Transition between Flow Regimes in Porous Media
Using Magnetic Resonance Velocimetry:
From Laminar to Turbulent

Meichen Lu
Churchill College

Department of Chemical Engineering and Biotechnology
University of Cambridge

A dissertation submitted for the degree of Doctor of Philosophy
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To my loving parents
Preface

This dissertation is my original work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. The research described herein was carried out in the Department of Chemical Engineering and Biotechnology, University of Cambridge. This dissertation contains no more than 65,000 words or 150 figures. It has not been previously submitted for consideration, in part or as a whole, for any other degree.

Meichen Lu
Cambridge
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Abstract

The primary aim of this thesis is to investigate the transition between different flow regimes in porous media. The complete transition spectrum of single-phase flow, from creeping flow to inertial, unsteady laminar, and turbulent flow regimes, was examined in sphere packings. Further understanding of the fundamental fluid dynamics was derived based on the pore-scale flow visualisation using magnetic resonance velocimetry (MRV). Spiral imaging was selected as the ultrafast imaging protocol to probe the transient phenomena, and the acquisition was further accelerated by combining subsampling and compressed sensing reconstruction.

In a random sphere packing column with column-to-diameter ratio of 3.44, the inertial effect and the onset of unsteady regime were examined with respect to the principal flow characteristics: the inertial core/channeling, backflow, and helical vortices. Helical vortices have been observed experimentally in a random packing for the first time, and the analogy between the swirling flow and helical vortices provides insight into the design and operation of packed bed reactors. Another new observation is that the transition to the unsteady regime is a highly heterogeneous process, where the evolution of the flow instability depends on the pore geometry. Moreover, pixelwise validation was achieved between the experimental and simulation results on three-dimensional velocity fields in the inertial regime; this is enabled by an image-based meshing pipeline, which reproduces the geometry of the random packing in MRV for the numerical simulation.

The unsteady regimes were further investigated using a regular sphere packing, the simple cubic packing (SCP). The spectral analysis, in both the random and regular packing, revealed a route to chaos from the steady to periodic, quasi-periodic, and chaotic dynamics, which was only predicted numerically before. During the transition to turbulence, the coherent structures were extracted using proper orthogonal decomposition (POD), which yields a coherent picture regarding the turbulent dynamics, when combined with the skewness, flatness, and quadrant analysis. Furthermore, it was found that the macroscopic properties converged at lower Reynolds number than the microscopic features.

In conclusion, the opportunity to measure flow fields at high spatial and temporal resolution will play an increasingly significant role in the advancement of fundamental fluid dynamics. In this thesis, MRV is used, which is particularly advantageous for non-invasive measurements in opaque systems. This thesis provides the experimental and analysis toolkits for such studies and
has demonstrated the contribution to characterising and understanding different flow regimes in porous media.
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Chapter 1 Introduction

1.1 Flow regimes in porous media

1.1.1 Overview of flow regimes

The understanding of fluid flow through porous media is of importance in many fields including chemical engineering, geohydrology, and mechanical engineering. One of the porous media of particular interest to chemical engineers is the packed bed reactor; accurate modelling of the flow field is crucial in determining the heat and mass transfer, which underpin the efficiency and operating cost of the reactor (Dixon et al., 2006). Packed beds of spheres are common configurations of nuclear reactors (Hassan & Dominguez-Ontiveros, 2008), adsorption columns in chromatography (Hlushkou & Tallarek, 2006) and fixed-bed reactors (Dixon & Nijemeisland, 2001). Moreover, sphere packings have been widely used as a model system. For example, random packing of monodispersed spheres has also been used to model soil because it creates a complex, heterogeneous geometry with a single control variable (Narsilio et al., 2009). In this thesis, we focus on the pore-scale flow phenomenon in sphere packings due to their ubiquitous applications and simplicity. This study aims at understanding the transition between different regimes. Because the physical process is determined by local pore structures, the observations and conclusions apply to porous media with impermeable solid phases at various scales, from \( \mu \text{m} \) to m.

Distinct phenomena have been observed at different flow regimes, and the understanding and characterisation of different flow regimes in porous media is critical in modelling and predicting macroscopic properties (Dixon et al., 2006). The transition between different flow regimes is demarcated by the Reynolds number \( (Re) \), and the most widely used definitions in packed beds are superficial Reynolds number, \( Re_{sf} \), and pore Reynolds number, \( Re_{p} \):

\[
Re_{sf} = \frac{U_{sf}D_{p}}{\nu}, \quad \text{and} \quad \tag{1.1}
\]

\[
Re_{p} = \left( \frac{U_{sf}}{\epsilon} \right) \frac{D_{p}}{\nu} = Re_{sf} \frac{1}{\epsilon}, \quad \tag{1.2}
\]

where \( U_{sf} \) is the superficial velocity, \( \nu \) is the kinematic viscosity, \( D_{p} \) is the particle diameter, and \( \epsilon \) is the porosity. Superficial velocity is the hypothetical mean velocity if only liquid were
present, \( U_{sf} = \frac{Q}{A} \), where \( Q \) is the volumetric flowrate and \( A \) is the cross-sectional area. Pores refer to the void space occupied by fluid, and \( Re_p \), which based on the mean velocity, is more characteristic than \( Re_{sf} \). The well-acknowledged classification of flow regimes has been proposed by Dybbs and Edwards (1984), who used laser anemometry and dye injection visualisation to study flow in a random packing of cylindrical rods. They identified four flow regimes:

1. \( Re_p \leq 1 \): The creeping or Darcian regime, where the flow is dominated by viscous forces and Darcy’s law is valid.
2. \( 1 < Re_p < 150 \): The steady nonlinear laminar or inertial flow regime featured by the development of inertial cores in the centre of the pores.
3. \( 150 < Re_p < 300 \): The unsteady laminar regime characterised by the onset of laminar wakes that travel with distinct periods, amplitudes, and growth rates.
4. \( Re_p \geq 300 \): The turbulent regime with highly unsteady and chaotic flow.

Selected previous work will be discussed in this section, and a more comprehensive review on this subject was given by Hlushkou & Tallarek (2006).

### 1.1.2 Transition from creeping to inertial regime

The creeping or Darcian flow often refers to flow obeying Darcy’s law, which states that the pressure drop in the flow direction is proportional to the flowrate for in a homogeneous porous medium (Nield & Bejan, 2006). The transition from the creeping to the inertial regime is characterised by the deviation from Darcy’s law, which has been investigated by experimentalists and theoreticians for decades (J Bear, 1972; Eisfeld & Schnitzlein, 2001). The mechanism of this transition is still an active research field (Panfilov & Fourar, 2006; Chaudhary et al., 2011). This topic is particularly challenging because of the heterogeneity of the porous structure and the flow fields. The key inertial flow characteristics include the channelling, development of inertial core, reversed flow, recirculation and stationary eddies/vortices. Sederman et al. (1998) first quantified the highly heterogeneous flow field in a sphere packing via pore segmentation: 8% of the pores account for 40% of volumetric flow rate. The transition to the inertial regime was shown by Johns et al. (2000) to be dependent on the local flow field. The development of an inertial core was characterised by the flattening of the velocity profiles and was quantified by the decrease in the variance of axial velocity. The
sharp decrease in the variance was associated with a local Re of about 30, and the local Re was defined by the pore length scale and the average velocity in the pore.

Several computational fluid dynamics (CFD) studies have revealed the importance of pore-scale vortices on the deviation of Darcy’s law in porous media. The stationary eddies in pores formed from simple cubic packings were shown by Cardenas (2008) to remain the same size and shape at Darcian flow regime with increasing Re. Chaudhary et al. (2011) examined the transition from Darcian flow regime on a converging and diverging channel formed by a staggered pattern of spheres. The eddies were observed to grow with increasing Re, which accounts for the deviation from Darcy’s law. The growth of eddies was later slowed down by the pore boundary and the increased pressure of the bulk flow. A survey of the different pore-scale characteristics in the transition to inertial regime is provided in §3.1.

1.1.3 Transition to unsteady regimes

Although the transition to the unsteady (i.e., turbulent) flow has been well characterised in pipe flow, the same process in porous media is not well understood. Earliest studies attributed the deviation from Darcy’s law to the onset of turbulence, whereas this misconception has been carefully pointed out in several textbooks (J Bear, 1972; Dullien, 1992). This phenomenon was first studied by flow visualisation (Jolls & Hanratty, 1966; Dybbs & Edwards, 1984; Masuoka et al., 2003) and then quantitatively using electrochemical microelectrodes (Latifi et al., 1989; Rode et al., 1994; Seguin, Montillet, & Comiti, 1998; Bu et al., 2014). The latter technique revealed a broad spectrum of critical Re_{sf} (Re_{crit}) that demarcates the onset of unsteady laminar (Re_{crit} = 100-150) and the turbulent regime (Re_{crit} = 250-550). Moreover, the unsteady flow is highly heterogeneous, regarding the Re_{crit} and the strength of fluctuation, in contrast to the transition in pipe flow.

Most recent advancements have been enabled by applying particle imaging velocimetry (PIV) in refractive index matched systems. Patil & Liburdy (2012, 2013a, 2013b) conducted a study using PIV on a random packed bed of spheres up to Re_{p} ≈ 4000, and Khayamyan et al. (2017) used stereoscopic PIV (sPIV) up to Re_{p}=3320. It is worth noting that Patil & Liburdy (2013a) successfully estimated the macroscopic mechanical dispersion using the pore-scale Eulerian statistics. They also emphasised the importance of heterogeneity in porous media with respect to different flow regions: tortuous channel-like flow, jet-like regions and recirculating regions.
Because of the complexity of the phenomenon, a regular packing is often chosen to characterise the unsteady behaviour and investigate the mechanism. The study using lattice-Boltzmann method (LBM) in a face-centered cubic (FCC) packing by Hill & Koch (2002) has provided important insight into the instability mechanism. The unsteady flow in simple cubic packing (SCP) has been examined by numerical and experimental studies, and vortex-shedding like phenomenon was predicted by Finn et al. (2012) at Re_p = 600. The onset of unsteady flow will be reviewed in more detail in §5.1 on random packings, §6.1 on a structured packing; §7.1 will review on the transition to turbulence in porous media.

1.1.4 From pore-scale to macro-scale

A recurring theme in the above literature is the significance of the pore-scale flow characteristics in the understanding of the fluid dynamics, especially in determining the flow regimes. From the application’s perspective, the pore-scale flow behaviours are crucial in the accurate modelling of pressure drop, heat transfer and reaction in various porous media flows. Pore-scale simulations have gained popularity in the past two decades, including the more coarse-grained pore-network models and the high-fidelity direct numerical simulations (DNS) (Meakin & Tartakovsky, 2009). However, in large-scale simulations, the computational cost of fully resolved DNS calculation is still formidable, and the pore-scale dynamics contribute to the macroscopic models mainly by enabling better estimation of parameters, such as permeability and dispersivity (Scheibe et al., 2015; Wood et al., 2015). The macroscopic properties can be estimated by spatial-averaging in the representative elementary volume (REV), defined to be the smallest differential volume that results in statistically meaningful local average properties (R. W. Johnson, 2016). REV often consists of a large number of much smaller inhomogeneities (e.g., pores) in micro-scale, whilst being much smaller compared to the macro-scale (K Markov, 2000). Because the structural details can be averaged on the order of REV, the macroscopic parameters can be extracted from REV based on experimental studies or pore-scale simulations. Fourie et al. (2007) have demonstrated that the hydraulic conductivity in Darcy’s law can be derived from pore-scale microscopic models that solve the Navier-Stokes equations directly.

1.2 Measuring single-phase flow in porous media

In this section, we introduce the operating principles and key elements of the major experimental techniques to study fluid dynamics in porous media, especially the unsteady
phenomenon. The scope is limited to single-phase flow, mainly liquid phase, although references to gas flow studies are also made. Some key studies are highlighted here; more detailed reviews can be found in the relevant sections §3.1, §5.1, §6.1 and §7.1.

1.2.1 Electrochemical microelectrode techniques

The transition to unsteady flow regime was first studied quantitatively by electrochemical microelectrode techniques. The electrochemical system consists of the reduction reaction, $\text{Fe(CN)}_6^{3-} + e^- \rightarrow \text{Fe(CN)}_4^{4-}$, occurring on the cathode and the reverse reaction takes place at the anode. The applied voltage is increased until the current flowing in the circuit reaches the limiting current, $I_{lim}$, controlled by the rate of diffusion. The relationship between the average limiting current and the average velocity gradient ($\bar{S}_x$) was shown to be (Seguin, Montillet, & Comiti, 1998):

$$(I_{lim}) \propto (\overline{S}_x)^{\frac{1}{3}}.$$  \hspace{1cm} (1.3)

Rode et al. (1994) stated that microelectrodes are particularly suited for studying extremely non-homogeneous turbulent flow with high amplitude fluctuations of local shear rate. The technique has been applied to study the onset of unsteady flow in sphere packings, and this was first demonstrated by Jolls & Hanratty (1966). The probes are glued at or embedded in the wall or the surface of the packing, and they are ground and polished to a smooth surface, to ensure that the measurement is non-invasive. To overcome the limitation in complex structures with no internal access for electrode gluing, grinding, polishing and cleaning, Altheimer et al. (2016) used a novel mounting technique to investigate the flow in a 3D-printed structure.

