

Modelling Powder Flow Into a Confined Space

Powder Flow 2018, London. 12th April 2018



Charley Wu

Chemical and Process Engineering
University of Surrey,
Guildford, UK

 @charleywu

 C.Y.WU@surrey.ac.uk



Introduction

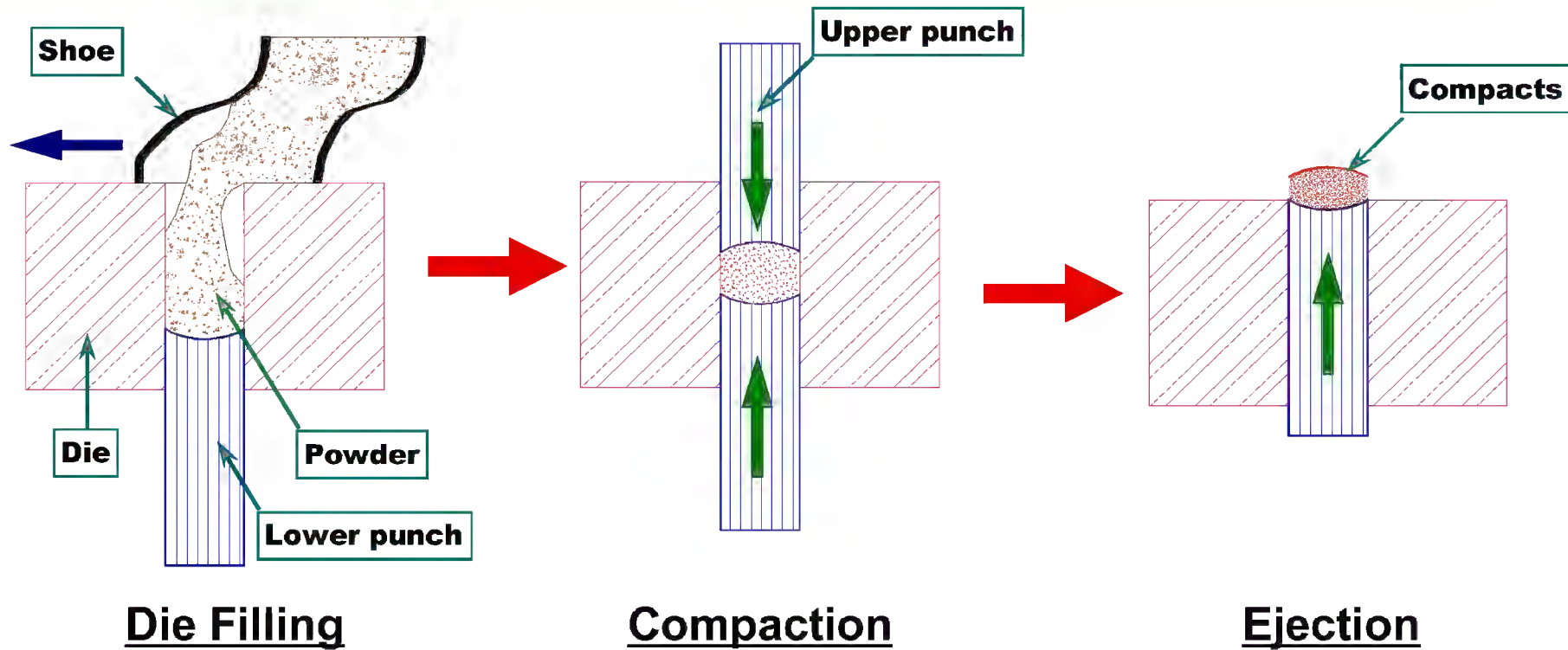
Many products are manufacturing through compaction of dry powders, involving powder flow into a confined space.



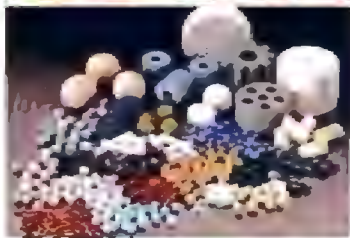
- Pharmaceutical
- Catalyst
- Automotive
- Chemical
- Ceramic
- Magnetic
- Food



Typical Manufacturing Process



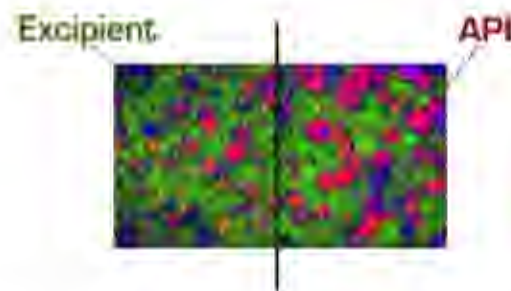
Why Die Filling Is Important?



Any problem during die filling will have a direct impact on the quality of the final products.

Failure during die filling can lead to

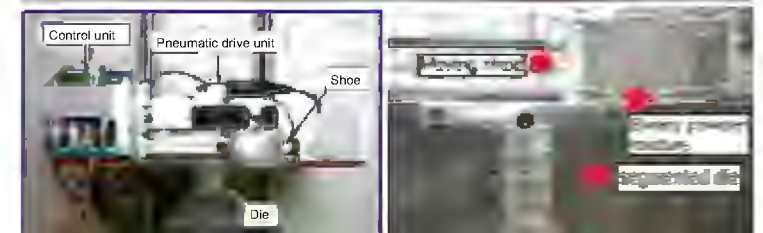
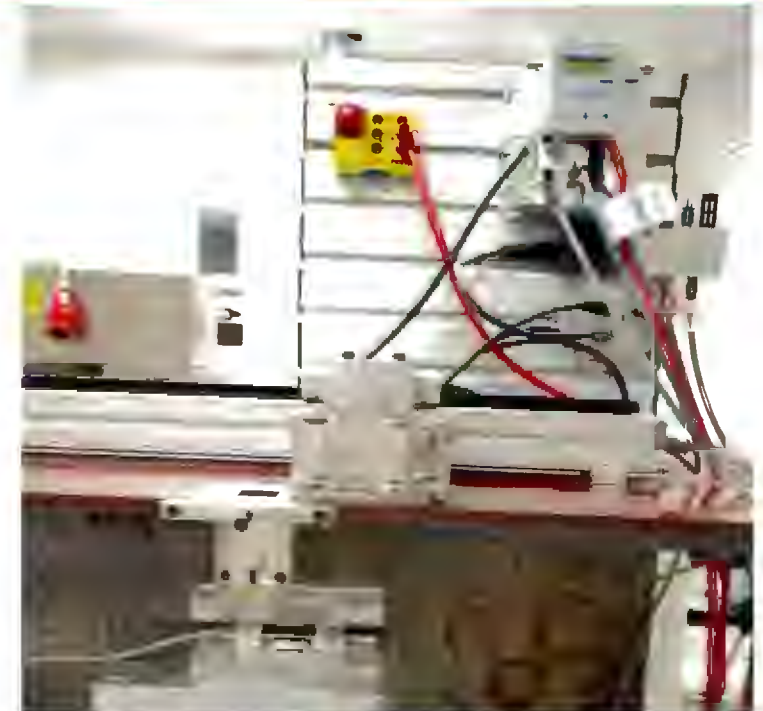
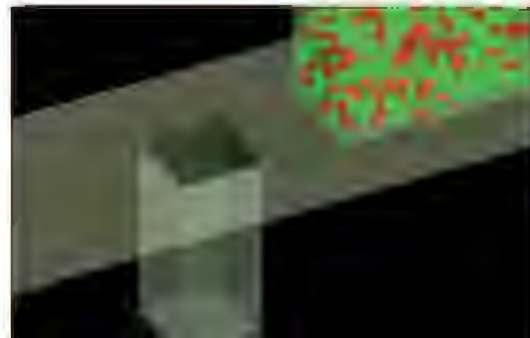
- Tablets of inaccurate dose!
- Products with large weight variation
- Products with non-uniform contents that detrimentally affect the functionality
- Gears of uneven strength and with weakest links.
- Distortion (and complete failure) during subsequent processes, such as sintering.



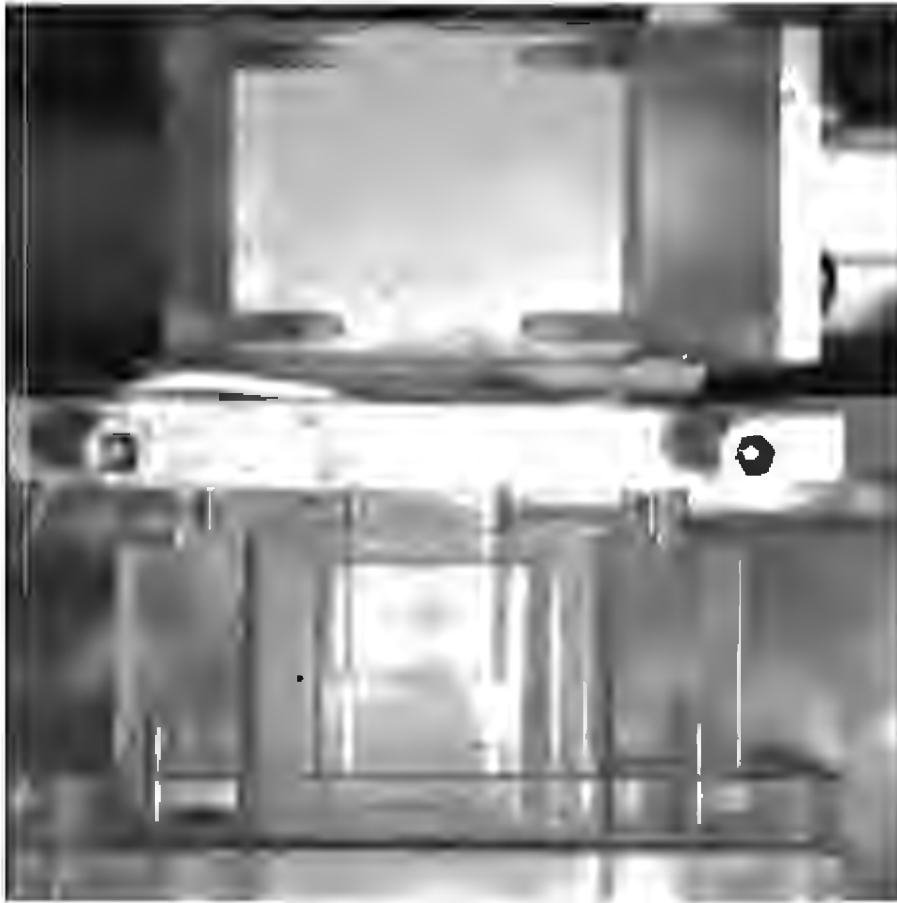
"If your doctor prescribed half a tablet a day, which half would you want to take?" (Malvern Instruments, 2008).

