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Visualising Shear Stress Distribution inside Flow Geometries Containing Pharmaceutical Powder Excipients Using Photo Stress Analysis Tomography and DEM Simulations

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Abstract. For the first time, photo stress analysis tomography (PSAT) is applied to probe the distribution of maximum shear stress and direction of major principal stress field within 'powder' assemblies inside hopper geometries, and further supported by discrete element model (DEM) simulations. The results show that for decrease in hopper angle, the direction of major principle stress aligns with the direction of gravity which could promote flow rate under dynamic conditions. Conversely, the propensity of developing relatively more non-homogeneous distribution of shear resistance zones inside powder assemblies increases with the hopper angle, which could subsequently decrease their macroscopic flow rate.

Keywords: Photonic stress analysis tomography (PSAT), discrete element modelling (DEM), granular flow, particulate processes.
PACS: 45.70.Cc, 45.70.Mg, 07.10.Lw

INTRODUCTION

Processing behaviours of materials in granular and powder form are well sought in several industrial applications though complex and not yet well established [1,2]. Their mechanical behaviour is different from other conventional state of materials viz., solids, liquids and gases [1-3]. For particulate materials subjected to external boundary loading, stresses propagation occurs through inter-particle contacts usually in a non-homogeneous manner. It has been shown that bulk shear strength of particulate materials originate from contributions of a small proportion of force-transmitting contacts referred to as strong force chains and their fabric features are influenced by single-particle scale properties and packing conditions [2]. Although previous studies based on photo stress analysis method showed non-homogenous characteristics of force-transmitting contacts inside particulate assemblies under external loading, such studies are performed with relatively bigger size of birefringent particles (in mm size range) and not yet widely known for powder assemblies with micron size distributions [4,5]. Recent developments of experimental techniques to analyse structure of particulates such as the X-ray Micro Tomography [6] and Nuclear Magnetic Resonance Imaging [7] are limited in providing density and velocity variations of granular particles. However, visualising shear stress distribution inside powder packing is not yet well established. In this paper, we report early results on shear stress field inside two dimensional powder assemblies of initial (static) random filling using experimental photo stress analysis tomography (PSAT). To enable this, we developed birefringent powders (with different cohesivity) of micron size distribution and characterised their particle-scale properties. Further, PSAT results for maximum shear stress distribution in powder assemblies are compared with DEM simulations as much as possible.

PSAT METHOD AND MATERIALS

PSAT analysis is based on opto-mechanical phenomenon known as birefringence of materials observed under circularly polarised light which can be related to the maximum shear stress using the well- known stress-optic law [4,5]. In this paper, the PSAT based studies are limited to 2-dimensional conditions. However, as supported later by results of 3d simulations for near-axisymmetric fillings in the hopper funnel geometry, 2d PSAT studies are found to be adequate and relevant. Novel pharmaceutical birefringent stress-responsive sensor powders with a particle size range of 300µm to 1000µm (normal size distribution) have been fabricated and developed in our laboratory using natural polymer

pharmaceutical excipient. These birefringent powders with different level of cohesivity are identified as JASA100 and JASA200 respectively as shown in Fig. 1

FIGURE 1. Birefringent powder samplers: JASA100 and JASA200

EXPERIMENTAL SETUP

The PSAT experimental rig consists of a linear polariser, two quarter wave plates, an analyser, light source and the birefringent sensor powder hopper (angle of hopper =θ) is held as shown in Fig. 2. The powder bed height (H) was kept constant for different hopper angles which are similar to that used in DEM simulations reported later (Fig. 6). More details, on the experimental set up can be found elsewhere [4].

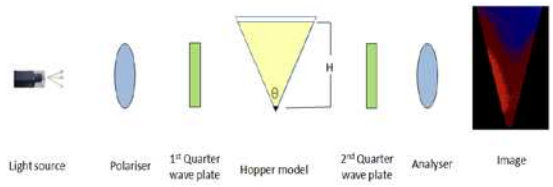

FIGURE 2. PSAT experimental setup

Different cases of hopper angle are considered in this study. All the hopper geometries were filled with birefringent powders using identical filling procedure in random packing. The light source emitted ordinary light and converted to a linear polarised light by the effect of the first polariser after which it changed to a circularly polarised light by passing through the quarter wave plate. When the circular polarised light passed though the fabricated birefringent sensors (JASA100 and JASA200), it is split into two components known as ordinary and extra-ordinary components. The retardation in the speed of light among these axes is subsequently measured and related to maximum shear stress at any point of interest inside hopper geometry. The thickness of the hopper geometry is 4mm and we have ensured that the thickness effects are minimised without compromising on the accuracy of the measurements.

