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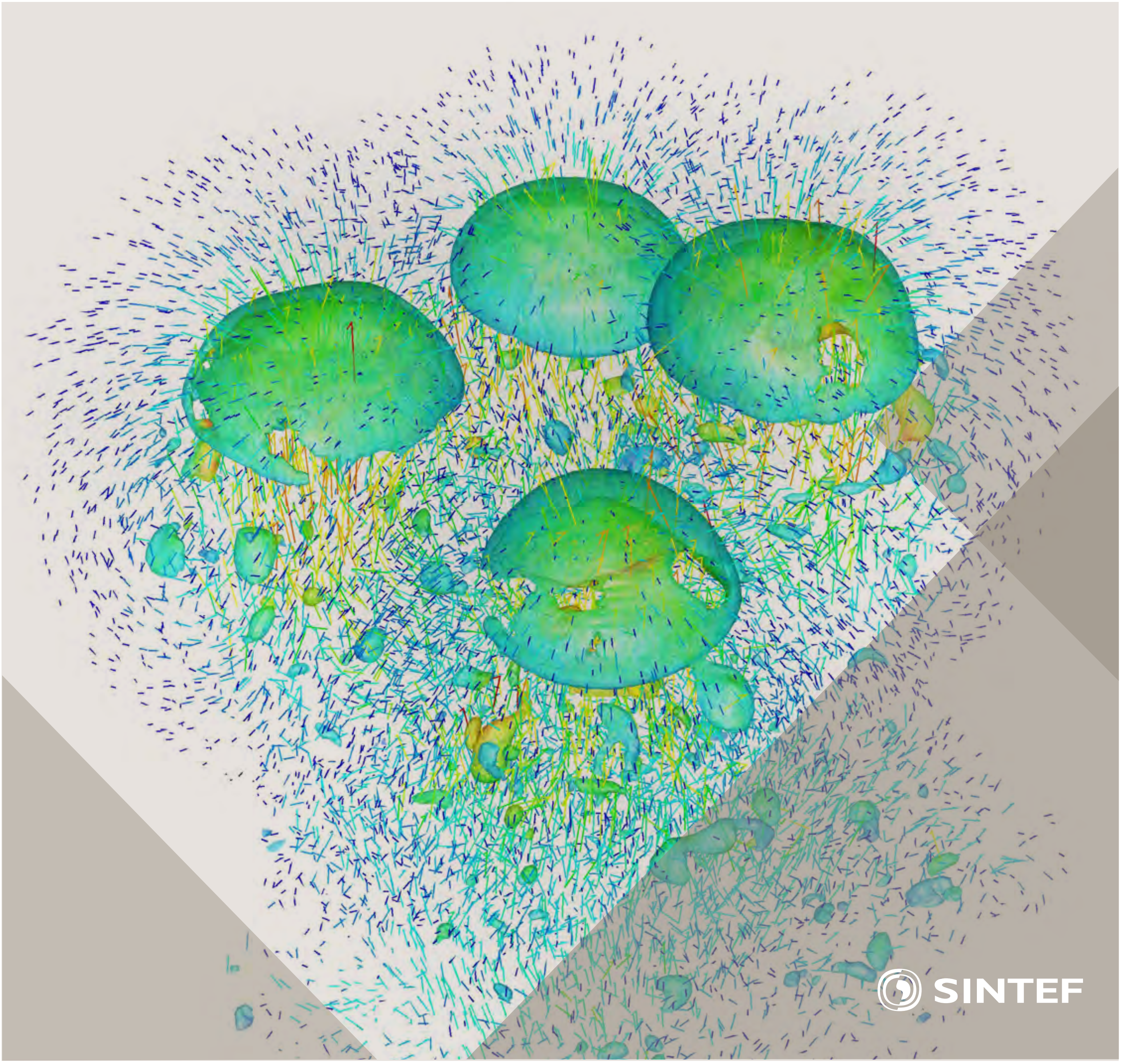
Progress in Applied CFD



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SINTEF Proceedings

Editors:
Jan Erik Olsen and Stein Tore Johansen

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SINTEF Academic Press

SINTEF Proceedings no 1
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Key words:
CFD, Flow, Modelling

Cover, illustration: Rising bubbles by Schalk Cloete

ISSN 2387-4287 (printed)
ISSN 2387-4295 (online)
ISBN 978-82-536-1432-8 (printed)
ISBN 978-82-536-1433-5 (pdf)