1.2.2 Hot-wire anemometry

Hot-wire anemometry (HWA) is one of the first quantitative techniques to study turbulence, and it measures mean and fluctuating-velocity components at a point. The wires are usually made of platinum or tungsten with diameters of the order of 5 microns (Bradshaw, 2013). The sensor is heated by an electric current and cooled by incident flow so that the velocity of the fluid can be deduced from its resistance (Comte-Bellot, 1976). By employing two or more sensors spaced closely in the flow field, HWA was the first technique to measure velocity-gradient tensors (Wallace & Vukoslavčević, 2010). Moreover, HWA was applied by Mickley et al. (1965) and Van der Merwe & Gauvin (Van der Merwe et al., 1971) to study turbulent air flow through a structured packing of spheres.
1.2.3 Laser-Doppler velocimetry

Laser-Doppler velocimetry (LDV), also known as Laser-Doppler anemometry (LDA), is based on the measurement of the Doppler shift of laser light scattered by the small particles, which are often smoke in gas and dye particles in liquid. The Doppler shift is related to the fluid velocity, \( \mathbf{u} \), by

\[
\omega_D = K \cdot \mathbf{u} = (K_s - K_i) \cdot \mathbf{u},
\]

where \( K_s \) and \( K_i \) are the wave vector of the scattered and incident light. The key element for the successful application in porous media is the refractive index matching, which minimises the disturbance from the solid phase to the incident and scattered laser light. LDV was first applied to measure creeping flow by Johnston (1975) in a structured sphere packing and later by Dybbs and Edwards (1984) in a random rod packing, and Giese et al. (1998) with four different packing particle shapes. The first pore-scale feature during the transition to the inertial regime was interpreted from the LDV results by Dybbs and Edwards (1984) and it has also been used to study turbulent flow in structured packings by Yevseyev et al. (1991).

1.2.4 Ultrasonic velocity profiler

Similar to LDV, the ultrasonic velocity profiler (UVP) is also based on the Doppler effect but, instead of lasers, ultrasound is used. UVP extends the point-based measurement of the instantaneous velocity to a 1D distribution and can also probe flow in opaque systems (Ozaki et al., 2002). In a UVP experiment, sinusoidal ultrasound pulses are emitted from a transducer, with short time intervals, along a measurement line. The same transducer is used to detect the echo signal reflected from the tracer particles. The position of the particle is calculated from the speed of the sound and the velocity deduced from the Doppler frequency shift (Manes et al., 2009). UVP was used to measure the axial velocity in SCP from the steady to the turbulent regime at a temporal resolution of 30 Hz (Horton & Pokrajac, 2009).

1.2.5 Particle-imaging velocimetry

HWA is well-known for its excellent signal-to-noise ratio and LDV can measure temporal statistics accurately; however, they provide limited spatial information, e.g., flow field measurements and spatial correlation (Westerweel et al., 2013). PIV has gradually become the dominant approach due to its high spatial and temporal resolution and is particularly suited to study turbulent flows. The standard setup is the planar PIV, whose key processes and elements
are shown in Fig 1.1. The flow is seeded with sub-micrometre particles that scatter the laser light sheet. A digital camera images the light scattered and the images are taken at discrete times, each called a frame. The frames are divided into small interrogation regions, and the displacement of the particles are computed from cross-correlation between adjacent frames. The temporal resolution has been sped up by the Nd:YLF lasers capable of generating pulses up to 10,000 Hz and complementary metal-oxide semiconductor cameras that can record 1024 × 1024-pixel images at 5,000 frames per second (Westerweel et al., 2013).

![Fig 1.1. Elements and processes in a planar, 2D PIV system. Figure taken from Adrian & Westerweel (2011).](image)

Two types of techniques, polarisation-based and colour-based systems, were proposed to measure all three velocity components for a two-dimensional (2D) plane using four cameras (Arroyo & Hinsch, 2008). More recently, the focus has shifted to temporally resolved measurements of three-dimensional (3D) three components velocity fields. There are three categories of 3D PIV experiments (Arroyo & Hinsch, 2008):

1. **Multiple-plane PIV**: the 3D region is illuminated with a number of evenly spaced light sheets; e.g., digital image plane holography.
2. **Adjustable-depth volume PIV**: the cross-sectional area of the illumination is increased in depth; e.g., defocus-evaluating PIV, tomographic PIV.
3. **Full-flow-depth volume PIV**: using forward or backward light scattering to image the entire volume; e.g., optical forward scattering holography, digital in-line holography.
Westerweel et al. (2013) also introduced some other advanced variants of PIV: Tomographic PIV as a more robust technique to acquire full 3D information, statistical PIV measuring the flow statistics instead of the instantaneous flow fields, and triple-pulse PIV, which can measure the acceleration directly and yields the velocity measurement with greater time accuracy. PIV has also found its applications in porous media by refractive index matching, from as early as Saleh et al. (1992) to the latest stereoscopic PIV by Khayamyan et al. (2017). Readers interested in PIV are referred to Schröder & Willert (2007) and Adrian & Westerweel (2011) for further details.

1.2.6 Magnetic resonance imaging

Magnetic resonance imaging (MRI) is a non-invasive technique, particularly suitable to study optically opaque systems, with multiple components and/or phases. Magnetic resonance velocimetry (MRV) extends the spatially resolved mapping capability of MRI to velocity measurements. The spatial resolution can reach ~10 µm, and recent advancements on the temporal resolution were enabled by numerous fast imaging techniques. MRV has provided invaluable insight into the flow in porous media (Sederman et al., 1997, 1998; Ren et al., 2005). MRI is the technique used in this work and its principles are introduced in Chapter 2. Relevant literature will be reviewed in later chapters.

1.3 Scope of the thesis

The primary aim of this thesis is to advance the fundamental understanding of the transition between different regimes of single-phase flow in porous media. The porous structure studied in this work is the commonly used packing of spheres, and experiments are focused on measurements of the pore-scale velocity field. Prior to this work, there has not been a systematic study for the transition between flow regimes in such packing. The roadmap for this study is shown in Fig 1.2. The experimental data are analysed to obtain insight into the transition processes, from the creeping regime to turbulent regime, and can contribute towards the theoretical studies and modelling of porous media flow. Imaging of the pore-scale flow is highly valuable for the development and validation of numerical models at a range of conditions, which could be scaled-up for the more accurate modelling of diverse applications, from laminar flow in rocks to turbulent flow in nuclear reactors.
1.4 Outline of thesis chapters

Chapter 1 gives an overview of the current understanding of the transition from the creeping to the turbulent regime of the single-phase flow in porous media. The primary experimental techniques to probe the hydrodynamic phenomenon are also reviewed. The aims of the thesis are stated, and a roadmap is provided.

Chapter 2 introduces the principles of NMR and MRI relevant to this work, in particular, the ultra-fast MRV techniques and theories of compressed sensing.

Chapter 3 first reviews the key flow characteristics in the inertial flow regime and identifies the lack of experimental evidence of helical vortices. The application of MRV to measure 3D velocity maps is demonstrated, and the developing inertial flow is analysed in detail with respect to the key flow features.

Chapter 4 demonstrates how the pore-scale information can be used to validate numerical solutions. The structure of the random packing is extracted from the 3D MRI images using image-based meshing, which enables the pixel-wise validation of simulation results. This study is the first direct validation of pore-scale simulation in the inertial regime. Building upon the
analysis of the previous chapter, further insight is derived by comparing the predicted and measured flow features.

Chapter 5 applies the ultra-fast spiral imaging technique to study the onset of unsteady flow in a random packing, which is further accelerated by combining subsampling and the state-of-the-art compressed sensing reconstruction. By pushing the limit of MRI in the challenging geometry, spatially resolved development of unsteady flow is revealed for the first time. Moreover, proper orthogonal decomposition has been applied for the first time to MRV data of unsteady flows to distil coherent structures.

Chapter 6 is a more in-depth investigation of the nature of instability using the same experimental techniques as Chapter 5, and the study is conducted on the SCP channel. Two bifurcations are identified, and a direct link with the exact coherent states has been established. Dynamic mode decomposition is implemented, and valuable insight is obtained from this novel analysis technique.

Chapter 7 extends the previous chapter to the transition to turbulence. The demarcation of the onset of turbulent flow and turbulent statistics from the literature are reviewed, and a detailed comparison is made with current data. The differentiation between the microscopic and macroscopic turbulence is pointed out, which has significant implications on the turbulent modelling. The coherent structures are extracted using proper orthogonal decomposition and their relationship with the turbulent statistics is addressed.

Chapter 8 summarises the main conclusions and draws readers’ attention to the promising areas of future research.

A special remark on the definition of $Re$ is needed: in random packed bed (Chapters 3-5), the default $Re$ is based on the superficial velocity, i.e., $Re = Re_{sf} = \frac{U_{sf}D_{p}}{\nu}$, following the convention of the majority of studies in random packings. In Chapters 6 and 7, the default $Re$ is $Re = Re_{p} = \left(\frac{U_{sf}}{\nu}\right)D_{H} = Re_{sf}\frac{1}{\epsilon}$ because: (1) there is a well-defined porosity ($\epsilon$) in the structured packing, (2) the mean velocity is more representative, and (3) $Re_{p}$ is commonly used in the studies in SCP.
Chapter 2 MRI theory

In this chapter, the underlying science of nuclear magnetic resonance (NMR) is first presented before introducing the basic principles of magnetic resonance imaging (MRI). Particular emphasis is given to fast velocity measurement protocols, especially spiral imaging. Only an introduction to the theory and techniques is provided, and more comprehensive treatment of the theory is given by standard texts, e.g., Callaghan (1993), Levitt (2001) and Brown et al. (2014). Finally, compressed sensing theory is briefly discussed.

2.1 Basic principles of NMR

2.1.1 Nuclear spin

Nuclear spin is an intrinsic property of sub-atomic particles, characterised by spin angular momentum. Spin angular momentum is parameterized by the nuclear spin quantum number, I, which is either zero or multiples of ½. There are 2I+1 possible states for a spin and they are degenerate in the absence of an external magnetic field. The energy levels of the states are different in a magnetic field (often referred to as the static magnetic field, \( B_0 \)) and the splitting between nuclear spin levels is known as Zeeman splitting. For example, the hydrogen atom (\(^1\)H) has a spin number I=½ and there exists two different energy levels: the high energy state (\(-½\)), when spins align against the external magnetic field \( B_0 \), and the low energy state (\(+½\)), when spins align with \( B_0 \). A diagram of spin ½ energy splitting is shown in Fig 2.1.

\[
\Delta E = \frac{1}{2\pi} h \gamma B_0
\]

\( I_z = -½ \) high energy state

\( I_z = +½ \) low energy state

**Fig 2.1.** Zeeman splitting for a \(^1\)H atom.

The transition between the two energy states is enabled by absorbing or emitting the energy, \( \Delta E \), provided by electromagnetic radiation:
\[ \Delta E = \frac{1}{2\pi} \hbar \gamma B_0, \tag{2.1} \]

where \( \hbar \) is Planck’s constant \((6.63 \times 10^{-34} \text{ J s})\), \( \gamma \) is the gyromagnetic ratio, \(2.68 \times 10^8 \text{ rad/(Tesla s)}\) for \(^1\text{H}\), and \( B_0 \) is the strength of magnetic field in Tesla. In thermal equilibrium, the population of spins in each state is given by a Boltzmann distribution:

\[ \frac{N_{-1/2}}{N_{1/2}} = \exp \left( - \frac{\Delta E}{k_B T} \right) = \exp \left( - \frac{1}{2\pi} \frac{\hbar \gamma B_0}{k_B T} \right), \tag{2.2} \]

where \( k_B \) is the Boltzmann constant \((1.38 \times 10^{-23} \text{ J/K})\) and \( T \) is the absolute temperature.

### 2.1.1.1 Bloch vector model

The ensemble of spins gives rise to a net magnetisation dipole and this net magnetic moment can be considered to be a vector \( \mathbf{M} \), allowing a simpler description of its motion by classical mechanics:

\[ \frac{d\mathbf{M}}{dt} = \gamma \mathbf{M} \times \mathbf{B}, \tag{2.3} \]

which is known as the Bloch vector model. In a static external magnetic field, Equation 2.3 indicates a gyroscopic precession of the magnetisation vector around the field, and the corresponding angular frequency is called the Larmor frequency, \( \omega_0 \):

\[ \omega_0 = \gamma B_0. \tag{2.4} \]

### 2.1.1.2 Excitation

Because the longitudinal nuclear spin magnetisation is too weak compared to the typical diamagnetism of the sample, most NMR experiments rely on the magnetic moment perpendicular to the magnetic field, called transverse magnetisation, \( M_{xy} \). The spins are perturbed from the thermal equilibrium by applying pulses of electromagnetic radiation, i.e., r.f. pulses, which generates a second magnetic field \( (\mathbf{B}_1) \) oscillating at the Larmor frequency. This oscillating field rotates the magnetisation vector into the transverse plane while the vector precesses at the Larmor frequency simultaneously, as shown in Fig 2.2(b). To isolate the effect of \( \mathbf{B}_1 \) from \( \mathbf{B}_0 \), a rotating frame of reference at the Larmor frequency can be used. In the rotating frame, the effect of the r.f. pulse is isolated as a pure circular motion towards the transverse
plane, around the axis of the induced magnetic field; see Fig 2.2(c). The final rotation angle, $\theta$, i.e., the tip angle, depends on the pulse duration, power, and time-profile shape.

![Fig 2.2. The behaviour of the net magnetisation $\mathbf{M}$ at different magnetic fields and reference frames. (a) In the laboratory frame $\mathbf{M}$ precesses about $\mathbf{B}_0$ at the Larmor frequency. (b) During the application of the r.f. pulse that generates the $\mathbf{B}_1$ field, $\mathbf{M}$ precesses about both $\mathbf{B}_0$ and $\mathbf{B}_1$. (c) The same precession motion in (b) observed in the rotating frame at the Larmor frequency.]

