Microstructure Evolution During Compaction of Powder Blends

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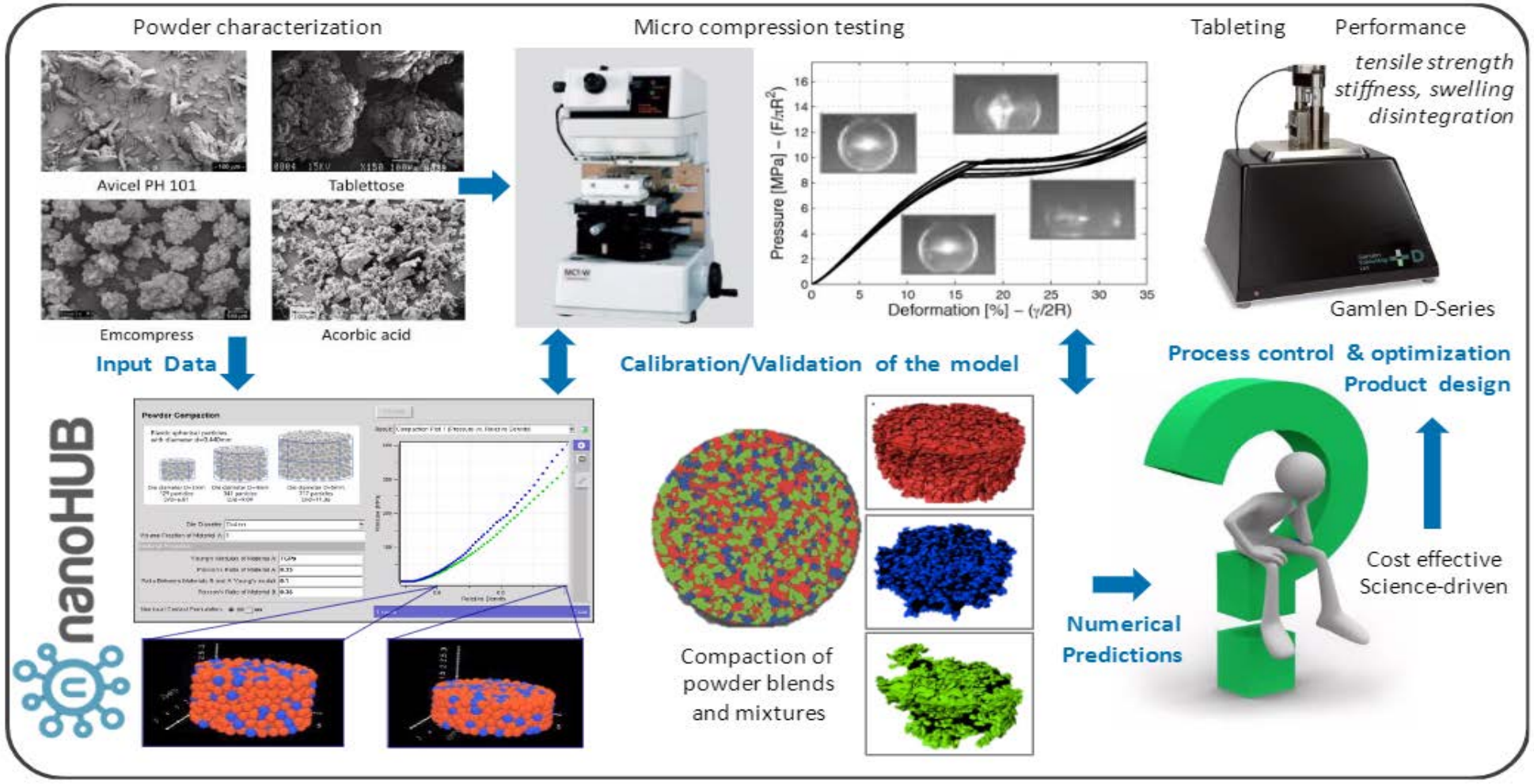
Background and motivation:

- In Pharmaceutical manufacturing of compressed tablets, crystalline or granular active materials (API) are compacted in combination with required expients to form tablets of different shapes.
- Improper compaction of pharmaceutical tablets can lead to capping/horizontal separation. Erroneous compaction of pharmaceutical tablets can also bring change in the chemical properties of their constituents!

