A comparison of measured and modeled velocity fields for a laminar flow in a porous medium

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Abstract

Obtaining highly-resolved velocity data from experimental measurements in porous media is a significant challenge. The goal of this work is to compare the velocity fields measured in a randomly-packed porous medium obtained from particle image velocimetry (PIV) with corresponding fields predicted from direct numerical simulation (DNS). Experimentally, the porous medium was comprised of 15 mm diameter spherical beads made of optical glass placed in a glass flow cell to create the packed bed. A solution of ammonium thiocyanate was refractive-index matched to the glass creating a medium that could be illuminated with a laser sheet without distortion. The bead center locations were quantified using the imaging system so that the geometry of the porous medium was known very accurately. Two-dimensional PIV data were collected and processed to provide high-resolution velocity fields at a single planes within the porous medium. A Cartesian-grid-based fictitious domain approach was adopted for the direct numerical simulation of flow through the same geometry as the experimental measurements and without any adjustable parameters. The uncertainties associated with characterization of the pore geometry, PIV measurements, and DNS predictions were all systematically quantified. Although uncertainties in bead position measurements led to minor discrepancies in the comparison of the velocity fields, the axial and normal velocity deviations exhibited normalized root mean squared deviations (*NRMSE*) of only 11.32% and 4.74% respectively. The high fidelity of both the experi-

mental and numerical methods have significant implications for understanding and even for engineering the micro-macro relationship in porous materials. The ability to measure and model sub-pore-scale flow features also has relevance to the development of upscaled models for flow in porous media, where physically reasonable closure models must be developed at the sub-pore scale. These results provide valuable data in support of that goal.

Key words: Porous media; Darcy’s Law; particle image velocimetry; direct numerical simulation; pore-scale

Nomenclature

$\mathcal{A}_{\gamma e}$	Fluid boundary not shared with a solid
$\mathcal{A}_{\gamma\kappa}$	Fluid-solid interface
d	Seed particle image size
$\mathbf{D}[\mathbf{v}]$	The deformation rate tensor
D_1, D_2	Actual sectional diameter of a spherical bead as defined in Fig. A.1
d_1, d_2	Image diameter of beads as defined in Fig. A.1
D_B	Bead diameter
D_ℓ	Characteristic length used to define the Reynolds number
d_p	Seed particle diameter
$\mathbf{f}$	Body force
F_s	Multiplicative factor of safety used to compute the GCI
$\mathbf{g}$	Gravitational acceleration
GCI	Grid convergence index
K_{yy}	yy –component of the hydraulic conductivity tensor (i.e., the hydraulic conductivity in the vertical direction)
L_{bed}	Height (approximate) of the porous medium within the test section

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L_c	Side length of cubes used in REV analysis
L_{in}	Height of the inlet section
L_{out}	Height of the outlet section
L_x	Test section width, x – direction
L_y	Test section width, y – direction
L_z	Test section height, z – direction
M	Magnification of optical system
M_1, M_2	Local magnification of the image as defined in Fig. A.1
n_γ	refractive index of the liquid phase (at $\lambda = 589.3$ nm)
$\mathbf{n}_{\gamma\kappa}$	unit normal vector pointing from the fluid toward the solid phase at the fluid-solid interface
n_κ	refractive index of the solid phase (at $\lambda = 589.3$ nm)
$NRMSD$	Normalized root mean square deviation of the velocity field
$NRMSD_x$	Normalized root mean square deviation of the x –component of the velocity field
$NRMSD_y$	Normalized root mean square deviation of the y –component of the velocity field
p_γ	Pressure
$\mathcal{P}$	Local order of convergence
$\mathcal{P}_G$	Global order of convergence
Q	Volumetric flow rate
r	Grid refinement ratio
r_{ij}	Distance between centers of two adjacent beads, where i and j index a unique bead number
Re_p	Pore Reynolds number
Stk_p	Stokes number for the seed particles
$\mathbf{v}$	The velocity vector for the fluid phase
$\hat{\mathbf{v}}$	The total velocity vector for the solid phase in the immersed boundary method
$\mathbf{v}^{RBM}$	The rigid body motion velocity vector within the solid phase in the immersed boundary method

$\tilde{\mathbf{v}}$	Residual of non-rigid body motion in the within the solid region in the immersed boundary method
v'_x, v'_y	Normalized deviation of velocities in x - and y - directions, respectively
v_x, v_y, v_z	Three components of velocity vector in x -, y -, and z -directions, respectively
$\langle v_y \rangle$	Superficial average (Darcy) axial (y -direction) velocity
$\langle v_y \rangle^\gamma$	Intrinsic average (pore) axial (y -direction) velocity
V	Volume of the porous bed
V_N	The normalized volume defined by Eq. 12
V_γ	Volume of the fluid phase
$\mathcal{V}$	Total domain for a DNS simulation
$\mathcal{V}_\gamma$	Fluid domain for a DNS simulation
$\mathcal{V}_\kappa$	Solid domain for a DNS simulation
z_0	Distance of the bead vertex from the wall
z_1, z_2	Distance along optic axis of object plane defined in Fig. A.1

Greek

ε_γ	$= \frac{V_\gamma}{V}$ Porosity
ε_{ij}	Variation of grid solution in the convergence analysis
ε_{REV}	Normalized metric defined by Eq. (13) for determining the size of an REV
Δ	(Preceding a variable) indicates a difference
Δ_i	The “ i^{th} ” grid size in the convergence analysis
$\Delta_{5\%}$	Grid size required for a 5% uncertainty level in the convergence analysis
Δ^*	Grid resolution to obtain a target level of uncertainty
μ_γ	Dynamic viscosity of the fluid phase
$\mu_{\Delta z_1}$	Uncertainty in the bead position
μ_d	Uncertainty in the bead diameter
μ_M	Uncertainty in the magnification
ρ_γ	Density of the fluid phase
ρ_p	bulk density of the seed particles

σ_{bias}	In-plane loss of image pairs (bias) error
σ_{DG}	Spatial gradients (displacement variations) error
σ_{mag}	Magnification error
σ_p	Out-of-plane motion (perspective) error
σ_{rms}	Finite number of image pairs error
σ_R	Refractive index mismatch error
σ_T	Total error for PIV method
ξ	Dummy variable to denote a parameter
ξ_∞	The (spatially) asymptotic value of the parameter ξ
Ψ	Normalized pressure drop
Ω	Angular velocity of rigid body motion within the solid region in the immersed boundary method

Subscript

DNS	A value extracted from a direct numerical simulation
PIV	A value extracted from a particle imaging velocimetry experiment
x	The x —component of a vector
y	The y —component of a vector
z	The z —component of a vector
γ	Fluid phase
κ	Solid phase

1. Introduction

The micro-macro coupling of transport phenomena in porous media is important for understanding a wide range of processes including such disparate areas as the fundamental underpinnings of Darcy’s law [69, 23], heat transfer in porous media [32], and mixing and reaction rates in porous media [2, 67, 66]. The understanding of porous media processes from the fundamental pore-scale physics has been attempted theoretically for more than a

century (an extensive history of this topic is available in the excellent review by Markov [39]). However, the ability to measure pore-scale processes in complex, three-dimensional porous media is a relatively new development, enabled in part by the advent of computational resources needed to collect and process the large amounts of data associated with complex media. A similar evolution has occurred for the capability to conduct properly resolved simulations of mass, momentum, or energy in representations of complex porous media. One of the drivers for seeking this level of understanding is, ultimately, to be able to engineer porous materials (via particle shape, matrix connectivity, external chemical functionality, etc.) to have desirable properties [17]. As an example, improving the connectivity of the pore structure in proton exchange membranes is of significant interest in the area of fuel cell design [71].

In this work, the pore scale velocity field in a porous medium is measured, with the goal of rectifying experimental velocity measurements with theory (as represented by numerical simulation) for Reynolds numbers at the start of the inertial range. This kind of comparison is important because it (1) provides validation that representing the details of flow within a porous medium by the Navier-Stokes equations is not a theoretical artifice, but can actually be done (with fidelity) in reality; (2) illustrates that the conventional numerical methods can be expected, when properly converged, to provide results for the velocity field that are very similar to those that are measurable (i.e., correspondence between theory and experiment); (3) provides information regarding the existence of a *representative* region of the porous material, and (4) provides direct information about the sensitivity of the flow to external boundary conditions imposed on the medium. These last two items, are topics that are difficult to address from a theoretical perspective, so direct experimental evidence is particularly useful.

Although the use of pore-scale simulation for scientific and engineering purposes is becoming much more commonplace [43], there have been very few studies to date that have directly compared experimental measurements of pore-scale flow in porous media with predictions from direct numerical simulation [53, 73]. The results obtained in this work are unique in two respects: (1) the high resolution of the measured data, and (2) the fidelity be-

tween the measured and simulated results. This paper is organized as follows. In §2, a brief review of the literature of (1) experimental methods for imaging velocity fields in porous media, and (2) the numerical methods for conducting sub-pore scale numerical simulation is provided. In §3, the particular experimental methods used in this study are presented; a presentation of the numerical methods appears in the following section (§4). In §5 the results are presented and the paper is concluded with a short review of the primary points in §6.

