

# 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

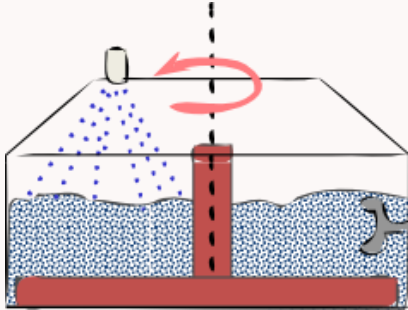
*Wednesday, November 11, 2015: 9:38 AM*

*254A (Salt Palace Convention Center)*



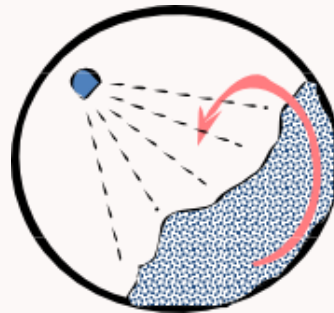
# Traditional to new granulation method

High-shear mixer



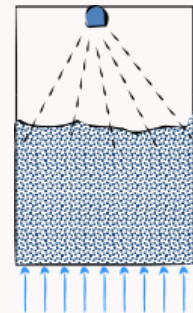
Batch

Drum



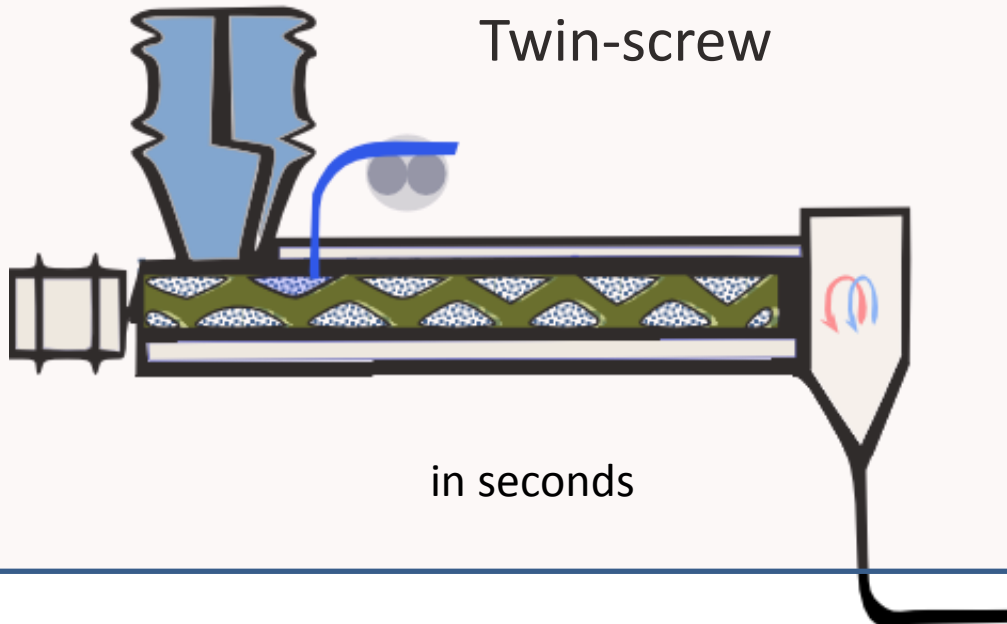
From minutes to hours

Fluidised-bed



Continuous

Twin-screw

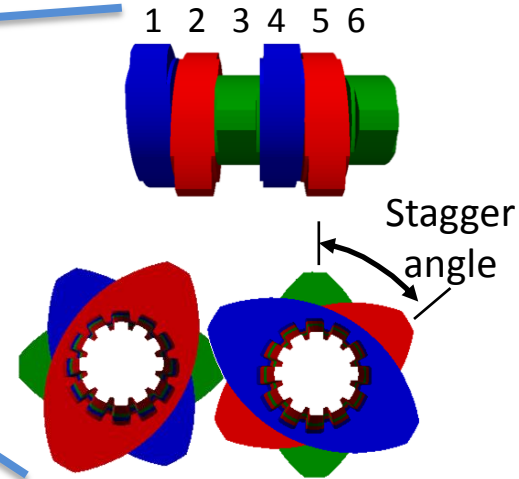


# Design of granulator screw, screw speed, material feed rate control granulation

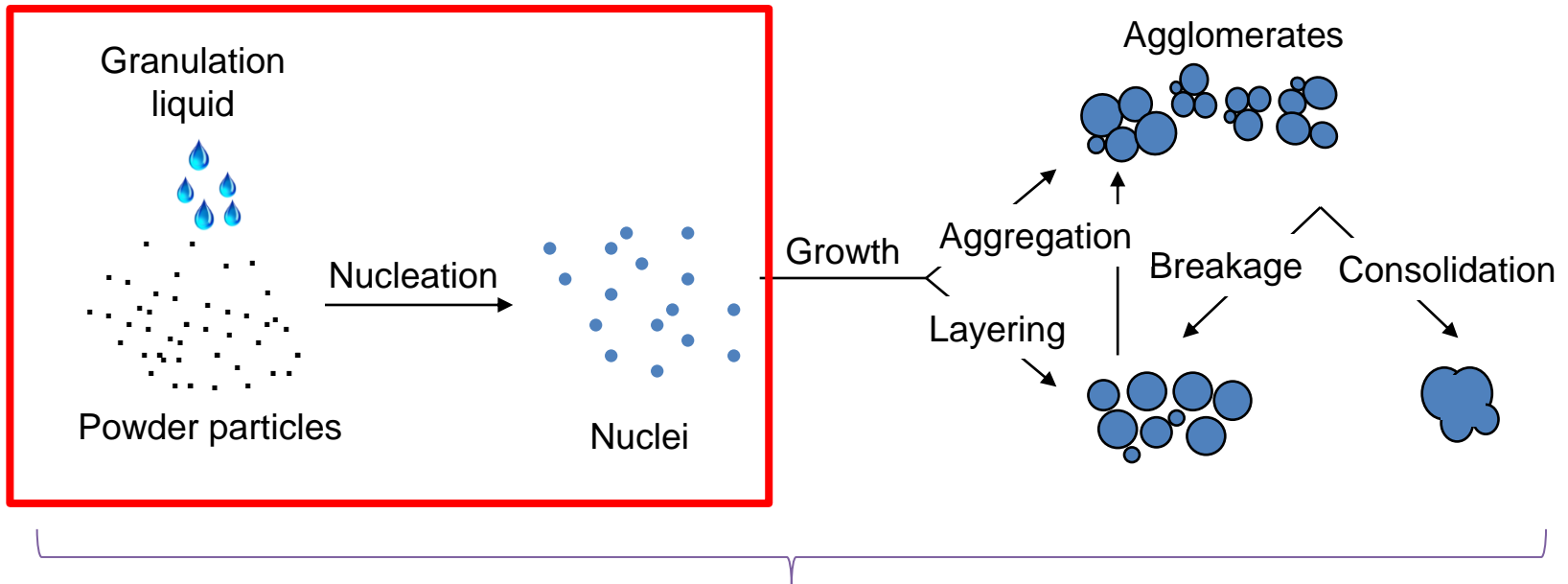