Methodology (Exp. + Modelling)

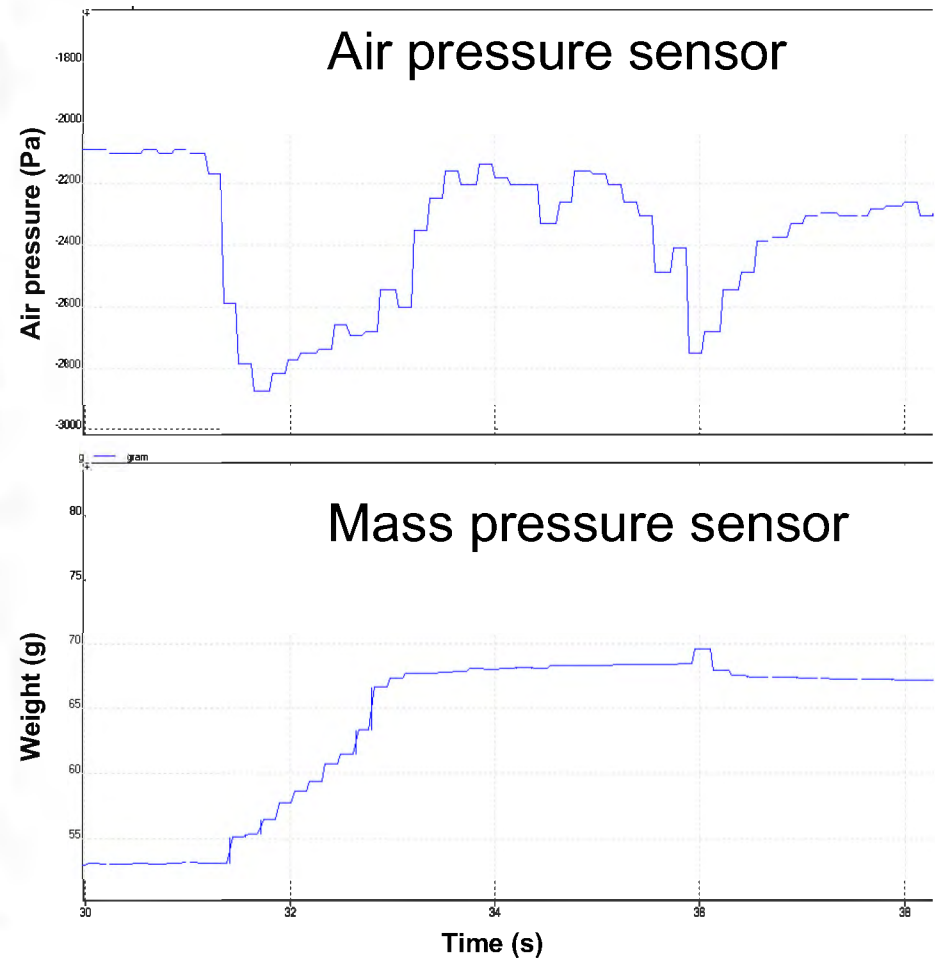
- ❑ A combined **experimental** and **numerical** approach was employed to understand the die filling process.
- ❑ A **model die filling system** was developed.
- ❑ Die filling behaviour was visualised using a **high speed video** system.
- ❑ Quantitative analysis was also performed using
 - **PEPT** -> particle velocity
 - A **pressure sensor** -> time evolution of deposited mass.
 - An **air pressure sensor** -> air pressure build-up
- ❑ Mechanistic analysis was performed using **DEM-CFD**



A typical experimental set-up



High speed video



PEPT Study

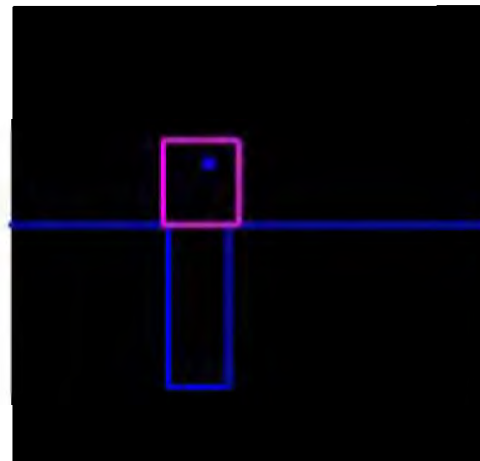
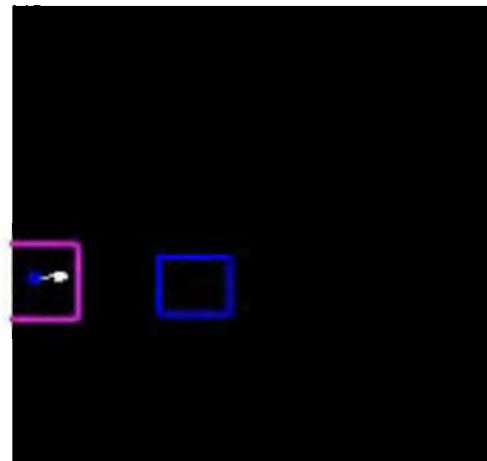
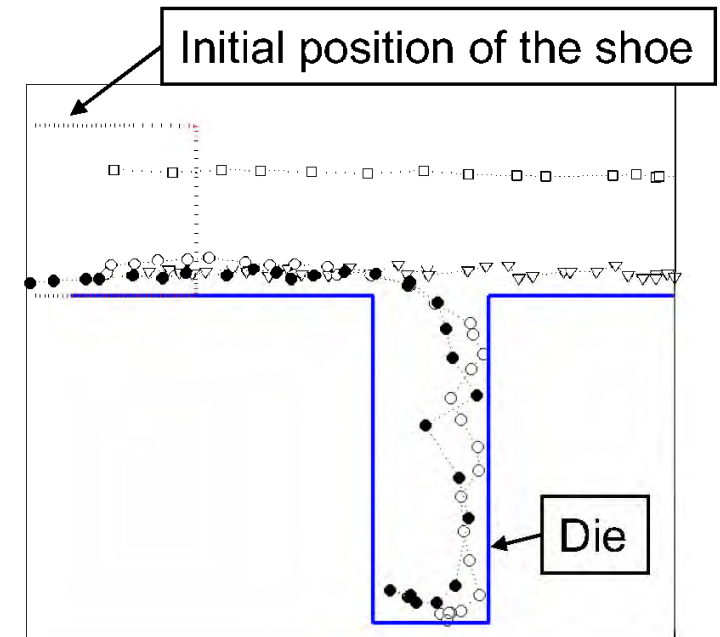
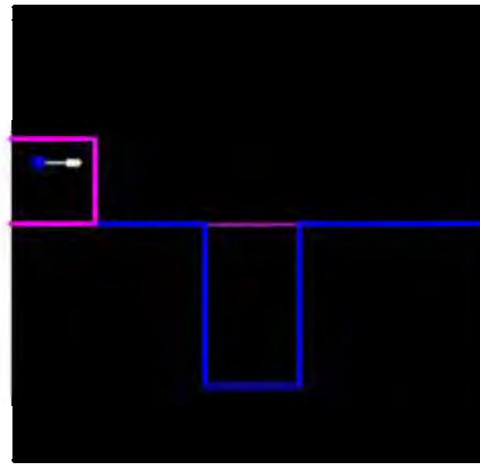
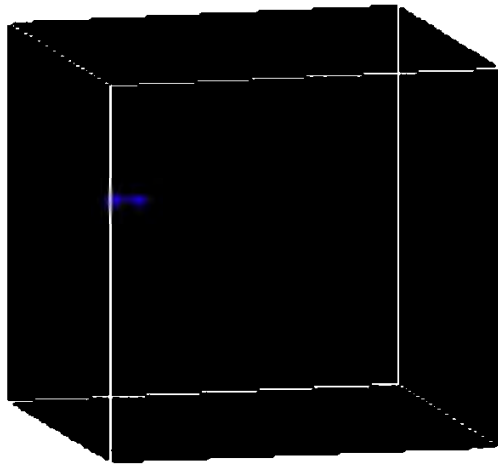
(Positron Emission Particle Tracking)