2. Background

A brief review of various pore-scale flow measurement techniques and direct numerical simulation (DNS) methods is given below.

2.1. *Measurement of pore-scale fluid velocity*

Non-invasive experimental methods for measuring fluid velocities in porous media have been attempted for several decades, but methods with an appropriate level of resolution have only been available somewhat recently. Among the non-invasive methods, the following techniques have each been used with some success (1) particle image velocimetry (PIV) (which measures the statistical behavior of groups of particles) [45, 76, 78, 47, 50], (2) particle tracking velocimetry (PTV) (which measures the behavior of individual particles) [13, 36, 41, 44, 51], (3) Laser Doppler Anemometry (LDA) [19, 23, 75, 74], (4) Magnetic Resonance Imaging (MRI) [35, 38, 46, 61, 62, 64], and (5) positron emission tomography (PET) [7, 10, 33]. The first three of these methods all involve using index-matched fluid-solid systems; these methods have recently been reviewed by Wiederseiner et al. [70] and Dijksman et al. [15]. The methods used for MRI velocimetry (including applications to porous media) have been reviewed by Elkins and Alley [20] and Gladden [24]. To date, the use of PET velocimetry has been limited to a very few studies, so no general review exists.

In this study a two-dimensional PIV measurement technique was used for reasons related to a combination of accuracy and control of error propagation, versatility in data acquisition throughout the bed (in both time scales and spatial region of interest), and relative ease

of experimental set-up and analysis. The use of PIV has developed very rapidly over the last two to three decades with the advent of very powerful commercially available systems; this has been primarily a function of the development of high-speed data collection and improvements in computational post-processing capabilities. Details of recently-developed techniques are reviewed in Raffel et al. [55] and Adrian and Westerweel [1].

Because PIV is very flexible in its ability to resolve both small and large domains through optical means, it has advantages of use for complex flow geometries. With the advent of high-speed and highly-resolved imaging systems, it is possible to obtain PIV data (for both two and three components of velocity) at scales of resolution that allow determination of even very small scales applicable to turbulent flow analysis. Since particle seeding is typically required for PIV, the choice of seed particles is important to assure high fidelity for the results. For seed particles, the goal is to minimize particle inertia and buoyancy effects, as well as any inherent fluid-particle interactions that may disrupt the flow field.

A number of index-matched PIV- and PTV-based studies have been previously reported for porous media (e.g., [45, 76, 78, 13, 36, 41, 44, 51]), and the methods used for these works can be found in the respective manuscripts. In relation to this particular work, a detailed reporting of the refractive-index matching method for this particular experiment was presented previously by Patil and Liburdy [47]. Unique to the work we report in Patil and Liburdy [47] and in this paper, particular care was taken to quantify the effects of image intensity distribution, imaging wavelength differences, signal to noise loss, and interfacial glare. The use of an optical imaging model to help predict refractive errors through a randomly packed porous bed have shown that uncertainties can be reduced beyond what has been done in past efforts though more exact refractive-index matching. Consequently, with careful experimental design, it is possible to construct a low-uncertainty PIV system that can be used to obtain high-resolution time-resolved velocity vector fields.

2.2. Direct numerical simulation of pore scale flow

Porous media present unique challenges to resolved simulation techniques, mostly due to the complexity of the geometry and the solid-fluid interface. Several alternative computa-

tional methods to simulate pore scale flow have been discussed and successfully applied in the field of porous media. For pore-scale flow studies, the most commonly employed techniques are (1) the Lattice-Boltzmann (LB) [28, 29, 31, 30, 37], which moves and collides the fluid particles on a fixed lattice, and at the same time enforces the time-averaged element motion following the Navier-Stokes equation by a particular rule; (2) the Smoothed Particle Hydrodynamics (SPH) method [65, 8], which is a mesh-free particle-based method; and (3) the DNS approach [42, 52, 68], which solves the Navier-Stokes equations using conventional numerical discretizations on a fine grid in which the complex geometry of the porous media is explicitly resolved.

In this paper, a DNS method is chosen as the simulation technique because of its higher computational efficiency and accuracy (when compared to SPH and LBM), especially for single-phase flows with many solid-fluid boundaries. The challenge with conventional finite-volume DNS methods for this application is the need to generate a high quality grid that conforms to the complex geometry of a porous medium. While the body-fitted approach has the ability to directly resolve the solid-fluid interface, generating and working with body-conformal meshes for contacting-sphere geometries can be extremely cumbersome. Most of the difficulty is due to the sphere-to-sphere contact points, which require careful treatment to avoid skewed, high-aspect-ratio control volumes [18]. The time required to generate a high quality unstructured mesh for a large scale, complex geometry like a packed bed can often take longer than performing the simulation itself. Importantly, the significant meshing overhead and unstructured nature of the body fitted meshes for this problem makes systematic uncertainty quantification more difficult. Nonetheless, successful simulations of these flows have been carried out for laboratory scale packings containing up to hundreds of spheres, most often using a body-fitted grid combined with a finite volume approach [26, 6, 16, 18], Lattice-Boltzmann approach [37], or a body-fitted finite-element approach [9].

The mesh-related pitfalls encountered in body fitted simulations can be avoided with immersed-boundary or fictitious domain approaches which use regular Cartesian grids over the entire domain, inclusive of the solid regions. In these types of approaches, a synthetic force is applied in or around the solid regions to satisfy the desired no-slip boundary condi-

tion. The way in which this force is computed and applied is a field of active research, and a number of formulations have been proposed [27]. In the fictitious domain (or distributed-Lagrange-multiplier) approach, the entire domain (including the solid regions) is treated as a single fluid, and the rigid motion of immersed solid objects is projected in one or more steps onto the flow field using Lagrangian force points within the rigid object. Simple Cartesian grids are used throughout the entire domain, making grid generation a trivial task. A fractional time-stepping algorithm is typically employed in these approaches wherein the incompressibility and rigidity constraints are applied in separate fractional steps.

A fictitious domain approach developed by Apte and co-workers [4, 5, 3] is employed in this work. A systematic study of the relative performance of a body-fitted unstructured grid solver and a Cartesian grid non-body conforming solver was investigated in considerable depth in prior work [22]. It was shown that, using the same second-order fractional time-stepping algorithm, the fictitious domain approach provides better quality solutions near the boundaries of a porous bed than do other methods. The use of high quality Cartesian mesh as opposed to skewed unstructured mesh near bead surfaces seems to give faster convergence rates and smaller uncertainties. A systematic uncertainty analysis was also conducted to estimate number of grid points necessary per bead diameter to accurately capture the flow field within 5% uncertainty for a range of Reynolds numbers, $5 \leq Re_p \leq 600$. Because it was not possible to directly measure the velocities in the inlet manifold, uncertainty due to the particular inlet condition imposed was also examined in detail to assure that the solution was not dramatically influenced by this boundary condition. A thorough analysis of uncertainty in the numerical method is essential in order to obtain a high-fidelity results for the complex geometries typically observed in randomly-packed porous media. It also facilitates direct evaluation of the uncertainty in PIV measurement techniques applied to such complex flows.

3. Experimental methodology

The experimental porous medium was designed to for the collection of high-resolution velocity data and to facilitate direct comparison between the experimental data and nu-

merical predictions. In the remainder of this section we describe (1) the geometry of the experimental porous medium, and (2) the experimental setup detailing the methods for collecting PIV measurement of fluid velocities in the index-of-refraction-matched porous media. A careful analysis of the effect of magnification on the PIV data was critical to obtaining quality results, and this analysis was presented separately Patil and Liburdy [49]. Because it is central to the work presented in this paper, the analysis of magnification effects is also briefly reviewed in Appendix A.

3.1. Porous medium and fluid

In Fig. 1, a highly schematic three-dimensional flow geometry and the plane of interest for experimental and computational analysis is illustrated; in Fig. 2 the test section is shown as it was actually constructed for the experimental work. The porous medium was constructed of optical-quality Pyrex[®] glass beads of 15 mm diameter. These were randomly packed in hexahedral a test section constructed of Pyrex[®] glass to a porosity of 0.44 (as determined by direct volume measurement). The apparatus was a 70 mm $\times$ 70 mm square in cross-section with a height 90 mm. At each end of the test section flow was controled by manifolds; these were 62 mm for the inlet, and 32 mm for the outlet. Although the top surface of the porous bed is not a sharply-defined value, the bed occupied approximately 60 mm of the test section height. The flow direction was from top to bottom, and fluid entered the test section through an inlet structure containing a distributor plate to help create uniform pressure and velocity conditions at the inlet. A perforated bottom plate supported the beads; the plate was fabricated to be 1.5 mm thick with holes of 5 mm diameter arranged in a honeycomb fashion, with a 6 mm center-to-center spacing. The porosity of this plate was significantly larger (plate porosity = 0.597) than that of the porous bed.