60 copies printed by AIT AS e-dit
Content: 100 g munken polar
Cover: 240 g trucard

SINTEF Academic Press
Address: Forskningsveien 3 B
PO Box 124 Blindern
N-0314 OSLO
Tel: +47 22 96 55 55
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PREFACE

This book contains selected papers from the 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in June 2014 and is also known as CFD2014 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focus on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. The papers in the conference proceedings and this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are presented in the conference proceedings. More than 100 papers were presented at the conference. Of these papers, 27 were chosen for this book and reviewed once more before being approved. These are well received papers fitting the scope of the book which has a slightly more focused scope than the conference. As many other good papers were presented at the conference, the interested reader is also encouraged to study the proceedings of the conference.

The organizing committee would like to thank everyone who has helped with paper review, those who promoted the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: FACE (the multiphase flow assurance centre), Total, ANSYS, CD-Adapco, Ascomp, Statoil and Elkem.

Stein Tore Johansen & Jan Erik Olsen

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CONTENTS

CFD SIMULATIONS OF FLOW IN RANDOM PACKED BEDS OF SPHERES AND CYLINDERS: ANALYSIS OF THE VELOCITY FIELD

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ABSTRACT

In this work, we aim to better understand the flow patterns in a random arrangement of particles that might affect local mass transfer and effective reactor performance.

Using the DEM code Grains3D, spherical or cylindrical particles are randomly inserted inside a horizontally bi-periodic container and fall under gravity. Hydrodynamic simulations are performed with PeliGRIFF, a Fictitious Domain/Finite Volume numerical model. Simulations parameters are the bed height and particulate Reynolds number. Effect of random packing on the flow field is analysed in terms of the probability distribution function (PDF) of the normalized vertical velocity.

A higher Reynolds number makes more backward flow zones and changes the PDF curves that we interpret as thinner boundary layers.

Unexpectedly, internal variability is independent of bed height. We propose that the probability of occurrence of random structures increases with bed volume in opposition with volume averaging effects.

Internal and external variability are similar for beds of spheres and cylinders of aspect ratio (< 2). However, for longer cylinders (higher aspect ratio), subdomains with same thickness are statistically different from one bed to another. We propose that the subdomain thickness required to average out sources of variability increases with high particle aspect ratio.

Keywords: Chemical Reactors, packed beds, velocity distribution, probability density function.

NOMENCLATURE

Greek Symbols

ρ Fluid density, [kg/m^3].

μ Dynamic viscosity, [kg/m.s].

ε Porosity (void fraction)

Latin Symbols

a Aspect ratio of a cylinder (length /diameter of cylinder)

d Particle equivalent diameter, [m].

l Cylinder length, [m].

P Pressure, [Pa].

$\mathbf{U}$ Velocity, [m/s].

Subscripts

c relative to a cylinder

s relative to a sphere

ls liquid, superficial

z vertical direction

INTRODUCTION

In this study, we are interested in small size fixed bed reactors which contain spherical or cylindrical catalysts with a characteristic size of 2-3 mm. These reactors are used to test small amounts of catalyst and are *a priori* more prone to random effects than industrial reactors.

Reactive testing performed inside these reactors involves complex mass transfer interactions between the fluid flow and reaction in the particles. In this paper, we are interested in the flow patterns in random packed beds. In literature, flow distributions are obtained using either an experimental approach (PIV (Particle Image Velocimetry), NMR (Nuclear Magnetic Resonance imaging), MRI (Magnetic Resonance Imaging) ...) or a numerical one. Concerning numerical works in random packing, Maier (1998) performed Lattice-Boltzmann simulations to study viscous fluid flow in a column of glass beads. He found that the velocity distribution is affected by bed porosity and Reynolds number. Rong (2013) performed also Lattice-Boltzmann simulations inside periodic randomly beds of mono-disperse spheres with porosity ranging from 0.37 to 0.8. However, the aforementioned studies do not study and quantify the local variability inside the bed.

The purpose of this work is to give a quantitative information of local velocity field and to link this information to internal and external structural variabilities. Internal variability is defined as variability within a bed, whereas external variability is defined as the difference arising between two random beds.

Numerical simulations for packed beds of spheres and cylinders are performed. We study the effect of Reynolds number, packed bed heights, and local random structure (repeatability) on velocity distributions.