Throughput

Screw  
Speed

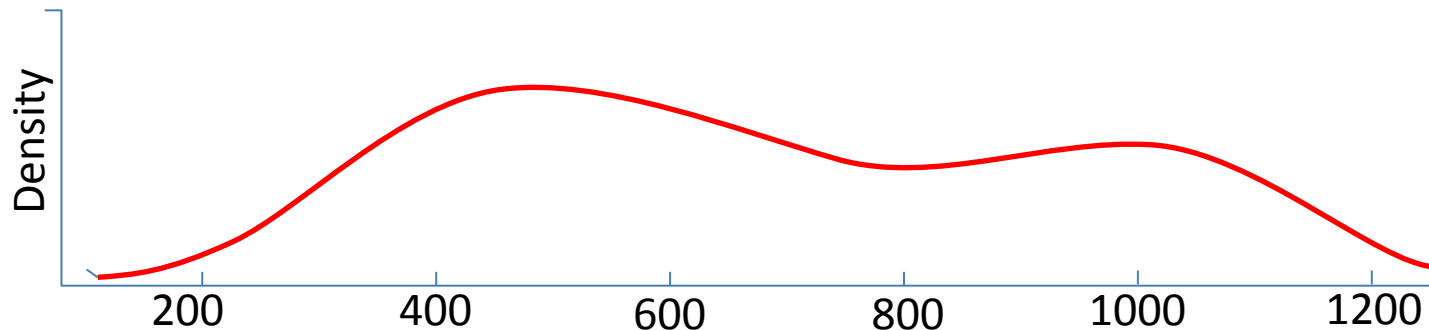
Kneading discs at  
certain stagger  
angle



# Wet Granulation involves different events which are *queueing*

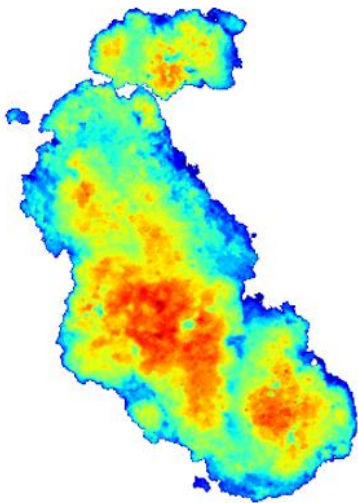


Granule Size Distribution



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

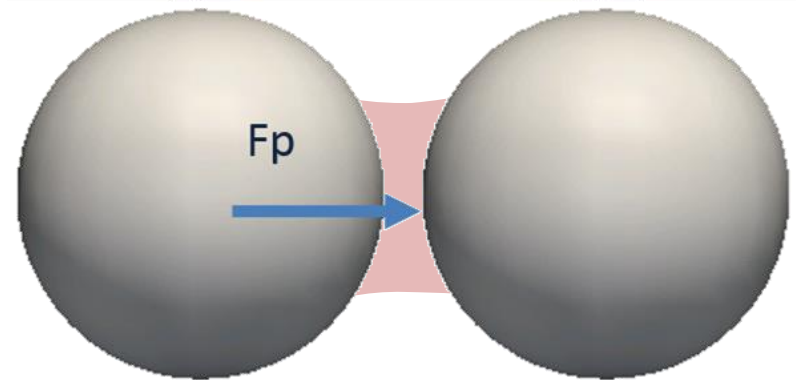
Experimental investigation  
(meso-scale)



Spectroscopy

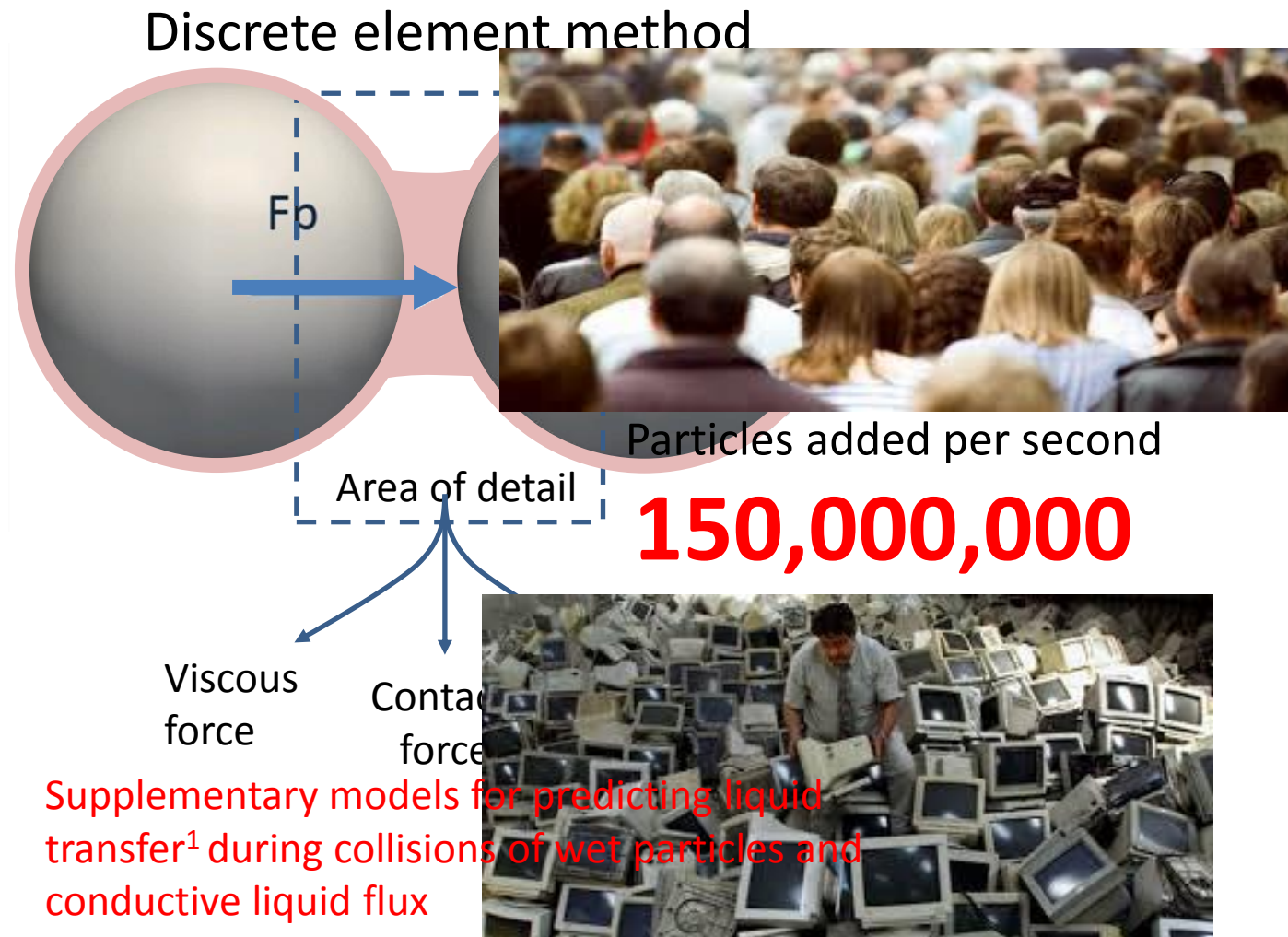
Abstract (572d), Presentation today at 4:25 PM  
Ballroom B (Salt Palace Convention Center)

