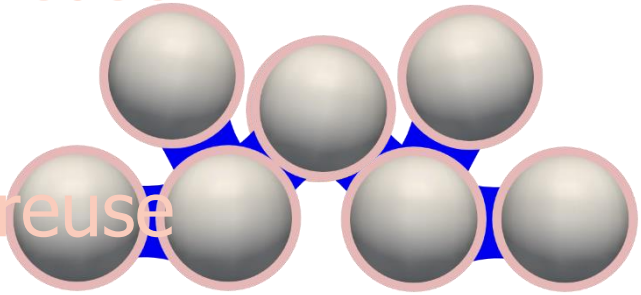
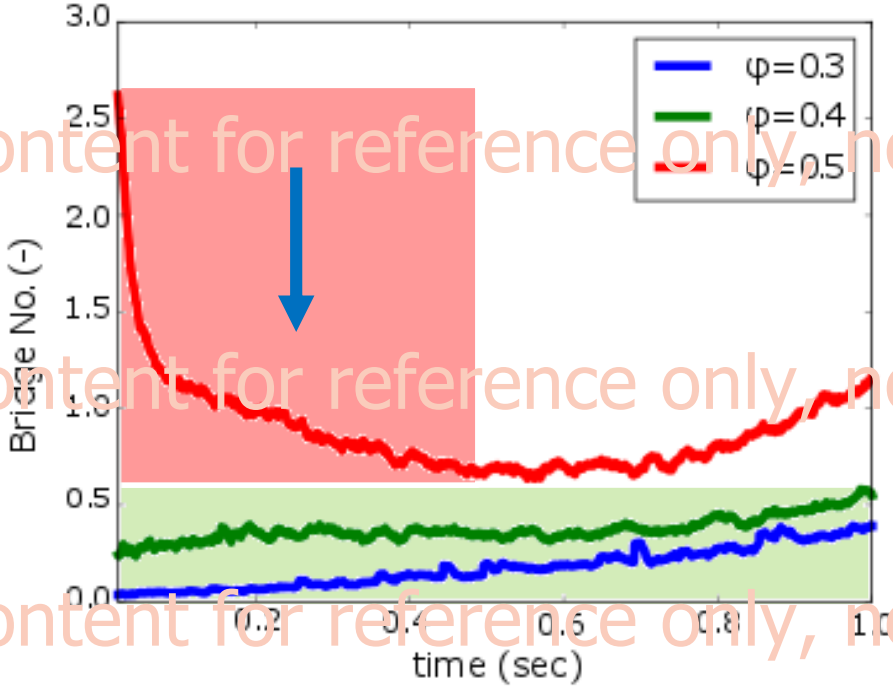
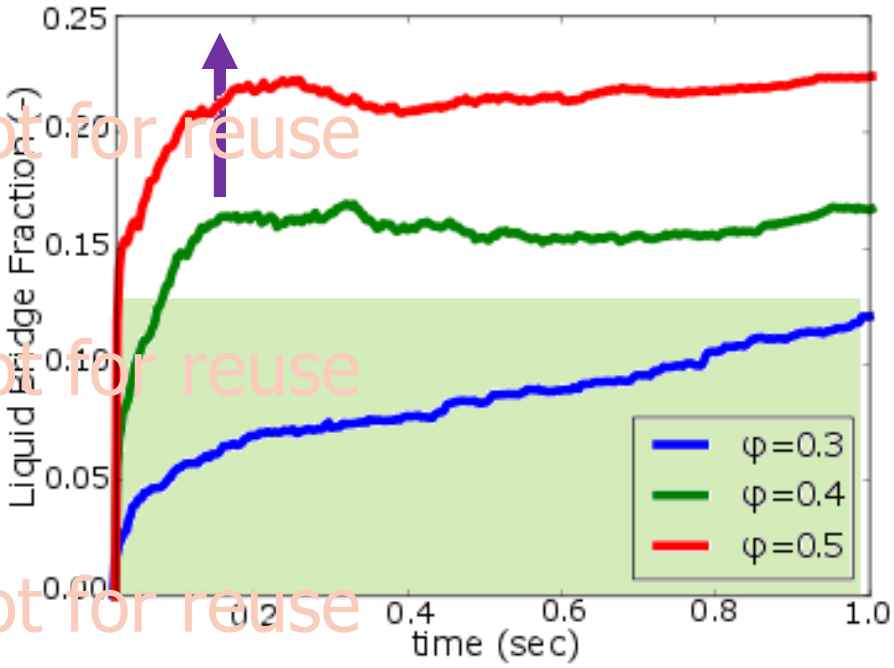
Weak liquid bridges break to transfer liquid to stronger bridges at a high fill ratio