SIMULATIONS DESCRIPTION

In order to examine the flow through packed beds of catalysts, simulations of packed beds of mono-disperse spheres and cylinders were performed in single phase flow in laminar regime (Re<15). The packing is created using the DEM (Discrete Element Method) code Grains3D (Wachs et al. (2012)). Particles are randomly inserted inside a container. They fall from the top under gravity and collide with each other and the bottom of the reactor. The boundary conditions used are periodic in the horizontal directions. Hydrodynamics simulations are performed with PeliGRIFF (Wachs (2010)), using the packing created with Grain3D. The meshing of the fluid domain is based on a cartesian structured grid with a constant grid size in the 3 directions. The CFD boundary conditions are: periodic boundary conditions in the same directions as the DEM simulations, uniform vertical upward velocity in the inlet (bottom wall of the domain) and uniform pressure in the outlet of the domain (top wall of the domain).
The simulations performed for spheres and cylinders are summarised in Table 1.

Table 1: Simulated cases for spheres and cylinders packed beds

Case Label	Particle size (mm)	Reynolds Number	Particles number	Number of repetitions of packing
S1-0.07	$d_s = 3$	0.07	540	1
S1-0.7	$d_s = 3$	0.7	540	1
S1-7	$d_s = 3$	7	540	10
S1-14	$d_s = 3$	14	540	1
S2	$d_s = 3$	7	1000	1
S3	$d_s = 3$	7	1500	1
S4	$d_s = 3$	7	2000	1
C2	$l_c = 2$ $d_c = 1.6$	0.37	380	3
C3	$l_c = 3$ $d_c = 1.6$	0.43	250	3
C4	$l_c = 4$ $d_c = 1.6$	0.47	180	3

Particulate Reynolds number is based on the equivalent diameter (diameter of a sphere of the same volume). It is defined as follows:

$$\mathrm{Re} = \frac{\rho U_{ls} d}{\mu} \tag{1}$$

In Figure 1-a and b, bed S1 is presented showing the CFD boundary conditions and the mesh used. For S1, the computational domain dimensions are $6d_s$*$6d_s$*$17d_s$ (which corresponds to 18 mm*18 mm*51 mm) with entry and exit zones. The spatial resolution used (20 points / particle diameter) gives a computational domain composed of about 5 millions of cells. This resolution has been set after a convergence study toward exact analytic solutions of pressure loss in various packed beds.

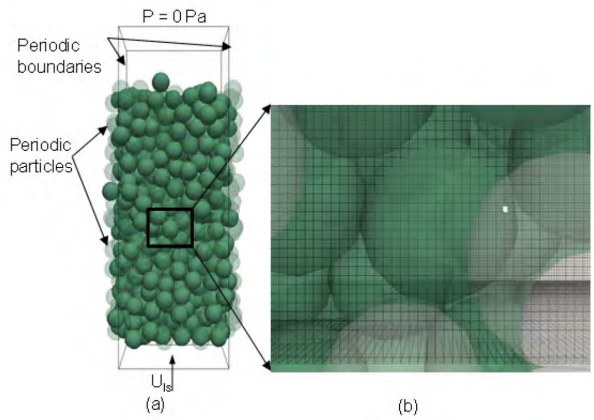

Figure 1: (a) Simulated packed bed of monodisperse spheres (S1) and (b) mesh of the geometry

For packed beds of cylinders, we considered 3 classes of cylinders with the same diameter d_c = 1.6 mm and an increasing length: 2 mm, 3 mm and 4 mm (Table 1). Each case was repeated three times. The bed height is approximately 40mm in all the cases (Figure 2). Particulate Reynolds number is below 0.5. The computational domain dimensions are 8 mm*8 mm*49 mm with entry and exit zones (below and above). The spatial resolution used (32 points / particle diameter) results in a computational domain composed of about 25 millions of cells. It has been chosen after a convergence study that showed that convergence was slower than for spheres Dorai et al. (2014).