Particle scale modelling  
(micro-scale)



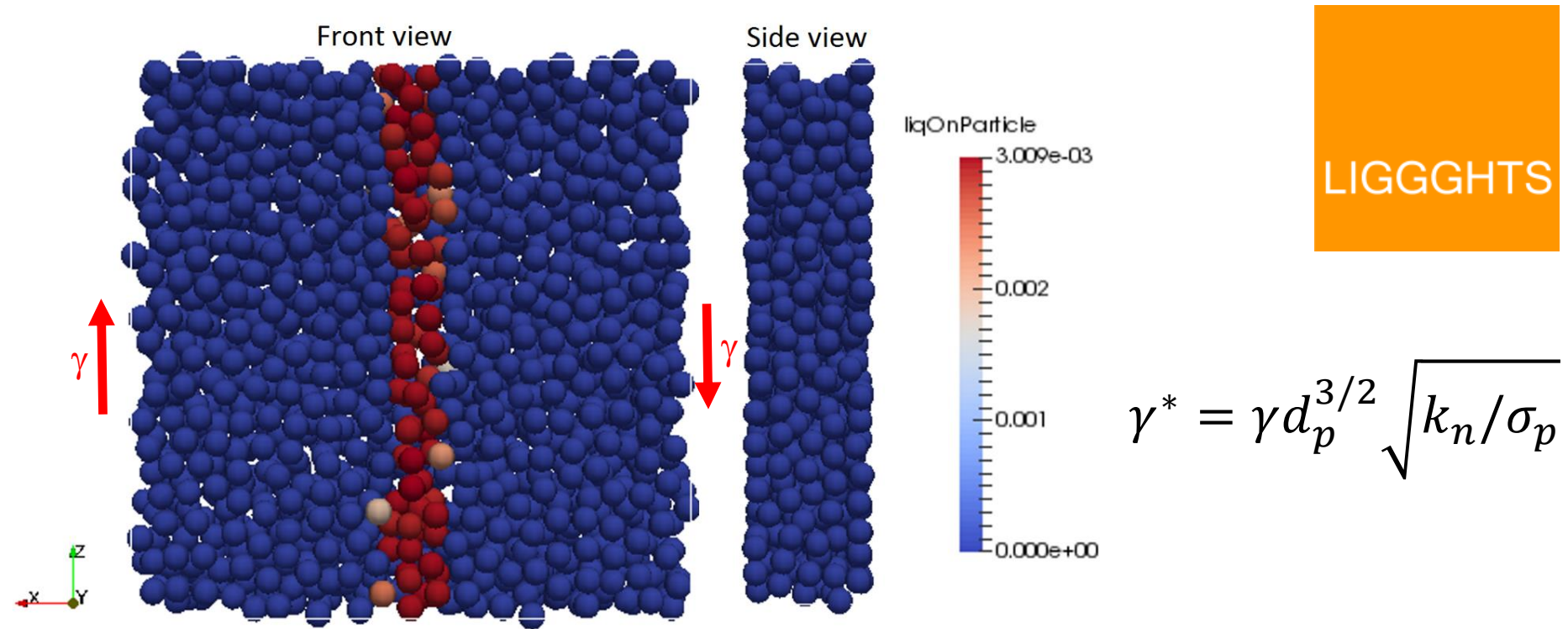
Discrete element method

# Particle scale for detailed investigation of liquid distribution



<sup>1</sup>Mohan et al., *Powder Technology*. (2014)

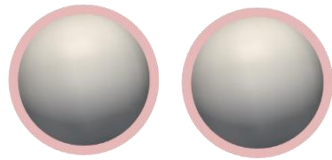
# Setup for simple shear simulation



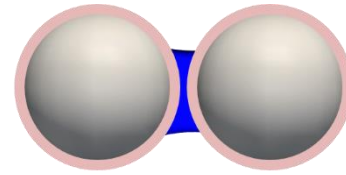
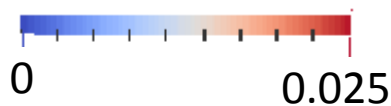
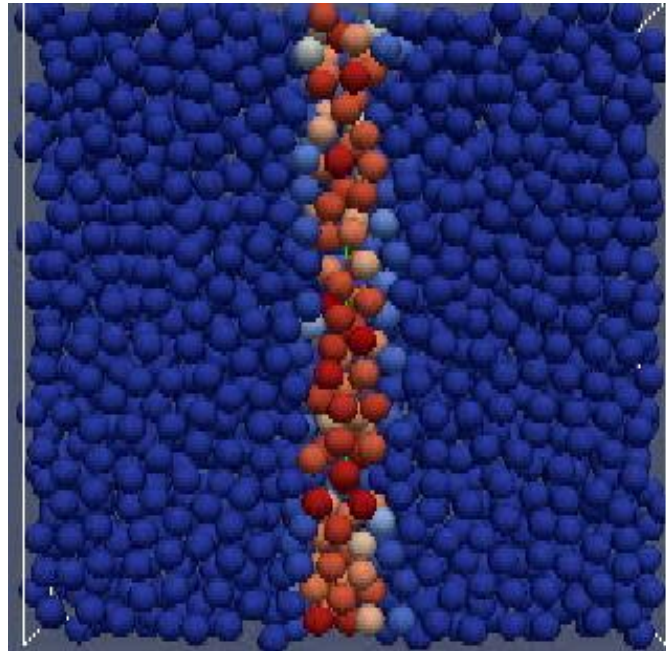
- » Approximately 1500 particles in a periodic box ( $S/D_p=15$ )
- » Shear gradient in x-direction (Lees–Edwards boundary conditions)
- » Stiffness based on dimensionless shear rate  $\gamma^*$
- » Particles in the center are **wet** ( $L_p^* = 1$ ) other **dry** ( $L_p^* = 0$ )