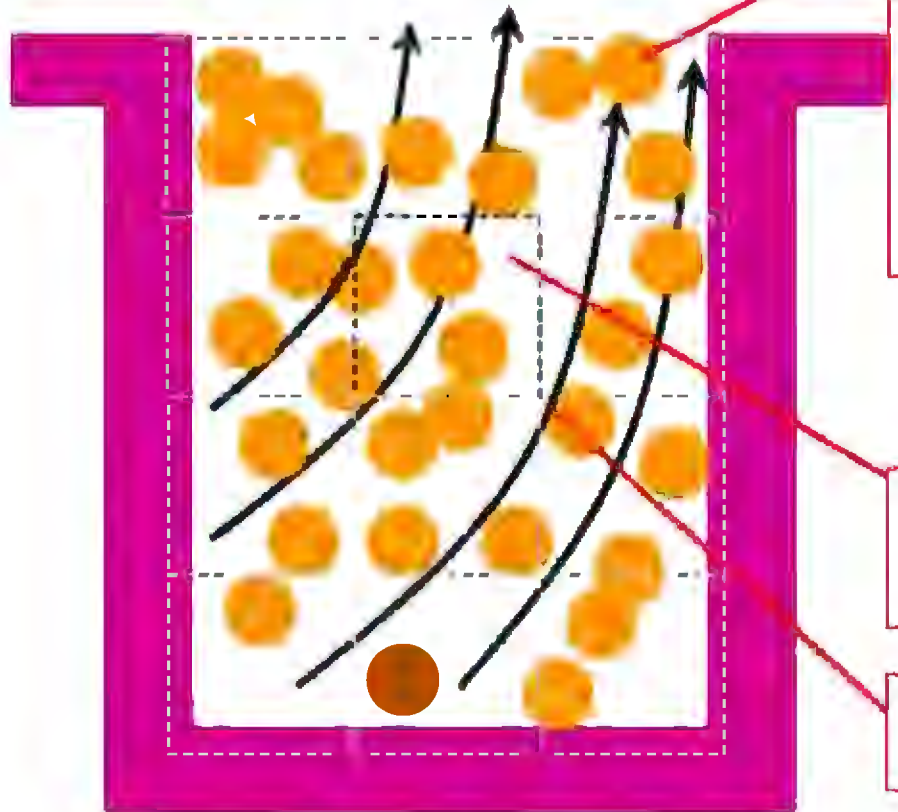
PEPT Study

3D trajectories of individual particles

Spherical microcrystalline cellulose (Celphere, CP102)



DEM-CFD



The flow of particles is modelled using **DEM**.

The interaction between particles are rigorously modelled using theoretical contact mechanics:

- **Hertz-Mindlin-Deresiewicz** for elastic particles
- **JKR** for adhesive particles

The interaction between air and particles is considered.

The flow of air is modelled using **CFD**.

Particle equations of motion:

$$F_i = F_i^c + \mathbf{F}_i^m + F_i^e + m_i g = m_i \ddot{x}_i$$

$$T_i = I_i \ddot{\theta}_i$$

fluid-particle interaction force

$$\mathbf{F}_i = -V_{pi} \nabla p + V_{pi} \nabla \cdot \boldsymbol{\tau}_f + \varepsilon f_{di}$$

Total fluid-particle interaction force per unit volume

$$\mathbf{F}_{fp} = \frac{\sum_{i=1}^N \mathbf{F}_i^{fp}}{\Delta V_c}$$

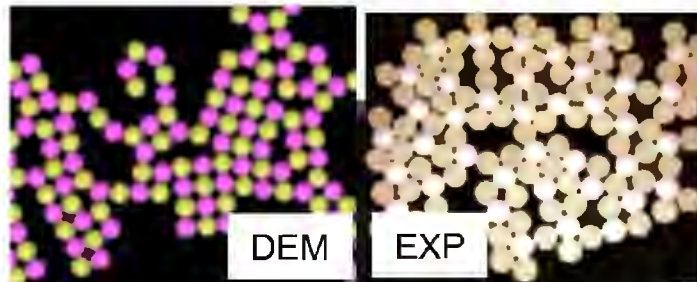
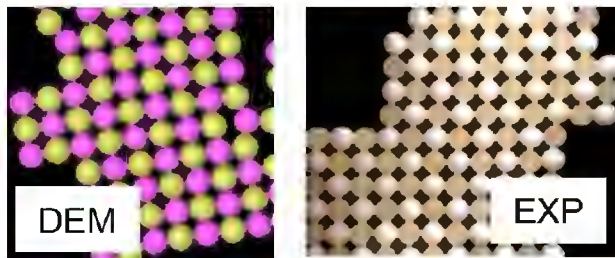
Fluid continuity and momentum equations

$$\frac{\partial(\varepsilon \rho_f)}{\partial t} + \nabla \cdot (\varepsilon \rho_f \mathbf{u}) = 0$$

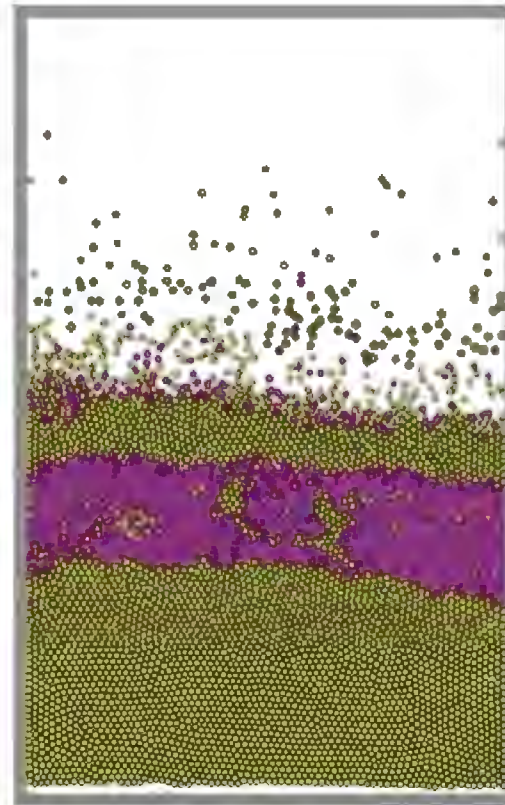
$$\frac{\partial(\varepsilon \rho_f \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon \rho_f \mathbf{u} \mathbf{u}) = -\nabla p_f + \nabla \cdot \boldsymbol{\tau}_f + \varepsilon \rho_f \mathbf{g}$$

DEM-CFD Validation

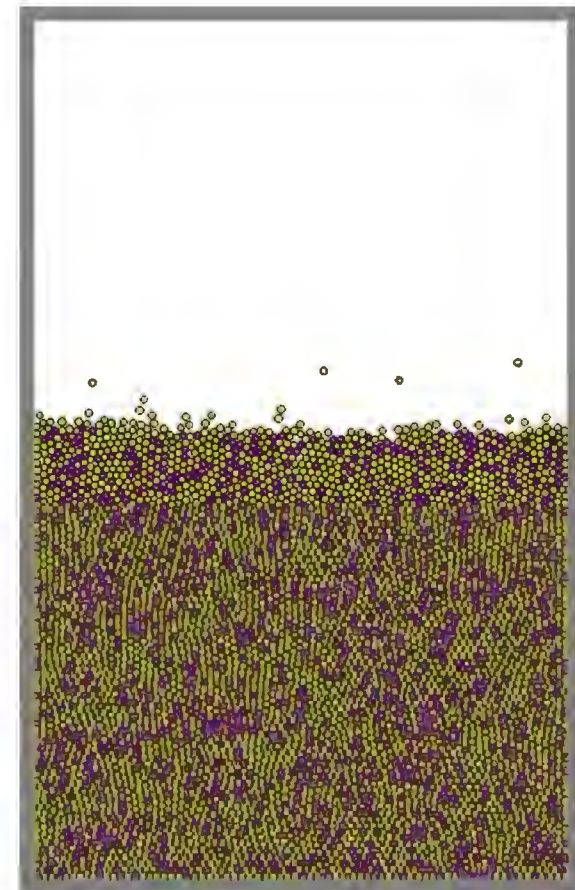
- ❑ Validation of DEM models is important.
- ❑ Qualitative validation is easy, is it convincing?
- ❑ Case-to-case quantitative validation is difficult.



Experimental

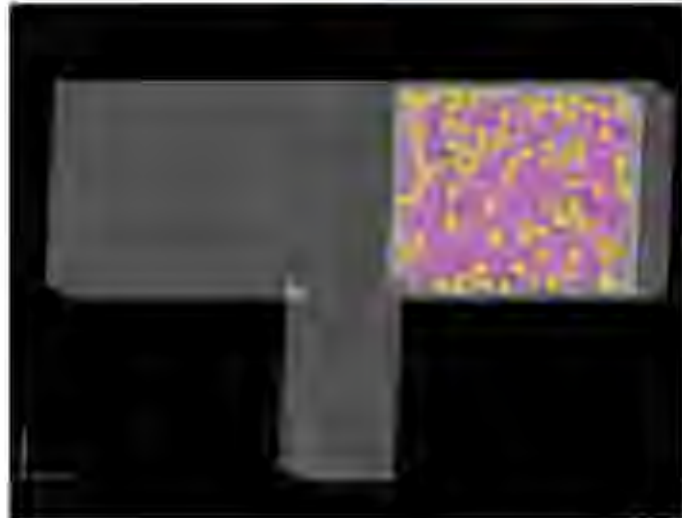


DEM-CFD

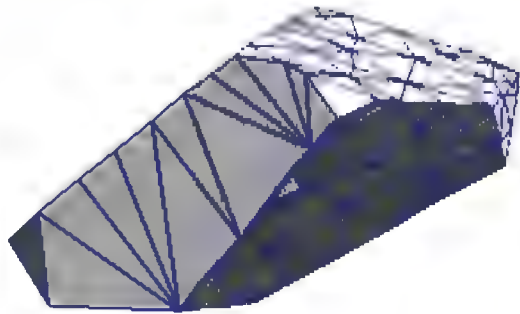


DEM-CFD with Non-spherical Particles

- ❑ Multi-sphere -> approximate particle shapes using clumped spheres.
- ❑ Utilize the rigorous contact laws for modelling particle-particle interaction