The working fluid used in the PIV setup was an aqueous solution of ammonium thiocyanate (NH_4SCN). Ammonium thiocyanate has particularly desirable properties for the experimental work. The density and viscosity are not dramatically different from that of water, and the refractive index can be adjusted (by adjusting the concentration of NH_4SCN) to match the index of refraction of the borosilicate glass beads. The liquid refractive in-

dex was measured using a refractometer (Atago co., model R5000) with light at a reference wavelength of 589.3 nm. The actual value used during experiments was set so that the absolute difference between the refractive index of the beads (n_κ) and the refractive index of the liquid (n_γ) was constrained by $|n_\kappa - n_\gamma| < 0.0005$ to minimize uncertainty due to image distortions. The index matching process itself is somewhat lengthy; however, it is described in detail in Patil and Liburdy [48]. Note that one assumption adopted in this study (and others) is that the absolute *difference* between the index of refraction and the fluid does not change appreciable with wavelength. Thus, it was not necessary to match the wavelength at which the refractive index was measured with the wavelength of the laser. Additionally, we note that index matching was conducted directly before each experiment, with both the solid and fluid phases both at the ambient temperature ($T = 21.1 \pm 0.06^\circ\text{C}$). Thus, although the index of refraction is a temperature-dependent property, this factor did not need to be accounted for because the temperature did not fluctuate appreciably during any one experiment. Table 1 gives additional details of the geometric and mechanical specifications of the test section, glass beads, and fluid.

A single $x - y$ plane located at ($Z_p/D_B = 1.1$) was imaged. This plane was chosen to simultaneously limit wall effects and to minimize the uncertainty in the bead locations. Sources of error for the experiment are discussed in detail in §3.2 and §5.6.

3.2. Measurement of velocities using PIV

The experimental set up is shown in Fig. 2. The pore Reynolds number was adopted as the measure of the inertial component of the flow field, and was defined by (cf. [28])

$$Re_p = \frac{\rho_\gamma \langle v_y \rangle^\gamma D_\ell}{\mu_\gamma} \quad (1)$$

$$D_\ell = \frac{\varepsilon_\gamma D_B}{1 - \varepsilon_\gamma} \quad (2)$$

Here, the porosity, ε_γ , is defined by

$$\varepsilon_\gamma = \frac{V_\gamma}{V} \quad (3)$$

Figure 1: A three-dimensional geometry of the randomly packed porous bed. The location of the image plane for PIV data collection is shown for reference.

Table 1: Flow setup parameters for experimental system. Bulk values represent averages over the entire experimental volume of the porous medium.

Parameter	Symbol	Value
Test section width, x -direction [m]	L_x	0.070
Test section width, z -direction [m]	L_y	0.070
Test section height, y -direction [m]	L_z	0.090
Inlet section height [m]	L_{in}	~ 0.032
Outlet section height [m]	L_{out}	~ 0.032
Porous medium height [m]	L_{bed}	~ 0.06
Bead diameter [m]	D_B	0.01500 ± 0.00001
Glass bead refractive Index (at $\lambda = 589.3$ nm)	n_κ	1.4740
Liquid refractive index (at $\lambda = 589.3$ nm)	n_γ	1.4740 ± 0.0005
Liquid dynamic viscosity [$\text{N} \cdot \text{s}/\text{m}^2$]	μ_γ	0.00144
Liquid density [kg/m^3]	ρ_γ	1118
Bulk porosity of medium	ϵ_γ	0.44
Intrinsic average (pore) velocity [m/s]	$\langle v_y \rangle^\gamma$	3.79×10^{-4}
Superficial average (Darcy) velocity [m/s]	$\langle v_y \rangle$	1.67×10^{-4}
Pore Reynolds number	Re_p	3.47
Volumetric flow rate [m^3/s]	Q	8.20×10^{-4}
Ambient temperature [$^\circ\text{C}$]	T	21.1 ± 0.06

where V is the volume of the porous bed within the flow cell (solids plus fluid) and V_γ is the volume of the fluid phase within the porous bed. The remaining parameters appearing in these expressions and other relevant experimental parameters are defined in Table 1. Note that there are several different forms for the pore Reynolds number in use, so particular care must be taken when comparing results across studies. During the experiments, the pore Reynolds number as defined by Eq. (1) was $Re_p = 3.47$. This is sufficiently low that the inertial effects are not significant and the flow is steady and laminar.

Figure 2: Schematic of the experimental flow loop and test section.

The imaging system, shown schematically in Figure 3, used a Nd – YLF laser, wavelength of 527 nm (New Wave Research, Pegasus PIV) and a CMOS camera (Integrated Design Tools Inc., model MotionPro X-3 with 1280×1024 pixel array, complete with image intensifier and 11 bit dynamic range) using an adjustable focusing lens (Nikon AF Micro-NIKKOR

Figure 3: The PIV imaging setup.

60 mm $f/2.8D$). All data were collected using an f -number setting of 8 for the optics. The light sheet was created using the Dantec Dynamic 9080 $\times$ 0651 light sheet module resulting in a 0.5 mm sheet thickness. By imaging the thickness at discrete locations along the sheet, the variation of this thickness was found to be negligible.

To access different vertical planes within the bed without moving the light sheet relative to the camera imaging plane, the test section was mounted on a two directional transverse stage (Parker Hannifin Corporation, model 4454). In order to be able to perform direct comparison between the PIV data and numerical predictions, the bead locations of the porous medium in the test section were accurately measured. Because the medium used in this study was composed of optical-quality monodispersed beads (with very low variance in the diameter), measuring the bead center locations was sufficient to fully describe the porous bed. The PIV imaging system was used to obtain the bead center locations, as follows. A laser sheet illuminated the bead pack at discrete locations along the optical axis in the bed. At each position, the glare from the surface of each bead was imaged, and the image diameter determined. The bead positions were determined using Eq. (A.3), as described in Appendix A. Using this arrangement results in a variation of magnification for

each measurement plane. The variation of magnification throughout the bed was determined to vary from 0.264 to 0.290. The local magnification was used to convert pixel displacements to object plane displacements depending on the particular object plane being imaged. This process is described in more detail in Patil and Liburdy [49].

The field of view for PIV measurements was approximately $55 \text{ mm} \times 44 \text{ mm}$ with a subregion interrogation window of 32×32 pixels, which, using 50% overlap, results in a velocity vector spacing of 0.688 mm. This is equivalent to 21.8 vectors per bead diameter for measurements taken at the bed centerplane. These data were analyzed using DynamicStudio version 3.40.0 software (Dantec) using a multi-grid, multi-pass adaptive correlation method with central differencing window offset coupled with a sub-pixel peak fitting algorithm. A 3×3 moving filter scheme was used to validate vectors with a rejection rate of less than 1%. To help reduce the overall uncertainty due to in-plane image loss, 1000 images were collected of a given imaged plane and used to form 999 image pairs. A correlation averaging method was used to determine the seed particle displacements [14, 40].

The fluid flow field was imaged using reflective seed particles, silver-coated hollow glass microspheres with nominal size of $10.7 \pm 3.5 \text{ } \mu\text{m}$ and a density of 1.3 g/cm^3 . The seed image density was approximately 5 seeds particles per interrogation window for all data. To assure that there the influence of the seed particle density was negligible, the Stokes number was computed by

$$Stk_p = \frac{\rho_p d_p^2 \langle v_y \rangle^\gamma}{18 \mu_\gamma D_B} \ll 1 \quad (4)$$

Here, Stk_p is the Stokes number for the seed particles. For our system, the Stokes number was computed to be $Stk_p = 1.50 \times 10^{-7}$, which is more than sufficiently small to assure that inertia effects due to particle density are negligible.

To determine the seed image size, d , we used the statistics of the particle image size as described by Adrian and Westerweel [1]. Briefly, a histogram of the correlation peak width, was used to determine the size distribution. This result indicated a peak width of 3.2 pixels which corresponds to a seed size, d , of approximately 2.3 pixels; this result helps to assure

no peak-locking error [55, 1]. To assure that seed particle motion in the absence of flow was not a significant source of error, the settling velocity of the seed particles was evaluated by obtaining PIV data under no flow conditions in the test bed. These results showed that the displacements were less than 0.1 pixels, which is close to the total uncertainty value of the measurements, as is detailed below.

The uncertainties associated with the PIV velocity data is presented in detail in Patil and Liburdy [48, 49]. A summary of these results are presented here, indicating the relative values of the sources of uncertainty and the overall results. The total uncertainty was determined based on the contributions from: (1) magnification, (2) refractive index mismatch, (3) in-plane loss of image pairs (bias), (4) finite number of image pairs (random), (5) out of plane motion (perspective), and (6) spatial gradients. The relative values of each of these uncertainties is provided in Table 2. As shown, results are given for both the cross stream and flow wise directions (x - and y -components of velocity). The overall uncertainty was 2.6% in the flow wise direction, and 7.5% in the cross stream direction. The largest contributions to this uncertainty is from the in plane loss of image pairs (4.8% of maximum displacement) and out of plane motion or the perspective error (4.96% of maximum displacement); together, these account for approximately 65% of the total error. The major sources of errors due to magnification (0.4% of maximum displacement) and index mismatch (0.32% of maximum displacement) have been reduced to small contributions, representing only about 5% each of the total uncertainty. This small value for the uncertainty was achieved by carefully determining the magnification distribution within the bed and by closely matching the index of refraction. Details on the refractive index mismatch, contained in [48] include refraction and image intensity distortion due to refractive mismatch. It was found previously that the index mismatch needs to be less than ± 0.0005 to reduce these errors below those attributable to other PIV conditions of seed imaging and cross correlation analysis; these conditions were maintained throughout the experiment.