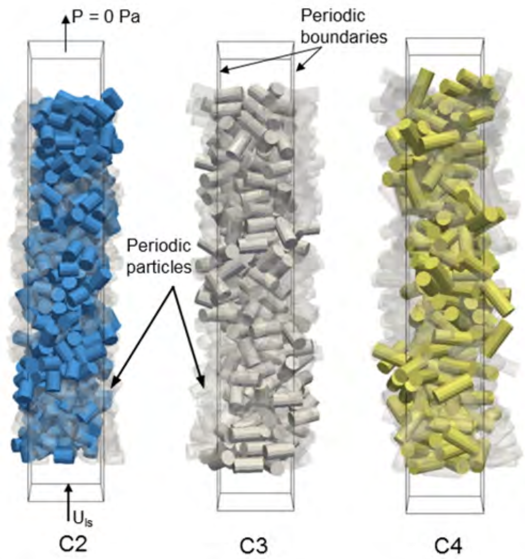

Figure 2: Simulated packed beds of monodisperse cylinders

ANALYSIS METHODOLOGY

Construction of PDF curves

The objective of this work is to compare the spatial velocity distributions for various cases and derive quantitative information for velocity fields in the case of random packed beds with low porosities (around 0.4). The analysis of the results is performed by considering the velocity field as the occurrence of a random variable such as described in Cedenese (1996), Rong (2013). Results are thus presented in the form probability

density functions (PDF) of the normalized vertical velocity (P (U_z / U_{ls})).
The PDF is constructed by first defining velocity classes, then, by counting the number of fluid cells whose velocity belongs to each class. At this step, we obtain a histogram that is converted to a PDF by normalizing the vertical velocity so that it satisfies equation (2).
As we use a large number of velocity classes (400), the information is better presented as a curve.

$$\int P(U_z / U_{ls}) dU = 1 \qquad (2)$$

All PDF curves present the same general features (Figure 3): (i) in the left side, the proportion of negative velocity is negligible (about 1% of all occurrences), (ii) sharp peak near U_z /U_{ls}= 0, (iii) gradual decrease for velocities U_z /U_{ls} > 1 (the curve becomes flatter). These observations were also reported by Maier (1998) and Rong et al., (2013) for packed structures (ε~0.36). Rong observed bimodal shapes for loose structures and high Reynolds number.

Effect of entrance and exit regions

By dividing the bed in non-overlapping sub-domains of equal thickness in the vertical direction (= 2*d_s), it is possible to compare the velocity fields within a bed. The PDFs obtained by dividing S1-7 in 7 zones are plotted in Figure 3. Zone 7 (outlet, top of the bed) and the lower extent zone 1 (inlet) have distinct PDF shapes. In zone 7, porosity is much higher as there are some vacancies in the lattice due to lower densification by lack of impacting particles. In zone 1, the rigid flat bottom constraints the packing that is not as random as in the other subdomains. This has been reported and discussed elsewhere (Dorai, 2012). From here on, we will exclude from analysis all subdomains near the top and bottom of the packed beds (excluded zone thickness = 2*d_s for spheres and 2*d_c for cylinders).

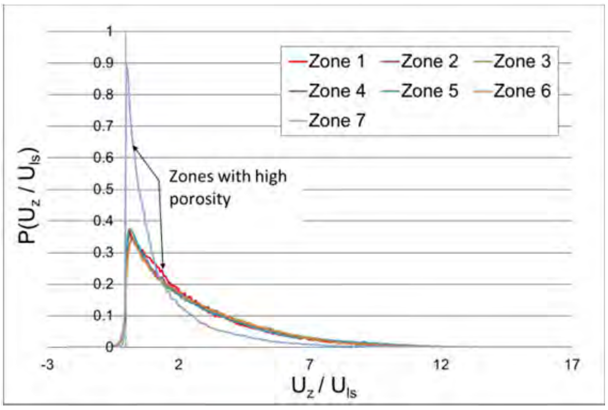

Figure 3: Effect of entrance and exit regions on PDF curves (bed S1-7)

PDFs comparison

Comparison of PDF curves has been performed with two methods: subtraction and statistical. Both methods require to have the same velocity classes for PDF curves. In the subtraction method, we compute the class to class difference between PDFs which is referred to as "PDF deviation" in the rest of the text. If the number of PDFs to compare is larger than 2, it is more convenient to subtract a common reference that should be chosen so as to represent some asymptotic or average case. When studying internal variability, the reference is the PDF of the whole bed (inlet and outlet excluded). If the focus is on external variability, the reference is chosen as the longest bed for length comparison or average of all PDF bed for repeatability. When comparing many PDF curves, after subtracting the reference, we calculate the "Maximum deviation function" that is constructed by choosing for each class the maximum deviation (absolute values) from the reference among all PDFs. Deviation functions are an indicator of the maximum variability within the domain studied. They do not respect equation (2).