RESULTS AND DISCUSSION

Physio-Mechanical Characteristics of Birefringent Sensors Particles.

The physio-mechanical properties of the fabricated birefringent sensors powders were evaluated including angle of repose, bulk density, tapped density, Carr's index and Hausner ratio. The angle of repose, Carr's index and Hausner ratio were 38^{o}, 16.4 and 1.19 for (JASA100) comparing to 34^{o}, 14.5 and 1.7 respectively for (JASA200). The results suggest that JASA100 is relatively more cohesive than JASA200 type birefringent powders.

X-ray diffraction analysis of both sensors powders was performed and the results though not presented here, showed that JASA200 type powder was more crystalline than JASA100, which also lead to better display of birefringence.

Distribution of Maximum Shear Stress and Direction of Major Principal Stress

The magnitude of the maximum shear stress (colour coded in relation to its magnitude) and the direction of major principal stress were evaluated within the whole hopper at different segments for both JASA100 and JASA200 though the results are presented here for JASA100 in Figure 3. However all the basic characteristics of the results of JASA200 were similar to that of JASA100.

In the plots, the arrows show the direction of major principal stress. The segments (images) are arranged in order of top, middle and bottom levels for each angle of hopper. In general, the direction of the major principal stress tends to be acting in the vertical direction in the case of hopper with 30° angle. However, for increase in hopper angle, the direction of major principal stress deviated from vertical direction and tends to act normal to wall boundaries. The maximum shear stress distribution of both particle sensors at different hopper heights are also evaluated (H/2, H/4 and H/∞).

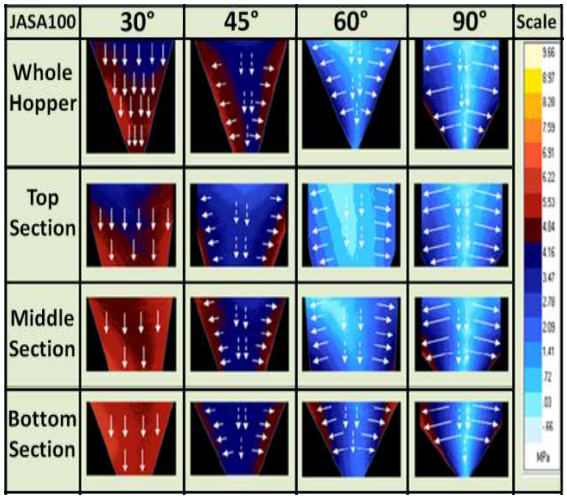

FIGURE 3. Maximum shear stress distribution and major stress principal direction inside hoppers of different opening angle

The result shown in Fig. 4 and 5 are for height H/2 and the results are normalised in relation to corresponding maximum shear stress at wall boundary.

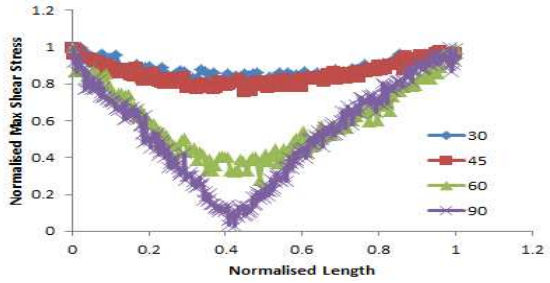

FIGURE 4. Normalised magnitude of maximum shear stress distribution across the width of JASA100 bed at H/2 inside different hopper geometries

These results indicate that, the maximum shear stress distribution is relatively more uniform across the width of the hopper for decrease in internal angle of the hopper and non-homogeneous for higher values of hopper angle.