Table 2: Uncertainty estimates for PIV measurement. All units are in fractions of pixels unless otherwise stated.

Error Source	Δx	Δy
Max Displacement	1.25	3.56
Magnification, σ_{mag}	0.005	0.014
Refractive index mismatch error, σ_R	0.004	0.004
In-plane loss of image pairs (bias), σ_{bias}	0.06	0.06
Finite number of image pairs (random), σ_{rms}	0.037	0.037
Out-of-plane motion (perspective), σ_p	0.062	0.056
Spatial gradients (Displacement variations), σ_{DG}	0.002	0.006
Total error, σ_T	0.094	0.091
Total error (% of max)	7.5%	2.6%

4. Computational approach

In this work, a simple uniform Cartesian grid is used for flow predictions. A detailed description of the fictitious domain method used in this study is available in the works of Apte and Patankar [5], Apte et al. [4] and Apte and Finn [3] is used for simulating the flow through a randomly packed bed. Description of the mathematical formulation of the method and the generation of the immersed-boundary objects is briefly summarized below. A detailed validation of the numerical method, specifically conducted for porous media, is reported in Appendix B.

4.1. Mathematical formulation

Let $\mathcal{V}$ be the computational domain which includes both the fluid ($\mathcal{V}_\gamma$) and the solid ($\mathcal{V}_\kappa$) domains. A structured Cartesian grid is generated throughout the fluid as well as solid domains. Let the fluid boundary not shared with the solid be denoted by $\mathcal{A}_{\gamma_e}$ and have a Dirichlet condition (generalization of boundary conditions is possible). The basis of fictitious-domain-based approach [25] is to extend the Navier-Stokes equations for fluid

motion over the entire domain $\mathcal{V}$ inclusive of particle regions. The natural choice is to assume that the particle region is filled with a Newtonian fluid. Both the fluid and the solid regions will be assumed as incompressible and thus incompressibility constraint applies over the entire region. In addition, as the solid is assumed to be rigid, the motion of the material inside the solid is constrained to be a rigid body motion.

The momentum equation for motion of the incompressible, constant density and viscosity fluid in the entire domain $\mathcal{V}$ is given by

$$\nabla \cdot \mathbf{v} = 0 \quad (5)$$

$$\rho_\gamma \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p_\gamma + \mu_\gamma \nabla^2 \mathbf{v} + \rho_\gamma \mathbf{g} + \mathbf{f} \quad (6)$$

where $\mathbf{v}$ is the velocity vector (with components given by $\mathbf{v} = (v_x, v_y, v_z)$), ρ_γ the fluid density, μ_γ the fluid viscosity, p_γ the pressure, $\mathbf{g}$ the gravitational acceleration, and $\mathbf{f}$, the additional body force, is used to impose the rigid condition for the solid phase part. Additionally, the particles are assumed to be rigid, the motion of the solid part is constrained as a rigid body motion. A non-zero forcing function, $\mathbf{f}$ is needed as a constraint to enforce the rigidity of the solid part. Inside the particle region, the rigid body motion, $\mathbf{v}^{RBM}$, implies a vanishing deformation-rate tensor [3]

$$\left. \begin{aligned} \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) &= \mathbf{D}[\mathbf{v}] = 0 \\ \Rightarrow \mathbf{v} &= \mathbf{v}^{RBM} = \mathbf{U} + \Omega \times \mathbf{r} \end{aligned} \right\} \text{ in } \mathcal{V}_\kappa \quad (7)$$

Here, $\mathbf{U}$ and Ω are the translational and angular velocities of the object, and $\mathbf{r}$ is the position vector of a point inside the object from its centroid. For the fixed-bed problems considered here, $\mathbf{v}^{RBM}$ is always zero. The vanishing deformation rate tensor for the rigidity constraint automatically ensures that the solid region is divergence free and incompressible. The incompressibility constraint of divergence-free velocity field is enforced by solving a Laplace equation for the pressure field. Similarly, the tensor constraint $\mathbf{D}[\mathbf{v}] = 0$ for rigid motion gives rise to a tensor field inside the solid region. Sharma and Patankar [63] proposed

an approach that provides the rigidity constraint explicitly, thus reducing the computational cost significantly. Note that the tensorial rigidity constraint can be reformulated to give

$$\nabla \cdot (\mathbf{D}[\mathbf{v}]) = 0 \text{ in } \mathcal{V}_\kappa \quad (8)$$

$$\mathbf{D}[\mathbf{v}] = 0 \text{ on solid/fluid interface, } \mathcal{A}_{\gamma\kappa}. \quad (9)$$

A fractional-step algorithm can be devised to solve the fictitious domain problem [4, 3, 63]. Knowing the solution at time level t^n the goal is to find $\mathbf{v}$ at time t^{n+1} . The algorithm can be outlined as follows.

1. In the first step, the rigidity constraint force $\mathbf{f}$ in Eq. 6 is set to zero and the equation together with the incompressibility constraint (Eq. 7) is solved by standard fractional-step schemes over the entire domain. Accordingly, a pressure Poisson equation is derived and used to project the velocity field onto an incompressible solution. The obtained velocity field is denoted as $\mathbf{v}^{n+1}$ inside the fluid domain and $\hat{\mathbf{v}}$ inside the solid object.
2. To solve for $\mathbf{v}^{n+1}$ inside the solid region $\mathbf{f}$ is needed. The constraint on the deformation rate tensor given by Eq. 7, along with the no-slip specification at the solid-fluid interface can be reformulated to obtain

$$\nabla \cdot (\mathbf{D}[\mathbf{v}^{n+1}]) = \nabla \cdot \left(\mathbf{D} \left[\hat{\mathbf{v}} + \frac{\mathbf{f}\Delta t}{\rho_\gamma} \right] \right) = 0 \quad (10)$$

$$\mathbf{D}[\mathbf{v}^{n+1}] \cdot \mathbf{n}_{\gamma\kappa} = \mathbf{D} \left[\hat{\mathbf{v}} + \frac{\mathbf{f}\Delta t}{\rho_\gamma} \right] \cdot \mathbf{n}_{\gamma\kappa} = 0 \quad (11)$$

The velocity field in the solid is zero for fixed beads. Thus $\hat{\mathbf{v}}$ is split into a rigid body motion ($\mathbf{v}^{RBM} = \mathbf{v} + \Omega \times \mathbf{r} = 0$) and residual non-rigid motion ($\tilde{\mathbf{v}}$). The above formulation can be easily generalized to solid bodies with *specified motion* by directly setting $\mathbf{v}^{RBM}$ to the specified velocity.

3. The rigidity constraint force is then simply obtained as $\mathbf{f} = \rho_\gamma(\mathbf{v}^{RBM} - \hat{\mathbf{v}})/\Delta t$. This sets $\mathbf{v}^{n+1} = \mathbf{v}^{RBM}$ in the solid domain. Note that the rigidity constraint is non-zero only inside the solid domain and zero everywhere else. This constraint is then imposed in a third fractional step.

For the pressure, a pressure Poisson equation was solved. Briefly, the momentum equation is solved without pressure term at first step. Then, the temporary velocity from step 1 is used in the Poisson equation to solve for pressure. Finally, the pressure from step 2 is applied to correct the velocity so it satisfies the continuity. In this process, ghost points are used to specify boundary conditions.

The set of equations is computed for the whole domain, including the fluid and solid regions, by using the fictitious domain approach. A fractional stepping algorithm together with an algebraic multigrid (AMG) solver for the pressure Poisson equation are implemented in a parallel three-dimensional version of the solver [4].

4.2. Generation of immersed objects

To generate immersed objects and their interfaces on the background Cartesian grid, a triangulated representation of the surface and the associated outward normals to this representation are first generated. These were generated using CAD software. Marker points were defined on the surface; knowing the marker point and sphere centers, an outward normal was determined for each marker point. Representing multiple bead surfaces was straightforward using this approach.

Figure 4: Schematic of material volumes within a circular object with subcell resolution.

Once the sphere surfaces were represented by marker points, the inside region of the particle is subdivided into cubic material volumes of size smaller than the background Cartesian mesh. This process helps to develop both a sharp representation of the boundary and an accurate representation of the rigidity constraint force. To illustrate the essential features of the process, an example of a circular interface with associated material volumes within the interface is provided in Fig. 4. The use of material volumes over the entire particle domain (as opposed to only around the particle surface) is advantageous as it simplifies calculation of the rigidity constraint force that is non-zero to only within the particle region. To preserve accuracy of the scheme, consistent and conservative interpolations are necessary between the centers of the material volumes and the centers of the background Cartesian cells. Accordingly, interpolations that have compact support are typically used in immersed boundary method [60].