**2.1.1.3 Signal detection**

A 90° pulse rotates $\mathbf{M}_0$ from equilibrium into the transverse plane, and the precession of the transverse magnetisation induces an oscillating electric voltage in the r.f. coil that is directly proportional to $M_{xy}$. In the absence of relaxation effect, the precession can be described as:

$$M_{xy} = M_0 \cos \omega_0 t + i M_0 \sin \omega_0 t = M_0 e^{i \omega_0 t},$$  

(2.5)

where $M_0$ is the bulk magnetisation at thermal equilibrium. In the r.f. receiver the signal is mixed in two separate channels with outputs from reference r.f. oscillators; the signals from the two channels are 90° out of phase from each other. This mixing separates the in-phase and quadrature phase output signals, often referred to as the ‘real’ and ‘imaginary’ part of the signal. This process is known as heterodyning. The heterodyned signal measures only the frequency difference $\Delta \omega$ from the reference frequency (i.e., $\Delta \omega = \omega_0 - \omega_r$), the same as detecting the signal in the rotating frame. Therefore, the NMR signal $S(t)$ in the time domain is:

$$S(t) = M_0 e^{i(\theta_0 + \Delta \omega t)},$$  

(2.6)

where $\theta_0$ is an arbitrary receiver phase. The resonant frequency can be identified by transforming the time-domain signal to the frequency domain via a Fourier transform:

$$S(\omega) = \int_{-\infty}^{\infty} S(t) \exp(i2\pi \omega t) \, dt.$$  

(2.7)

In practice, the signal is sampled digitally with a time delay, $t_d$, between the alternating real and imaginary part of complex data points, and the range of frequency is determined by $t_d$.
according to Nyquist-Shannon sampling theorem. Often, signal averaging over \( n \) repeated experiments is employed to improve the signal-to-noise ratio (SNR), which scales as \( \sqrt{n} \).

### 2.1.2 Relaxation

The process of excited magnetisation returning to equilibrium is called relaxation. There are two relaxation processes occurring simultaneously:

(a) The spin-lattice relaxation is the return of the longitudinal magnetisation \( (M_z) \) to its equilibrium value \( (M_0) \) due to the interaction of molecules (spins) with their environments (lattice). This process is also referred to as longitudinal relaxation and is characterised by the time constant \( T_1 \):

\[
\frac{dM_z}{dt} = - \frac{M_z - M_0}{T_1}.
\]  

(2.8)

(b) The spin-spin relaxation results from the dephasing of transverse magnetisation in the XY-plane because of the variation of the magnetic field experienced by the individual spins. As the spins precess at slightly different Larmor frequencies, they lose phase coherence gradually, resulting in decaying \( M_{xy} \) governed by the time constant \( T_2 \):

\[
\frac{dM_{xy}}{dt} = - \frac{M_{xy}}{T_2}.
\]  

(2.9)

After we integrate the above equation, it can be found that the transverse magnetisation decays exponentially with time:

\[
M_{xy}(t) = M_{xy}(0) \exp \left( - \frac{t}{T_2} \right).
\]  

(2.10)

In reality, \( M_{xy} \) decays faster than the prediction of Equation 2.10 because an extra dephasing is always present due to the inhomogeneity in the static magnetic field. This extra dephasing is characterised by \( T_2^\prime \); both \( T_2 \) and \( T_2^\prime \) contributes to the apparent transverse relaxation constant, \( T_2^* \):

\[
\frac{1}{T_2^*} = \frac{1}{T_2} + \frac{1}{T_2^\prime}.
\]  

(2.11)

The time constant \( T_2^* \) governs the decay rate of the NMR signal, such as in a pulse-acquire experiment, as shown by the decaying signal in Fig 2.3. \( T_2^* \) determines the frequency-domain line width and assuming the peak is approximately a Lorentzian distribution, \( T_2^* \) can be calculated using:

\[
T_2^* = \frac{1}{\pi \cdot \Delta \nu_{\text{FWHM}}},
\]  

(2.12)
where $\Delta v_{\text{FWHM}}$ is the peak width at half of the maximum height of the peak (Fig 2.3), measured in Hz.

![Fourier transform diagram](image)

**Fig 2.3.** The pulse program for a pulse-acquire experiment. The Fourier transform of the pulse-acquire signal yields a frequency spectrum.

The $T_1$ relaxation can be quantified by saturation recovery, which employs only 90° excitation pulses, or inversion recovery, where the magnetisation is first inverted by a 180° pulse, as shown in Fig 2.4. The subsequent 90° pulse returns the longitudinal magnetisation to the XY-plane after some time, $\tau$, and the solution of Equation 2.8 with initial condition $M_z(0) = -M_0$ is:

$$M_z(\tau) = M_0[1 - 2\exp\left(-\frac{\tau}{T_1}\right)].$$  \tag{2.13}

Therefore, $T_1$ can be found via fitting the $M_z(\tau)$ of multiple acquisitions obtained at different values of $\tau$.

![Spin echo diagram](image)

**Fig 2.4.** The inversion-recovery pulse sequence for the measurement of $T_1$.

### 2.1.3 Spin echo

$T_2^*$ can impose challenging short timescales for imaging; thus, the magnetic field homogeneity is first optimised using a secondary ‘shim’ magnetic field. However, it is difficult to render $B_0$ homogeneous, especially for samples consisting of phase interfaces between materials with different susceptibilities. One of the tools to overcome this problem is the spin echo, which was first discovered by Hahn (1950). At a time $\tau$ after the 90° pulse, a 180° refocusing pulse is applied to rotate the magnetisation into the opposite half of the transverse plane. The refocusing pulse reverses the phase offsets but does not affect the precession rate of each spin. From time
τ to 2τ, the magnetic field inhomogeneity acts to rephase the magnetisation, and an echo is produced at \( t = 2\tau \), as demonstrated in Fig 2.5. If the movement of spins is negligible during this time, 2τ, the echo signal intensity obeys the true spin-spin relaxation decay. Spin echo is the basic theory behind the CPMG (Carr-Purcell-Meiboom-Gill) pulse sequence in measuring \( T_2 \) (Carr & Purcell, 1954; Meiboom & Gill, 1958).

![Figure 2.5](image)

**Fig 2.5.** Pulse sequence for the formation of a spin echo and the behaviour of the magnetisation vector during the process. The spins are rotated into the transverse plane by a 90° r.f. pulse and dephase due to the inhomogeneity in \( B_0 \). A 180° r.f. pulse applied after time \( \tau \) refocuses the spins and a spin echo is formed at time 2τ, often referred to as the echo time.

### 2.2 MRI principles

#### 2.2.1 Image encoding and \( k \)-space

In MRI, the locations of the spins are labelled by imposing an additional magnetic field gradient (\( \mathbf{G} \)), and in this work, \( \mathbf{G} \) will be referred to as the gradient. The Larmor frequency of a nuclear spin, \( \omega(\mathbf{r}) \), at a certain position, \( \mathbf{r} \), is determined by the external magnetic field, \( B_0 \), and the imposed gradient, \( \mathbf{G} \):

\[
\omega(\mathbf{r}) = \gamma (B_0 + \mathbf{G} \cdot \mathbf{r}).
\] (2.14)

The NMR signal at time \( t \) from the local element \( dV \) is

\[
dS(\mathbf{G}, t) \propto \rho(\mathbf{r}) \exp[i\omega(\mathbf{r})t] \, dV = \rho(\mathbf{r}) \exp[i\gamma (B_0 + \mathbf{G} \cdot \mathbf{r})t] \, dV,
\] (2.15)

where \( \rho(\mathbf{r}) \) is the spin density function. If the spin-spin relaxation effects are ignored, the signal is proportional to the spin density integrated over the sample and the phase of the spin is given in the rotating frame of reference (at Larmor frequency \( \omega_0 = \gamma B_0 \)):

\[
S(\mathbf{G}, t) \propto \iiint \rho(\mathbf{r}) \exp[i\gamma \mathbf{G} \cdot \mathbf{r}t] \, dV.
\] (2.16)
Mansfield (1973) introduced the concept of $k$-space,

$$k = \frac{\gamma G t}{2\pi}. \quad (2.17)$$

Thus, the relationship in Equation 2.16 can be rewritten as a conjugate Fourier transform pair between $k$ and $r$ (assuming that the constant of proportionality in Equation 2.16 is 1):

$$\begin{align*}
S(k) &= \iiint \rho(r) \exp[i2\pi k \cdot r] \, dr \\
\rho(r) &= \iiint S(k) \exp[-i2\pi k \cdot r] \, dk.
\end{align*} \quad (2.18)$$

Therefore, a map of spin densities $\rho(r)$ can be obtained by Fourier transform of the acquisition signal, $S(k)$. Because $k$-space is the reciprocal of the true space, the field-of-view (FOV) of an image is determined by the spacing between adjacent points in the $k$-space and the image resolution is determined by the width of the $k$-space.

### 2.2.2 Spin-warp imaging

Many pulse sequences can be used to acquire the $k$-space data, and one of the most common methods is the spin-warp technique, first proposed by Edelstein et al. (1980). As shown in Fig 2.6(a), it combines spin echoes with frequency and phase-encodings to traverse through $k$-space in a raster pattern. The sampling of one line in $k$-space is demonstrated in Fig 2.6(b).

![Fig 2.6. (a) The spin-warp imaging pulse sequence with slice selection: The read gradient provides spatial encoding in the $x$-direction, the phase gradient is in the $y$-direction. TE is the echo time and TR is the recycle time, i.e. time for one phase encoding cycle. (b) The corresponding $k$-space raster shows the movement in one phase encoding cycle.](image)
In this example, the phase-encoding direction is along the y-axis, and the frequency-encoding is along the x-axis. A constant gradient in the y-direction is applied for a fixed time to impose dephasing along y, corresponding to a fixed $k_y$, and this gradient is called the phase-encoding gradient, $G_{\text{phase}}$. On the other hand, the frequency-encoding gradient is applied during the acquisition so that $k_x$ varies from $k_{\text{min}}$ to $k_{\text{max}}$; thus, this gradient is termed the read/readout gradient, $G_{\text{read}}$, and x is the read direction. In the subsequent passes, the magnitude of the phase encoding gradient is varied to sample all the lines in $k$-space. The timings of the acquisition and gradients are tuned such that spin-echo is refocused when $k_x = 0$, thus maximising the signal intensity. The signal intensity is governed by $T_2$, often referred to as $T_2$-weighted.

### 2.2.3 Slice selection

To selectively excite spins within a small frequency range, we often use a ‘soft’ pulse with relatively long duration and low power. Because the bandwidth of frequencies in the excitation pulse is inversely proportional to the pulse duration, the ‘soft’ pulse can selectively excite a narrow bandwidth, $\Delta \omega_s$. By applying a gradient (the slice gradient, $G_{\text{slice}}$) simultaneously, as shown in Fig 2.7 (a), the Larmor frequencies of the spins are rendered spatially dependent, enabling the excitation of a specific slice of the sample. For a soft pulse with a narrow bandwidth, $\Delta \omega_s$, the thickness of the slice excited, $\Delta z$, can be calculated by:

$$\Delta z = \Delta \omega_s / \gamma G_{\text{slice}}.$$  \hspace{1cm} (2.19)

Because $G_{\text{slice}}$ also acts as an image encoding gradient, it dephases the magnetisation that exists in the transverse plane, resulting in reduced image intensity. Thus, measures could be taken to rephase the magnetisation, such as the pulse sequences proposed by Pope and Yao (1993). Assuming that the magnetisation reaches the transverse plane half-way through the soft pulse, the second half of the slice gradient acts to dephase the magnetisation and can be balanced by a refocusing gradient. The most common one is that in Fig 2.7 (b), where a gradient in the opposite direction, with half the duration and equal magnitude, is appended to $G_{\text{slice}}$. 
2.3 Flow measurements using MRI

2.3.1 Phase contrast velocity imaging

In addition to obtaining spatial information about the spin density, NMR can also be used to measure coherent molecular motion, also known as magnetic resonance velocimetry (MRV). The first technique to measure the coherent motion is Time-of-Flight imaging, which is limited by low spatial resolution; the phase contrast method is more robust and quantitative (Mantle & Sederman, 2003). The principle of phase contrast imaging is derived considering spins with a constant velocity along the direction of the applied gradient. The phase shift in the rotating frame at Larmor frequency, induced by a constant gradient applied from 0 to \( t \), is:

\[
\zeta(t) = \int_0^t \gamma (\mathbf{G} \cdot \mathbf{r}) dt, \tag{2.20}
\]

If the applied gradient is along the z-axis, the phase is only relevant to the position and motion in the z-axis, which can be expressed by Taylor’s expansion:

\[
r_z(t) = r_{0z} + v_z t + \frac{1}{2} a_z t^2 + \cdots, \tag{2.21}
\]

where \( r_{0z} \) is the location of the spin at \( t = 0 \), \( v_z \) is the velocity and \( a_z \) is the acceleration, all along the z-direction. Thus, the resulting change in phase is:

\[
\zeta(t) = \int_0^t \gamma (\mathbf{G} \cdot \mathbf{r}) dt = \int_0^t \gamma [\mathbf{G} \cdot (r_0 + v_z t + \frac{1}{2} a_z t^2 + \cdots)] dt. \tag{2.22}
\]

Two gradient pulses with the same pulse length (\( \delta \)) and amplitudes, but opposite directions, separated by time, \( \Delta \), are often utilised to measure the velocity, as shown in Fig 2.8. These gradients are called flow/velocity encoding gradients, \( G_{vel} \), and pulsed field gradients (PFGs).
PFG was first proposed by Stejskal and Tanner (1965) to measure diffusion and was first used to measure velocity by Moran (1982).