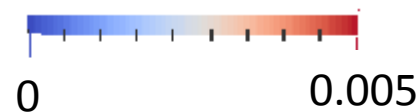
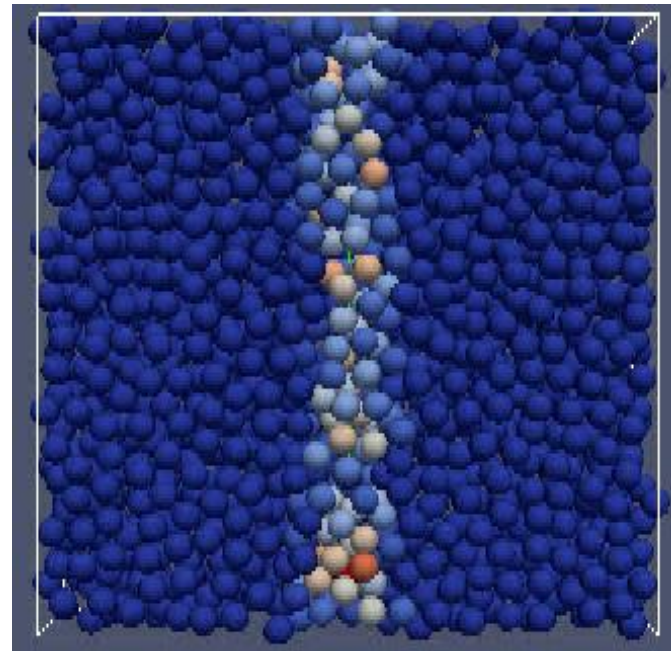
# Liquid distribution was tracked applying simple shear to particles in a periodic box



Liquid on Particle surface

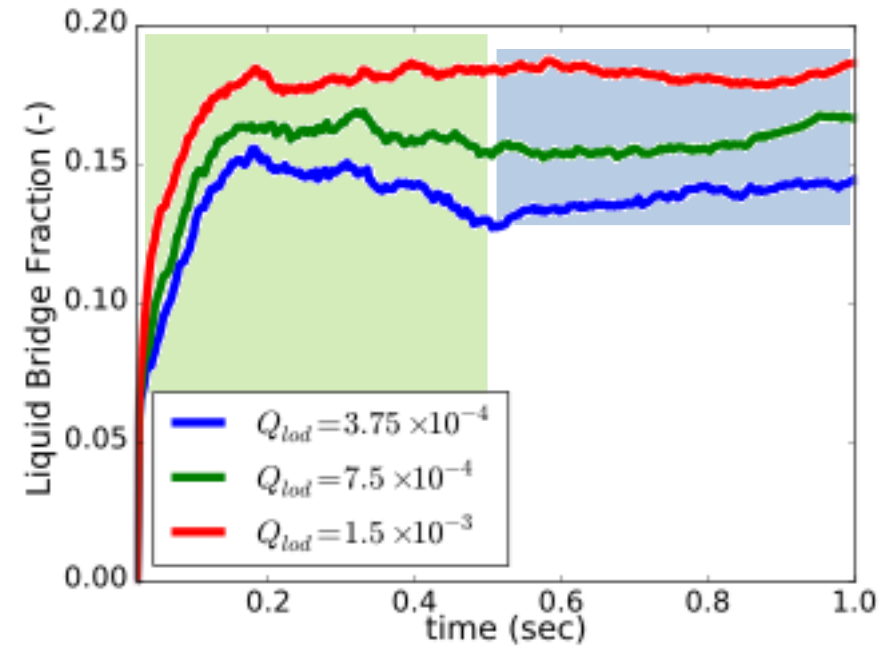
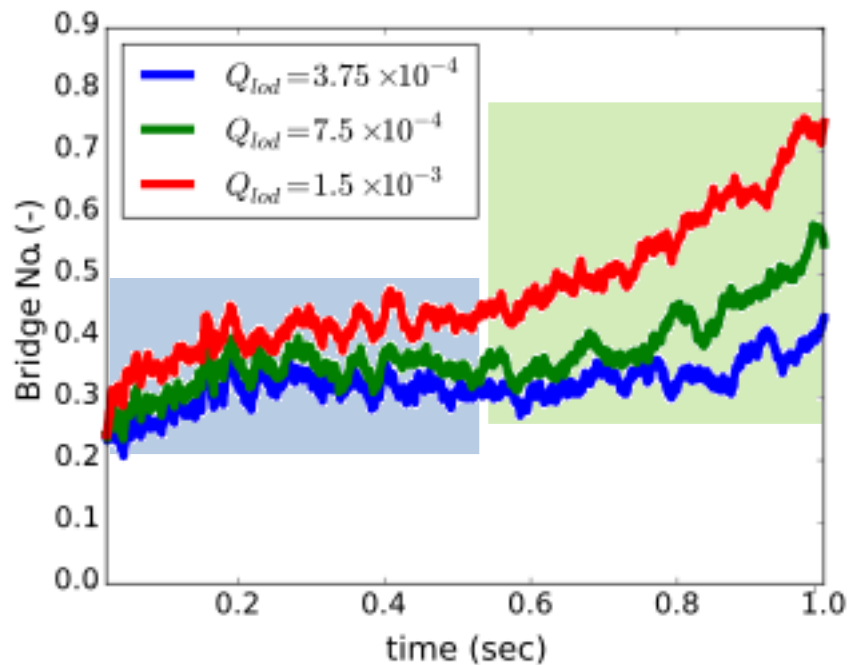
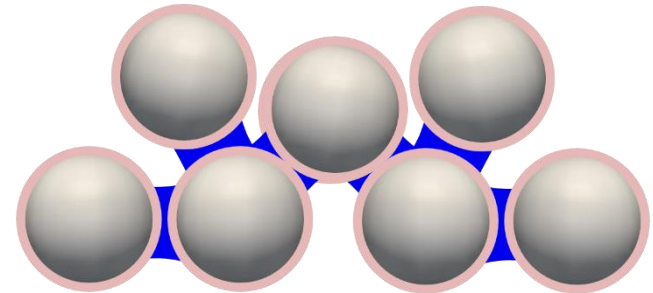
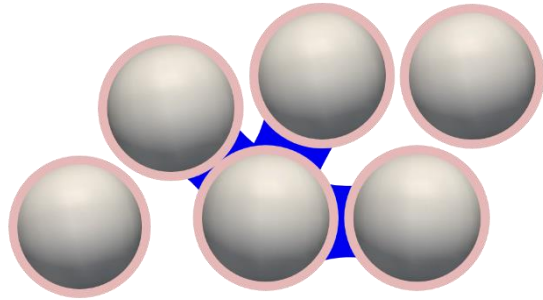