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Knowledge transferred from simple shear to complex shear field in TSG mixing zone

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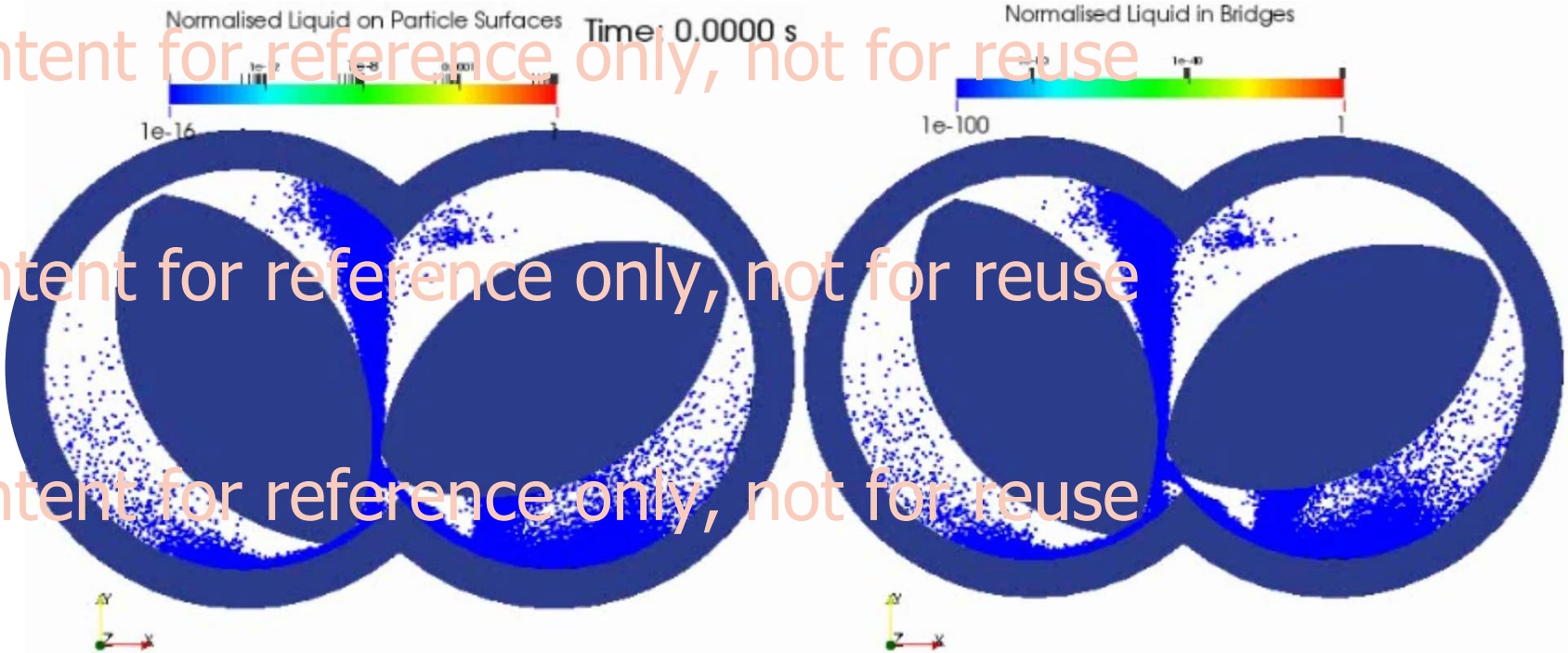
Approximately 45000 particles



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More liquid resulted stronger bridges, but coordination number remained same