Assuming the fluid velocity is constant, $v_z = v$ along the direction of the gradient, and self-diffusion is negligible, the result of integrating Equation (2.22) for the bipolar gradient pair is:

$$
\zeta(t) = \int_0^\Delta \omega(t) dt
$$

$$
= \gamma r_0 \left( \int_0^\delta G dt + \int_\Delta^{\Delta+\delta} \gamma (-G) dt \right) + \gamma v \left( \int_0^\delta G dt + \int_\Delta^{\Delta+\delta} (-G) dt \right)
$$

$$
= -\gamma v G \delta \Delta. \tag{2.23}
$$

PFG nullifies the zeroth moment phase shift but imparts a first moment phase shift that is proportional to the velocity. In practice, there are other sources of first moment phase accrual and off-resonance phase change, such as phase accrual due to other gradients and the susceptibility difference. Therefore, two flow images with different $G_{vel}$ are acquired and subtracting the two flow images will remove any phase offset other than the flow-induced phase offset. To remove flow-induced offset, such as those induced by the eddy currents due to velocity encoding gradients (Johns et al., 2000), we usually acquire reference experiments for the static fluid with the same pulse sequences and compute the flow-induced phase offset. Another practical limitation is the phase wrapping when the dynamical range of motion-induced phase change exceeds the effective range from $-\pi$ to $\pi$ rad. For a simple flow field, such as the pipe flow, the phase wrapping can be corrected by adding or subtracting integer multiples of $2\pi$ where appropriate, but this correction is not straightforward for flow in an irregular structure, especially porous media flow. Therefore, the effective dynamic range of $(-\pi, \pi)$ should be fully utilised with prior knowledge about the maximum and minimum velocities in the system, in order to maximise the velocity-to-noise ratio.
2.3.2 Propagator measurement

The same principle can be used to measure the probability distribution of velocity. The signal attenuation can be considered as a superposition of all the spins, weighted with the probability \( P_s(r|\mathbf{r}', \Delta) \) of the spin at \( r \) with respect to its final position \( r' \) over the observation time \( \Delta \) (Callaghan, 1993):

\[
S(G_{vel}) = \int \rho(r) \int P_s(r|\mathbf{r}', \Delta) \exp \left[ i\gamma G_{vel}\delta \cdot (r - \mathbf{r}') \right] \, d\mathbf{r}' \, dr.
\] (2.24)

By representing the displacement as a vector \( \mathbf{R} = r - \mathbf{r}' \), the previous integration can be rewritten as:

\[
S(G_{vel}) = \int \bar{P_s}(\mathbf{R}, \Delta) \exp \left[ i\gamma G_{vel}\delta \cdot \mathbf{R} \right] \, d\mathbf{R},
\] (2.25)

where \( \bar{P_s}(\mathbf{R}, \Delta) \) is the probability distribution of the displacement averaged over the sample over the time scale \( \Delta \). Similar to \( k \)-space, Kärger & Heink (1983) introduced \( q \)-space by defining,

\[
q = \gamma G_{vel}\delta / 2\pi,
\] (2.26)

such that \( q \) and \( \mathbf{R} \) also form a Fourier transform pair:

\[
S(q) = \int \bar{P_s}(\mathbf{R}, \Delta) \exp \left[ i2\pi q \cdot \mathbf{R} \right] \, d\mathbf{R}.
\] (2.27)

\( \bar{P_s}(\mathbf{R}, \Delta) \), known as the propagator, can be obtained by Fourier transform of the \( q \)-space data, \( S(q) \) and a spatially resolved propagator profile can be achieved by combining \( q \)-space with \( k \)-space. The measurement of self-diffusion is similar to a propagator and is based on the theory of Stejskal and Tanner (1965).

2.3.3 Velocity compensation

Following the derivation of (2.23), first moment phase accrual not only arises from velocity encoding gradients but can also be caused by other gradients. In the unsteady flow, the undesirable first moment phase accrual due to other gradients results in artefacts for instantaneous velocity measurements (Callaghan, 1993). Therefore, the first moment phase accrual should be prevented during the design of pulse sequences, and such gradient waveforms are called velocity compensated waveforms. Some examples given by Pope and Yao (1993) are shown in Fig 2.9, where the timing and magnitude of the gradients are tuned to nullify the first moment accrual of the slice gradient. This approach effectively reduces the motion-sensitive artefacts, especially intravoxel phase dispersion but the addition of extra gradients will increase
the sensitivity to the acceleration of fluid flow and elongate the acquisition time (Elkins & Alley, 2007).

![Gradient waveforms for flow compensated (a) slice selective excitation pulse and (b) slice selective refocusing pulse.](image)

**Fig 2.9.** Gradient waveforms for flow compensated (a) slice selective excitation pulse and (b) slice selective refocusing pulse.

### 2.4 Fast imaging

#### 2.4.1 FLASH

One of the earliest fast imaging techniques is the FLASH (Fast Low Angle Shot) sequence developed by Haase *et al.* (1986), as shown in Fig 2.10(a,b). The high temporal resolution is enabled by the low tip angles (5° < θ < 10°), which allows rapid successive excitations given the short recycle time $T_R$ for signal recovery. During the repeated excitation and recovery, the longitudinal magnetisation will reach an equilibrium at:

$$M_z = M_0 \frac{1 - \exp (-T_R/T_1)}{1 - \cos \theta \exp (-T_R/T_1)} \sin \theta. \quad (2.28)$$

Therefore, the pulse angle that gives the optimum SNR, called the Ernst angle, $\theta_E$, can be derived:

$$\cos \theta_E = \exp (-T_R/T_1). \quad (2.29)$$

Because the transverse magnetisation is proportional to $\sin(\theta)$, FLASH suffers from inherently low SNR. As a result, FLASH is often used for low spatial resolution imaging. On the other hand, thanks to the short readout time, FLASH is reasonably insensitive to susceptibility and motion artefacts, but signal contrast is induced by inflow into the imaging slice (Mantle & Sederman, 2003). Velocity imaging using FLASH has been achieved in arterial blood flow by Sakuma *et al.* (1999).
Fig 2.10. Pulse sequences and $k$-space rasters for (a) FLASH, (b) RARE and (c) EPI. The traversing motion in $k$-space due to the corresponding gradient are highlighted with the same colour and line type.
2.4.2 RARE

The Rapid Acquisition with Relaxation Enhancement (RARE) imaging (Hennig et al., 1986) is an extension of spin-warp imaging where multiple lines of $k$-space are acquired from a single excitation. Fig 2.10(c,d) shows the pulse sequence and $k$-space raster for single-shot RARE. The magnetisation is refocused by 180° refocusing pulses, forming a spin-echo, and the number of spin-echoes per excitation is called the RARE factor. Because the pulse offsets due to field inhomogeneity are refocused, the phase artefacts are not cumulative, and the signal decay is $T_2$-weighted instead of $T_2^*$-weighted. As FLASH yields $T_2^*$-weighted signal, RARE is more suited for systems with short $T_2^*$ than FLASH. Although multiple r.f. pulses would generate undesired echoes, it can be overcome by using soft r.f. pulses and homospoil gradients, enabling the spin and stimulated echoes to add coherently.

Although adding a pair of velocity encoding gradients before the imaging module is feasible for measuring the flow fields, RARE is not suitable for high velocity and high acceleration systems. Moreover, it is difficult to preserve the phase shift during the entire RARE sequence as the r.f. field is not perfectly homogeneous. Amar et al. (2010) proposed a new design based on RARE called ‘FLow Imaging Employing Single-Shot ENcoding (FLIESSEN)’, which incorporates independent velocity encoding and decoding before and after each echo. Although the time of the sequence is about 1.5 times the length of RARE, limiting its application to systems with long $T_2$, FLIESSEN demonstrated its advantage in studying flow with high constant acceleration, i.e. vortical motion.

2.4.3 EPI

Echo Planar Imaging (EPI) was first described by Mansfield (Mansfield, 1977) and the simplest and most commonly used type is called blipped-EPI (Elkins & Alley, 2007). The entire $k$-space is acquired after a single excitation in a rectilinear fashion as shown in Fig 2.10(e,f). The read gradient oscillates continuously to refocus the transverse magnetisation into successive gradient echoes and the phase gradient is increased slightly, or “blipped”, after each line, to move to the subsequent line in $k$-space. One major drawback is that the acquired signal is $T_2^*$-weighted so EPI is not suitable in magnetically heterogeneous systems (Mantle & Sederman, 2003). The acquisition time is also constrained by $T_2^*$, resulting in a limited resolution. Moreover, any asymmetry between positive and negative read gradients would result in a ghost image in the phase direction, known as the odd-even echo artefact. It has been widely used to probe the
transient flow phenomenon, both qualitatively (Kose, 1991a, 1992) and quantitatively (Kose, 1991b; Gatenby & Gore, 1996). An EPI based technique called Gradient Echo Velocity and Acceleration Imaging Sequence was proposed by Sederman et al. (2004) and was used to measure instantaneous three-component velocity vectors in turbulent pipe flow.

2.5 Spiral imaging

2.5.1 Principles of spiral imaging

Spiral imaging, first implemented by Ahn et al. (1986), traverses through the $k$-space with a single excitation similar to RARE and EPI. By applying oscillating gradient waveforms in both in-plane directions, the resulting movement in $k$-space, initiating at the centre of $k$-space, spirals out in a circular motion as demonstrated in Fig 2.11(a). This path is often referred to as the $k$-space trajectory. Because the centre of $k$-space is sampled at the beginning of the trajectory, there is the least signal loss and smallest off-resonance phase shift. As a result, the early sampling of the centre of $k$-space improves the SNR and reduces the off-resonance artefacts. Furthermore, as the four quadrants of $k$-space are sampled in an interleaved fashion, the first moment phase shift is refocused periodically; in comparison, the first moment phase shift is accumulated in EPI. Therefore, spiral imaging is more robust to artefacts due to flow, whereas EPI shows significant shear-induced loss of signal intensity (Tayler et al., 2011). Spiral imaging is also more robust to aliasing artefacts due to its capability to oversample the centre of $k$-space (Delattre et al., 2010). On the other hand, spiral imaging is more susceptible to field inhomogeneity because phase offsets are accumulated in both directions. The details and the remedies of the imaging artefacts are given in §2.5.2.

Fig 2.11(b) shows the pulse sequence used to measure the flow field in the XY-plane and two things are worth noting: first the slice gradient in the z-direction is velocity compensated, and second, the velocity encoding gradient is applied simultaneously to minimise the acquisition time. Usually, a $64 \times 64$ image takes about 10-13 ms and a $32 \times 32$ image takes half that time; by harnessing the advancements in compressed sensing, the subsampled spiral achieved an acquisition time of 5.3 ms for a $64 \times 64$ image (Tayler et al., 2012). To track the transient flow phenomena and accommodate such high temporal resolution, the authors used a low tip-angle Gaussian excitation pulse.
**Fig 2.11.** (a) The corresponding $k$-space trajectory. (b) Pulse program for spiral imaging.

### 2.5.2 Spiral imaging artefacts

Blurring and distortions are induced by field inhomogeneities, such as the $B_0$ inhomogeneity, eddy currents, chemical shift effects, and susceptibility difference. Moreover, the actual $k$-space trajectory deviates from the designed trajectory due to gradient imperfections and eddy currents. The knowledge of the exact locations of sampled $k$-space points is necessary for a satisfactory reconstruction of spiral images, which can be derived from magnetic field gradient waveforms measurements. One technique was proposed by Duyn et al. (1998) based on the spin echo imaging sequence. The phase offsets, $\theta$, are acquired in the two read directions separately. After subtracting the reference measurements, the gradient is calculated according to:

\[
\theta = \gamma G t_p z_0,
\]

where $t_p$ is the phase encoding time, and $z_0$ is the distance of the source of signal from the gradient isocentre. A modified method implemented by Tayler (2011) has incorporated a third slice selective pulse to isolate a 3D cube of spins, and this method is more robust to $B_0$ and $B_1$ inhomogeneities. One way method to correct for the field inhomogeneity is the conjugate phase reconstruction where the phase shift, $\zeta(r,k)$, was measured and corrected for, before image reconstruction by the Fourier transform (Nilsson et al., 2015):
The other significant artefact is the in-plane flow artefact. The in-plane motion was shown to cause fringes around the leading edge, a common ringing artefact due to spins moving during readout by Nishimura et al. (1995) and Gatehouse and Firmin (1994). Nishimura et al. (1995) also demonstrated that the in-plane flow artefact was more significant in EPI. The effect of a moving point source can be modelled as a velocity point spread function (PSF) and the resulting image is given by the convolution of the static and velocity PSF. Simulations were conducted to visualise the effect of in-plane motion and the dimensionless velocity is defined as (Tayler, 2011):

$$v^* = \frac{vt_d N_p}{dx},$$  \hspace{1cm} (2.32)

where $t_d$ is the sampling increment time, $N_p$ is the number of pixels in one spatial dimension, and $dx$ is the image resolution. For a point source with constant velocity in the y-direction, the spatial blurring in the x- and y-directions with increasing velocity are summarised in Fig 2.12. The fringing artefact and the misregistration of the signal intensity are more significant in the flow direction, as shown in Fig 2.12 (b). In particular, the maximum intensity is registered incorrectly when the dimensionless velocity exceeds $1.15 \times 10^{-2}$, i.e. when the pixel velocity is higher than 30 cm/s for a $64 \times 64$ image with FOV = 2 cm. The phase offset is proportional to the readout time and it was demonstrated that the subsampled trajectory can minimise this artefact (Tayler et al., 2011).

![Fig 2.12.](image-url) The blurring of PSF as a function of flow velocity integrated in the (a) x-direction and (b) y-direction.
2.5.3 Trajectory design

The spiral trajectory can be best described in a complex plane with polar coordinates as:

\[ k = \lambda \tau^\alpha e^{i \omega \tau}, \]  

(2.33)

where \( \lambda \) is a scale factor for the correct FOV, \( \tau \) is a function of time, \( \alpha \) is the variable density parameter, and \( \omega \) is the radial velocity of the trajectory. The most common spiral scheme is the Archimedean spiral, featuring a linear increase in radial position with constant angular velocity, i.e., \( \alpha = 1 \). The corresponding gradient waveform, \( G(t) \), and gradient slew rates, \( S(t) \), are defined as

\[
\begin{align*}
\frac{G(t)}{2\pi} &= \frac{\dot{k}(t)}{\gamma} = \frac{\dot{\tau}}{\gamma} \frac{dk}{d\tau}, \quad \text{and} \\
\frac{S(t)}{2\pi} &= \frac{\dot{G}(t)}{2\pi} = \frac{\ddot{\tau}}{\gamma} \frac{d^2k}{d\tau^2} + \frac{\dot{\tau}}{\gamma} \frac{dk}{d\tau},
\end{align*}
\]

(2.34)

where \( G(t) = G_x(t) + iG_y(t) \) for the gradient amplitude in the two directions. Duyn et al. (1998) proposed a simple analytical solution for the Archimedean spiral for the slew-rate limited case, which was later extended by Glover et al. (1999) for both the slew-rate and gradient amplitude limited scenarios. There is flexibility to adapt the trajectory design with radially varying density, known as variable density spiral (VDS). Tsai and Nishimura (2000) showed that because the high-frequency components in the \( k \)-space contain little energy, the aliasing artefact can be reduced by oversampling the low-frequency center of the \( k \)-space.