4.3. Parameters, initial, and boundary conditions for the DNS simulations

Direct numerical simulations were conducted on the geometry that was measured in the experiments; the system dimensions and other parameters are listed Table 1, and a schematic of the computational domain is given in Fig. 1. The outlet section was placed at 35 mm below the bottom surface of the beads section. A conventional convective outflow condition was used as the outlet boundary condition; the distance between the convective outlet and the top of the porous bed was sufficient to prevent significant influences on the velocity field. The inlet section (L_{in}) was 35mm long and located above the top surface of the porous medium. The perforated plate used in the experiments was not simulated in the computations because it had much higher porosity than the porous medium; its influence on the flow in the pore regions was assumed to be small. The outlet section (L_{out}) was located below the bottom of the porous medium and was also 35 mm long. The sensitivity of the solution to the inlet condition was examined, and is discussed further in §5.5 where it is shown to have a negligible influence on the velocity field within the porous medium. At the exit, the simulation domain was extended below the bead section and a conventional convective outlet boundary condition was applied. No-slip conditions were imposed at all

fluid-solid interfaces.

The only additional information used for the DNS study from the experimental results were the inlet mass flow rate, the fluid viscosity, and the fluid density. The flow was assumed to be incompressible and isothermal, and the inlet velocity was taken to be a uniform field set such that the a pore-scale Reynolds number of $Re_p = 3.47$ was achieved.

Three different grid resolutions were tested, corresponding to coarse, medium, and fine grids, to conduct a systematic grid refinement study. Additional details are results from the grid convergence study appear in §5.3.

5. Results and discussion

5.1. Experimentally-measured velocity field: Raw data for the entire image plane

The PIV method adopted for this work allows for high-resolution measurement of the velocity field within the porous medium. In Fig. 5, a color contour plot of the in-plane velocity magnitude and associated streamlines are illustrated for the image plane $z/D_B = 1.1$. The in-plane velocity magnitude was computed from $\|\mathbf{v}\|_{x,y} = (v_x^2 + v_y^2)^{\frac{1}{2}}$ (where, recall, $\mathbf{v} = (v_x, v_y, v_z)$). For the low Reynolds number flow, the velocity field remains attached and flow separation is absent. The maximum flow velocity within the pores in this plane is about 1.4 mm/s, which is roughly 3.7 times the interstitial velocity indicating that the flow speed increases in some open pore regions. The velocity field in this plane is analyzed further through global flow features such as the pressure drop and hydraulic conductivity, and compared in detail with the DNS predictions.

5.2. Determination of the REV

Part of the intent of this work was to examine a volume of porous media that was *representative*, in some sense, of the medium as a whole. Although clear definitions of the concept of a representative elementary volume (REV) exist [72], measuring them experimentally is challenging, and depends strongly upon the process being measured as well as the structure of the porous medium. Most of the efforts to date have focussed on measuring first-order

Figure 5: Streamlines and velocity magnitude contours obtained from PIV measurements of the two-dimensional flow field in the measurement plane $z/D_B = 1.1$.

statistics of the medium to determine its representativeness [77, 11, 56]. Because of the limited size of the experimental system, only first-order statistics of porous medium properties were measured in our examination of the REV.

Several global properties of the porous medium structure and the momentum transport processes were evaluated. For this effort, the DNS results were used because full three-dimensional data was available for the analysis. The properties evaluated were the porosity, ε_γ , the superficial average (Darcy) velocity, $\langle v_y \rangle$, the pressure drop per unit length, $\Delta p_\gamma / L_c$, and the diagonal component of the hydraulic conductivity in the direction of mean flow (the y -direction), K_{yy} . Because the direction of the average velocity was parallel to the y -axis, the only component of the hydraulic conductivity tensor that is relevant to this work is the diagonal component K_{yy} . Variation of these properties within the bed are obtained by considering a series of cubical regions with increasing size for property evaluation. Starting from a central location (the point (-1, 24.6, 2.65)), cubes with side lengths ranging between $0.4D_B$ to $3.7D_B$ in $0.1D_B$ increments were considered. An example of two such volumes are illustrated in Fig. 6.

Figure 7 shows the variation of the pressure drop per unit length ($\Delta p_\gamma / L_c$), the average velocity ($\langle v_y \rangle$), and the porosity within the bed (ε_γ), with respect to the size of cubic region. The corresponding hydraulic conductivity, K_{yy} , is plotted in Fig. 8. The hydraulic conductivity variation depends on the changes in the average velocity as well as the pressure drop per unit length as, $K_{yy} = \langle v_y \rangle \frac{\rho_\gamma g L_c}{\Delta p_\gamma}$. For data within cubes smaller than two bead diameters, rapid variation in these properties is observed. The porosity for this region approaches a value of 0.43 and compares well with the experimentally measured value of 0.44. The average velocity reaches a value of around 0.16 mm/s and the pressure drop per unit length of about 0.6 Pa/m. The average velocity is related to the interstitial velocity through the porosity, $\langle v_y \rangle = \langle v_y \rangle^\gamma \varepsilon_\gamma$. For this size of the cubic box, the interstitial velocity can be calculated as 0.372 mm/s, which is very close to the interstitial velocity based on inlet flow conditions (0.379 mm/s, see Table 1).

For cubical regions larger than about 3.2 bead diameters, these properties show some variation owing to the effect of the wall boundaries of the test section. However, these

Figure 6: Illustration of two (of many) regions used for the REV analysis, each centered within the experimental image plane ($z/D_B = 1.1$). In subsequent analyses, these volumes will be called the “large” (40×40 mm) and “small” (30×30 mm) REV’s. Note that the coordinate system was imposed for experimental convenience; thus the investigated region is not located at the origin of the domain. Beads are color-coded by the overlapping percentage for beads in this plane, as describe in §5.6.

Figure 7: Variation of pressure drop per length ($\diamond$), average velocity ($\triangle$) and porosity ($\blacksquare$) as a function of the length of the cubic box (L_{Cubic}) used to calculate them. The vertical lines — and — · — represent medium and large box lengths of 30 and 40 mm, respectively.

Figure 8: Variation of hydraulic conductivity (○) and porosity (■) as a function of the length of the cubic box (L_{Cubic}) used to calculate them. The vertical lines — and - · - represent medium and large box lengths of 30 and 40 mm, respectively.

variations have little effect on the determination of the REV. To compute the size of the REV, the volumetric derivative of each of the quantities shown in Figs. 7 and 8 was computed as described by Brown et al. [11]; these results are shown in Fig. 9. In these figures, for convenience we have defined ϵ_{REV} as the fractional variation for any parameter, ξ , from its asymptotic value, ξ_∞

$$\epsilon_{REV}(\xi) = \frac{1}{\xi_\infty} \frac{\partial \xi}{\partial V_N} \quad (12)$$

$$V_N = \left(\frac{L_c}{B_D} \right)^3 \quad (13)$$

Each of the global properties tend toward a well-defined asymptotic value as the volume becomes large enough (at approximately $L_c/D_B = 2.7$, as illustrated in the figure). From these results, we find that cubic volumes with sides between about 30 mm and 40 mm can be considered to be an REV with a less than 0.005 (0.5%) variation in this metric; direct observation of the quantities plotted in Figs. 7 and 8 suggest that the cube with side equal to 40 mm is perhaps more consistently representative for all of the macroscale parameters considered.

5.3. Comparison of PIV and DNS velocities

The REV analysis provides appropriate volumes with which meaningful comparisons between the PIV and DNS data can be made. For a direct comparison between the two datasets, the DNS results (obtained on the fine grid) are interpolated to the grid locations used in the PIV data (which is slightly coarser than the fine grid used in DNS). A higher-order consistent interpolation scheme is used so that interpolation errors are minimized.

Using the REV results as a guide, the large (40 mm $\times$ 40 mm) region illustrated in Fig. 6 was selected for further analysis. The large region most closely corresponds to the representative length of the porous bed as obtained from the variation of global measures such as the porosity, pressure drop per unit length, and average velocity.

Figures 10 a,b show the contour plots of the axial velocity (v_y) in the measurement plane and within the large binning box. The orientation is such that the flow going from the top

Figure 9: The volumetric derivative of the properties analyzed to determine the REV. The vertical lines — and - · - represent medium and large box lengths of 30 and 40 mm, respectively.

Figure 10: Comparison of axial velocity (v_y) between PIV and DNS; (a) contour plot from PIV (velocity in (mm/s)), (b) contour plot from DNS (velocity in (mm/s)), (c) distribution of axial velocity obtained from PIV, (d) distribution of axial velocity obtained from DNS.

to bottom. Also shown in Figs. 10 c,d are the distributions of v_y obtained from PIV and DNS, respectively. Qualitatively the contour plots obtained from PIV measurements and DNS predictions match well, except in the top and bottom right corner regions, where the PIV data seems to record larger velocity magnitudes than the DNS. The range of the axial velocity is slightly larger in the PIV data than in the DNS data as is also seen from the histograms. However, both the PIV and DNS show very similar plots with positive velocity values. This suggests that there is no reverse flow, which is expected for the low Reynolds number investigated here. It is observed that the axial flow velocity is very small around the beads and small gaps between the beads. In the top right corner, there is marked difference in the axial velocity, with PIV registering maximum velocities of around 1.6 mm/s, whereas DNS predicting maximum values of 1.2 mm/s. As will be shown later, this difference may be related to the fact that the top right corner of the plot is close to the region where there the bead location has the largest uncertainty (and, hence, large overlapping percentage).