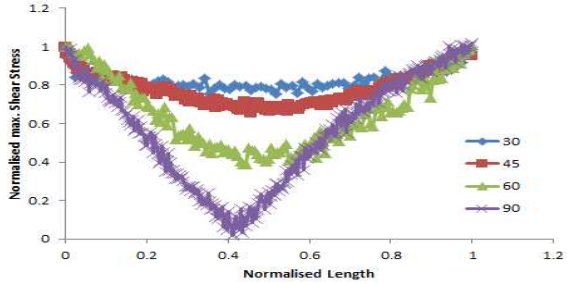

FIGURE 5. Normalised magnitude of maximum shear stress distribution across the width of JASA200 bed at H/2 inside different hopper geometries

DEM Results

Inter-particle interactions between grains of the above mentioned particle assemblies are modelled by DEM methods [2, 8]. The contact model used is the linear contact model and it is defined by the normal and shear stiffness (force/displacement) of the two contacting entities (particle-to-particle or particle-to-wall). This method has been widely adopted in DEM simulations of granular materials. Maximum shear test within conical hoppers is carried out using PFC3D for granular materials of identical properties used in PSAT analysis as shown below for different hopper angles.

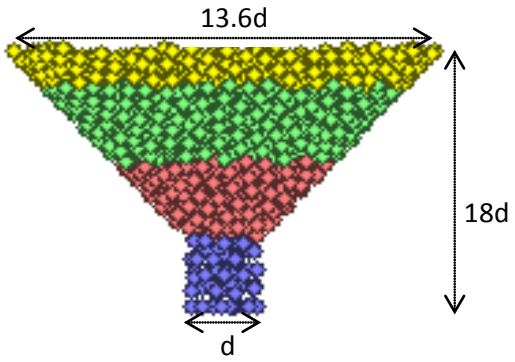

FIGURE 6. Cross section of the hopper (schematic) and the confinement of particles

Where d = 0.005m which is the hopper width and the major properties used are given in table 1.

Table 1. Properties of particles used in DEM simulations

Quantity	Value	Quantity	Value
Gravity m/s^2	9.8	Particle average radius (µm)	650
Density kg/m^3	708	Particle radius ratio	3.3
Initial porosity	0.16	Friction coefficient	0.3
Particle minimum radius(µm)	300	Stiffness (N/m)	1e7

The samples are created randomly and consistently in all the runs. The particles were allowed to reach equilibrium after which the maximum shear stress is tracked along different scanning points at a selected height (H/2) within the hopper and presented in Fig. 6.

The DEM-based results are compared with experimental results obtained from PSAT technology for hopper angles 60^o and 90^o. The simulation results show that stress is higher along the walls of the hopper and tend to decrease

towards the middle of the hopper for different angle of opening. Higher shear stress field was experienced at lower internal angle of the hopper across the width of the hopper. This trend of shear stress across the powder bed obtained from DEM is similar to what was obtained using PSAT as shown in Fig. 7.

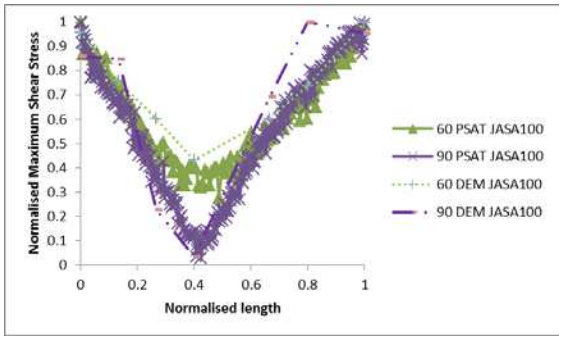

FIGURE 7. Maximum shear stress distribution for granular bed using DEM simulation and PSAT (hopper angles = 60^{o} and 90^{o})

The current results help to understand the nature of shear stress field in static packing of powders inside hopper geometries. Further studies are required to evaluate the dynamic characteristics of powders through hoppers and their dependence on the initial shear resistance zones inside powder packing.

CONCLUSION

For the first time, PSAT is applied to probe the local distribution of maximum shear stress field within actual powder assemblies inside different hopper geometries. The obtained PSAT and DEM results indicate that the magnitude of maximum shear stress distribution across the width of the hopper tends to be more uniform, as well as the direction of the major principal stress acts along the direction of gravity for decrease in internal angle of the hopper. This indicates that hoppers with small opening angles could be the preferred candidate for designing devices with uniform powder flow.

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