2.5.4 Image reconstruction

Because the sampling points are not located in a rectangular grid, the fast Fourier transform (FFT) algorithm cannot be used, and the category of reconstruction algorithm called non-uniform FFT (NUFFT) must be used instead. Before the inversion, density compensation is necessary to minimise the intensity distortion due to the variation of sampling density. The most flexible and widely-adopted method is the Voronoi diagram, which computes the weighting from the measured trajectory directly (Pauly, 2012). The first class of NUFFT method is the augmented matrix that interpolates the data onto an oversampled rectangular grid and the increased FOV due to the oversampling was later corrected. The most widely used method relies on regridding, which was first introduced by O’Sullivan (1985) for computed tomography. The principle is similar to the augmented matrix, while better-quality interpolation onto the Cartesian grid is achieved by first convolving the data with a kernel function. Jackson
et al. (1991) compared several kernel functions and proposed the optimised Kaiser-Bessel kernel. Fessler and Sutton (2003) proposed an iterative optimization algorithm, the min-max framework for the interpolation step of NUFFT methods, which can be used with different convolution kernels. The reconstruction for VDS subsampled acquisition is particularly challenging due to the strong violation of the Nyquist-Shannon theorem, which can be effectively formulated as a compressed sensing (CS) reconstruction problem. CS was also applied to overcome the chemical shift artefact in a water-oil mixture (Tayler et al., 2014). The principles and algorithms of CS will be introduced next.

2.6 Compressed sensing

As mentioned, compressed sensing (CS) enables the recovery of the spin density map with significantly fewer data points than the fully sampled data. The fully sampled $k$-space follows the Nyquist-Shannon sampling theorem that the highest frequency recovered is half of the sampling frequency of the digital signal, and CS allows us to overcome this limitation while preserving the measurement quality. In this section, the fundamental principles of the CS, its formulation in MRI, and the special treatments regarding the phase information will be introduced. A more comprehensive review of the application of CS in MRI can be found in Lustig et al. (2008) and Sandilya et al. (2017).

2.6.1 Theory

CS is motivated by data compression and relies on the sparsity of the signal. A high $N$-dimensional signal can be represented by a vector $x$ in $\mathbb{R}^N$ and, the projection of the signal onto a $N \times N$ orthonormal basis matrix $\Psi = [\psi_1 | \psi_2 | ... | \psi_N]$ is:

$$x = \sum_{i=1}^{N} u_i \psi_i = \Psi u,$$

where $\psi_i$ are the basis vectors and $u$ is the representation of $x$ in the $\Psi$ domain. By definition, the signal is $S$-sparse if there are $S$ non-zero entries in the vector $u$. Instead of acquiring all $N$ data and compressing the signal $x$ to the smaller size, $S$, as in data compression, compressed sensing aims at acquiring a compressed signal representation in the first place. Without prior knowledge of the data, this sampling pattern is not adaptive and two conditions need to be satisfied for designing a stable measurement matrix $\Phi$. Consider a linear measurement process.
of the original signal, represented by the measurement matrix $\Phi = [\phi_1 | \phi_2 | \ldots | \phi_M]$ that yields a lower-dimensional output $y$ in $\mathbb{R}^M$ ($M < N$), the measurement $y$ is related to $x$ by

$$y = \Phi x = \Phi \Psi u = Au,$$  \hspace{1cm} (2.36)

where $A = \Phi \Psi$. The transform matrix, $A$ must satisfy the restricted isometry property (RIP) condition, which states that for any vector, $v$, sharing the same nonzero entries as $u$ and for some $\delta_S > 0$, the following relationship must be valid

$$(1 - \delta_S) \|v\|_2^2 \leq \|A v\|_2^2 \leq (1 + \delta_S) \|v\|_2^2.$$  \hspace{1cm} (2.37)

In other words, the transform matrix, $A$, preserves the Euclidean length of the particular $S$-sparse vectors, which implies that these vectors cannot be in the null space of $A$. The other requirement is the incoherence of undersampling artefacts, which states that the artefacts in the linear reconstruction due to undersampling should be incoherent (noise-like) in the sparsifying transform domain. The coherence, $\mu$, between the measurement matrix, $\Phi$, and the sparsifying transform matrix, $\Psi$, is defined by the following:

$$\mu(\Phi, \Psi) = \sqrt{N} \max_{1 \leq k \leq N} \left| \langle \phi_k, \psi_j \rangle \right|$$  \hspace{1cm} (2.38)

where $\langle \cdot, \cdot \rangle$ is the inner product. A lower coherence, $\mu$, means fewer sample that can guarantee a perfect reconstruction theoretically (Candès & Wakin, 2008). It has been shown that random matrices are largely incoherent with any fixed representation basis $\Psi$ (Candès et al., 2006).

Given that the sampling pattern satisfies the RIP and is incoherent with the given sparsifying transform, a reconstruction algorithm is needed to recover the sparse signal $u$ from the $M$-dimensional measurement $y$. The most straightforward formulation is an $\ell_0$-minimization, whose solution is numerically unstable; moreover, $\ell_0$-minimization belongs to the Non-deterministic polynomial hardness class in complexity theory. Candès, Romberg and Tao (2006) have shown that the recovery via the following $\ell_1$-minimization is exact with high probability and the formulation is:

$$\hat{u} = \min \|u'\|_1 \text{ s.t. } Au = y,$$  \hspace{1cm} (2.39)

where

$$\|x\|_p = \left( \sum_{i=1}^{N} |x_i|^p \right)^{\frac{1}{p}}$$  \hspace{1cm} (2.40)

is the $\ell_p$ norm. Given noisy measurements, relaxed constraints are applied:
where $\epsilon$ bounds the amount of noise in the data. This formulation can be solved using convex optimization techniques and has been the most popular approach. Overall, there are five major classes of computational algorithms to solve the reconstruction (Tropp & Wright, 2010):

1. Convex relaxation that solves Equation 2.40, such as the least absolute shrinkage and selection operator and Lagrangian multiplier.
2. Greedy pursuit that identifies one or more components of the sparse solution iteratively, such as iterative thresholding and orthogonal matching pursuit.
3. Bayesian method that assumes a prior distribution for the unknown coefficients favouring sparsity.
5. Brute force method.

Convex optimisation and greedy pursuit are the most widely used because they are computationally practical and yield theoretical optimal guarantees under certain conditions. Bayesian methods and nonconvex optimization do not currently offer theoretical guarantees and brute force is only plausible for small-scale problems. The majority of the MRI reconstruction work adopts convex optimisation formulations.

### 2.6.2 CS in MRI

MRI is a significant medical imaging method but the acquisition process is inherently slow and CS has offered significant reduction to MRI, in both medical applications and beyond (Lustig et al., 2008). For MRI, the subsampling is applied in the $k$-space, i.e., the frequency domain, and the natural images are sparse in a certain transform domain, e.g., the medical images are compressible via wavelet transform. Therefore, in the context of MRI, the optimization can be written as:

$$\hat{u} = \arg\min \|u\|_1 \text{ s.t. } \|Au - y\|_2 < \epsilon,$$  

where $u$ is the spin density map, $y$ is the subsampled signal in $k$-space, $\hat{u}$ is some function, called regulariser, which promotes sparsity, and $F$ is a subsampled Fourier transform operator. It could be solved via the following convex optimization problem,

$$\hat{u} = \arg\min \left\{ \frac{1}{2} \|Fu - y\|_2^2 + \alpha f(u) \right\},$$  

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where $\alpha$ is called the regularisation or smoothing parameter. The most common regularisers include the wavelet, total variation (TV) and total generalised variation (TGV). TV is most suitable for piecewise constant images with sharp edges because it promotes the sparsity in the gradient of the image. Isotropic TV, for the image domain with size $n_1 \times n_2$, is defined as:

$$TV(x) = \|\nabla u\|_{2,1} = \sum_{i=1}^{n_1-1} \sum_{j=1}^{n_2-1} \sqrt{|\nabla_1 u(i,j)|^2 + |\nabla_2 u(i,j)|^2},$$  

where $\nabla u$ is the finite difference approximation of the two-dimensional gradient. With zero Neumann boundary conditions, $\nabla u$ is calculated as:

$$\nabla_1 u(i,j) = \begin{cases} u(i+1,j) - u(i,j) & \text{if } i < n_1, \\ 0 & \text{if } i = n_1, \text{ and} \end{cases}$$

$$\nabla_2 u(i,j) = \begin{cases} u(i,j+1) - u(i,j) & \text{if } j < n_2, \\ 0 & \text{if } j = n_1. \end{cases}$$  \tag{2.45}

The first term in Equation 2.43 controls the fidelity of the reconstruction to the measured data and $J(u)$ is the sparsity-promoting term; $\alpha$ balances the two terms. Benning et al. (2014) addressed the challenge to determine the regularisation parameter objectively and showed the effectiveness of Morozov’s discrepancy principle. According to the criterion, the iterative solver should halt when the following is satisfied:

$$\|F u - y\|_2 \leq \sigma \sqrt{M},$$  \tag{2.46}

where $\sigma$ is the standard deviation of the normally distributed noise.

### 2.6.3 CS in MRV

Because the MRV is the major experimental technique used in this thesis, we are particularly interested in how the phase of the complex MRI image affects the performance of CS. The majority of reconstruction algorithms are based on the sparsity of the magnitude image in the transformed domain while in low magnitude regions the phase image can have very low signal-to-noise ratio (Zhao et al., 2012; Benning et al., 2014). Without separating the phase information, thus preserving the convexity of the optimisation problem, Benning et al. (2014) surveyed the performance of different regularisers on their ability to recover phase and magnitude information during CS reconstruction. Stair-casing artefacts are present in the reconstruction using TV, while the total generalised variation (TGV) demonstrated its advantage in recovering the velocity map for the liquid flow in a packed bed because it provides a good compromise between the smooth phase variation and sharp boundaries in the magnitude.
data. The other method to handle the phase information is to reconstruct the real and imaginary intensity images separately and computed the phase afterwards (Holland et al., 2010).

The alternative approach is to exploit the sparsity in the phase image. Fessler and Noll (2004) proposed an iterative algorithm that reconstructs the phase and magnitude separately and a similar approach was applied by Zibetti and De Pierro (2010) to exploit the sparsity in magnitude and the smoothness of the phase. Zhao et al. (2012) pointed out that the previous method could not handle big jumps in wrapped phase maps due to the nonconvexity of the cost function. They compared several different regularisers to overcome the phase-wrapping issue and accommodate rapid changes in phase maps. Most recently, a novel technique to overcome phase-wrapping has been proposed by Ong et al. (2018) called phase cycling, where a different and random phase shift has been applied during each iteration to avoid the accrual of the artefacts due to phase wrapping.

A novel technique based on Bregman-iteration was described in Benning et al. (2016) based on the prior knowledge that (1) the magnitude image does not change for the single phase flow and (2) the velocity distribution is smooth. Given two images $u_1$ and $u_2$, their magnitude images are precomputed as $m_1$ and $m_2$ and phase maps are $\zeta_1$ and $\zeta_2$ respectively. The velocity is represented by the difference of two phase maps; therefore, the regularisation function given the prior knowledge of smooth velocity distribution is $\|\nabla (\zeta_1 - \zeta_2)\|_2$ and the cost function for reconstructing the phase image is:

$$
(\zeta_1, \zeta_2) \in \min \left\{ \frac{1}{2} \| (Fm_1 e^{i\zeta_1} - y_1) + (Fm_2 e^{i\zeta_2} - y_2) \|_2^2 \\
+ \alpha \|\nabla (\zeta_1 - \zeta_2)\|_2 \right\}.
$$

(2.47)

The magnitude image could either be found via a separate CS reconstruction or could be measured by other means.
Chapter 3 Inertial effects in random packed beds of spheres

3.1 Introduction

With the advancement of experimental techniques, pore-scale flow profiles in porous media have become more accessible, which provide significant insight into understanding the fluid dynamics. However, the majority of the studies are in the creeping flow regime, and the transition from the creeping to the inertial regime is not very well understood. In this chapter, the focus is to investigate the flow features in the inertial regime based on three-dimensional (3D) spatially resolved flow fields measured by magnetic resonance velocimetry (MRV). The introduction reviews the relevant literature, organised according to three key flow characteristics in random packed beds: (1) channelling, (2) backflow, and (3) helical vortices.

3.1.1 Flow heterogeneity and channelling

Flow heterogeneity is a widely observed phenomenon, with one of its characteristics being the presence of high axial velocity regions, known as channelling. The strong correlation of channelling with the structure of the packed bed has been revealed by numerous experimental observations. One of the earliest observations is made by Johnston et al. (1975) using laser Doppler anemometry (LDA) on a hexagonal close packing (HCP) arrangement, where channelling was shown at the wall due to inefficient packing. The relationship between high porosity and channelling is further supported by the study of random packings (Giese et al., 1998). The radially-averaged velocity profiles match the porosity profiles for random packings of spheres, deformed spheres, cylinders, and Raschig rings (aspect ratio, N≈10), especially near the wall regions; this effect is more significant for spherical particles. Aspect ratio, N, is the ratio of the column diameter to the particle diameter.