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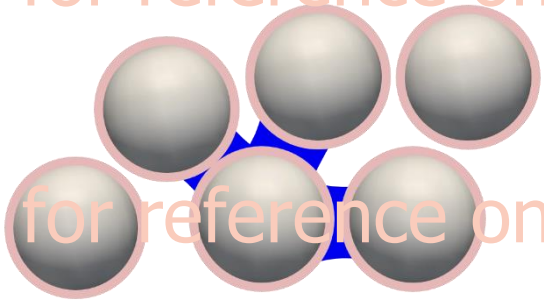

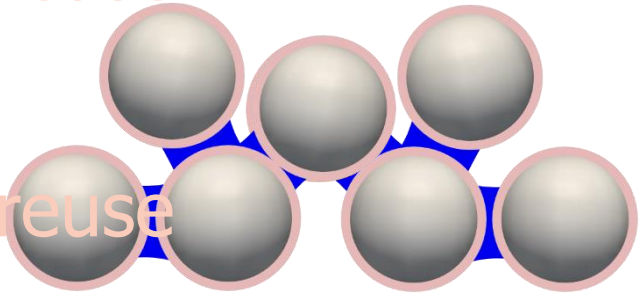

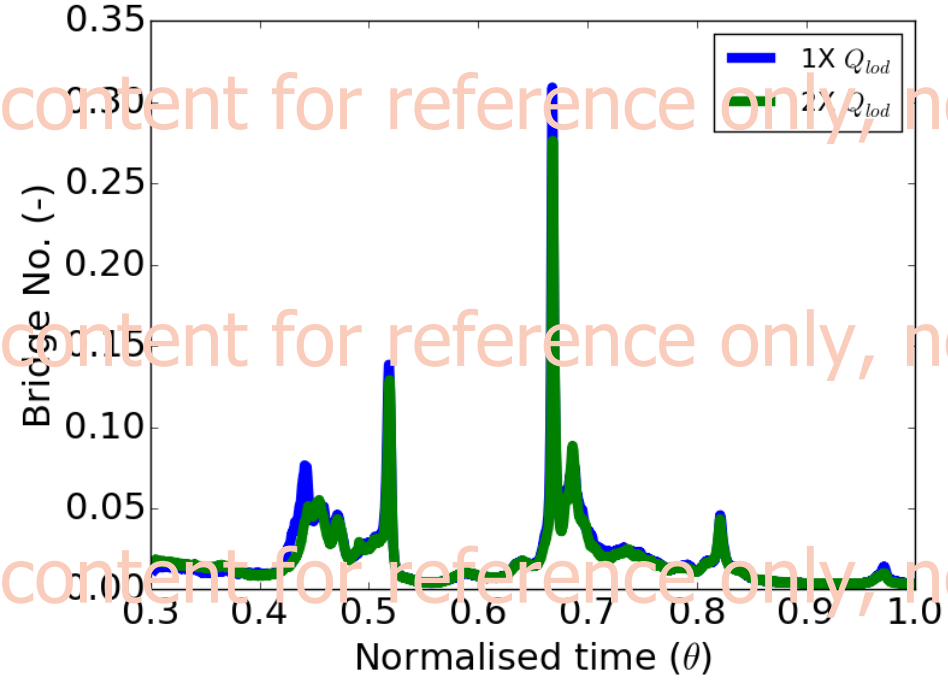