Another way to compare PDF functions is to use the statistical "variance test" (Fischer test) that tests the hypothesis H_0 "PDF is identical for all domains". The statistical test is run for each velocity class. The variance test has been used to determine whether domains extracted from different beds present significant differences or not. In other words, can we distinguish a sub domain from another when they do not belong to the same bed.

RESULTS

Simulations with different Reynolds numbers

In this section, the effect of Reynolds number is studied in the same packed bed of spheres in laminar regime (S1, ε = 0.39). PDF curves are presented in Figure 4.

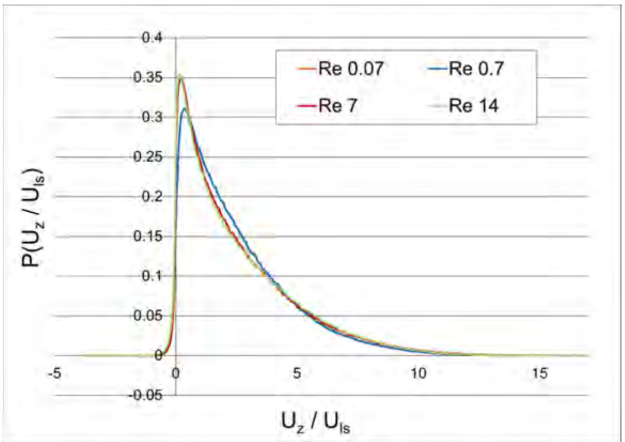

Figure 4: PDFs for different Reynolds numbers, bed S1

At very low Reynolds numbers 0.07 and 0.7 (creeping flow), curves are identical. The peak near 0 is more important for higher Reynolds number, which has also been reported in Rong et al. for ε = 0.5. In all cases, highest velocity can exceed 8*U_{ls}. At higher Reynolds number (7 and 14), there are more fluid cells with important velocity U_z / U_{ls} > 7 and less cells with small velocity (U_z / U_{ls} between 1 and 4) (Figure 5). We propose that increasing the Reynolds number leads to thinner boundary layers and increased number of fluid cells with high velocities.

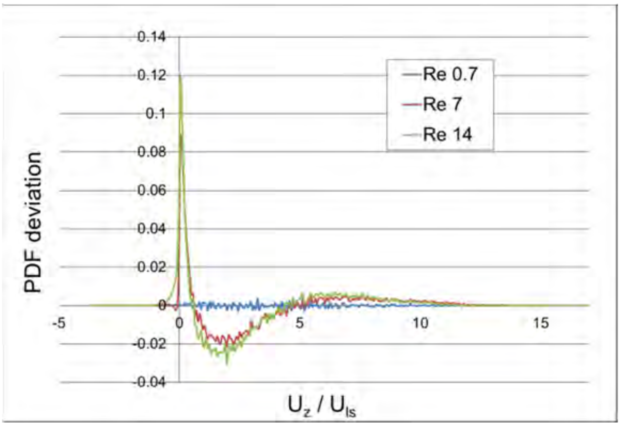

Figure 5: PDFs deviations calculated to PDF of lowest Reynolds number (0.07)

The proportion of negative vertical velocity (backward flow) is higher for higher Reynolds number (Figure 5 and Figure 6). This increase in proportion is more due to an increase in the number of backward flow zones rather than an increase in their size. For S1-14, the backward flow zones are homogeneously distributed in all domains.