Further insight has been provided by spatially resolved velocity profiles measured by MRV in random sphere packings. Sederman et al. (1997) showed the effect of pore geometry, illustrating that channelling is more exaggerated when the packing is more structured, compared with the other packing of the same aspect ratio (N = 9.2). The relationship between channelling and the local structure was studied by segmenting the cross-section of a packed bed into individual pores using the local minimum hydraulic radius. Sederman et al. (1998) have
quantified that 8% of the pores carry 40% of the volumetric flowrates. Moreover, the pores with high volumetric flowrates were reported to be located towards the exterior of the bed and tend to have larger cross-sectional areas (CSA) and interfacial surface area to adjoining pores.

Besides the experimental evidence, many numerical studies have shown that channelling is most effective at wall due to wall-induced structures (Atmakidis & Kenig, 2009; Eppinger et al., 2011; Khirevich et al., 2012). More accurate prediction of pressure drop can be obtained from correlations taking the wall effect into account in both regular and irregular packings (Atmakidis & Kenig 2009). High-speed channels are characterised by the inertial core as the key phenomenon during the transition from creeping to inertial flow regime (Dybbs & Edwards, 1984) and further quantitative study has revealed that the transition occurs at a local Reynolds number of approximately 30 (Johns et al., 2000).

### 3.1.2 Backflow and recirculating vortices

A number of experimental studies have reported the presence of backflow in packed beds. The amount of counter-current flow has been observed to increase in packed beds of large aspect ratio with increasing Reynolds number \((Re = \frac{U_{st}D_p}{\nu}, U_{st} \) is the superficial velocity, \(D_p \) is the particle diameter, and \(\nu \) is the kinematic viscosity). For example, Kutsovsky et al. (1996) demonstrated the increase in backflow from \(Re = 15, 30 \) to 45, Moroni & Cushman (2001) from \(Re = 0.05 \) to 0.13, and Johns et al. (2000) from \(Re = 3.6, 7.3 \), to 14.5. Various numerical studies using the lattice-Boltzmann method (LBM) (Hill et al., 2001a) and the finite volume method (Magnico, 2003; Eppinger et al., 2011) have made similar predictions. Eppinger et al. (2011) quantified this phenomenon where the volume fraction of cells with zero or negative velocity being 1, 11 to 12.5% at \(Re = 1, 100 \) and 1000 for a random packed bed of spheres of \(N = 8.\)

Using particle imaging velocimetry (PIV) with a refractive index matched system, Khayamyan et al. (2016) showed an increase in the area of backflow region from \(Re = 8 \) to 33. However, there was a slight decrease at \(Re = 100 \) before reaching an asymptote, which contradicts the observation from the previous numerical study.

The mechanism of backflow will be examined next. The region of backflow reported in computational fluid dynamics (CFD) studies are mainly located downstream of the spherical particles (Dixon & Nijemeisland, 2001; Eppinger et al., 2011). Similarly, the study by Dixon et al. (2006) on Raschig ring has observed backflow to be in the wake of an obstruction and at the contact points. These observations can be explained by the separation of the boundary layer,
where the boundary layer separates or breaks away from the solid boundary when the solid surface begins to diverge from the direction of the mean flow. The point where the boundary layer detaches from the solid surface is called a separation point. One of the most widely seen examples of boundary layer separation is the recirculation vortex at the wake of a sphere in an unbounded fluid. In the wake of a sphere, due to the symmetry, the recirculation vortices form a vortex ring structure, whose size grows in proportion to the logarithm of $Re$ (Taneda, 1956).

The flow separation pattern is more complicated in a sphere packing. Based on the visualisation of the velocity pattern on the sphere surface in a face-centered cubic (FCC) packing, Wegner et al. (1971) observed nine reverse flow regions, due to boundary layer separation. The nine regions are close to the contact points of the sphere, consisting of four regions at a polar angle of 45° ($0°$ is defined to be the upstream end of a sphere), four at 90° and one larger region behind the four contact points at 135°. Symmetrical recirculating zones have been predicted in structured packings by numerical studies, including FCC, simple-cubic packing (SCP) and hexagonal close-packed (HCP) structures (Hill et al., 2001a; Hill & Koch, 2002; Gunjal, Ranade, et al., 2005; Finn et al., 2012). The prediction in SCP has been confirmed experimentally (Suekane et al., 2003).

Recirculating flow is observed much less in random packings. For example, in the CFD study by Finn et al. (2012), they reported that there are few if any of the vortex-ring like structures in the $N = 5.96$ random packing with 326 spheres. Based on the LBM simulation in a dilute random packing of spheres at a solid volume fraction of 0.096, Hill et al. (2001) commented that the lack of recirculating flow could be due to the interaction between neighbouring spheres at random locations. Despite the importance of recirculation vortices, experimental evidence of recirculation vortices in random packings is scarce. Hassan & Dominguez-Ontiveros (2008) reported the increased number and size of vortices with pore size using PIV, while only one recirculating vortex was observed.

Moreover, recirculation vortices have been predicted to influence heat and mass transfer in CFD studies. Dalman et al. (1986) simulated flow in a long pipe with two spheres located along the axial axis in the middle of the pipe and noted that the occurrence of stationary eddies at the wake of the sphere accounted for reduced heat transfer. Moreover, the growth of eddy size caused a further decrease in heat transfer. Edwards et al. (1990) related the reduction in the permeability in an array of cylinders with the development of vortices with increasing $Re$. 

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Therefore, the presence and evolution of vortices can be crucial to the operation of heat exchangers and reactors.

3.1.3 Helical vortices

The eddies around the contact points and in the wake of the spherical particle constitute a major contributing factor towards backflow. The other significant vortical motion is the helical vortices and the relevant CFD studies are presented next. We refer to the regions with helical streamlines, where the velocity and vorticity vectors are roughly aligned, as helical vortices. The transverse flow features shown by numerical studies for FCC and SCP packings consist of 4 pairs of counter-rotating helical vortices through the channel (Hill & Koch, 2002; Gunjal, Ranade, et al., 2005; Finn et al., 2012). Finn et al. (2012) examined both the structured and random sphere packings and concluded that the prominent vortical feature is the helical structures that spiral through the pore space in a corkscrew motion. Similarly, eddies with large axial velocity were predicted numerically by Magnico (2003) in a random sphere packing, especially in the inertial regime. Helical vortices are more widely observed in regular packings. Helical vortices are highly relevant to inertial effect given their relevance with flow instability. Hill & Koch (2002) have quantified the helical flow features using the helicity and emphasised the strong influence of the helical vortices at the onset of unsteady flow in packed bed. Additionally, the unsteady features reported by Finn et al. (2012) include the stretching of helical vortices, multiple vortices swirling around each other and the translational motion of the helical core. They commented that the size and mean location of the vortices remained constant.

The only experimental evidence is by Suekane et al. (2003), who measured the flow fields in a single array of SCP unit cells using MRV. Although there is little experimental evidence on the helical vortices in random packed bed structure, stream-wise helical vortices have been widely observed in swirling flow (Alekseenko et al., 1999) and channel flow, such as in a curved pipe (Weston et al., 1998) and bifurcating pipes (Evegren et al., 2010). As a significant secondary flow feature, helical vortices are crucial in naturally occurring flow, e.g., heart valves (Kilner et al., 1993), and industrial configurations, such as heat exchangers (Elkins et al., 2003).

3.1.4 Aims

In summary, there has not been a study on the inertial effect regarding the flow features, which are critical in determining the performance of packed bed reactors. Moreover, there is a lack of experimental evidence on the vortical features in random packing. Therefore, high-resolution
3D velocity measurements are essential for investigating the unknown aspects in porous media flow. The aims of this chapter are the following:

1. To compare different imaging pulse sequences for 3D velocimetry.
2. To characterise the key flow features: channelling, backflow, and helical vortices.
3. To discuss the inertial effect with respect to the flow features.

### 3.2 Experimental method

#### 3.2.1 Flow rig and materials

![Image of experimental setup](image.png)

**Fig 3.1.** The schematic diagram of the experimental setup of the flow loop for MRV.

A flow rig driven by a peristaltic pump (Watson Marlow 505s) was built for flow visualisation experiments. The major part is a glass tube (inner diameter = 16.4 mm) packed with spherical particles, as shown in Fig 3.1. The resulting aspect ratio is 3.44. A plastic porous flat plate was fixed at the bottom of the 1.5 m column to stop the particles from falling. The column was first filled with glass beads of 5 mm diameter, then 4.76 mm diameter Polystyrene plastic spheres within the imaging region, followed by glass beads on the top. The glass beads ensured that the flow pattern being measured in the imaging region is free from entrance effects (Kataoka et al., 1972). Glass beads are used because they are heavier than water and lower-cost compared with polystyrene beads. The material of the packing in the imaging section was chosen to minimise the susceptibility difference required for spiral imaging and will be justified in Chapter 5. The packing should be tapped for close packing during the filling but this has not been done while preparing this packed bed so some beads were loose and shifted positions during the flow. The bead shift was small in range and the majority of the flow field was not affected. This problem
was fixed for the second random packing constructed by tapping the outside of the glass tube to induce a closer packing structure. The volumetric flowrate was tuned using the rotational speed of the peristaltic pump and measured using a graduated cylinder and a stopwatch. Five different readings were taken for each flowrate during the study before and after the full 3D acquisition.

The liquid phase used in the experiments was a 0.27 mM Gd$^{3+}$ solution. This concentration was to balance the effects of relaxation, quantified by the longitudinal relaxation time ($T_1 = 106$ ms) and the signal to noise ratio (SNR), as the signal drops exponentially according to the spin-spin relaxation ($T_2 = 88$ ms). The MRI flow experiments were performed using a Bruker AV 400 NMR spectrometer with a 9.5 T vertical magnet, operating at a $^1$H frequency of 400.25 MHz. The spectrometer was equipped with a three-axis, shielded gradient coil with a maximum gradient strength of 146.15 G/cm. A bird-cage radio-frequency coil of diameter 25 mm was used for excitation and signal reception.

### 3.2.2 Pulse sequence optimisation

![Pulse sequence](image)

**Fig 3.2.** The pulse sequence for 2D velocimetry.

2D velocimetry was measured for XY- and YZ-planes to estimate the maximum flowrate present such that phase wrapping can be avoided for the 3D MRV experiments. 2D velocimetry was performed using the pulse sequence shown in Fig 3.2. A $^1$H 90° pulse of duration 57 μs was used for excitation and a soft 180° pulse with a duration of 512 ms was used to select a 1 mm slice. The timings of the velocity encoding gradients ($\delta$) and the separation ($\Delta$) were varied.
to change the range of velocity measurement for different flowrate and other parameters of the 2D experiments are given in Table 3.1.

In the 3D velocimetry experiments, four 3D images were acquired to obtain the velocity measurements in the three directions z, y, x, which we will refer to as \( u, v, \) and \( w \), the velocity encoding gradients applied were \((0, 0, 0), (0, 0, G_{vel,z}), (0, G_{vel,y}, 0), \) and \((G_{vel,x}, 0, 0)\), respectively. Four different 3D MRV pulse sequences (PP1 to PP4) were tested on a packed bed of glass spheres to optimise the outcome. The first pulse sequence, shown in Fig 3.3, applies the read and phase encoding right before the hard excitation pulse and the time lag between the phase encoding gradients and acquisition time caused significant motion artefacts, as demonstrated in Fig 3.5. The bright and dark patterns stem from phase dispersion due to high shear in the transverse velocity and the region with complete loss of signal may be caused by the wash-out effect resulting from high axial velocity. When the lag between the phase encoding gradients and acquisition was reduced as in PP2 to PP4, the motion artefacts were significantly reduced.

![Fig 3.3. Pulse sequence 1 (PP1) for 3D velocimetry.](image)

The differences between PP2 to PP4 are the velocity encoding, which consists of a pair of gradients with zeroth moment nullified and the first moment proportional to the velocity. In PP2 (Fig 3.4(a)), a pair of gradients with equal length but opposite sign was applied before the hard 180° pulse. Conversely, two gradients with the same signs were applied before and after the refocusing pulse for PP3 and PP4 (Fig 3.4(b,c)). The timing for PP4 was optimized to reduce
the time from excitation to acquisition, resulting in an asymmetrical pair with respect to the refocusing pulse, compared to the symmetrical pair in PP3.

![Pulse sequence diagrams](image)

**Fig 3.4.** (a) Pulse sequence 2 (PP2) for 3D velocimetry. (b,c) Selected part of the pulse sequence 3 (PP3) and the pulse sequence 4 (PP4) for 3D velocimetry (the rest are the same as PP2).

Reference velocity images were acquired with stagnant liquid to correct the phase offset induced by the velocity encoding gradients and eddy currents. The phase difference in the reference images is much higher for PP2 than PP3 and PP4, as shown in Fig 3.6. The maximum velocity encoding gradient therefore applicable to avoid phase wrapping would be much smaller.
for PP2, potentially reducing the sensitivity to velocity by about 30%. The asymmetry in the hardware for generating positive and negative gradients may be the source of such large phase offset. Finally, comparing PP3 and PP4, loss of signal intensity was observed (Fig 3.5) and the flowrates were shown to be overestimated for PP4, as emphasized in Fig 3.7. Therefore, PP3 was selected for the 3D velocimetry measurements and the measurement parameters are summarised in Table 3.1.