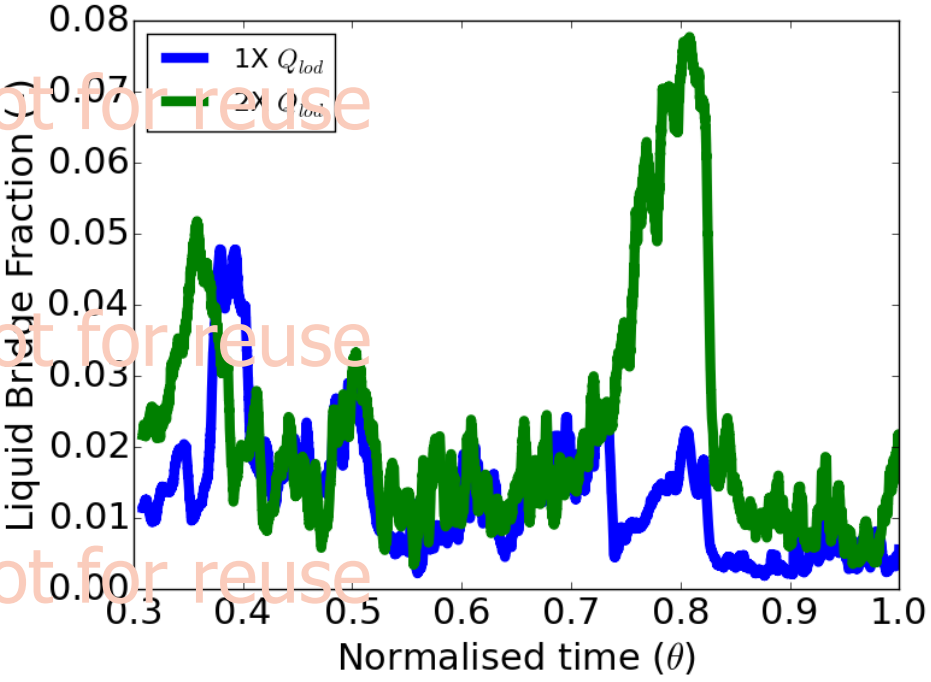

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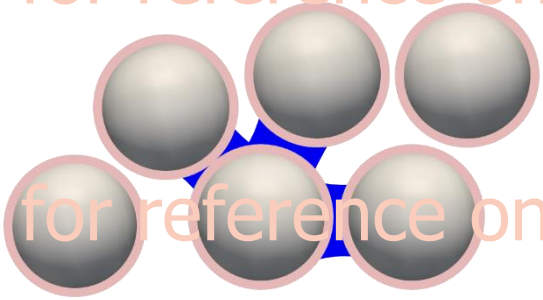
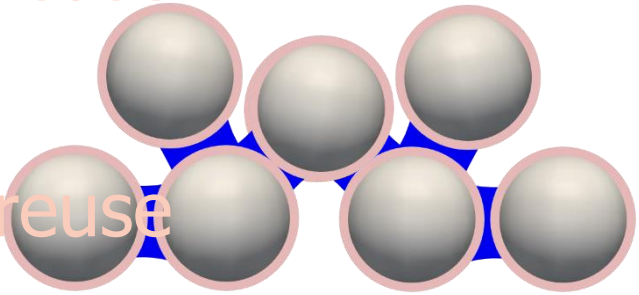