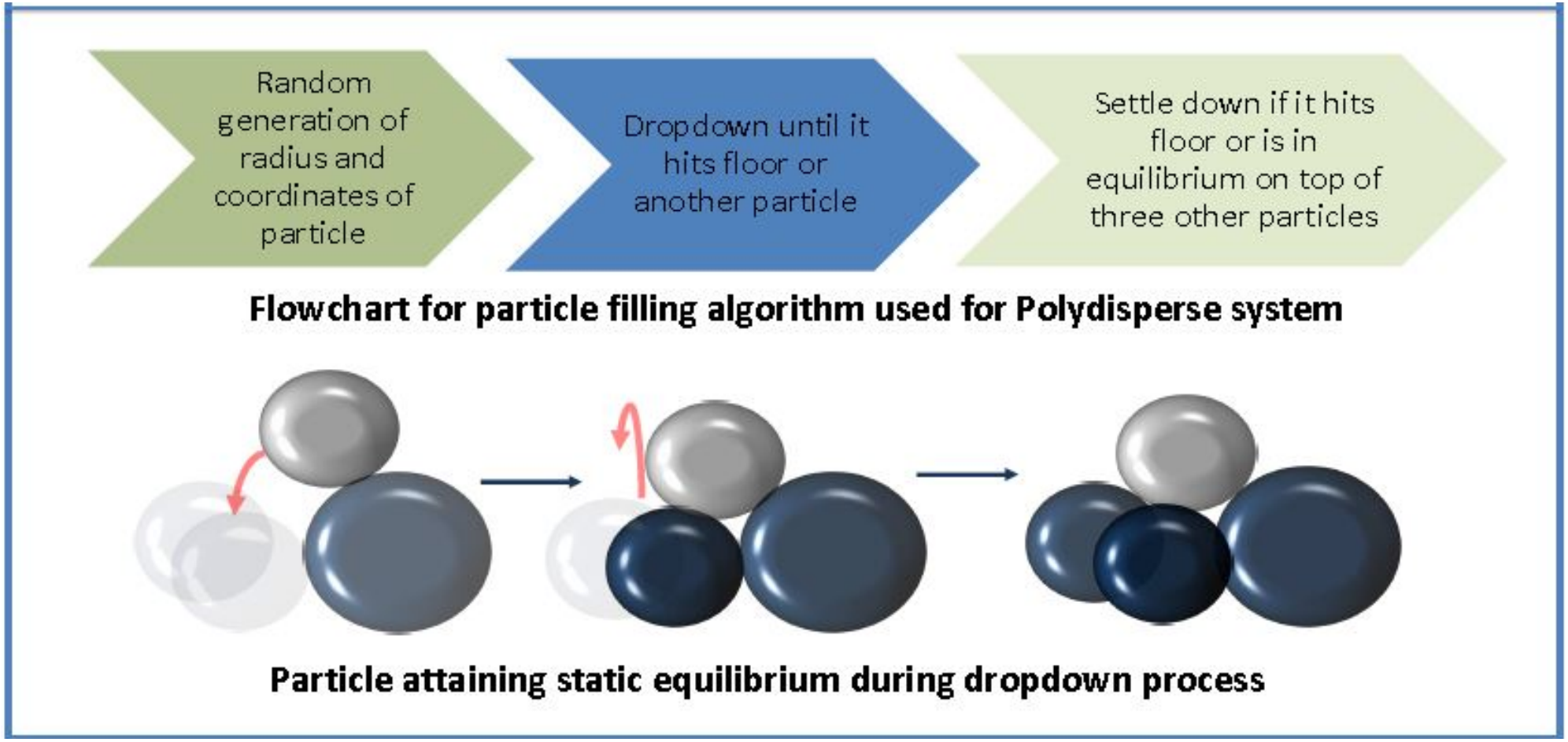
Capping of Tablets

Methods:



Results from nanoHUB simulation tool are used to predict and validate experimental results.

Methods continued:



Flowchart for particle filling algorithm used for Polydisperse system

Particle attaining static equilibrium during dropdown process

Static based algorithm used for particle packing.