Figures 11 a,b show the contour plots of the normal velocity (v_x) in the measurement plane. Also shown in Figs. 11 c,d are the distributions of the normal velocity field obtained from PIV and DNS, respectively. Again the two techniques provide a good qualitative match between the normal velocity distribution. The histogram of the normal velocity is reasonably symmetric, and this is to be expected because there is no mean flow in the x - direction. The frequency of near zero velocity is observed to be higher in the PIV data, which may be due to the inability of the PIV to accurately resolve the data very close to the bead surfaces and small gaps, as well as masking of the data in this region. Again, the range of the PIV data for normal velocity is slightly larger between $[-0.6, 0.6]$ mm/s compared to that of DNS $[-0.45, 0.45]$ mm/s. The discrepancy is again seen mostly right side of the plot where the bead surface overlap is relatively large.

The normalized differences of the two velocity components between PIV and DNS data are presented in Fig. 12 as both histograms and contour plots. Denoting the maximum velocities of each PIV component by $v_{x,max}$ and $v_{y,max}$ and the corresponding minimums by

Figure 11: Comparison of normal velocity (v_x) between PIV and DNS; (a) contour plot from PIV (velocity in (mm/s)), (b) contour plot from DNS (velocity in (mm/s)), (c) distribution of normal velocity obtained from PIV, (d) distribution of normal velocity obtained from DNS.

Figure 12: Normalized deviation data (PIV value minus DNS value) for each of the velocity components. (a) Color contours for the absolute axial ($|v'_y|$) data. (b) Color contours for the absolute normal ($|v'_x|$) data. (c) Histogram for the axial velocity deviations (v'_y). (d) Histogram for the normal velocity deviations (v'_x). All variables in these plots are unitless.

$v_{x,min}$ and $v_{y,min}$, the deviations were computed by

$$v'_x = \frac{v_{x,PIV} - v_{x,DNS}}{v_{x,max} - v_{x,min}} \quad (14)$$

$$v'_y = \frac{v_{y,PIV} - v_{y,DNS}}{v_{y,max} - v_{y,min}} \quad (15)$$

so that the deviations are normalized by the range of the velocity field measured in the experiments. For presentation purposes, the absolute value of the normalized difference is used for the color contour plots.

The color contour plots show that the deviations are small in the pore regions and large in small gaps between beads. Also, the upper right region of the plot shows large deviations owing to proximity to the overlapping beads. This difference is possibly because of the difficulty of resolving the velocity field near the fluid-solid interface in PIV; however, the error in bead position is a more likely source of the deviations. The normal velocity (v'_x) deviation exhibits a symmetric distribution centered at zero. The axial component (v'_y) deviation shows a much wider distribution centered distinctly around a small negative value of approximately -0.01 . This indicates that the axial velocity tends to have lower values in the PIV measurements than those predicted by DNS simulation. The contour plots indicate that the maximum difference in the axial velocity is almost twice as large as that of the normal component.

To further quantify the differences between the PIV and the DNS, a normalized root mean square deviation ($NRMSD$) value was calculated as

$$NRMSD_x = \frac{\sqrt{\frac{\sum (v_{x,PIV} - v_{x,DNS})^2}{N}}}{v_{x,max} - v_{x,min}} \quad (16)$$

$$NRMSD_y = \frac{\sqrt{\frac{\sum (v_{y,PIV} - v_{y,DNS})^2}{N}}}{v_{y,max} - v_{y,min}} \quad (17)$$

For the measurement plane and with the large box region investigated here, the $NRMSD$ for the axial (v_y) and normal (v_x) components of velocity were 11.32% and 4.74%, respectively. The higher value in the $NRMSD$ for the axial component of the velocity field is due to larger velocity mismatch observed near the top and bottom right corners of the plot, where

the predicted flow may be affected by the increased uncertainty in the bead locations in that region.

To better understand the differences between the PIV and DNS results, it was important to quantify potential sources of error in both in the PIV and the DNS data. The sources within the PIV method itself were already described in §3.2, and the total error reported there (7.5% in the x -direction and 2.6% in the y - direction, respectively) is much smaller than the *NRMSD* errors reported above. Thus, we examined several additional sources of error to describe these differences, including (1) numerical uncertainty in the DNS, (2) errors due to the incompletely-resolved inlet condition, and (3) errors due to uncertainty in bead locations within the packed bed.

5.4. Numerical uncertainty in DNS

The uncertainty in the DNS predictions were quantified by looking at the global convergence index (*GCI*) index as defined in Appendix B. Table 3 shows the uncertainties in DNS studies for both velocity components. Three grid resolutions coarse ($\Delta/D_B = 24$), medium ($\Delta/D_B = 36$), and fine ($\Delta/D_B = 48$) were used to quantifying these uncertainties. The global uncertainty obtained from GCI_G in predicting the axial and normal component of velocities is less than 4.5%, with the axial velocity component having slightly more uncertainty than the normal component. Slightly higher than second-order convergence is obtained in the present grid convergence study as indicated by global convergence order, $\mathcal{P}_G$.

The ratio $D_B/\Delta_{5\%}$ was computed from the convergence analysis, and it provides the number of grid points needed per bead diameter for an uncertainty of less than 5% in either velocity component. Thus, the uncertainty in the DNS simulations is roughly the same size as those inherent in the PIV data. Based on this ratio, the grid resolution requirement for the two components indicates that even the medium grid offers sufficient resolution; however, in order to have similar resolution as the PIV, the fine grid was used in calculating RMS deviations. With such a refined grid, the bead boundaries are approximated very accurately in the present simulation technique. The results of the analysis of numerical uncertainty suggest that it is a smaller source of uncertainty than the uncertainty in the PIV data, and

Table 3: Grid convergence and uncertainty quantification for flow through the packed bed at pore Reynolds number of $Re_p = 3.47$.

	$\mathcal{P}_G$	GCI_G [mm/s]	GCI_G [%]	$D_B/\Delta_{5\%}$
v_x	2.68	0.014	2.94	28
v_y	3.12	0.017	4.38	34

neither of these sources can explain the value of the $NRMSD$ observed in the comparison between the PIV and DNS data.

5.5. Influence of the inlet boundary conditions

As discussed above, the uncertainty in the inlet boundary condition was investigated as a potential source of error leading to small amount of mismatch between the PIV and DNS velocity data. The sensitivity of the DNS solution to the particular type of conditions imposed at the inlet was investigated by comparing the influence of two different inlet boundary conditions on the DNS velocity field. Two physically reasonable inlet conditions were constructed: (1) a fully-developed flow profile for a square duct [54], and (2) a uniform-velocity inflow.

Changing the inlet velocity profile did (obviously) change the flow field in the entrance region upstream of the porous bed; however, within the porous medium, the effect on the values for $NRMSD_x$ and $NRMSD_y$ is very small. There was less than 0.5% difference in the $NRMSD$ between the uniform and fully-developed velocity profiles. This strongly suggests that the inlet flow condition does not significantly affect the velocity field within the porous medium for this value of the Reynolds number.

5.6. Bead location and associated uncertainty

In the material above, the potential sources of error examined thus far can not explain the observed $NRMSD$ values for the comparison between the PIV and DNS data. Thus, the hypothesis that errors in the bead location data was posed. The uncertainty in estimating the bead center locations depends on both the magnification error and the uncertainty in

the image itself. The method of Kline and McClintock [34] was used to find the uncertainty in the bead position, $\mu_{\Delta z_1}$, as

$$\mu_{\Delta z_1} = \frac{1}{2} \frac{D_1}{M_1} \sqrt{\frac{\mu_d^2 + D_1^2 \mu_M^2}{D_B^2 - D_1^2}} \quad (18)$$

where, μ_M and μ_d are the uncertainties of the magnification and the diameter of each bead in the image, respectively. This results in an uncertainty of bead position of approximately 2.8% of the bead diameter.

Experimental uncertainties in measuring the bead centers in some cases lead to spheres that appeared to be overlapping. To examine how much error influenced sphere overlap, the number of spheres that have overlapping surfaces were determined, and a parameter was generated to assess the degree of overlap. The parameter, called the *overlapping percentage* for the purposes of this work, is defined by $(1 - r_{ij}/D_B) \times 100$, where r_{ij} the distance between centers of two adjacent beads and D_B the sphere diameter. For our system, more than 65% of the spheres show less than 1% overlapping percentage, and there are no spheres with overlapping percentage of more than 5% (Fig. 13).

Figure 13: Histogram of the overlapping percentage for the bead pack.

To visualize the distribution of overlapping beads, a color-coded three dimensional map of spheres is created as shown in Fig. 14 a (the flow direction for the orientation shown is

from top to bottom). The plane of interest, $z/D_B = 1.1$, where the PIV measurements were collected is also shown for reference. Figure 14 b shows the color-coded bead distribution for spheres with more than 2% bead overlapping percentage.

In order to see how the overlapping beads may affect predictions in the plane of interest ($z/D_B = 1.1$), a two-dimensional plot of the overlapping percentage is presented in Fig. 6 where the bead cross-sections at the plane of interest are shown. Note that the coordinate system was fixed for experimental convenience, and thus the origin is not at the center of the domain. To examine the influence of bead overlap on the deviation between the PIV and DNS data, two different regions of interest were identified as shown by the square boxes within the two-dimensional map. The first of these is a 40×40 mm region (large) which is very near to beads with some of the highest bead overlap errors; the second of these is a 30×30 mm region (small), chosen specifically to eliminate the highest overlap errors. These boxes are centered around the point (0, 5, 16.5) mm. The size of the large square binning box was determined initially by the fact that it represents an REV as described in §5.2.