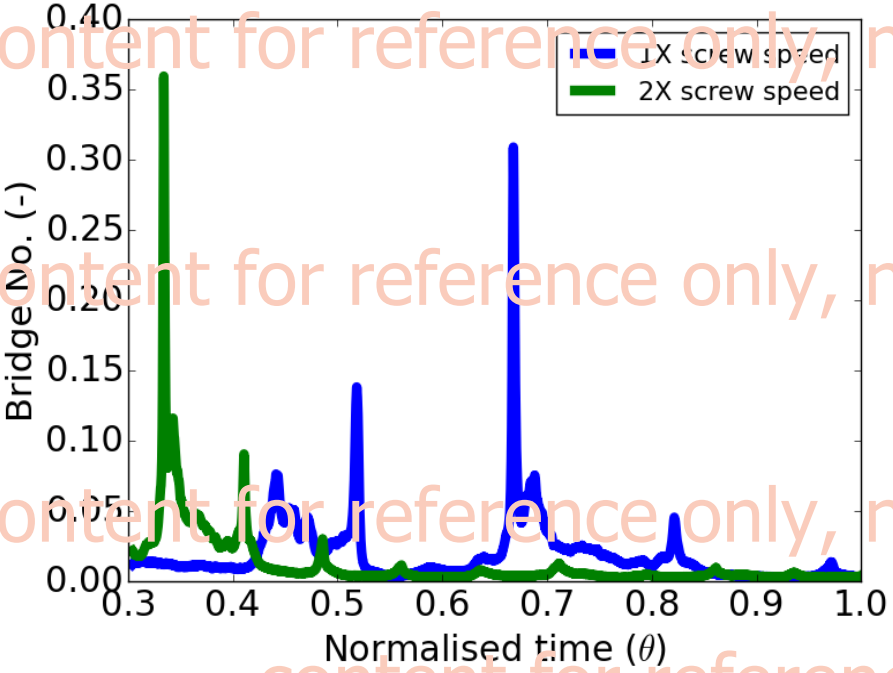
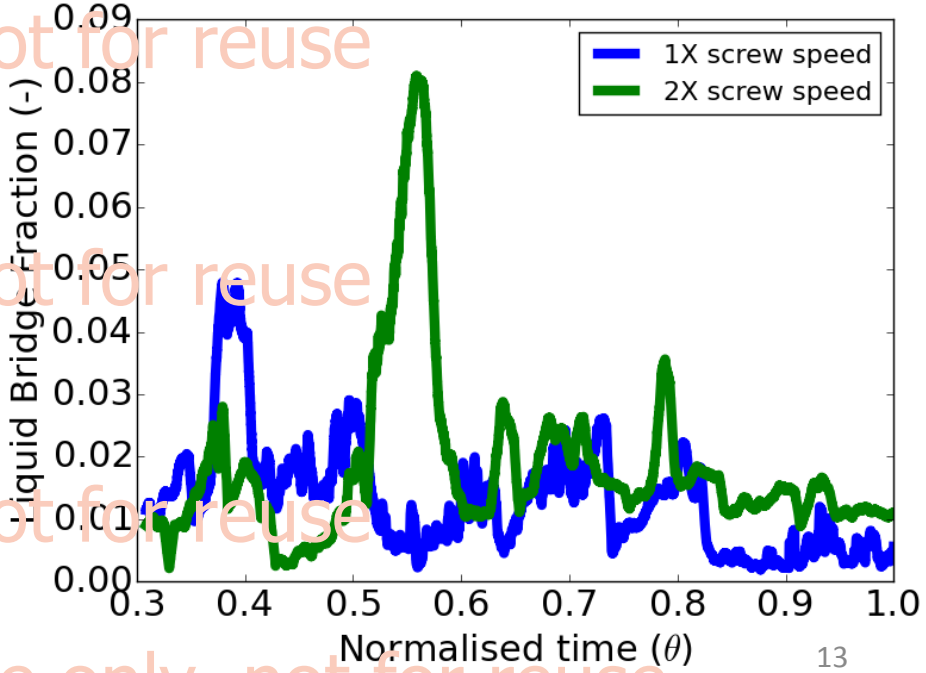
Higher shear resulted rapid liquid transfer from surface to bridges, but also breakage