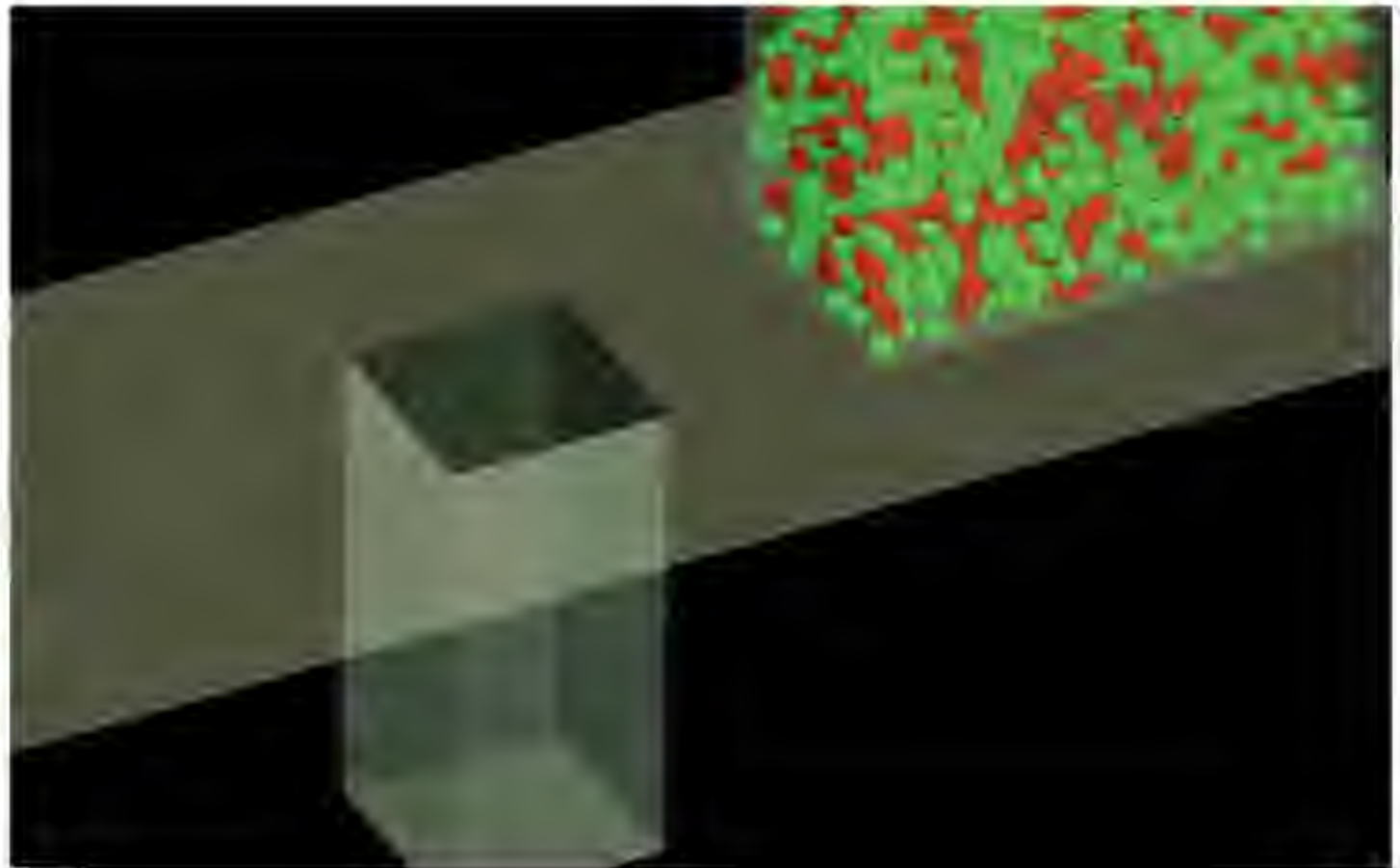
Die filling with real particles (Wu et al. 2016)