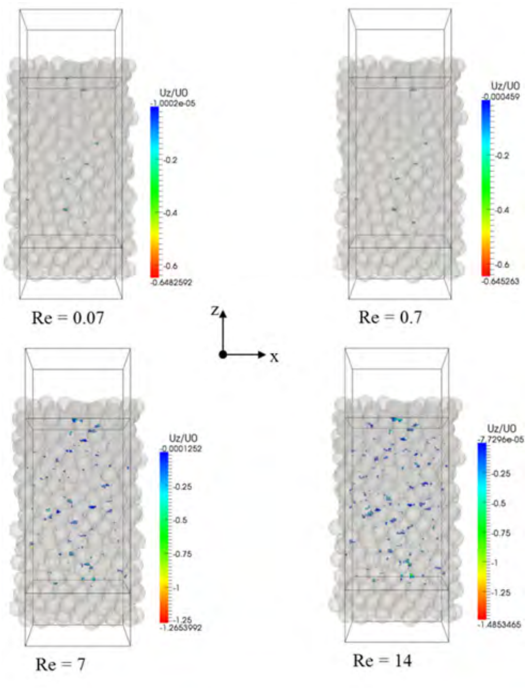

Figure 6: Zones with negative vertical velocity

Comparison of beds with different heights

Four packed beds of spheres (S1, S2, S3 and S4) are divided into regions with equal thickness (2*d_s). We calculated the deviation of PDFs in every region to the PDFs of longest packed bed (S4). We expected that maximum PDF variations would be higher for the shortest packed bed and that a longer bed would provide more averaging, which is not the case (Figure 7).

Moreover, the shortest bed (S1) presents less internal variability than the others. An explanation could be that increasing bed length increases the probability of occurrence of sources of variability, may-be from average random structures (tightly packed or loosely packed for example). In conclusion, bi-periodic long beds present the same internal variability as short ones.

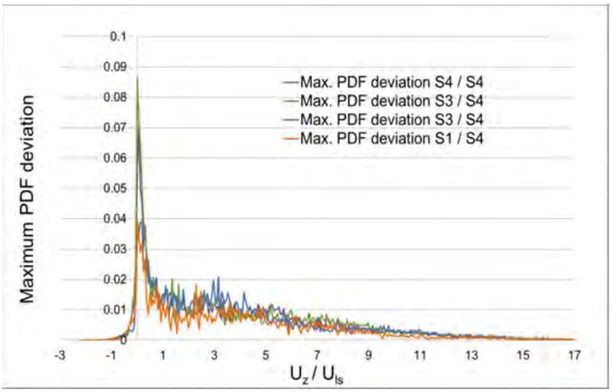

Figure 7: Maximum deviation functions calculated for S1, S2, S3 and S4 to mean PDFs of S4

External and internal variability for spheres

In this section, we want to know if there are any differences in flow structure in random packed beds composed of the same number of spheres (repetition of packing), and if these variations can be compared to the variations inside a given packed bed.

To answer the first question, we performed CFD simulation on 10 randomly packed beds with the same number of spheres; each bed has a different structure from the other. PDF deviation to the average PDF of all repeated cases indicate that some variability between beds is visible (Figure 8), for example “repeat5” bed present less “low velocity” cells and more “high velocity” cells than the average. Except near 0, deviation of all beds remains within a value of 0.003. It would be interesting to compare this value to the internal PDF variations (inside a single packed bed).

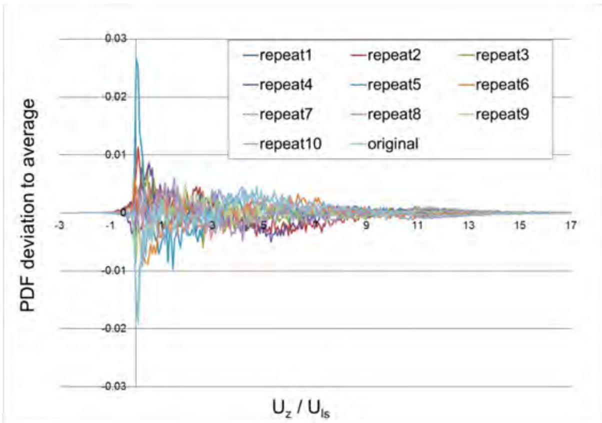

Figure 8: PDFs deviation to the average PDF of all repeated cases

To examine variability inside a bed, S1-7 is divided into domains of equal thickness (2*d_S) and PDFs deviations are calculated using the PDF of S1-7 as reference (Figure 9). In this case, except near 0, deviations are within a value of less than 0.01. Before comparing with the variations induced by repetitions (Figure 8), it is worth mentioning that the deviation to the average tends to decrease linearly with the number of sub-domains used. For example, if we would use two sub-domains instead of five to produce Figure 9, then the deviation would be 2.5 times lower. As the external variability value of 0.003 has been obtained on domains of thickness 10*d_S, and internal variability value of 0.01 has been estimated of domains of 2*d_S, the external variability value on 10*ds subdomains in the order of 0.003*5, which is quite similar to the internal variability. We conclude that internal and external variabilities are very similar.