Powder Compaction simulation inputs:

Powder Compaction Simulation Inputs

Size:

- Number of particles
- Volume fraction

Particle Size Distribution:

- Distribution type
- Mean radii
- Std. Deviations

Particle Size Cutoff:

- Minimum and Maximum radii

Material Properties:

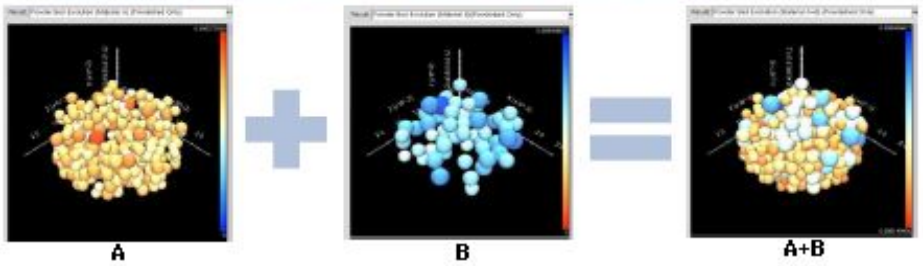
- Young's moduli of elasticity
- Poisson's ratios

Simulation Inputs

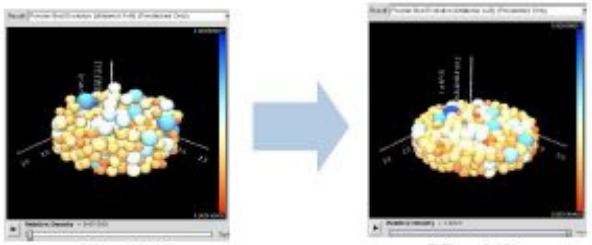
Powder Compaction simulation outputs:

Powder Compaction Simulation Outputs

Powder bed with binary mixture of materials:

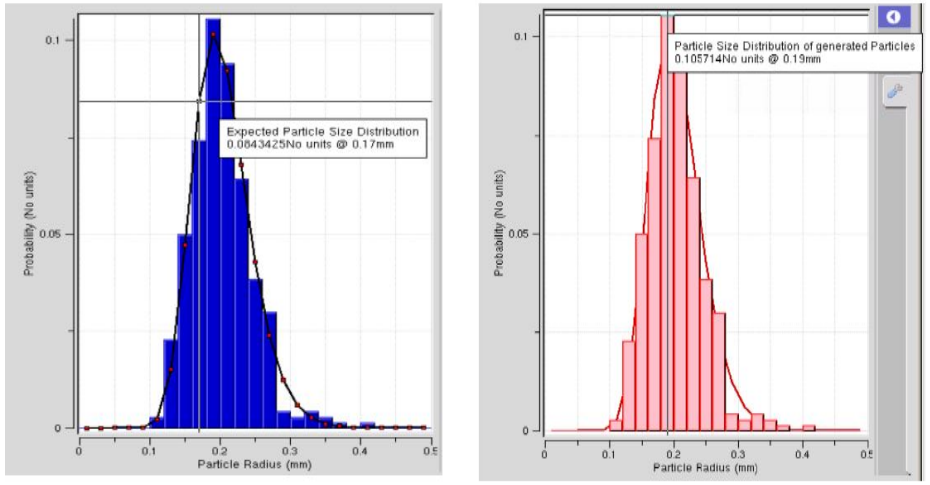


Particle Filling for individual materials and their binary mixture with a volume fraction ratio of 3:2



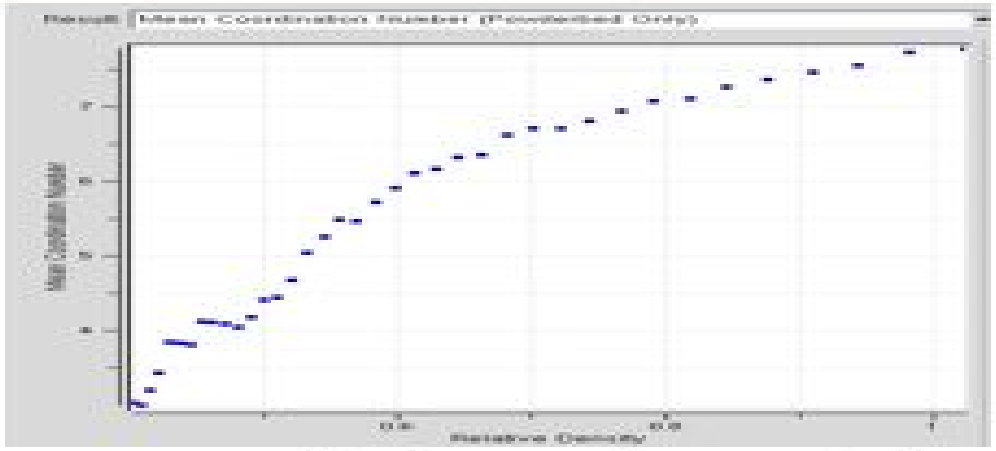
Compaction of powder bed with the change in relative density