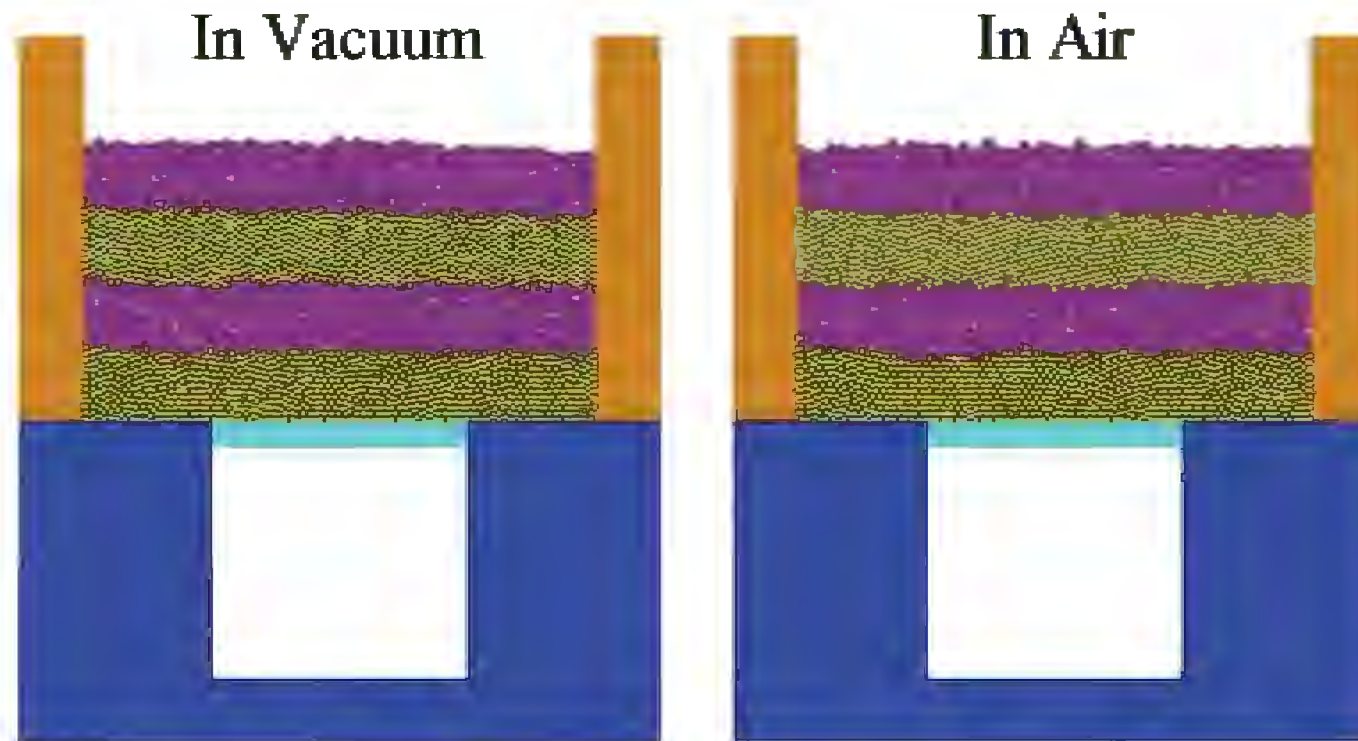
Real crystal



DEM approximation



Flow from a stationary feeder

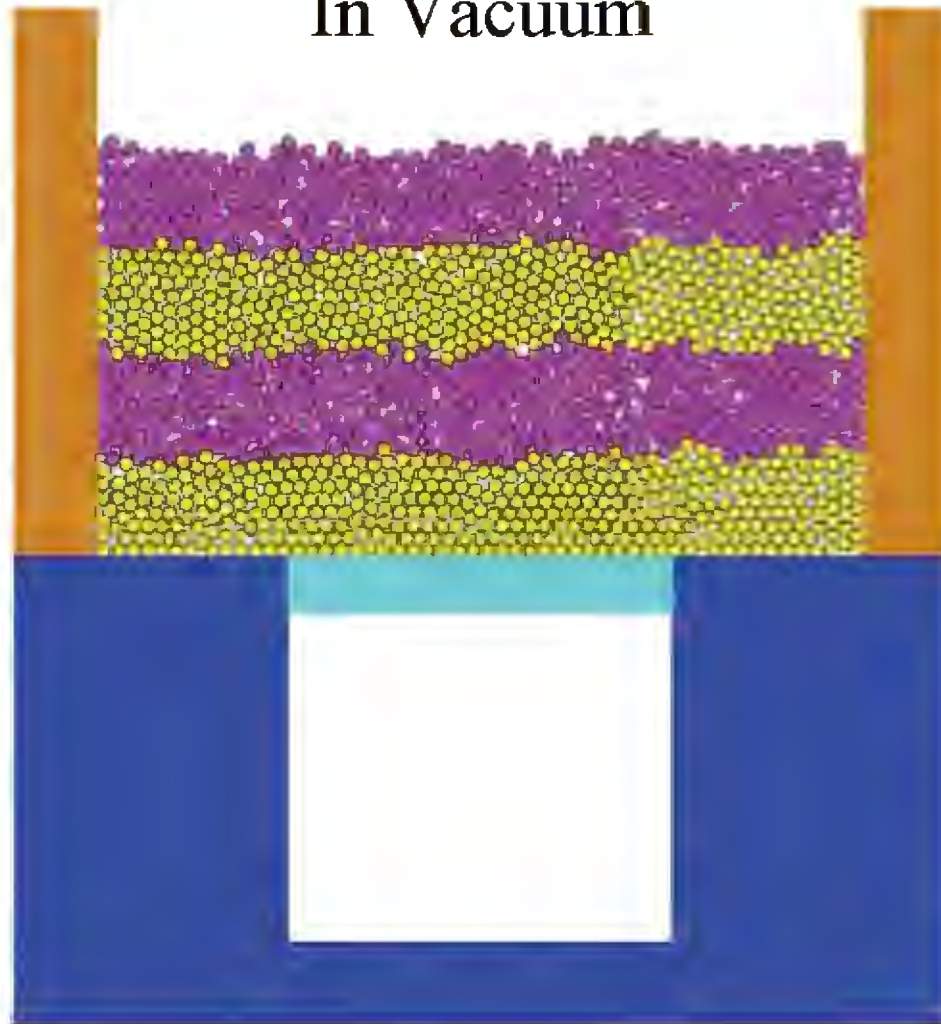


$$\rho_s = 1500 \text{ kg/m}^3, d_p = 50 \text{ }\mu\text{m}$$

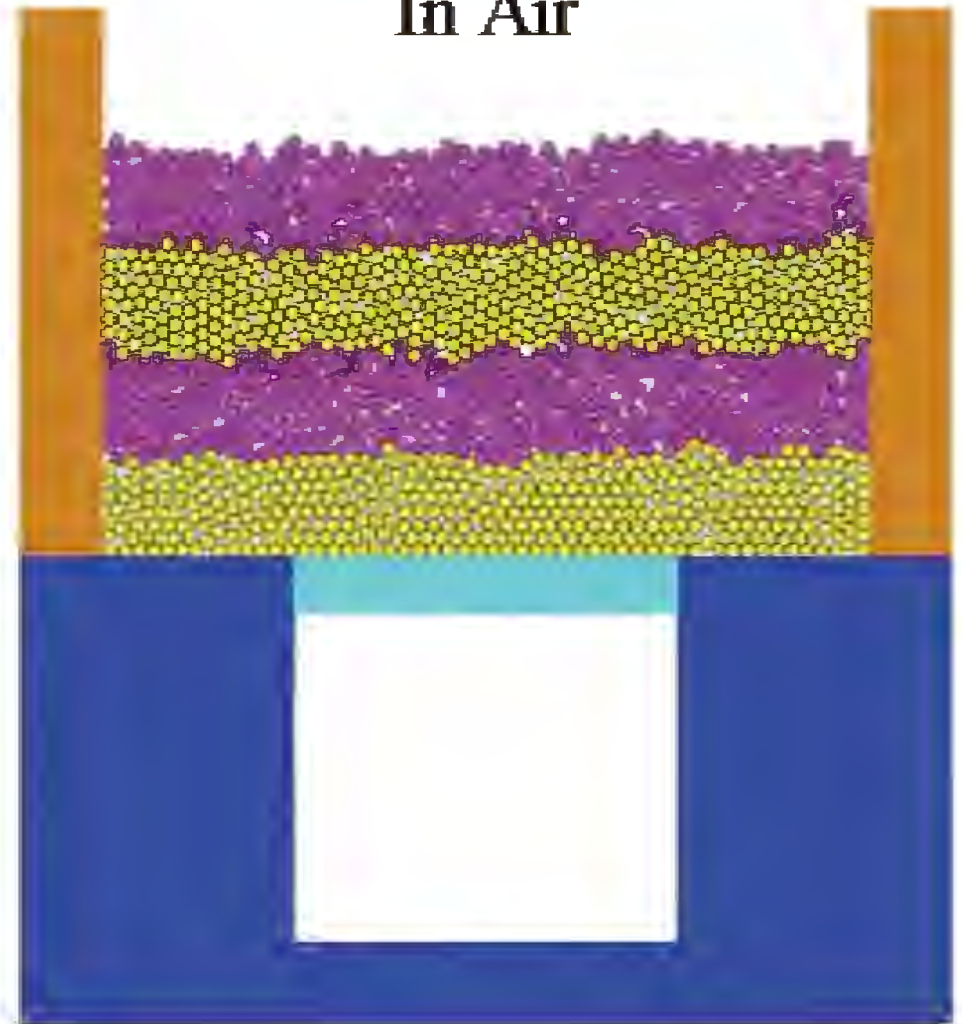


Flow from a stationary feeder

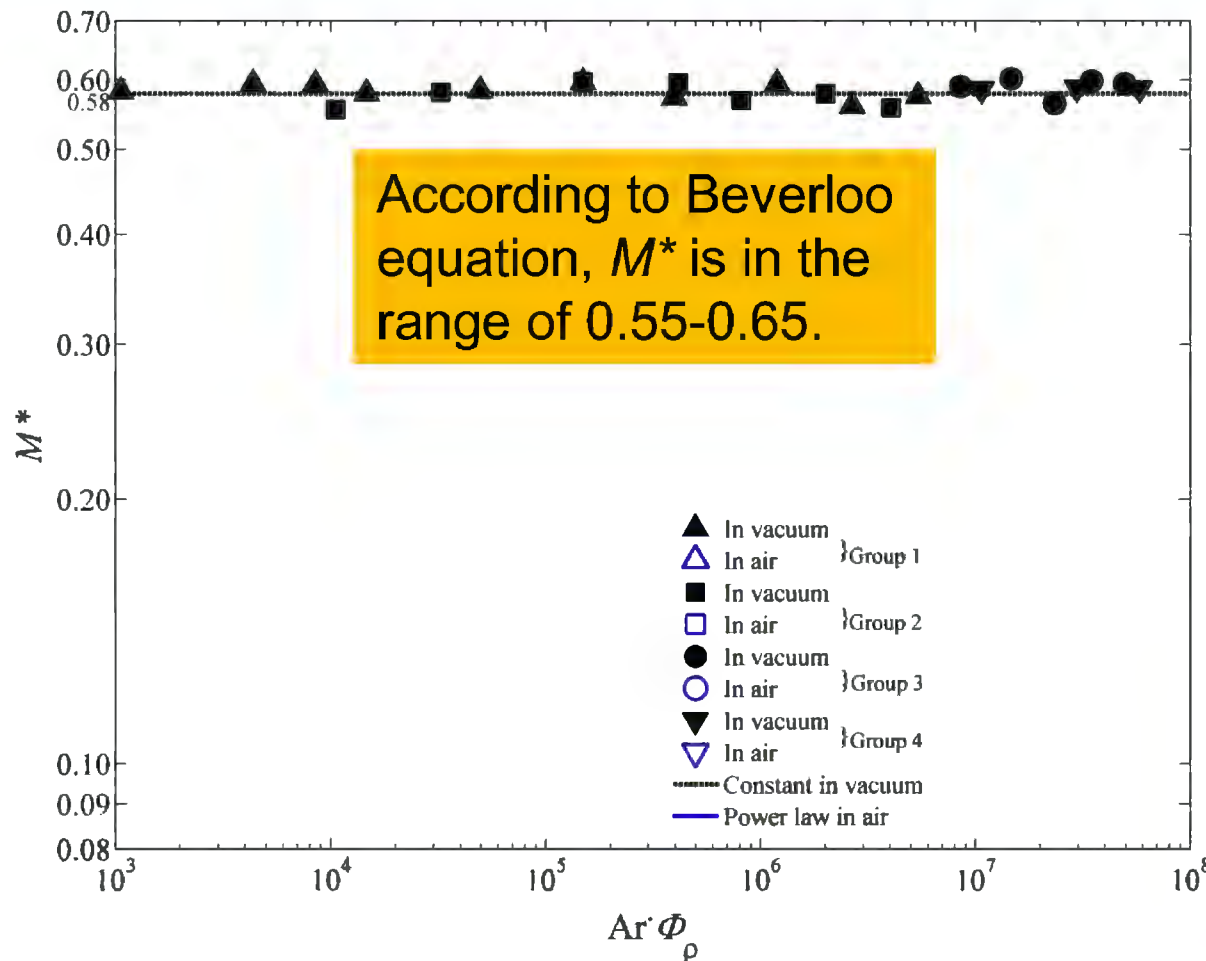
In Vacuum



In Air



Flow from a stationary feeder



Normalised mass flowrate

$$M^* = \frac{\bar{M}}{\rho_b g^{1/2} b^{3/2} l}$$

Normalised particle density