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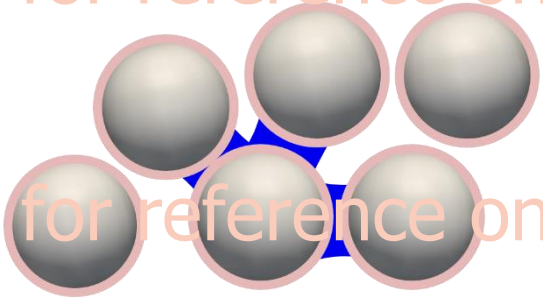
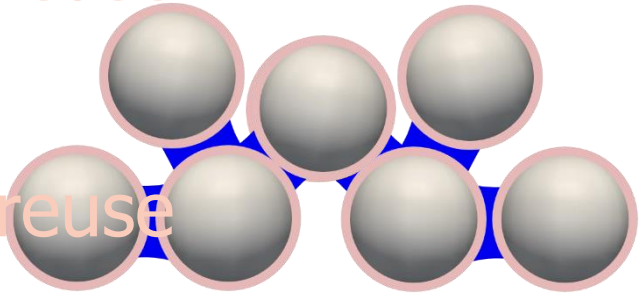
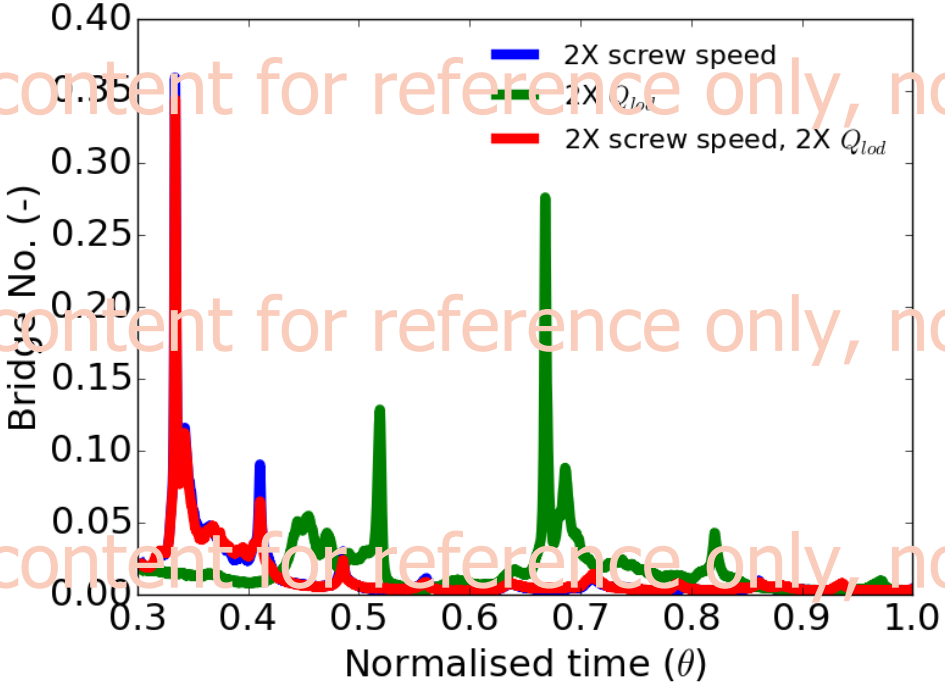
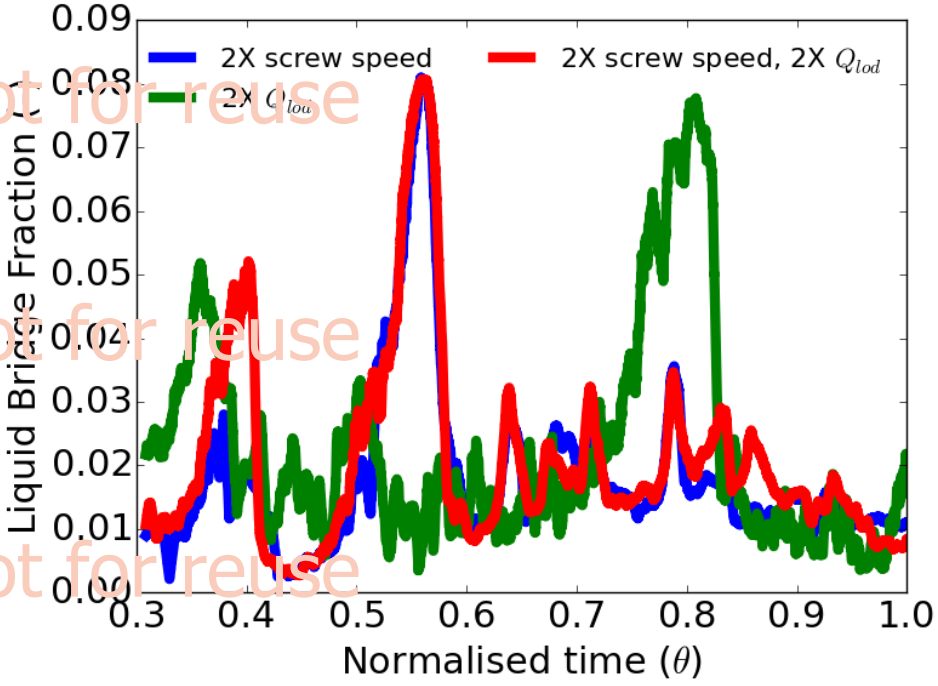
Higher shear and liquid loading resulted rapid and stronger liquid bridge formation









