
# Characterization of packed beds formed via Sequential Ballistic Deposition

Nikhil Agrawal[1], Prapanch Nair[2], Thorsten Pöschel[2] and Shantanu Roy[1]*

*1 Department of Chemical Engineering, Indian Institute of Technology – Delhi, Hauz, Khas, New Delhi 110016, India.*

*2 Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstrasse 49b, 91052 Erlangen, Germany.*

**Corresponding author: roys@chemical.iitd.ac.in*

***Highlights***

- Packed beds are created by sedimenting particles through different sources, using Sequential Ballistic Deposition.
- Grain-scale heterogeneity in the beds is characterized using Minkowski scalars and tensors
- Spatial void fraction and local isotropy distribution in the packed bed is shown to be a strong function of history

## 1. Introduction

Climate change concerns have elicited governments all over the world to introduce stringent norms for fossil fuel composition. As a result, refineries are compelled to increase conversion rates in hydrodesulphurization (HDS) reactors, and other applications which require "deep" processing. The reactor efficiency, in  is related to efficiency of the flow in the catalytic porous media, constructed by deposition of catalyst pellets. A detailed modeling of this porous media that takes into account directional properties, pellet geometry and method of packing the pellets are crucial to predict the reactive flow accurately. Minkowski scalars and tensors are known to be suitable in capturing pore scale directional properties [1] in granular packing. We characterize packings obtained by Sequential Ballistic Deposition (SBD) simulation of a large number of grains using Minkowski scalars and tensors. We show that the characteristics of the packings are related to the source of deposition of the grains, suggesting that a catalyst bed may be optimized by modifying the deposition geometry.

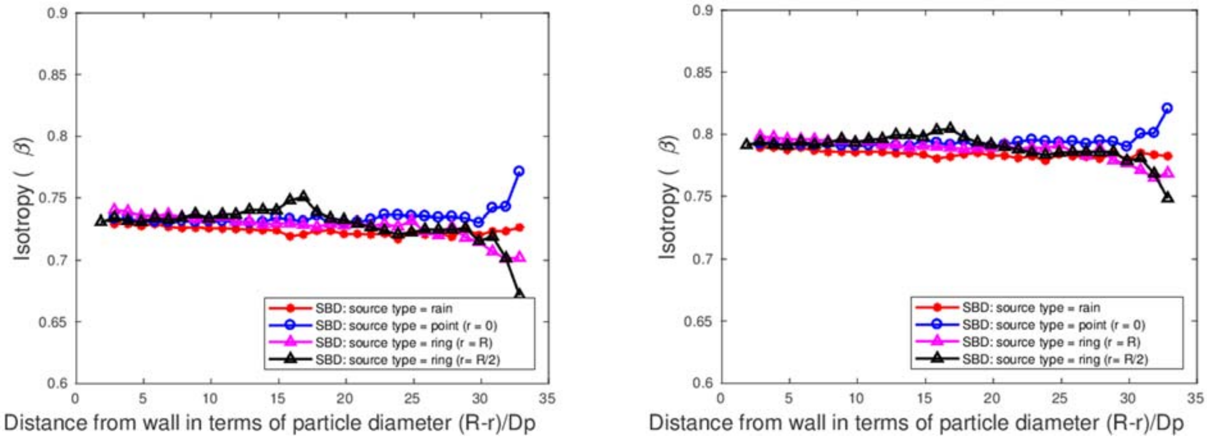
## 2. Methods

Since well-known simulation algorithms like DEM and Monte Carlo are not particularly efficient in simulating number of particles in the order of millions, we have used Sequential Ballistic Deposition (SBD), introduced by Visscher and Bolsterli [2], and implemented by Topic [3] in its current version. Spheres are deposited in a confined cylinder through 4 different kinds of deposition source geometries--a point source at a point along the axis of the cylinder, homogeneous rain of particles from a circular area normal to the axis of the cylinder, a circular ring source with a radius slightly smaller than that of the cylindrical confinement and a circular ring source of radius half that of the confining cylinder. The reason to conduct these simulations is to relate the history of the deposition to the characteristics of the packing.

We characterize these packings by calculating Minkowski tensors for the representative cells generated after partitioning the porous structure using Voronoi tessellation -- a detailed explanation for these tensors is given in [4]. Packings are examined via spatial isotropy with respect to two tensors namely Volume Moment Tensor (VMT) and Surface Orientation Tensor (SOT). The tensors were calculated using publicly available software package *Karambola* [5].

## 3. Results and discussion

The radial isotropy (β) profiles with respect to VMT ($W_0^{2,0}$) and SOT ($W_1^{0,2}$) are given in Figure 1a and 1b respectively. A strong dependence of radial isotropy on the particle source can be clearly seen; region directly beneath the particle source have a significantly higher isotropy (for both tensors) than other points in the packed bed. Interestingly, the radial void fraction profile (Figure 2) also shows a strong dependence on the particle source, with region directly beneath the source having the least void fraction or the highest density. A lower isotropy value concerning VMT means that the Voronoi cells are elongated to a greater extent while the width of the Voronoi cells are same (width of a Voronoi cell would obviously be equal to the diameter of a sphere). Thus, a cell with lower isotropy would necessarily have more volume, and hence, a higher void fraction is observed for such packed structures, which is in agreement with the calculated results.


(a) (b)

**Figure 1.** Variation in radial isotropy with respect to (a) Volume Moment tensor ($W_0^{2,0}$) and (b) Surface Orientation Tensor ($W_1^{0,2}$), where R is Radius of cylindrical confinement, r is distance from axis of cylinder and $D_p$ is diameter of particle

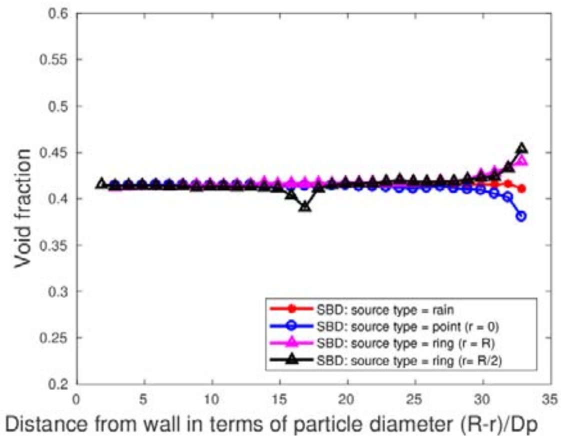



**Figure 2**. Variation in radial void fraction where R is Radius of cylindrical confinement, r is distance from axis of cylinder and $D_p$ is diameter of particle

## 4. Conclusions

We have identified a strong relationship between history of packing and the grain-scale properties of the packing; the local anisotropy in the system (with respect to both VMT and SOT) is a strong function of deposition source. In case of a circular ring source of radius half that of the confining cylinder a significant drop in void fraction is observed, such changes in density can have significant impact on fluid flow.

## References

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***Keywords***
Minkowski tensors, granular packings, grain deposition.