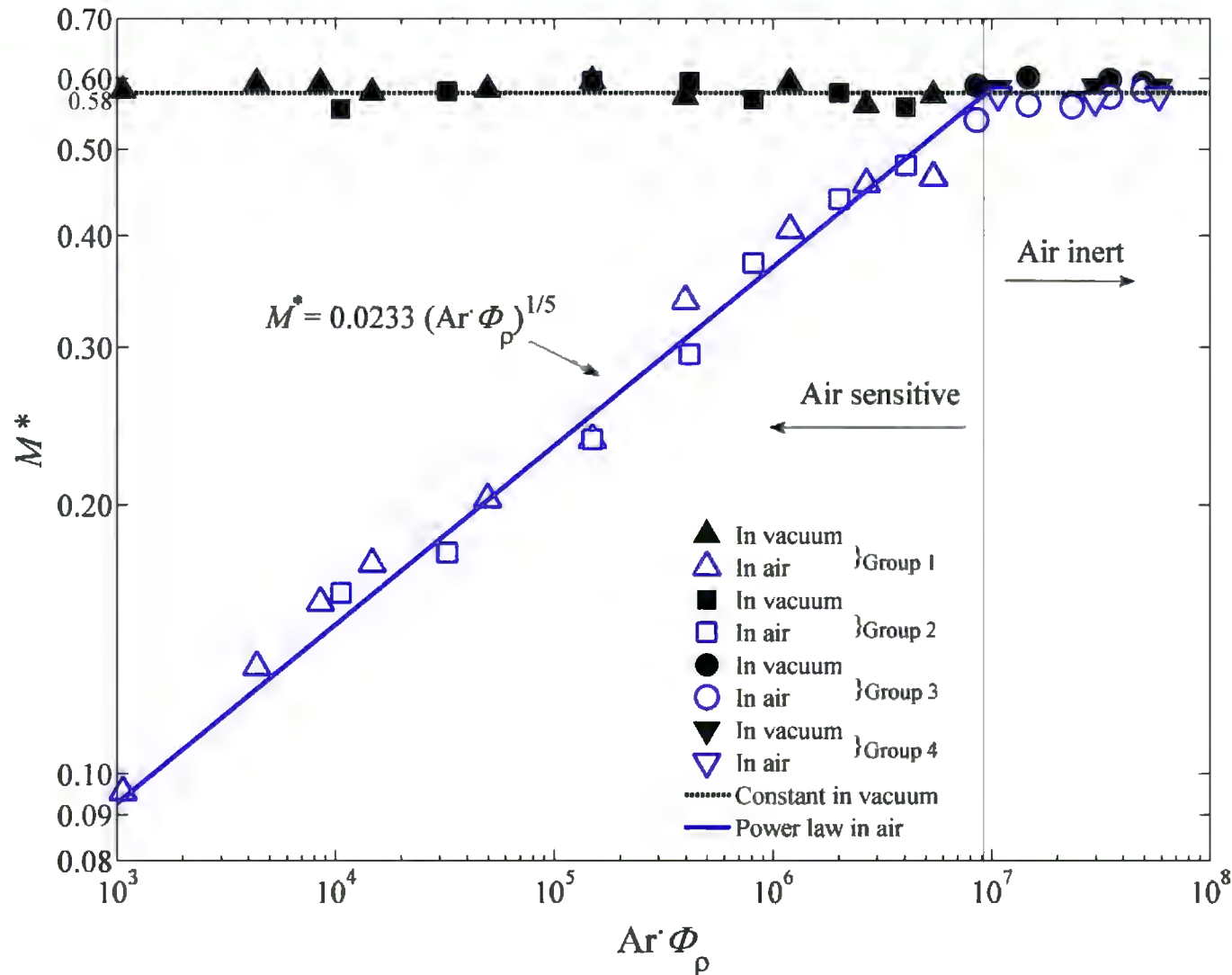
$$\Phi_\rho = \frac{\rho_s}{\rho_a}$$

Archimedes Number

$$A_r = \frac{\rho_a (\rho_s - \rho_a) g d_p^3}{\eta^2}$$

- This is in excellent agreement with Beverloo constants obtained experimentally (C is in the range of 0.55-0.65, for spherical particle $C \approx 0.58$, see Seville et al. 1997).

Flow from a stationary feeder



Flow from a moving feeder



(Fine sand, $V_{\text{shoe}} = 300$ mm/s)



(MCC, $V_{\text{shoe}} = 50$ mm/s)