It can be observed that the large box region used for analysis excludes the spheres with large overlapping percentage (over 3%); however, the proximity of these spheres to the outer edges of the box, can still affect the predicted flow fields as is shown later. The small region completely excludes the large overlapping spheres, and is also placed further away from them, thus minimizing the errors in flow prediction due to sphere overlap. The small region contains spheres with minimal overlapping percentage of less than 2%. The two binning sizes allow isolation of the effects of the overlapping region on the flow characterization and uncertainty estimates while comparing the PIV and DNS data. The influence of various sources of error, especially the bead overlap error, on the observed data is discussed in §5.3.

To examine the hypothesis that uncertainty in bead location was a significant source in the *NRMSD* error, an analysis was conducted in which the highest error beads were excluded. To accomplish this, a small domain of size 30×30 mm was chosen to evaluate the velocity deviations and their statistics (see Fig. 6). Although this volume was still an REV as established in the REV analysis, the superficial average velocity for this box size is slightly lower 0.120 mm/s and porosity ($\varepsilon_\gamma = 0.327$) are slightly lower; these yield an

Figure 14: Porous medium color-coded by the overlapping percentage, $(1 - r_{ij}/D_B) \times 100$. Also shown is the plane of interest $z/D_B = 1.1$ used for comparison of PIV flow measurements and numerical predictions. (a) showing all beads composing the porous medium, (b) showing all beads with an overlapping percentage of more than 2%, (c) showing only the beads touching the plane of interest. Flow orientation is from top to bottom.

intrinsic average velocity of 0.367 mm/s for the small domain.

The *NRMSD* values in deviations between the PIV and DNS data for axial and normal velocity components for the large (40 mm $\times$ 40 mm) binning region was 11.32% and 4.74%, respectively. When computed on the smaller (30 mm $\times$ 30 mm) binning region, the *NRMSD* gave values of 6.4% and 5.9%, respectively. The results show that the *NRMSD_y* decreases substantially in the axial velocity component when the region close to large overlapping spheres is eliminated. The deviation in normal velocity component increases very slightly; however, this may be related to the change in the range of the data used for normalization owing to reduced box size. Both components show that the *NRMSD* is less than 7%, which is very close to the uncertainties in the PIV and DNS techniques, respectively. Figure 15 shows color contour plots of the absolute deviation fields between the PIV and DNS data for the v'_x and v'_y velocity components in the small region. The histograms representing the distribution of v'_x and v'_y are given as well. The results of this analysis suggests strongly that the error in the bead position data is primarily responsible for the additional amount of *NRMSD* that is above what is inherent in the PIV and DNS data themselves.

6. Conclusions

The main goal of this study was to compare the experimentally measured (via PIV) velocity field at the sub-pore scale with the results of direct numerical simulation for a porous medium. The geometrical structure was identical (within experimental error) for both the experimentally-measured and numerically-computed velocity fields, so it was possible to directly compare the two results. There are several challenges in attempting this kind of direct comparison, including (1) uncertainty in the bead location and medium geometry, (2) appropriate representation of the inlet and boundary conditions, and (3) mismatch of PIV and DNS grids and resolution. The primary conclusions of this work are summarized as follows.

1. The principal conclusion from this work is that it is possible to develop high-resolution simulations of the velocity field in a porous medium that match the measured velocity

Figure 15: Normalized deviation data (PIV value minus DNS value) for each of the velocity components in the reduced domain (30×30 mm). (a) Color contours for the absolute axial ($|v'_y|$) data. (b) Color contours for the absolute normal ($|v'_x|$) data. (c) Histogram for the axial velocity deviations (v'_y). (d) Histogram for the normal velocity deviations (v'_x).

field with high fidelity. The deviations between the PIV and DNS data sets were within about 10% or less (11.32% for v_y and 4.74% for v_x) as measured by the (global) *NRMSE* metrics defined in the body of the paper. This has important ramifications both for upscaling in porous materials and for engineering design of porous materials at the pore scale by providing direct validation that DNS of porous materials can match the actual physical processes of interest with accuracy.

2. The index-matched fluid-solid porous medium allowed for velocity data collection with high resolution and high fidelity within the porous medium. However, the experimental process to obtain good data from this technique is more sensitive to experimental errors- particularly with regard to index-of-refraction mismatch between the solid and fluid phases- than has been implied in previous work. In this work, the index of refraction mismatch was poised such that $|n_\kappa - n_\gamma| < 0.0005$ in order to keep mismatch errors acceptably low.
3. Accurate measurement of the porous medium geometry was found to have an important role in the ability to accurately predict the velocity field. In this effort, particular care was taken to locate bead centers, and the resulting uncertainty was relatively small (2.76% uncertainty or within 0.1 mm of 15 mm diameter beads). However, even with an exceptional effort to carefully characterize the geometry, the numerical model contained overlapping spheres, which is physically unreasonable. Although most of the beads negligible overlap (65% of the them had less than 1% overlap percentage), there were some regions with overlap percentages as high as 3-5%. Comparison of the PIV and DNS data suggest that even this small percentage of position uncertainty could significantly influence the velocity fields predicted by DNS, leading to larger *NRMSE* errors.
4. It was possible to determine an REV for the porosity (ε_γ), the hydraulic conductivity (K_{yy}), the superficial average velocity ($\langle v_y \rangle$), and the pressure drop per unit length ($\Delta p_\gamma / L_c$) on the basis of first-order statistics (i.e., the average value). This was done by examining the average value with increasingly large averaging volumes. Although the results show that none of the fields were perfectly stationary, the values of the

fields for the $40 \text{ mm} \times 40 \text{ mm}$ averaging window showed that the assumption of an REV with a characteristic length of greater than or equal to 40 mm is a reasonable one. These results are consistent with other observations from the literature [77]. Our results showed that the asymptotic value of porosity determined this way was consistent with the measured value (0.43 versus 0.44), and that the hydraulic conductivity estimated this way was equal to approximately $K_{yy} = 2.5 \text{ m/s}$.

5. It was possible to show that the resulting velocity field, as measured by global *NRMSD* error statistics, was significantly influenced by the error in the bead position data. Bead position error appears to be the largest error source, being perhaps more important than the error inherent in the PIV and DNS data themselves. The uncertainty in the inlet boundary condition was largely eliminated as a significant source of error, which is in itself a significant result. The proposal that boundary conditions, under many circumstances, may not strongly influence global measures of porous medium properties has been discussed extensively (e.g., [72, §5.2]), but there has been little experimental evidence to date. Thus, this study adds useful experimental evidence that the integral porous media properties (e.g., such as the *NRMSD* statistic) are not significantly affected by the particular inlet boundary condition imposed.

This study represents the first step at comparing experimental versus computational results within a randomly packed porous medium. It was shown that with carefully-constructed experiments and well-resolved numerical simulations, it is possible to obtain good fidelity between the measured and numerically simulated velocity field in a randomly-packed porous media. Further investigation of these techniques for higher Reynolds numbers involving inertial flow, unsteady flow, and transitional or turbulent flows in porous media are ultimately necessary to expand these results to other flow regimes.

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A. Experimental details for magnification

In this study, it was required that the test section be moved in order to view various planes within the test bed. Moving the test bed results in a change of local magnification; this influences the ability to determine the local seed particle displacement in the object plane, and in determining bead centers for reconstructing the geometry. Usually, the magnification is estimated by introducing a calibration target in the object domain, Adrian and Westerweel [1], which is difficult to do in a porous bed. To overcome this problem, an *in-situ* method was used to determine the local magnification which is useful when the porous bed is a distribution of solid phase spherical beads of known uniform diameter. Further details of the magnification estimation procedure is given in Patil and Liburdy [49].

Figure A.1: Schematic showing laser light sheets used to image two different sections of a bead (at distances z_1 and z_2 from the cell wall) to estimate local magnification and also the center of beads. Also shown are sectional cuts of diameters, D_1 and D_2 of a spherical bead, the corresponding imaged diameters d_1 and d_2 associated with laser light sheet positions at 1 and 2, respectively.