Liquid in Bridges

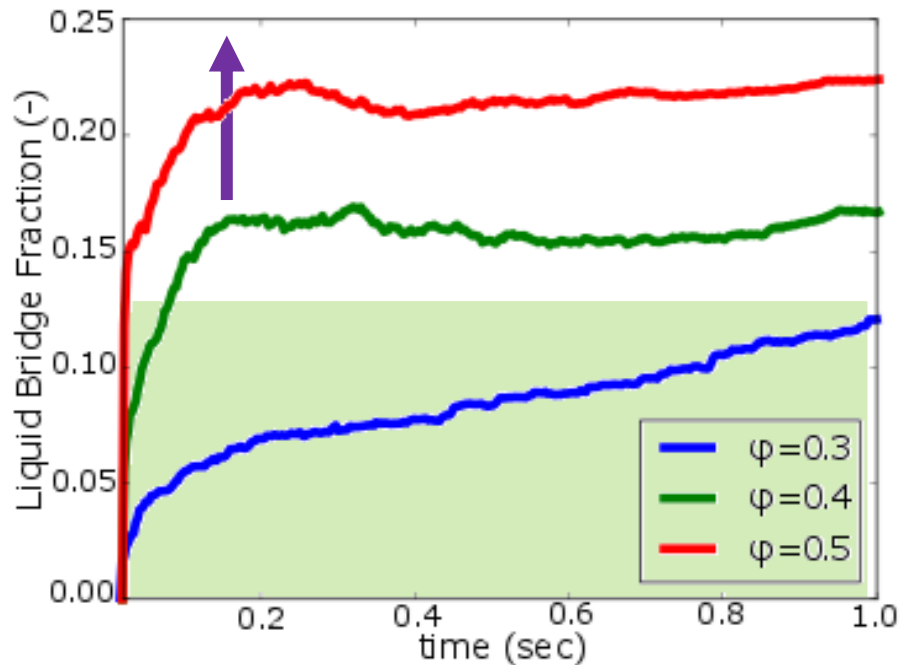
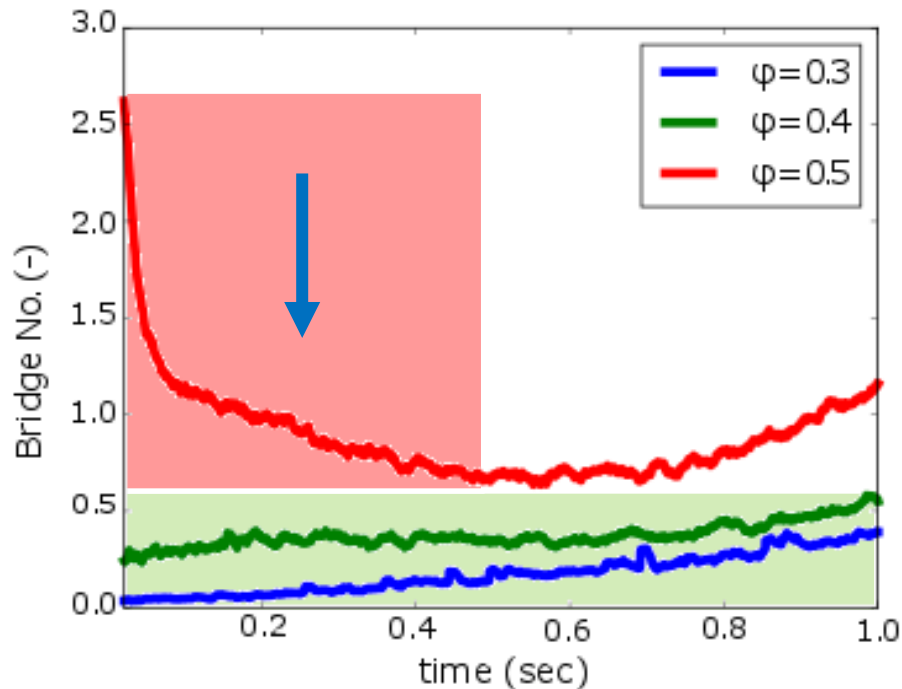
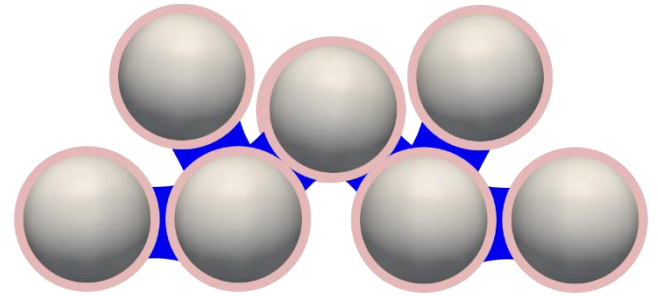
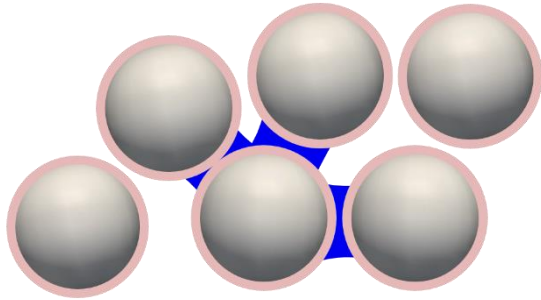