Flow from a moving feeder

In Air

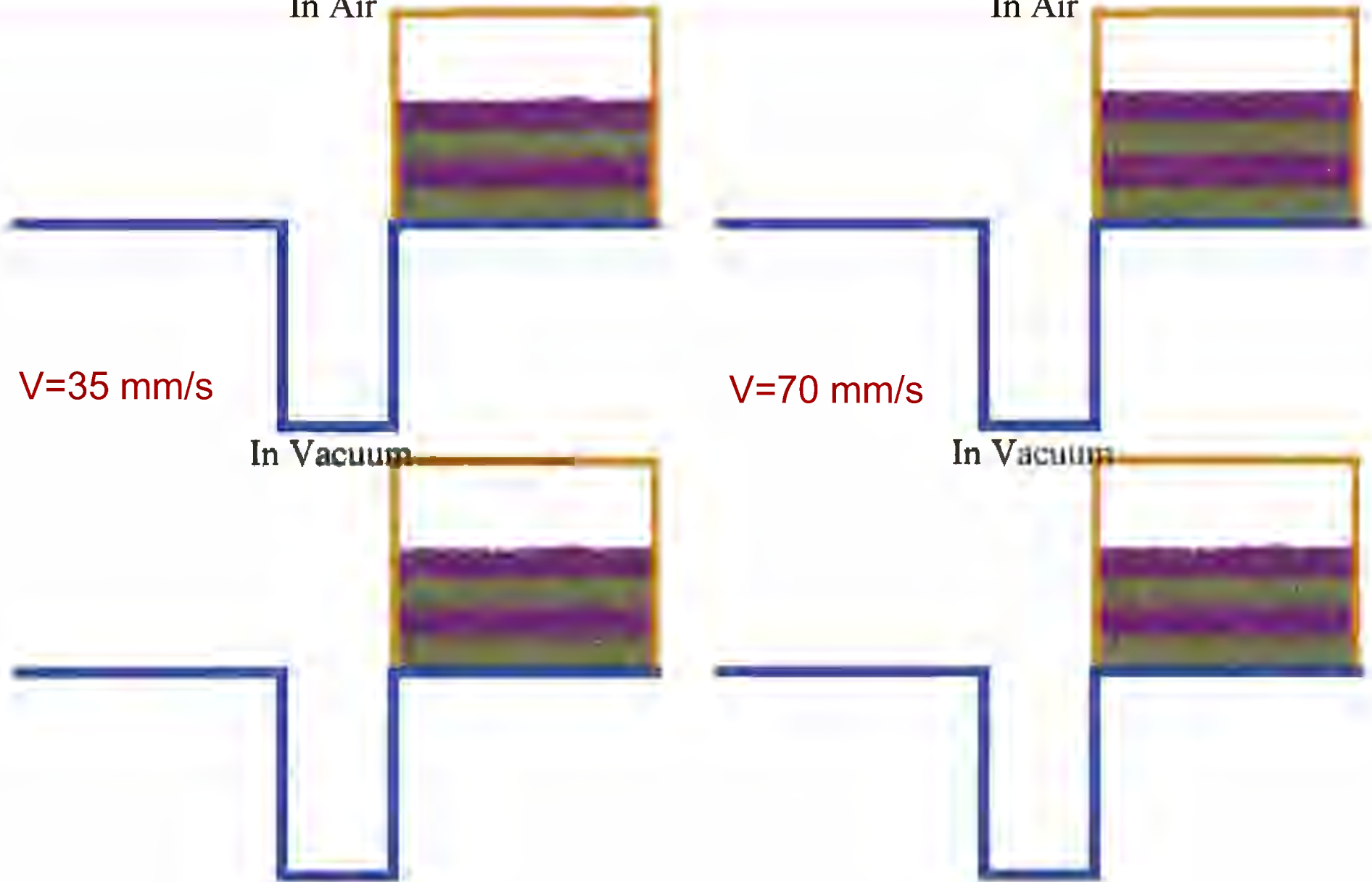
In Air

$V=35$ mm/s

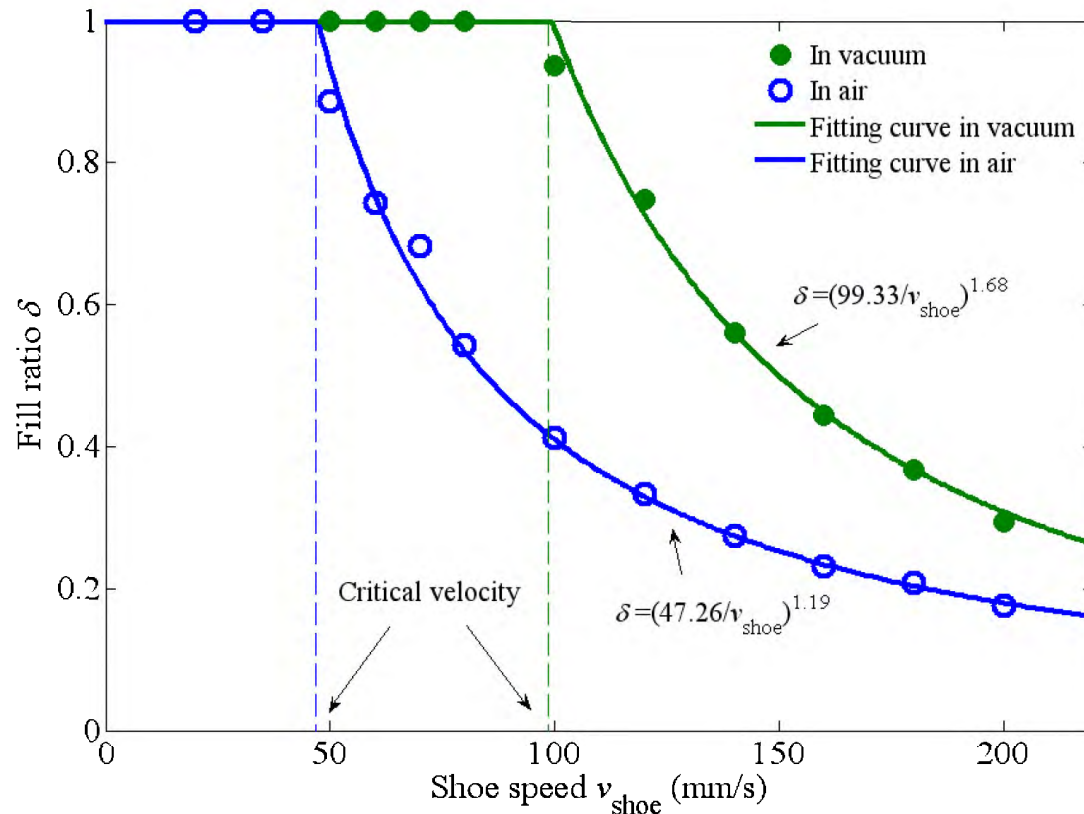
$V=70$ mm/s

In Vacuum

In Vacuum

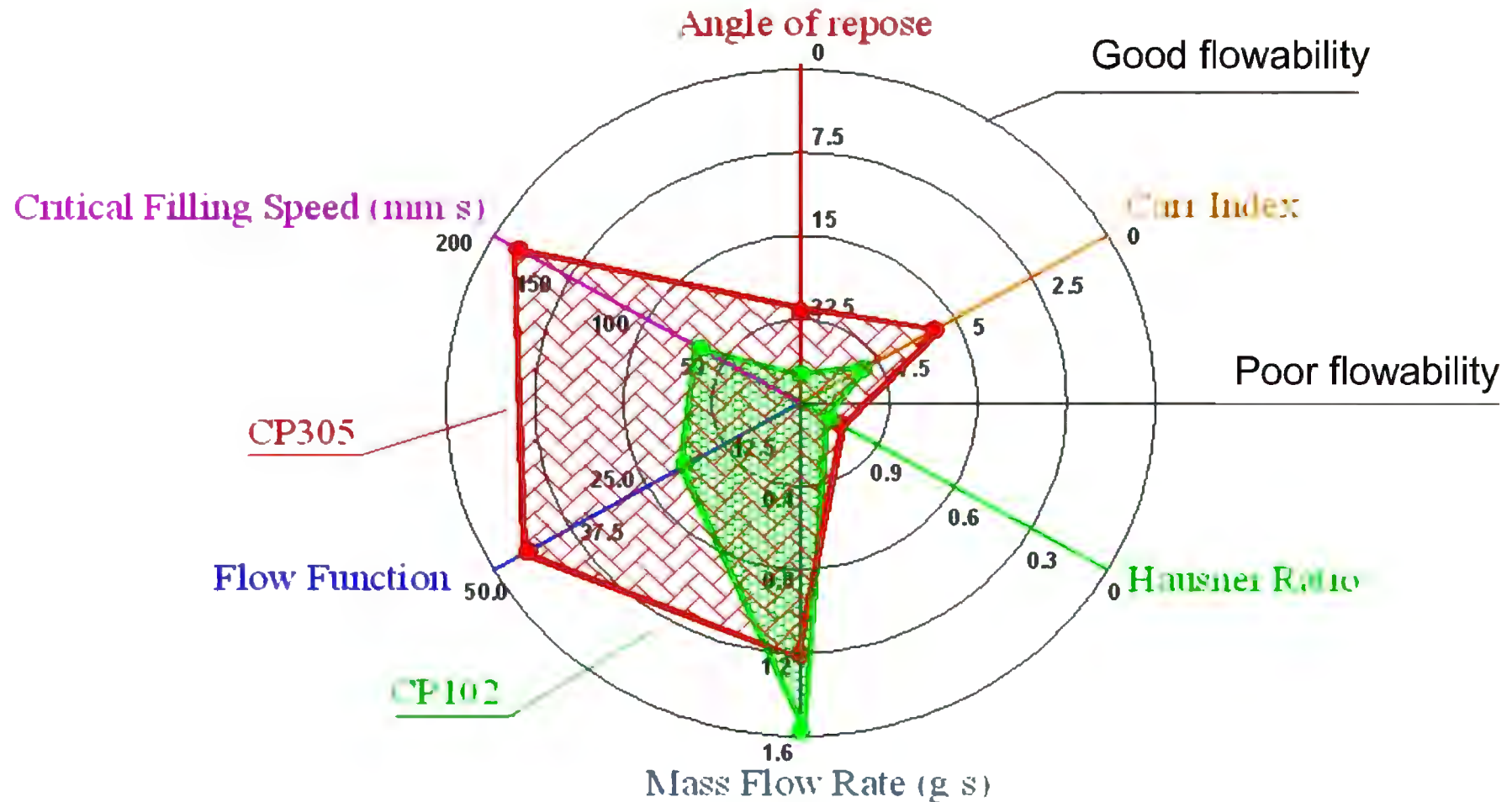


Flow from a moving feeder

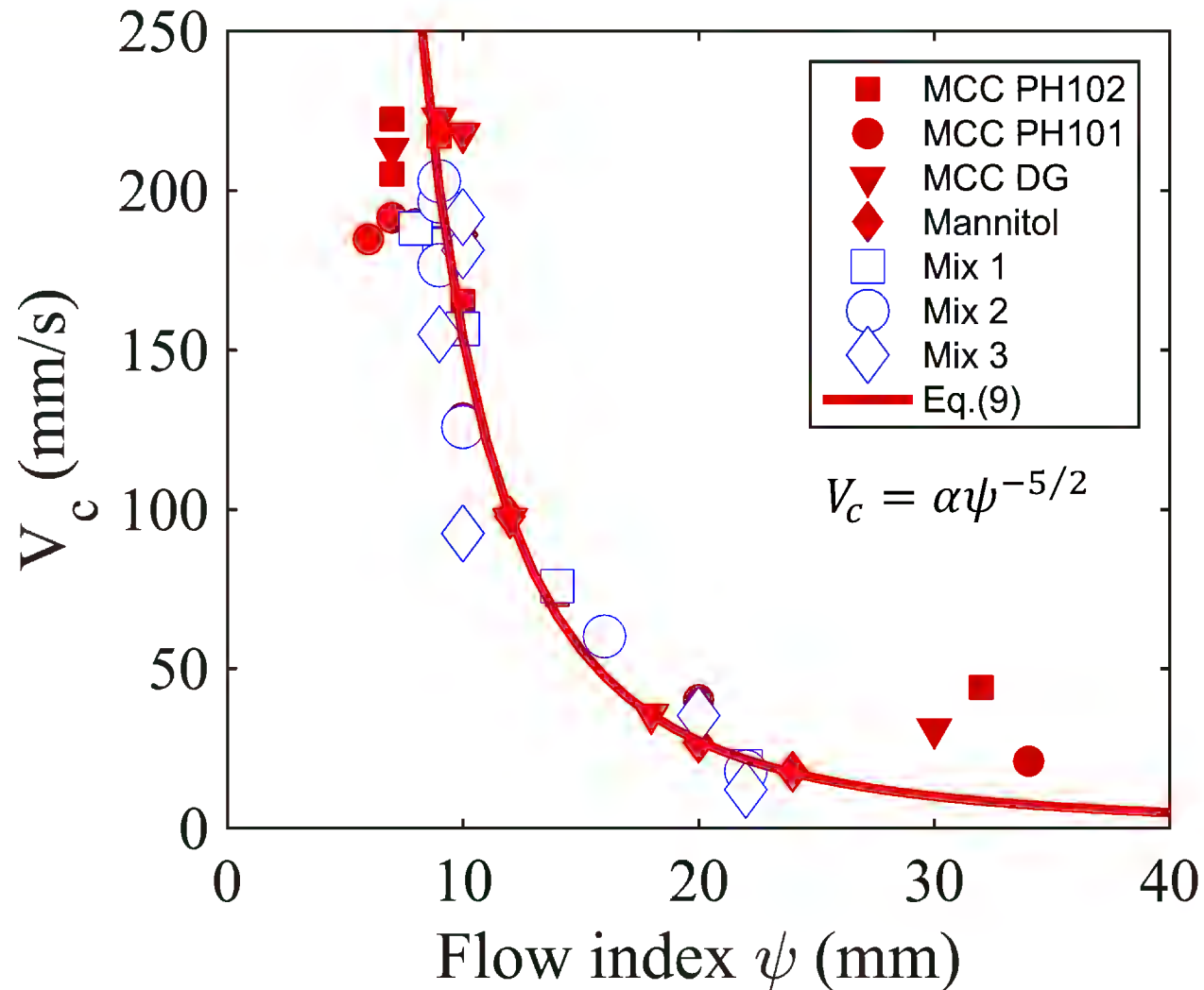


- ❑ There is a critical filling speed during die filling, above which the die cannot be completely filled.
- ❑ The critical filling speed is a function of powder properties, and process system parameters
- ❑ For a given process system, the critical filling speed is dominated by powder properties. This can also be used to assess powder flowability.