A single plane within the bed will image bead particles of different diameters depending on the location of the bead centers along the optical axis, as shown in Fig. A.1. The ratio of imaged bead diameters at two different planes separated by a small distance ($|z_1 - z_2|$)

along the optical axis are denoted as d_1 and d_2 , and can be given as

$$\frac{d_1}{d_2} = \frac{M_1 D_1}{M_2 D_2} = \frac{M_1 \sqrt{D_B^2 - (D_B - 2(z_1 - z_0))^2}}{M_2 \sqrt{D_B^2 - (D_B - 2(z_2 - z_0))^2}} \quad (\text{A.1})$$

where M_1 and M_2 are the local magnifications, and D_1 and D_2 are sectional diameters of beads imaged at z_1 and z_2 , respectively. By using small displacements, $(z_2 - z_1)$ of approximately 1 mm, so that M_1 is approximately equal to M_2 , then the ratio of imaged diameters, d_1/d_2 , is a function of D_B , z_1 and $(z_2 - z_1)$. Consequently the above equation allows the determination of z_1 based on the measured bead diameters within the plane. The magnification, M_1 , at the object plane z_1 is expressed as

$$M_1 = \frac{d_1}{\sqrt{D_B^2 - (D_B - 2(z_1 - z_0))^2}} \quad (\text{A.2})$$

This quantity specifies the variation of magnification along the optical axis through the porous bed. Imaging software was used to calculate the bead diameter at each plane based on the circular image of the bead. Since multiple bead diameters were observed in each image plane within the bed the local magnification was taken as the average of calculations of all beads within the plane. As shown in Patil and Liburdy [49] the standard deviation among trials using the average value for each case is 0.001. After computing the magnification for 9 separate planes, a linear regression curve was generated for the magnification factor as a function of location of the plane (z); this function was given by $M = 0.0002z + 0.2171$.

The expression developed above can also be used to determine the centers of the beads when one knows the magnification, M_1 , and the imaged bead diameter, d_1 . By inverting Eq. (A.2), this expression is

$$z_1 - z_0 = \Delta z_1 = \frac{D_B}{2} - \frac{1}{2} \sqrt{D_B^2 - D_1^2}; \quad D_1 = \frac{d_1}{M_1} \quad (\text{A.3})$$

B. Validation of the numerical method

The numerical approach used in this work has been extensively verified and validated for a range of canonical problems involving flow over stationary cylinder as well as sphere for a wide range of Reynolds numbers, flow over two contacting spheres at different orientations,

among others. The detailed verification tests can be found in [3]. In addition, the results predicted by this approach have also been compared with resolved simulations for body-conforming unstructured grid solvers to show very good predictive capability Finn and Apte [22]. Overall the numerical approach is second-order accurate in space and time.

Figure B.2: Computational configuration and comparison of interstitial velocity profiles with the data of Suekane et al. [64] along the $y = 0$, $z = 0$ line probe. (a) The experimental Geometry. (b) Solutions for (—) Fine Grid (with error bars), (---) Medium Grid, (- · -) Coarse Grid, ● Experiment.

A validation study was conducted comparing experimental measurements for a simple cubic lattice structure [64] with numerical results generated from the numerical code on the same geometry (see Fig. B.2a). Suekane et al. [64] applied MRI techniques to make detailed three-dimensional measurements of the pore-scale velocity field for a range of Reynolds numbers in the inertial flow regime. The geometry consists of six layers of diameter $D_B =$

28 mm quarter spheres located in the corners of the channel, with no-slip boundaries enforced on the exterior channel walls, and a porosity of $\varepsilon_\gamma = 0.476$. The flow field at a Reynolds numbers of $Re_p = 11$ was computed to compare directly with the experimental results (N.B., we have corrected Reynolds numbers reported in [64] to be consistent with the definition of the pore Reynolds number adopted in this paper). A constant inflow boundary was applied $5D$ upstream of the first sphere (not shown in the figure). A convective outlet is located $5D$ downstream of the last sphere. Cartesian grids were used for both the fluid and solid parts of the configuration. Three meshes were generated with mean spacing, $D_B/\Delta = 16, 32, 64$ and representing the coarse, medium and fine grids, respectively.

The fine, medium, and coarse grid predictions of streamwise (for the work of Suekane et al. [64], this was the z -direction) velocity along the $y = 0, z = 0$ line is plotted in Fig. B.2b. In Fig. B.2b, only the fine grid result with error bars is plotted alongside the experimental data of [64]. In the inset, the fine, medium, and coarse grid solutions are shown for the region near $|x/D_B| \lesssim 0.15$ to more clearly illustrate the convergence with grid refinement. In all cases there was good agreement between the experimental data and the medium- and fine-grid solutions. As part of the validation effort, a normalized pressure drop was computed as per Ergun [21]

$$\Psi = \frac{\Delta p_\gamma}{L} \frac{D_B}{\rho U_p^2} \frac{\varepsilon_\gamma^3}{1 - \varepsilon_\gamma} \quad (\text{B.4})$$

The computed non-dimensional pressure drop of 13.85 was in reasonable agreement with the Ergun relation value of 13.83. Higher Reynolds numbers (not reported here) up to $Re_p = 181.6$ for steady flow as well as up to $Re_p = 544.8$ for unsteady flows have also been studied on finer grid resolutions to show consistently good convergence and predictive capability [22].

In the absence of an analytic solution, it is important to be able to estimate and report the uncertainty associated with numerical predictions. The *grid convergence index* (*GCI*), originally proposed by Roache [57] was used to quantify the uncertainty associated with the present numerical results. To compute an uncertainty band for any flow variable, ξ , the solution is first obtained on at least three grids with (not necessarily equal) refinement

ratios $r_{21} = \Delta_2/\Delta_1$ and $r_{32} = \Delta_3/\Delta_2$. The fine and medium grid solutions, ξ_1 and ξ_2 , are then interpolated to the coarse grid, where the variations, $\epsilon_{32}(\mathbf{x}) = \xi_3(\mathbf{x}) - \xi_2(\mathbf{x})$, and $\epsilon_{21}(\mathbf{x}) = \xi_2(\mathbf{x}) - \xi_1(\mathbf{x})$, are computed. From $\epsilon_{32}(\mathbf{x})$ and $\epsilon_{21}(\mathbf{x})$, the *local* apparent order of accuracy, $\mathcal{P}(\mathbf{x})$, may be calculated, using the following equation [12].

$$\mathcal{P}(\mathbf{x}) = \frac{1}{\ln(r_{21})} \left| \ln |\epsilon_{32}(\mathbf{x})/\epsilon_{21}(\mathbf{x})| + \ln \left(\frac{r_{21}^{\mathcal{P}(\mathbf{x})} - \text{sign}(\epsilon_{32}/\epsilon_{21})}{r_{32}^{\mathcal{P}(\mathbf{x})} - \text{sign}(\epsilon_{32}/\epsilon_{21})} \right) \right| \quad (\text{B.5})$$

In the event that $r_{21} \neq r_{32}$, a straightforward iteration of equation B.5 can be used to determine $\mathcal{P}(\mathbf{x})$. The global order of convergence, $\mathcal{P}_G$, is then computed by averaging $\mathcal{P}(\mathbf{x})$ at nodes where monotone convergence is observed, indicated by $\text{sign}(\epsilon_{32}/\epsilon_{21}) > 0$.

Using the global order of convergence, the *GCI* of the fine grid solution is then computed as

$$GCI(\mathbf{x}) = F_s \left| \frac{\xi_1(\mathbf{x}) - \xi_2(\mathbf{x})}{1 - r_{21}^{\mathcal{P}_G}} \right| \quad (\text{B.6})$$

where $F_s = 1.25$ is a conservative factor of safety for a three grid refinement study [59]. In this form, the *GCI* has the same units as ξ , and may be taken as a local uncertainty band. A dimensionless relative uncertainty can also be obtained if the *GCI* is normalized by some appropriate ξ_{ref} value. Here the non-dimensional global uncertainty, GCI_G , is reported as the node averaged percent relative uncertainty with ξ_{ref} equal to the spatial average of $RMS(\xi(\mathbf{x}))$. Boundary nodes, or nodes where ξ is fixed (such as within rigid bodies in fictitious domain computations), are excluded from the global averages. Finally, the grid resolution required to obtain some target level of uncertainty, denoted GCI^* , may be estimated by [58]

$$\Delta^* = \Delta_1 \cdot \left(\frac{GCI^*}{GCI_G} \right)^{1/\mathcal{P}_G} \quad (\text{B.7})$$

This is useful for determining minimum resolution requirements for a given simulation.

The grid convergence properties were computed for the stream-wise velocity component, $\xi = u_z$, as well as the non-dimensional macroscale pressure gradient, $\xi = \Psi$. For $\xi = u_z$ the convergence of the pore-scale velocity field was directly assessed, while for $\xi = \Psi$, the convergence of a macroscale integrated property (the pressure drop) was assessed. Key results of the analysis are reported in Table B.1. The global apparent rate of convergence,

$\mathcal{P}_G$, was bound by the formal second order accuracy of the spatial discretization schemes, and was observed to be between 1.4 and 1.7 for this case. The global uncertainty for the pore-scale velocity field was 1.6% and for the non-dimensional pressure drop was approximately 3.7%. It was observed that the global measure (the pressure drop) has slightly more uncertainty than the pore-scale measure (velocity). Based on this, for a general 5% uncertainty level, the grid requirements for pore-scale velocity was around 28 control volumes per bead diameter, whereas, for pressure drop convergence it was almost twice as much. The higher uncertainty in pressure drop may be related to the way it was calculated. To estimate the pressure drop, the pressure field was spatially averaged at planes located $L = 2D$ apart in the flow direction, once the flow was fully developed.

Table B.1: Grid convergence and uncertainty quantification for flow through the simple cubic lattice at $Re = 11$.

Re_p	ξ	$\mathcal{P}_G$	$GCI_G[\%]$	$D/\Delta_{5\%}$
11	u_z	1.45	1.60	28
11	Ψ	1.67	3.69	53

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