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Summary

1. Particle scale simulations studies using simplified geometry can be used for **detailed analysis of liquid transfer**.
2. Simulating complete TSG is difficult, but particle scale simulation of **a 2D-section** is useful for a first understanding.
3. Simultaneous increase in **screw speed** and **liquid-solid ratio** was identified to be important for solid-liquid mixing and granulation in TSGs.

Perspective

1. Development of closures **population balance models**.
2. Exploring non-conventional **screw element geometries.**

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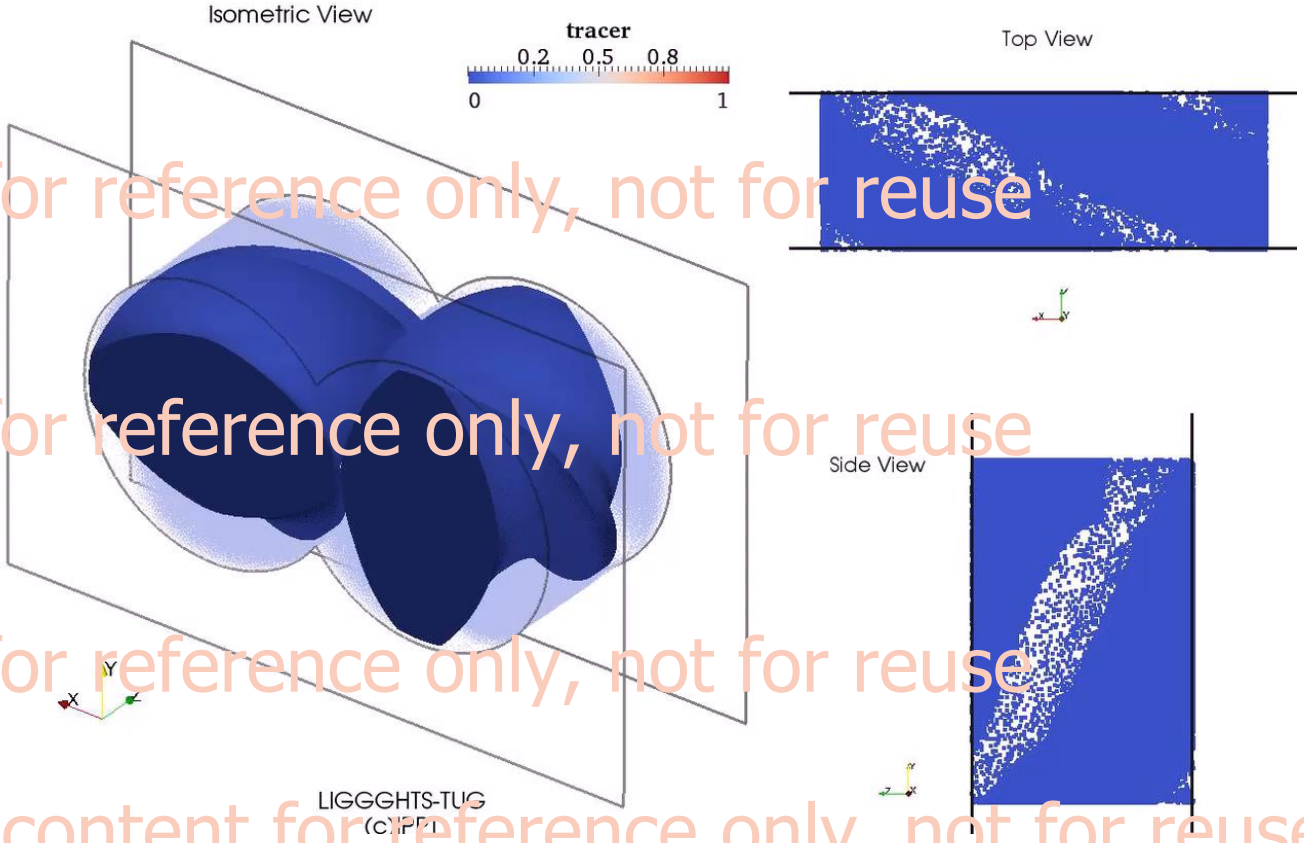
Outlook

Particle scale simulations allow the analysis of particle mixing rates (and hence final product quality) **in a screw section** (movie shows **non-cohesive system,** a force is applied in the axial direction to model the effect of a pressure gradient)



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Aknowledgements

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