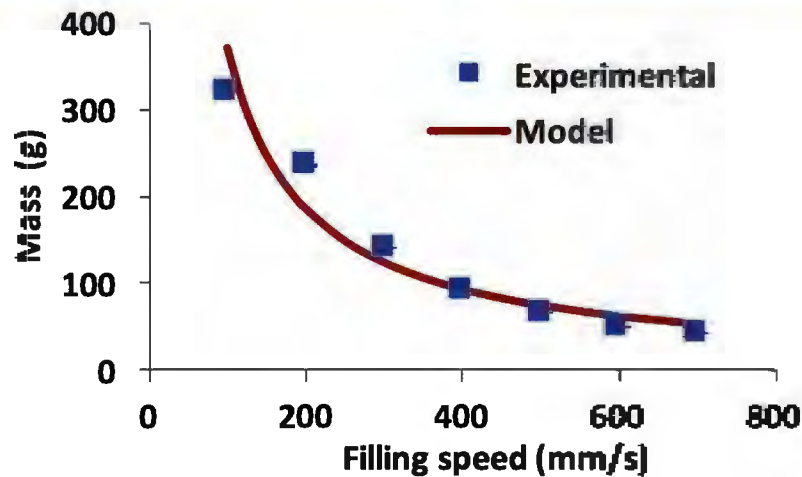
Flow from a moving feeder



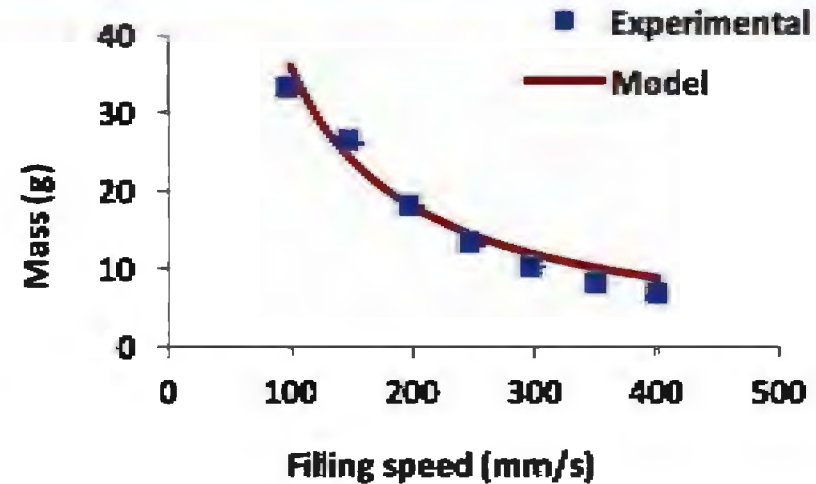
Flow from a moving feeder



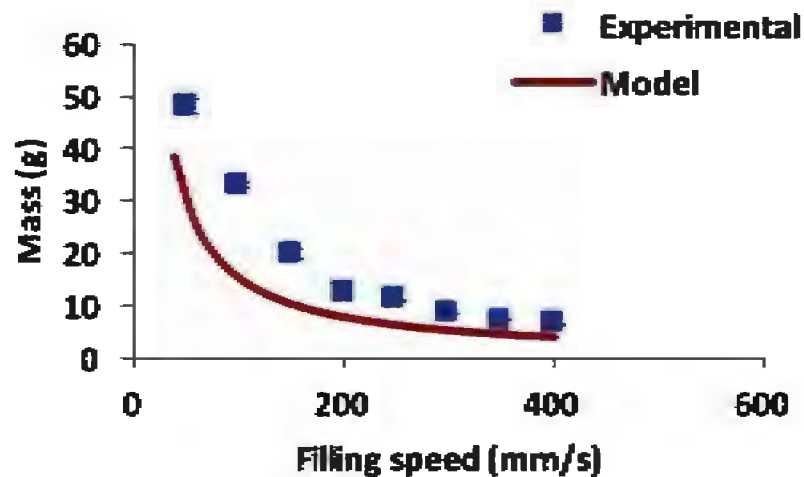
A Mathematical Model for Die Filling



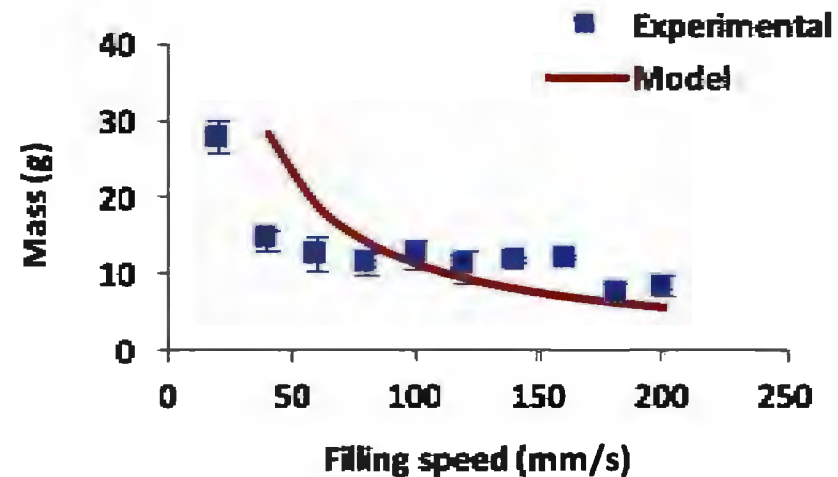
(a)



(b)



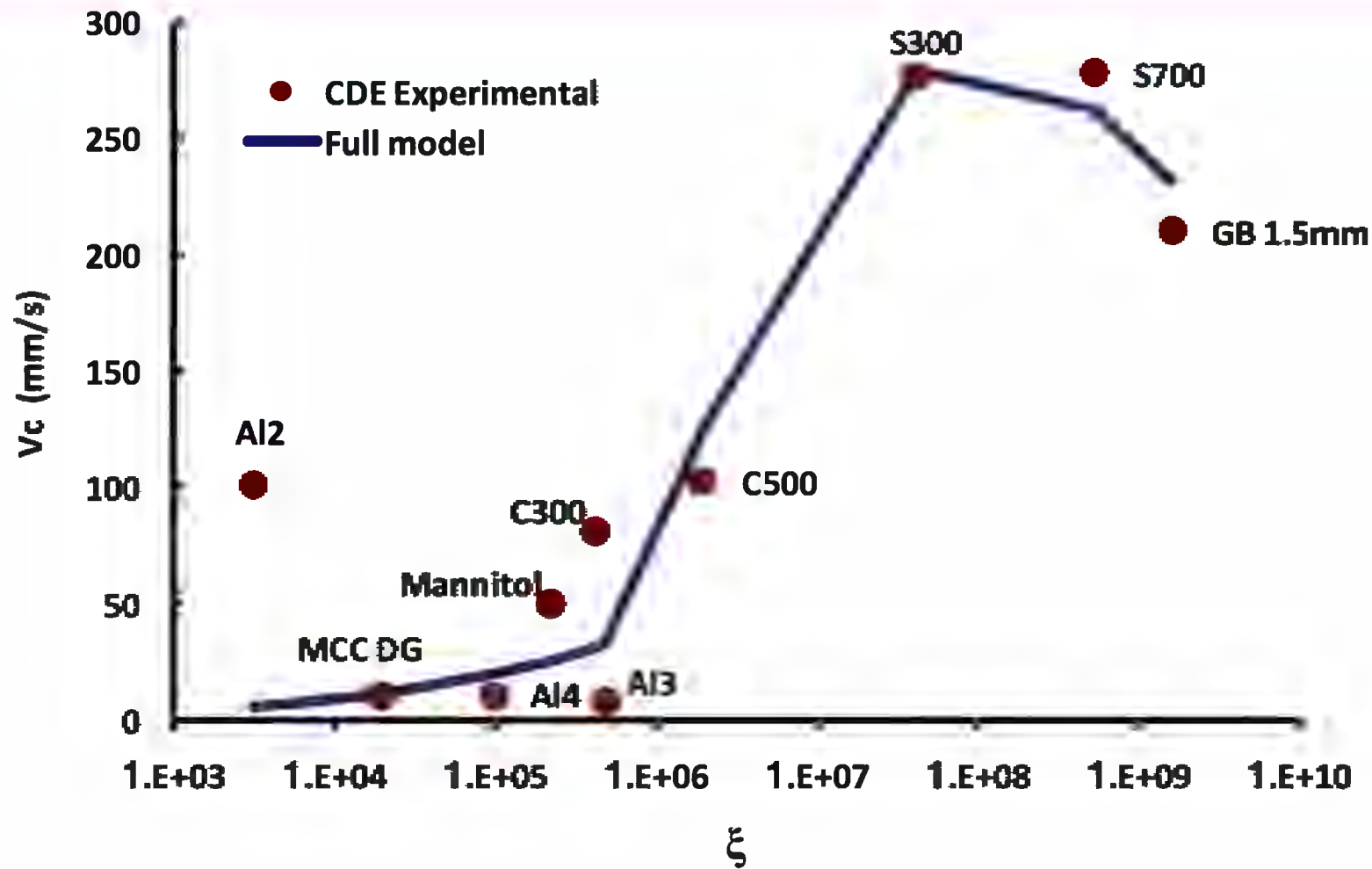
(c)



(d)

The variation of the *deposited mass* with the filling speeds for a) Silibeads 300; b) Cenopheres 500; c) Mannitol and d) Alumina 4.

A Mathematical Model for Die Filling



The critical filling speed obtained in the closed die experiments as a function of ξ ($=Ar \cdot \Phi$)

$$Ar = \frac{\rho_a \rho_s g d_p^3}{\eta^2} \quad \Phi = \frac{\rho_p}{\rho_a}$$

Conclusions

- ❑ Powder into a confined space depends upon powder properties, die geometry and filling conditions.
- ❑ The influence of air presence can be significant.
- ❑ DEM-CFD is capable of capturing the major features during die filling.
- ❑ Critical filling speed could be used to characterise powder flowability.
- ❑ Based on air sensitivity classification obtained by Guo et al. (2010), a model was developed to predict the deposited mass and the critical filling speed.



Acknowledgements

EPSRC
IFPRI
AstraZeneca
Sanofi
Pfizer

Dr. Yu Guo
Dr. Chunlei Pei
Dr. Serena Schiano
Mr. Joesry El Hebieshy
Ms. Anastasiya Zakhvatayeva
Dr. Colin Thornton
Dr. Ling Zhang

EPSRC

Engineering and Physical Sciences
Research Council