![Fig 3.5. Comparison between the images acquired from different 3D MRV pulse sequences.](image)

![Fig 3.6. Comparison between the phase maps measured in the reference experiments across the central XZ slice for PP2, PP3, and PP4.](image)

![Fig 3.7. Comparison between the flowrates measured by different pulse sequences.](image)
### Table 3.1 2D and 3D acquisition parameters for MRV.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>2D MRV</th>
<th>3D MRV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix size (read × phase) [-]</td>
<td>256 × 128</td>
<td>256 × 128 × 128</td>
</tr>
<tr>
<td>Field-of-view (read × phase) [mm]</td>
<td>18 × 18</td>
<td>36 × 18 × 18</td>
</tr>
<tr>
<td>In-plane spatial resolution [µm]</td>
<td>70 × 141 × 1000</td>
<td>141 × 141 × 141</td>
</tr>
<tr>
<td>Spectral width [kHz]</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Read gradient strength [G cm⁻¹]</td>
<td>13.05</td>
<td>6.53</td>
</tr>
<tr>
<td>Maximum phase gradient strength [G cm⁻¹]</td>
<td>5.74</td>
<td>5.94</td>
</tr>
<tr>
<td>δ [ms]</td>
<td>0.2 - 0.5</td>
<td>0.8 - 1</td>
</tr>
<tr>
<td>Δ [ms]</td>
<td>4 - 5</td>
<td>2.5</td>
</tr>
<tr>
<td>TR [ms]</td>
<td>250</td>
<td>150</td>
</tr>
<tr>
<td>Signal averages [-]</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Typical experimental time</td>
<td>2 min</td>
<td>12 h</td>
</tr>
</tbody>
</table>

### 3.3 Data analysis

#### 3.3.1 Packing defect

![Magnitude images of the 3D MRV data for a vertical slice at different flowrates](image)

**Fig 3.8.** Magnitude images of the 3D MRV data for a vertical slice at different flowrates, the magnitude being an arbitrary unit. The FOV is 18.0 × 36.0 mm². The FOV for all the figures are given in the horizontal (x) and vertical (y) axes of the figures as x × y.

It is worth noting that there are two beads that shifted locations with increasing flow, as highlighted in the magnitude image without flow. The upper one shifts up from Re = 29 and the lower one only moves for the highest two flowrates. Because the movement is relatively small, there is negligible influence on the macroscopic statistics and the flow features extracted are also not affected.
3.3.2 Correction of 3D velocimetry

Fig 3.9. The velocity measured in reference experiments at the three middle planes for (a) u and (b) v and the corrected reference velocity for (c) u and (d) v. The FOV are 18.0 × 18.0 mm² for XY slices and 18.0 × 36.0 mm² for XZ and YZ slices.

Fig 3.9 demonstrates the correction of phase offsets using the reference experiments acquired with stagnant liquid. Linear dependencies in all three directions can be observed for u and v, as shown in Fig 3.9(a,b); however, the reference velocity is only dependent on the slice direction for w. A correction velocity map was computed by first taking into account the linear dependency in z, then adding the correction in x and y-directions by fitting a function $f(x, y) =$
The corrected velocity of the reference experiments are shown in Fig 3.9(c,d), where the spatial dependency has been removed.

### 3.3.3 Binary gating

A binary map differentiating the fluid region and the packing structure is needed for further data analysis and generating the geometry for CFD simulation. When the pixel is located at the solid/liquid boundary, the image intensity of the pixel is between that of noise and fully occupied by water, known as the partial volume effect. A threshold has been chosen based on the distribution of image intensity at each slice, as shown in Fig 3.10(a). The signal intensity for liquid pixels is Gaussian distributed and the noise intensity obeys a Rayleigh distribution. The two distributions were fitted to the pixels with high signal intensity (higher than half of the maximum signal present) and the pixels outside the tube, as demonstrated in Fig 3.10(b).

Assuming the noise has a threshold $I_N = \mu_N + 3\sigma_N$ and the signal is characterised by a lower bound $I_S = \mu_S - 3\sigma_S$, a reasonable threshold to differentiate the two types of signal is $\frac{I_N + I_S}{2}$.

---

**Fig 3.10.** (a) Signal distribution and the fitting used to select the threshold for slice 100 of the MRI image. (b) Demonstration of the input data for the fitting. The FOV is $18.0 \times 18.0 \text{ mm}^2$. 

$ax + by + c$ to the data.
Fig 3.11. Demonstration of the different types of pixels: black pixels are at the edge and gray pixels are fully occupied with liquid. The FOV is $18.0 \times 9.0 \text{ mm}^2$.

The error in the velocity measurements can be evaluated from the reference measurements with stagnant liquid. To evaluate the partial volume effects on the phase data, errors were also evaluated for pixels at the edge and those occupied fully with liquid, as demonstrated in Fig 3.11. As can be seen from Table 3.2 that there is negligible difference between the fully and partially filled pixels for the first reference experiments, whereas slightly higher noise level is observed in the pixels at the edge for the second group.

<table>
<thead>
<tr>
<th></th>
<th>Ref 1, $u$</th>
<th>Ref 1, $v$</th>
<th>Ref 1, $w$</th>
<th>Ref 2, $u$</th>
<th>Ref 2, $v$</th>
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<td>0.126</td>
<td>0.242</td>
<td>0.317</td>
<td>0.456</td>
<td>0.662</td>
</tr>
<tr>
<td>Liquid</td>
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<td>0.126</td>
<td>0.248</td>
<td>0.289</td>
<td>0.315</td>
<td>0.575</td>
</tr>
</tbody>
</table>

### 3.3.4 Streamline visualisation

The streamlines are visualised using MATLAB’s built-in function ‘streamline’ and the inputs include the 3D velocity fields, the corresponding Cartesian coordinates, and the starting points. The streamlines are computed by integration using a step size of $1/10^{th}$ of the length-scale of the 3D cell. The velocity fields between the grid points are approximated by linear interpolation. Two types of streamline plots are shown, one is rendered with the same colour and the other is rendered with varying colour according to the magnitude of the velocity.

### 3.4 Results

In this chapter, all the velocities are normalised with respect to the superficial velocity $U_{sf} = Q/A$ unless otherwise stated.
3.4.1 Velocity distribution

The probability distribution functions (PDFs) are shown in Fig 3.12 and the transverse velocity distribution is represented by $u$ as the distribution in $v$ is nearly identical. The PDF for the transverse velocity is symmetrical, and the average transverse velocity becomes higher with increasing $Re$. There is more contrast in the axial velocity: the backflow velocity also increases and the stagnant area decreases significantly with higher $Re$, accompanied by a more homogeneous distribution. Both the positive axial velocity and the transverse velocity in positive and negative directions show an exponential decay, as highlighted in Fig 3.12(c,d).

![Fig 3.12. PDFs for the normalised (a) the transverse velocity $u$ and (b) the axial velocity $w$ for $Re = 29, 60$ and $115$. (c,d) are the equivalents in log scale.](image-url)
3.4.2 Channelling and inertial core

![Graph](image)

**Fig 3.13.** Radial distributions of the axially and azimuthally-averaged axial velocity $w$ for $Re = 29$ to 145.

Fig 3.13 shows the axially and azimuthally averaged axial velocity profile, which has been most widely used for quantifying flow heterogeneity and the wall effect. The first velocity maximum is located at $0.1 \, D_p$ and the second one about $1.1 \, D_p$ from the wall. Furthermore, the profiles are nearly identical with increasing $Re$.

The channelling behaviour can be examined in more detail at the two transverse planes and the axial plane YZ, shown in Fig 3.14. The channelling occurs at either the voids close to the wall or within $0.1 \, D_p$ from the wall, which is consistent with the radial velocity distribution. The higher axial velocity at $1.1 \, D_p$ can be attributed to the presence of large voids as demonstrated in the YZ-plane (Fig 3.14(c)), which results from wall-induced packing structure of the first layer of particles besides the wall. Comparing the velocity profiles for increasing $Re$, the maximum normalised velocity of the major channels decreases and the distribution of axial velocity becomes more even, which is consistent with the development of inertial core. The shapes of the channelling flow are more irregular due to the interaction of helical vortices with the high-velocity channel. This interaction is demonstrated in Fig 3.15 for the bottom channel at $Z = -6.75 \, mm$ (highlighted by the red square in Fig 3.14(a)). The channelling is reduced due to the development of the counter-rotating vortices at the centre of the inertial core.
**Fig 3.14.** Contour maps of normalised axial velocity at the transverse planes (a) $Z = -6.8$ mm (b) $Z = 0.0$ mm and the axial plane YZ at the centre for $Re = 29$ to 145. The FOV is $16.6 \times 16.6$ mm$^2$ for (a,b) and The FOV is $18.0 \times 30.0$ mm$^2$ for (c).

**Fig 3.15.** Normalised axial velocity (colour scale) and transverse velocity vector (arrows) plots for $Re = 29$ to 145 at the bottom pore at $Z = -6.8$ mm, highlighted by the red square in Fig 3.14(a). The FOV is $4.1 \times 3.9$ mm$^2$.

A case study of a converging-diverging flow channel formed by two adjacent spheres and the wall has been conducted. Fig 3.16 shows the evolution of the axial velocity distribution across the flow channel for different $Re$. The acceleration due to the converging section is
demonstrated, in particular the acceleration extends to the diverging section of the pore from $Z = 0.4$ mm.

![Contour maps of normalised axial velocity](image)

**Fig 3.16.** Contour maps of normalised axial velocity for a converging-diverging pore at $Z = -0.2$ to 2.6 mm for $Re = 29$ to 115. The position in the title is measured in mm and the convention is followed in the rest of the chapter. The FOV is $4.6 \times 4.2$ mm$^2$.

This acceleration is quantified by the peak velocity in the inertial core, which is computed as an average of 16 pixels containing highest velocities within the region. The evolution of the peak velocity, along the area of pore, is shown in **Fig 3.17**. At $Re = 29$, the peak velocity reaches a maximum at $Z = 1$ mm, slightly downstream of the pore neck (location with minimum area) and the peak velocity decreases as the channel expands further. For higher $Re$, the axial velocity reaches the maximum further downstream and no decreasing trend is seen.

![Normalised peak axial velocity profiles](image)

**Fig 3.17.** Normalised peak axial velocity profiles within the inertial core shown in **Fig 3.16** from -0.7 to 2.6 mm for $Re = 29$ to 145. The number of pixels in the pore at different axial locations is shown by the black-dotted line.

The velocity distribution across the channel has been examined in **Fig 3.18** at $Re = 29$ and 115 at four different axial positions, including the one-dimensional profile along the red lines. The
velocity maxima for different positions confirmed that the peak velocity is further downstream of the pore neck for $Re = 115$. Furthermore, the transition from the parabolic to top-hat shape can be observed for higher $Re$, which is consistent with the inertial core characteristics.

Fig 3.18. Normalised axial velocity (colour scale) and transverse velocity vector (arrows) plots for $Re = (a) 29$ and (c) 115 at the converging-diverging pore at $Z = 0.4, 0.9, 1.5$, and $2.0$ mm. The FOV is $4.6 \times 4.2$ mm$^2$. Normalised axial velocity profiles along the highlighted line are shown for $Re = (b) 29$ and (d) 115.
3.4.3 Backflow and recirculation vortices

![Fig 3.19](image)

**Fig 3.19.** Normalised vorticity (colour scale) and transverse velocity vector (arrows) plots for (a, b) the two axial slices for $Re = 115$. The highlighted red and green rectangle are shown in (c) and (d), respectively; (e) shows a close-up view of the red rectangle in (b). The FOV are (a) $18.0 \times 18.0$ mm$^2$, (b) $18.0 \times 16.9$ mm$^2$, (c) $2.0 \times 1.8$ mm$^2$, (d) $2.5 \times 1.8$ mm$^2$, and (e) $4.5 \times 3.7$ mm$^2$.

To study the evolution of recirculation vortices, the recirculation vortices highlighted in Fig 3.19(a,b) are examined. The recirculating vortices in Fig 3.19(c,d) are similar to those shown by Hill *et al.* (2001b) in the wake of the contact points. There is no apparent vortical motion at $Re = 29$ in Fig 3.19(c), and, with increasing $Re$, the vortices become tighter and stronger given the increasing normalised vorticity. From $Re = 115$ to 145, the vortex in Fig 3.19(d) become smaller in size. Larger recirculation regions have also been identified and one example is shown
in Fig 3.19(e). From \( Re = 29 \) to 60, the recirculating vortex grows in size and the backflow becomes stronger. For \( Re = 115 \) and 145, strongest vorticity is observed at the edge of the region instead of the core of the vortices which occurs at lower \( Re \) and the entire pore is occupied by the recirculation vortex.

Further information is derived from the 3D visualisation of the streamlines. An example is given for a large recirculating region in Fig 3.20. At \( Re = 29 \), there are only small recirculation vortices, as shown by the blue streamlines at \( Z = 3.3 \) mm in Fig 3.20(a). The backflow induced by the downstream sphere is relatively weak, as indicated by the red streamlines at \( Z = 2.5 \) and 2.6 mm. However, at \( Re = 145 \), the blue streamlines originating from the centre of the recirculating region, at \( Z = 3.3 \) mm in Fig 3.20(b), indicate the presence of a tight vortex core. Further downstream, the blue streamlines travel around the edge of the recirculation cell, which almost spans the entire pore. This expansion of the recirculation region is similar to the scenario shown in Fig 3.19(e).

**Fig 3.20.** The streamlines originated at different axial positions (the red is more upstream than the blue ones) for (a) \( Re = 29 \) and (b) \( Re = 145 \). The FOV is \( 5.2 \times 4.1 \times 4.4 \) mm\(^3\).

### 3.4.4 Helical vortices

Fig 3.21 demonstrates the evolution of a typical helical vortex at a wall-bounded pore. The swirling motion is negligible at \( Re = 29 \) and 60, and the axial velocity is dominant. Strong swirling motion is observed for \( Re = 115 \) and 145, especially at the entrance to the pore because of the momentum influx from the side jet formed at the edge of the pore. As suggested by the wider span of the vortical streamline, the size of the vortex increases at \( Re = 145 \) compared to \( Re = 115 \).
**Fig 3.21.** The streamlines for a helical vortex in a wall-bounded pore for $Re = 29$ to 145. The streamlines are coloured by the velocity magnitude. The FOV is $3.7 \times 4.4 \times 5.1$ mm$^3$.