# Overfilled-liquid bridges formed quickly which formed more liquid bridges later

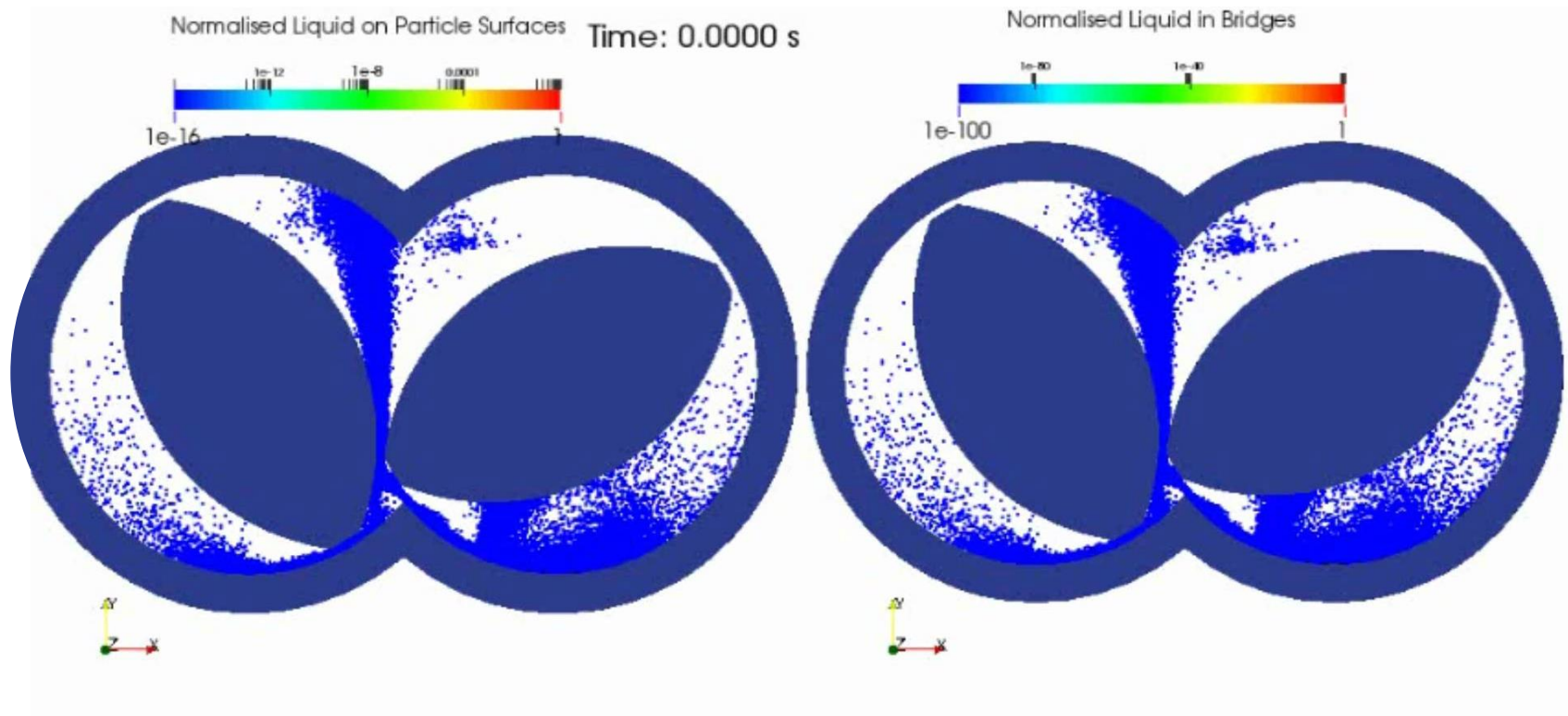


# Weak liquid bridges break to transfer liquid to stronger bridges at a high fill ratio

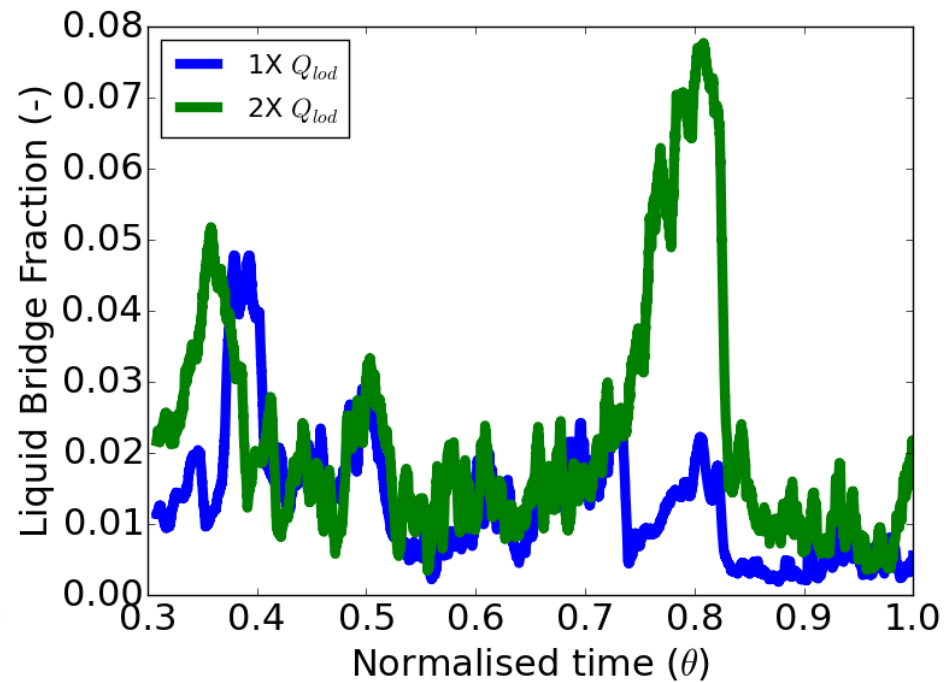
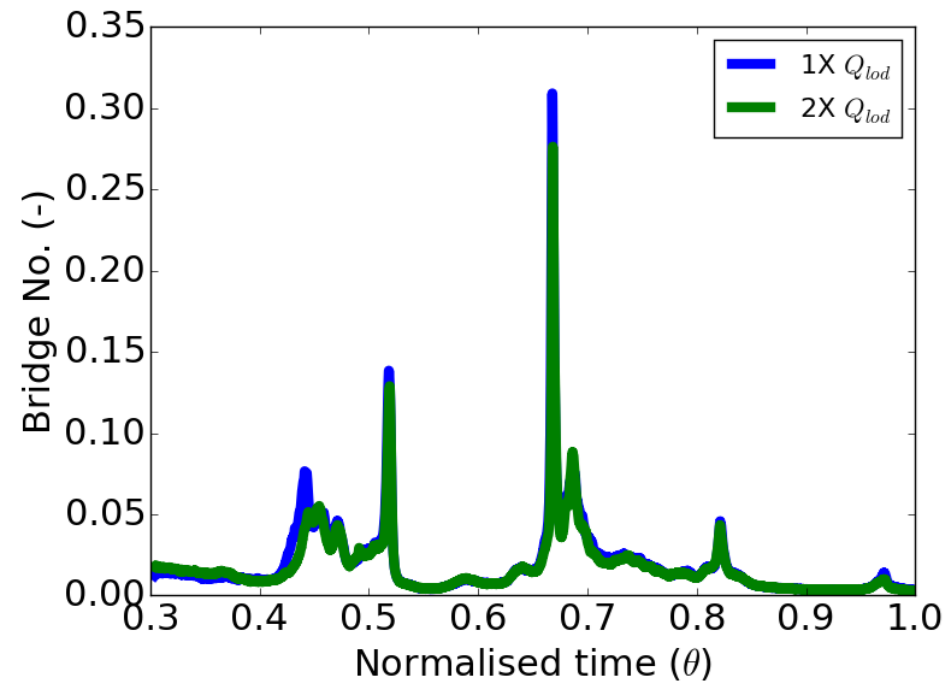
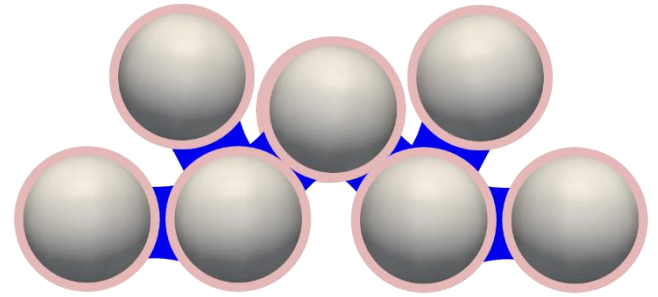
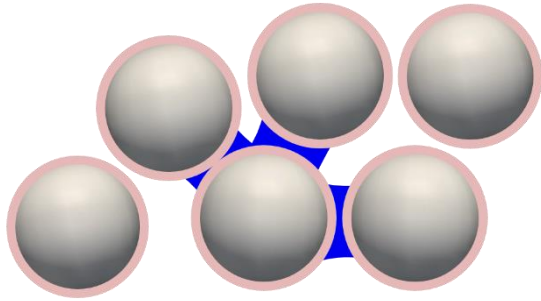


