

# PREDICTING THE STATIC LIQUID HOLDUP IN TRICKLE BED REACTORS IN TERMS OF THE LOCAL STRUCTURE OF THE PACKED BED

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## Summary

A new fluid dynamic model has been developed predicting the static liquid holdup in trickle bed reactors based on liquid/solid physical and local structural properties of a packed bed. The model predictions have been compared to experimental data covering a wide range of relevant physical properties. A notably good agreement between prediction and experiments is observed.

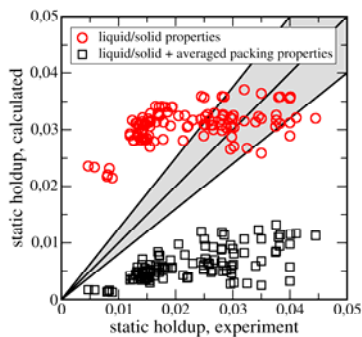
## Keywords

multiphase and particulate reactors, multiscale analysis

## Introduction

The static liquid holdup is an important performance parameter for designing and operating trickle bed reactors. In the past several models for predicting static holdup were proposed which are based either on liquid/solid properties and averaged properties of the packed bed or on liquid/solid properties alone. A comparison with experimental data recently obtained in our laboratory for a variety of liquid/solid systems and packing properties is shown in Fig.1. The poor agreement between calculated and experimental data may be regarded as indication that a significant factor of the liquid/solid systems is not accounted for in these models. As will be shown in this paper, the missing factors are identified as the local structural properties of the packed bed.

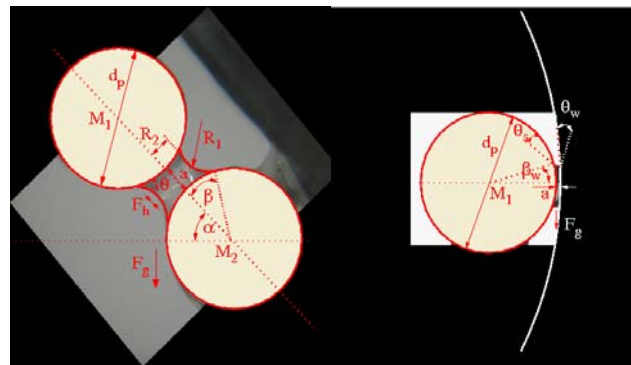
## Model Development



**Figure 1:** Comparison between measured static liquid holdup (this work) and correlations from literature (20% variance)

In principle, the static holdup can be calculated knowing the sum of volumes of all pendular liquid bonds between two neighboring spheres. In order to establish such a liquid bond the two spheres need not to be in close contact to each other. As long as the distance between the centers of two spheres does not exceed a critical threshold a liquid bond can form. This threshold depends on the liquid properties as well as on the inclination angle of the line connecting the centers of two neighboring spheres. Liquid bonds can occur between the cylinder wall and neighboring particles, too. In this case, the curvature of the cylinder wall and the respective angle has to be accounted for additionally.

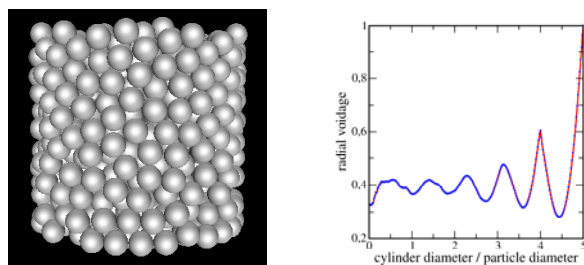
In order to represent the geometry of a single liquid bond the model of Pietsch and Rumpf (1967) is used due to its versatility. As shown in Fig. 2 the volume of the liquid bond can be represented very well in terms of geometrical properties (sphere diameters and distance) and contact and filling angles. This applies to liquid bonds between the



**Figure 2:** Model of a single liquid bond between two spheres (left) and between a sphere and the cylinder wall (right) in comparison with observed geometry wall and the particle as well.

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Generally, the local geometric arrangement of a sphere with respect to its neighbors as well as to the cylinder wall inside the packing is unknown. It was demonstrated before that computer simulated sphere packings closely resemble real packings (Schnitzlein, 2001). Therefore, the local geometric properties (distance between the centers of two spheres, inclination angle) are retrieved from such simulated sphere packings (Fig.3). By calculating the volume for each individual bond in terms of the local geometrical properties the static liquid holdup can then be obtained.

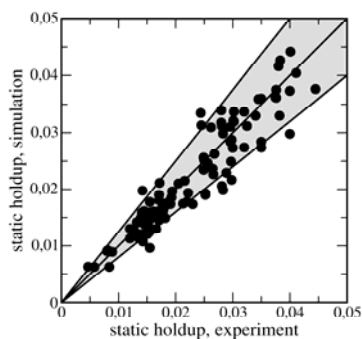


**Figure 3:** left - computer generated sphere packing, right – respective radial voidage distribution

## Experimental Setup

Experiments were carried out for different liquid/solid systems covering a wide range of liquid properties (density, viscosity, surface tension) and different solid particles (glass, polyoxymethylen, vitrified clay) to determine contact and filling angles by image analysis. Moreover, the respective surface energy which is characteristic for the wettability of the solid particles was obtained by means of tensiometric measurements. Finally, the critical threshold was measured for a simple arrangement of two single spheres as a function of the inclination angle of the line connecting the centers of the two spheres towards the horizontal.

The model space of the sphere packing including the containing tube was computationally generated, varying the diameter of the spheres and the cylindrical tube as



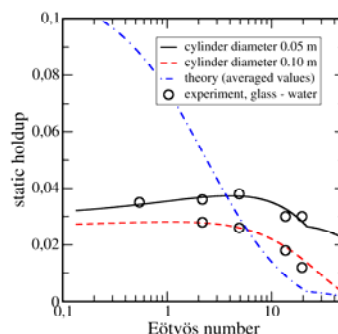
**Figure 4:** Measured and simulated static holdup for different liquid/solid systems and geometric properties (20% variance)

well. Thus, all relevant data necessary for the prediction of static liquid holdup were provided.

## Results

Predicted values for the static liquid holdup are compared to experimental data as obtained by the drainage method covering a wide range of liquids and solids as well as packing parameters. It is noted that the model predictions did not require the adjustment of a single parameter. The good agreement between experiment and simulation shown in Fig. 4 can be regarded as indication that the additional geometric parameters considered, are essential for describing the influence of the local structure for a reliable prediction of static liquid holdup in packed beds. It is noted that the same experimental data were used for the comparison shown in Fig.1.

A further evidence for this statement can be obtained by inspection of Fig. 5, where computed and measured static liquid holdups for the same liquid/solid system are plotted in terms of Eötvös number for two different cylinder diameters. By comparison with theoretical predictions based on averaged properties of the packing it is clearly seen that the experimentally observed behavior of static liquid holdup can only be reproduced by taking into account the local structural properties of the packed bed.



**Figure 5:** Static holdup vs. Eötvös number for different cylinder diameters

## Acknowledgment

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## References

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