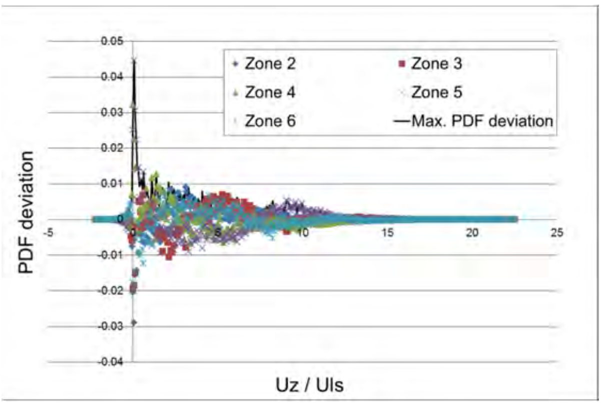

Figure 9: PDFs deviation calculated to the average PDF of all regions in S1

This conclusion is coherent with a variance analysis test performed on 5 sub-domains of S1-7 and 5 sub-domains of S1-7-repeat1. The analysis shows that for 99.5% of classes there is no statistical difference (at 5% risk) between S1-7 and S1-7-repeat1 sub-domains based on flow patterns.

External and internal variability for cylinders

Identical methodology has been applied to packed beds of cylinders with 3 repetitions on each cylinder length case. Variability between repeated beds is similar to that of spheres (Figure 10). Variability inside one bed is also of the same order of magnitude.

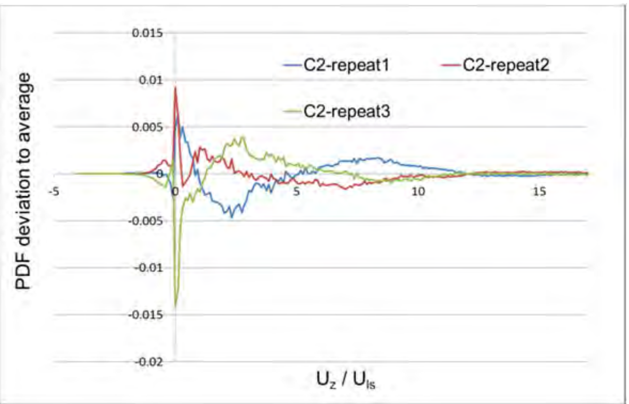

Figure 10: PDF deviation calculated to average PDF of repeated simulations of C2

The variance analysis gives a slightly more precise information. More classes are found to present difference between repetitions: 12.5 % of classes for C4 (a = 2.5), compared to 1.25 % and 0.25 % for C2 (a = 1.25) and C3 (a = 1.875) respectively. C2 and C3 appear to behave like packed beds of spheres: for aspect ratio up to 1.875, subdomains of thickness of 2*d_c present the same variability regardless of their origin (any location in any bed). On the opposite, for the highest aspect ratio case, subdomains of the same thickness are statistically different from one bed to another. It may be that higher particle anisotropy increases the minimum volume required to average out the sources of variability, also called Representative Elementary Volume (REV).

CONCLUSION

Simulations of fluid flow in bi-periodic packed beds of mono-disperse spheres and cylinders have been performed using a Fictitious Domain/Finite Volume numerical model. The simulations provide detailed information on the hydrodynamics and local velocity fields. Effect of random packing on the flow field is analysed by considering the velocity field as the occurrence of a random variable characterized by its probability distribution function (PDF).

- Top and bottom part of the packing are excluded from the analysis as they do not present the same flow patterns, due to lack of densification (top) and due to the presence of a flat surface (bottom) that prevents random positioning of particles on a layer of about two particle diameters.
- PDF curves for packed beds of spheres and cylinders have the same overall shape.
- A higher Reynolds number results in the presence of more backward flow zones and change in the PDF curves that we interpret as thinner boundary layers.
- Unexpectedly, internal variability is independent of bed height. We propose that the probability of occurrence of random structures increases with bed volume in opposition with volume averaging effects.
- Internal and external variability are similar for beds of spheres and cylinders of aspect ratio lower than 2. However, for longer cylinders (higher aspect ratio), sub-domains of the same thickness (2*d_c) are statistically different from one bed to another. We propose that the subdomain thickness required to average out sources of variability increases with high particles aspect ratio.

Perspectives are: to explore the link between shape and Representative Elementary Volume dimensions, to focus on how the presence of walls may change the results presented in this work and to perform simulations of reactive transport and study the link between structure, flow and reactivity variations in random packed beds.

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