Probability distribution curves:

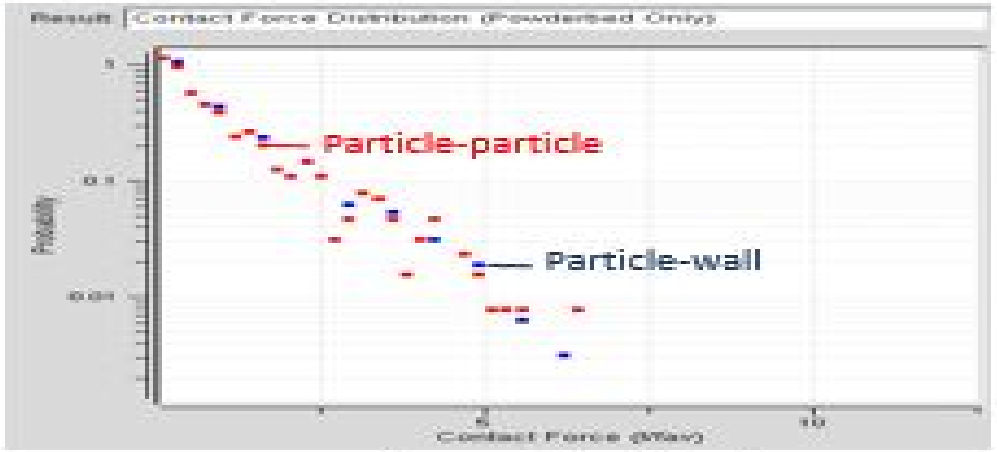


Comparison of Probability distribution of generated particles (bar) vs User Inputted Probability distribution function (line)

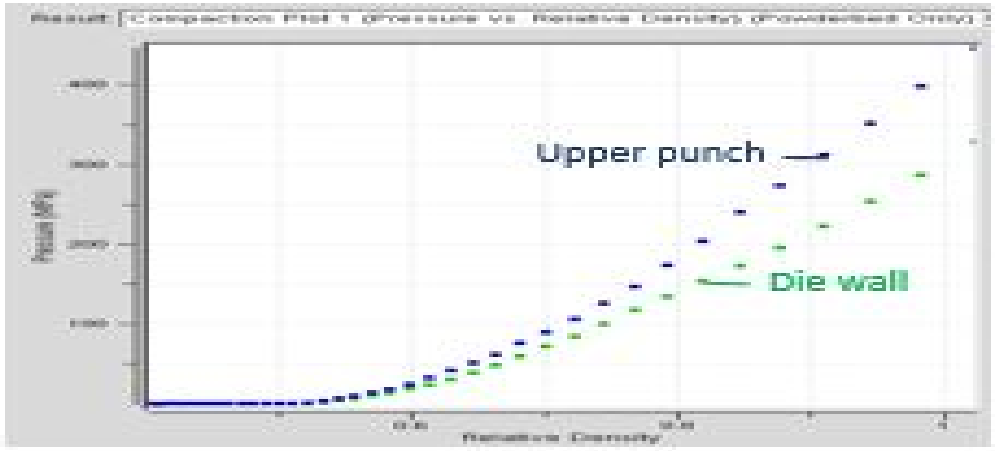
Powder Compaction Simulation outputs:



Mean coordination number vs relative density



Contact force distribution



Pressure vs relative density

Pressure vs tablet height

Conclusions:

- A new version of the nanoHUB Powder Compaction tool was developed.
- The new feature allows users to create powder bed with binary mixture of particles of different sizes.
- Users can select distribution types for each material type to better mimic practical composition of powder bed.
- Simulation tool can be made more effective by extending polydisperse mixture to mixture of three or more powders.
- The tool can be accessed using the following link:

  https://nanohub.org/resources/gscompaction