# Knowledge transferred from simple shear to complex shear field in TSG mixing zone

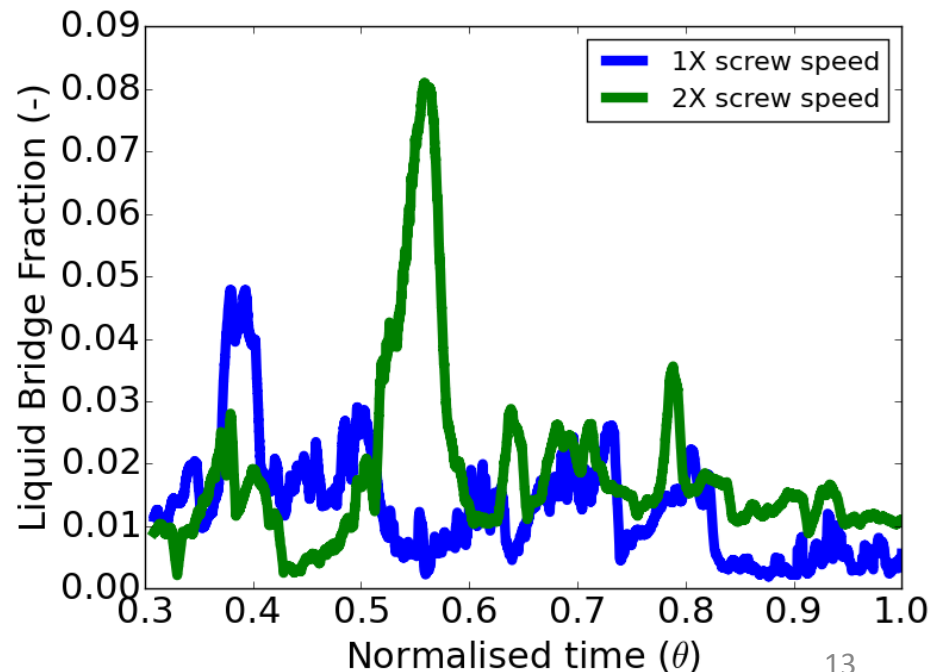
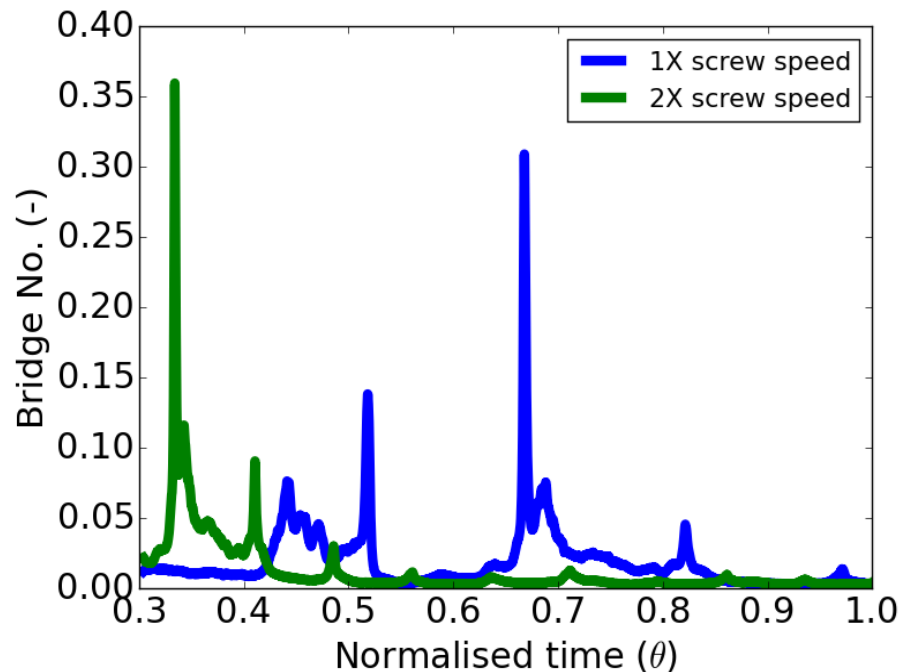
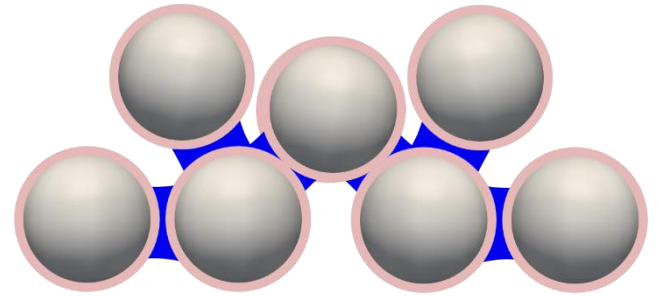
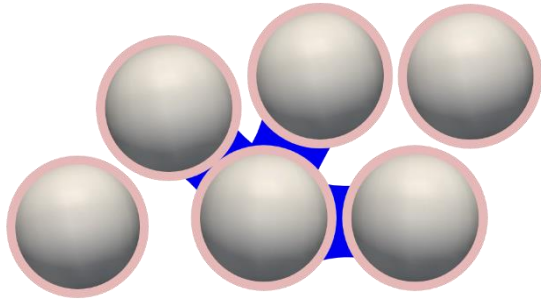
Approximately 45000 particles



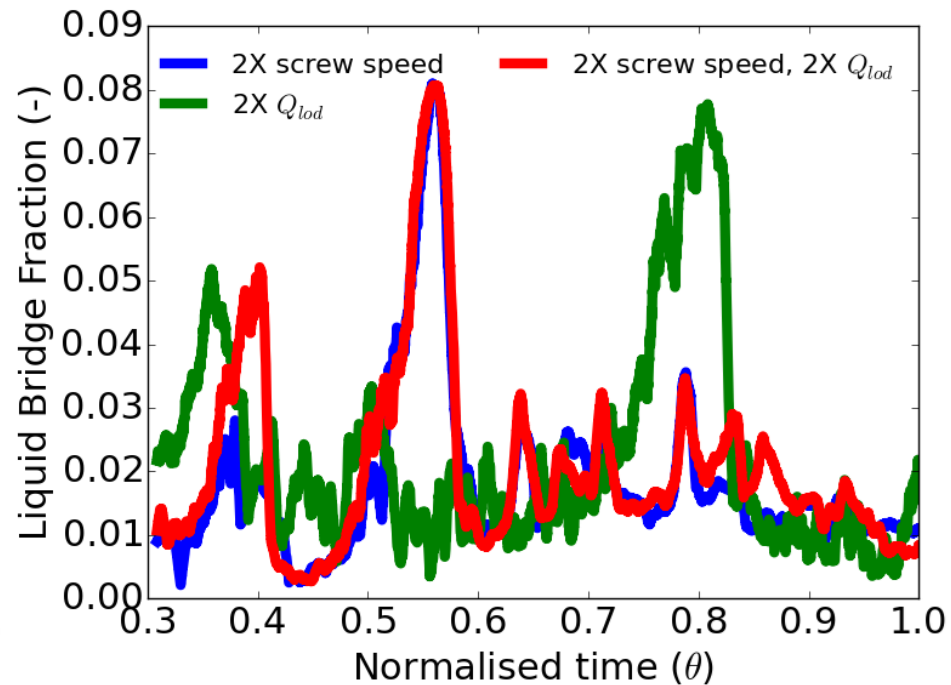
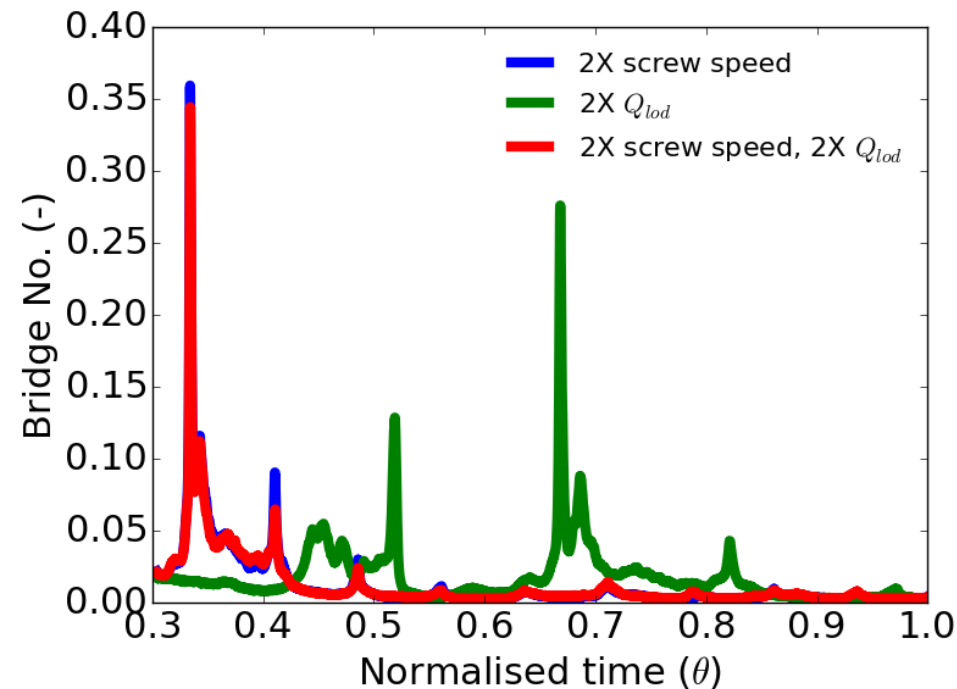
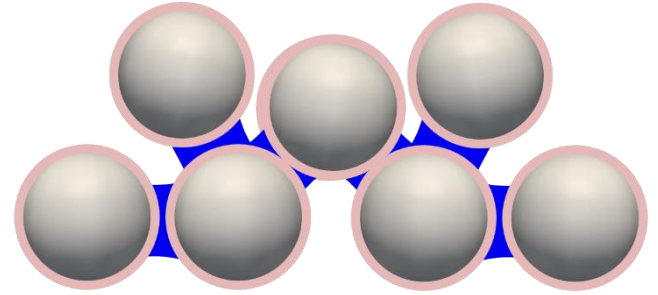
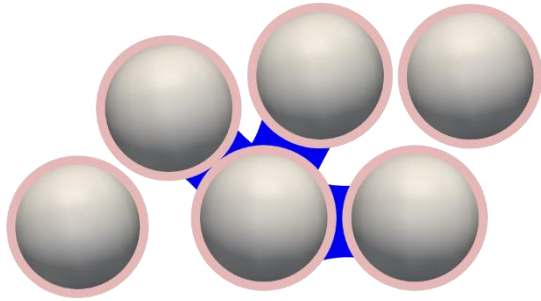
# More liquid resulted stronger bridges, but coordination number remained same



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



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





# Summary

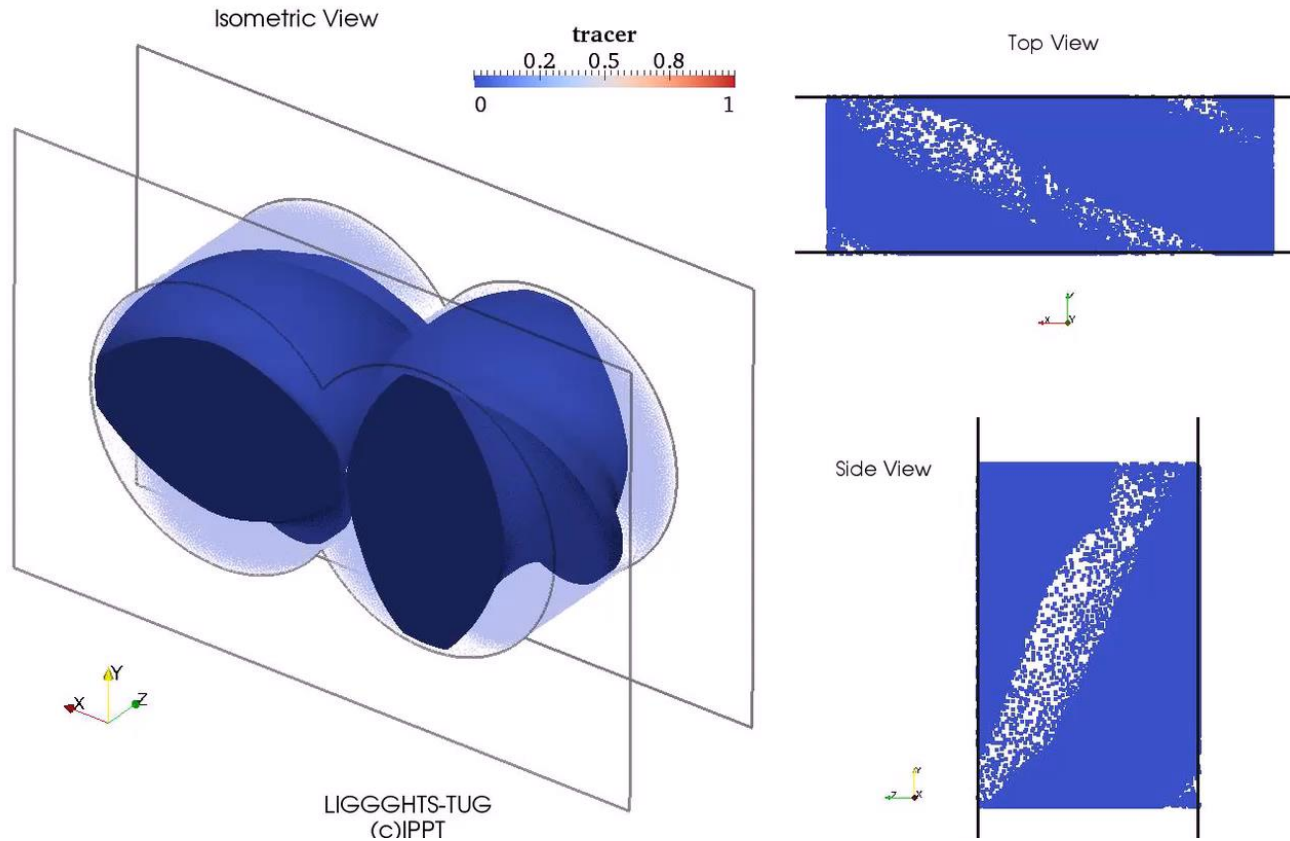
1. Particle scale simulations studies using simplified geometry can be used for **detailed analysis of liquid transfer**.
2. Simulating complete TSG is difficult, but particle scale simulation of **a 2D-section** is useful for a first understanding.
3. Simultaneous increase in **screw speed** and **liquid-solid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

# 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)



# Aknowledgements

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Prof. Stefan Radl

Prof. Johannes G Khinast



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