For flow within larger voids, especially at the centre of the packing, multiple helical vortices can be observed for $Re = 115$ and 145, where a stronger helical vortex is often accompanied by a weaker vortex adjacent to it. Two pairs of counter-rotating vortices are visualised Fig 3.22 and the vortex with stronger radial motion is in red while the weaker one is in blue. In Fig 3.22(a), the vortical motion is not observed for $Re = 29$ and is very weak at $Re = 60$. Similar to that shown in Fig 3.21, the strong vorticity is present at $Re \geq 115$, especially at pore entrance in Fig 3.22(b). In both examples, the streamlines from the weaker vortex join the stronger helical vortex, which might be due to the interactions of the two vortices or the two vortices merging.

**Fig 3.22.** The streamlines of two counter-rotating vortices for $Re = 29$ to 145. The FOV are (a) $6.6 \times 6.5 \times 7.9$ mm$^3$ and (b) $5.3 \times 7.0 \times 7.2$ mm$^3$. 
The evolution of a helical vortex in the axial direction is shown in Fig 3.23 and its formation is due to the high momentum side jets at the corners of the pore, as a result of converging pore geometry. The vorticity increases with angular momentum accumulation along the converging pore from \( Z = -1.5 \) to 0.2 mm and decreases in the diverging section. The major difference is the strength of the helical vortex: at \( Re = 60 \), the maximum normalised vorticity is about 40 while it exceeds 80 at \( Re = 115 \). Furthermore, at \( Z = 1.6 \) mm, the helical vortex cannot be seen at \( Re = 60 \) while it is still notable at \( Re = 115 \). The stronger vorticity and slower decay are due to the inertial effect being dominant at higher \( Re \) while the viscous force induces the decay of vorticity.

**Fig 3.23.** Normalised vorticity (colour scale) and transverse velocity vector (arrows) plots for a wall-bounded helical vortex at different axial positions for (a) \( Re = 60 \) and (b) \( Re = 115 \). The FOV is 3.0 × 2.4 mm².

### 3.5 Discussion

#### 3.5.1 Velocity distribution

The exponential decay of the population density for the positive part of the axial velocity has been observed in a number of experimental studies: Kutsovsky *et al.* (1996) at \( Re = 14.9, 29.9, \) and 44.8, Johns *et al.* (2000) at \( Re = 0.84-14.52, \) Moroni & Cushman (2001) at \( Re = 0.05-0.13, \)
and Sederman & Gladden (2001a) at $Re = 2.8$. Sederman & Gladden (2001a) further showed that the positive and negative number densities for the transverse velocities also decay exponentially. Similarly, in the inertial regime examined here, the exponential decays in the positive axial velocity and transverse velocities have been demonstrated in Fig 3.12(c,d).

In the LBM simulation by Reynolds et al. (2000), the exponential decay was predicted in the number density of the kinetic energy, $E = (u^2 + v^2 + w^2)/2$. The same relationship was examined in a random 2D porous media using finite difference numerical methods by Andrade et al. (1997) in the creeping ($Re = 0.0156, 0.156, and 1.56$) and inertial ($Re = 156$) regimes. On the plot of $\log(n(E/E_{max}))$ versus $\ln(E)$, where $n(E/E_{max})$ is the number density at normalised kinetic energy $E/E_{max}$, a gradient of $0.90 \pm 0.03$ is consistently observed at the creeping flow regime but the equivalent is $0.79 \pm 0.03$ for the inertial one (Andrade et al., 1997). The authors accounted the difference to the dramatic change of direction and magnitude of the mainstream velocity at the highest $Re$. The decreased gradient with increasing $Re$ predicted by Andrade et al. (1997) is validated in Fig 3.12(d), which shows that the gradients for all velocity components decrease with $Re$. In the same figure, there is a deviation from the linear trend in the axial velocity at $Re = 115$, which needs further investigation due to the lack of theoretical support and similar observations.

### 3.5.2 Channelling and inertial core

The wall effect on the channelling phenomena is highly consistent with the previous studies. Eppinger et al. (2011) examined packings with $N = 5, 6, 7$, and $8$, and observed the first velocity maximum ($\sim 3U_{sf}$) at about $0.25D_p$ and second maximum ($\sim 1.5U_{sf}$) at $D_p$. For two axial locations in the random packing with $N = 5$, the two maxima closest to the wall were shown to be at $0.25D_p$ and $1.25D_p$ by Atmakidis & Kenig (2009). Very similar features have been shown in other experimental (Giese et al., 1998) and numerical studies (Augier et al., 2010; Khirevich et al., 2012) for random sphere packings. The locations of channelling shown in Fig 3.13 are similar to literature results, but the magnitude of the axial velocity at the second maximum is different compared to the higher N packings observed previously. In literature, the second maximum is about half of the one at the wall because the internal packing is more disordered compared to the wall layer. In contrast, in this study, the ordering is enhanced locally, resulting in even higher channelling velocities. This evidence further reinforces the sensitivity of the flow maldistribution to the morphological features of the packing structure.
Therefore, care must be taken while using phenomenological models for narrow packing structures, such as pressure drop correlations.

The evolution of the inertial core in the converging-diverging pore will be compared with the behaviour of the central jet in SCP (Suekane et al., 2003), where the Reynold number is given by \( \text{Re}_{\text{int}} = \frac{U_{\text{int}} D_p}{v} \) (\( U_{\text{int}} \) is the interstitial velocity). At the lowest \( \text{Re}_{\text{int}} = 12.17 \), there is periodic variation of the peak velocity along the axial direction whilst the maximum velocity does not vary at different CSA for the highest \( \text{Re}_{\text{int}} \) (204.74). Regarding the location of the peak velocity, with increased inertia effect, the velocity reaches a maximum at a point further downstream of the pore neck for \( \text{Re}_{\text{int}} \geq 12.17 \). The evolution of maximum velocity in the inertial core in this study follows the same trend, as shown in Fig 3.17: (1) At \( \text{Re} = 29 \), the maximum is observed at the pore neck, after which a decreasing trend is observed; (2) At \( \text{Re} > 29 \), the maxima occur further downstream and persist along the inertial core.

There is one discrepancy regarding the inertial core profile in the literature. Parabolic profiles were observed at all \( \text{Re}_{\text{int}} \) in SCP (Suekane et al., 2003) but Johns et al. (2000) identified that the axial velocity featured a top-hat shape when the local \( \text{Re} \) exceeded a threshold. It was explained by Suekane et al. (2003) that a parabolic profile was developed in SCP as the inertial core penetrated through the pore without changing direction. They proposed that the inertial effect is more significant in a random packed bed because of the tortuosity. The proposal by Suekane et al. (2003) that the flattening of velocity profile stems from the development of boundary the layer thickness, \( \delta \), is supported by theory. We can approximate the development of \( \delta \) using the derivation by Blasius (Blasius, 1907):

\[
\delta \propto \frac{x}{\sqrt{\text{Re}}} = \frac{\sqrt{vx}}{u_0},
\]

(3.1)

where \( x \) is the position from the initiation of boundary layer and \( u_0 \) is the far field velocity. The equation justifies that with higher \( \text{Re} \), i.e., increased \( u_0 \), the distance from the initiation, \( x \), will increase for a full parabolic profile to develop (\( \delta \approx 1/2 \) the pore size) in a pore. This is the same phenomenon as the inertia effect at the pipe entrance, which results in a longer entrance length with increasing \( \text{Re} \).

In the random packing examined, parabolic profiles can persist in inertial cores while the transition from a parabolic profile to a top-hat one is also observed, such as in the converging-diverging pore (Fig 3.18). In the infrequent scenarios where the high-velocity channel spans a
longer axial span, a parabolic profile can persist in the inertial flow regime, although it takes longer to develop at higher $Re$. Therefore, it can be concluded that the inertial core is determined not only by the local $Re$, but also by the topology of the pore.

3.5.3 Vortical motion

The porescale velocity profiles in this work suggest that the underlying mechanism of the increased backflow at higher $Re$, reported in the majority of the literature, is the expansion and strengthening of the recirculation vortices. This phenomenon has been shown experimentally in the vortex ring downstream of the sphere (Taneda, 1956), and numerically between two spheres (Dalman et al., 1986), and in a converging-diverging channel (Chaudhary et al., 2011). Using CFD, Chaudhary et al. (2011) proposed that the reason for the growth of vortices to be the increased inertia force surpassing surrounding pressure force. After a critical point, this growth was shown to slow down due to the limiting pore boundary and increased pressure from the bulk flow. A similar trend is shown in Fig 3.19(d), where the size of the recirculation vortex grows from $Re = 29$ to 115 and then plateaus afterwards. Following the speculation by Chaudhary et al. (2011), the decreased vortex size from $Re = 60$ to 145 in Fig 3.19(c) may be caused by the increased pressure from the bulk flow. Besides recirculation at the contact points, large recirculation cells also exist in random packing and their influence on the heat and mass transfer in random packing is worth investigating.

Given that helical vortex is characteristic of random sphere packing, some insights can be drawn from their influence on the heat and mass transfer from the literature. Although most studies are on turbulent flow, the analysis is still useful because: (1) the helical vortex at steady state is a backbone of the secondary turbulent flow feature, such as the Dean vortices in a curved pipe (Kalpakli & Örlü, 2013) and vortices in a square duct (Owolabi et al., 2016), (2) the influence of heat and mass transfer due to the flow topology could be extrapolated to the laminar regime. Helical vortices were introduced in cylindrical rod bundles by inserting vanes. Here, the swirling flow enhances heat transfer (Yao et al., 1982; Holloway et al., 2004), which is useful for nuclear fuel bundle design. However, care should be taken while designing the swirling flow because two types of helical vortices exist: the left-handed vortices with wake-like velocity profiles increase heat and mass transfer whereas the right-handed ones with jet-like profiles are less efficient, even detrimental (Martemianov & Okulov, 2002, 2004). In this study, the helical vortices are likely to be left-handed, thus improving the heat transfer. The reasons for this speculation are: (i) there is slight backflow where the helical vortices form and (ii) the axial
velocity at the wall is enhanced due to the presence of helical vortex; both phenomena are the characteristic features of the left-handed vortices.

To summarise, the inertial effect has important implications on the heat and mass transfer. Thus, the correct prediction of the detailed flow features under a strong inertial effect is useful for designing packed bed reactors or heat exchangers.

3.6 Conclusions

In this chapter, the inertial effect in porous media has been analysed based on 3D flow visualisation using MRV. Different designs of 3D velocimetry pulse sequences have been tested and validated with mass conservation. The inertial effects have been demonstrated by the key flow characteristics:

1) Channelling due to the wall-induced packing has been observed. The development of the inertial core, characterised by the transition from the parabolic to top-hat velocity profile, was shown to be determined by both the inertial effect and the pore topology.

2) A catalogue of vortical features were visualised in 2D and 3D. The evolutions of the recirculation vortices have been analysed and the large recirculation zones have been reported in a random packing for the first time.

3) The helical vortices predicted by simulations were shown experimentally and the swirling motion was most prominent at relatively high $Re$ in the inertial regime.

The flow features are not only important in understanding the inertial effect, but also critical for the performance of packed bed reactors. With the increased dependency on simulations for reactor design and optimisation, it is crucial that the detailed flow features are reproduced with reasonable accuracy. In next chapter, the results will be used to validate a computational fluid dynamics model.
Chapter 4 Validation of computational fluid dynamics in random packed beds of spheres

4.1 Introduction

Computational Fluid Dynamics (CFD) is becoming increasingly important as a standard tool for analysing chemically-reacting flows and the methods for multiphase reactors, e.g., packed bed reactors, are under active development (Dixon et al., 2006; Y. Wang et al., 2013). Experimental validations of CFD models are crucial, especially for the accurate prediction of pore-scale flow features. In this chapter, the pipeline for the direct comparison between numerical and experimental data is introduced, with a focus on validating the prediction of macroscopic and pore-scale flow fields. In this section, different modelling strategies are briefly introduced, followed by a detailed description of the pore-scale modelling methods. The validation studies are reviewed, and, finally, the literature related to image-based meshing are discussed.

4.1.1 CFD methods

4.1.1.1 CFD overview in packed bed reactors

Fig 4.1. (a) Demonstration of the mesh in the effective porous medium approach, where the domain is modelled as blocks with varying porosity (Jiang et al., 2000). (b) Surface mesh used in a discrete particle approach study, where the true geometry is explicitly meshed (Dixon & Nijemeisland, 2001).

Strategies of modelling single-phase flows in packed bed reactors vary from simple empirical correlations to complete direct numerical simulations. For decades, chemical engineers have relied on empirical or semi-empirical correlations, such as the Ergun equation, which correlates
the pressure drop with the geometry and operating condition of a packed bed, assuming a homogeneous flow field. The homogeneity assumption is inherently flawed, and the effective porous medium approach was proposed in order to improve the modelling. In this approach, the bed is treated as a macroscopically inhomogeneous medium, as shown in Fig 4.1 (a). For single phase flow, the bed is treated as being composed of two phases, each with its own set of effective parameters as well as interphase coefficients. The bed is often generated using empirical correlations that describe the radial porosity distribution (Jiang et al., 2000; Gunjal, Kashid, et al., 2005; Y. Wang et al., 2013). However, such approaches rely on lumped parameters, e.g., for dispersion or heat transfer, and do not consider the accurate reproduction of the internal flow field.

The discrete particle approach models interstitial flow by taking into account the packing structure and has gained popularity with the advancement of computing power (Dixon & Nijemeisland 2001; Dixon et al. 2007). For example, the packing geometry was resolved explicitly by Dixon & Nijemeisland (2001), as shown in Fig 4.1 (b). In this strategy, the relationship between the bed geometry and the flow field can be directly interpreted. Discrete particle simulations have also been used to derive macroscopic correlations. Moreover, such models extend the ability to simulate heat and mass transfer, which are difficult or impractical to measure experimentally. However, the geometric modelling and mesh generation are cumbersome, and a significant computational cost is required (Y. Wang et al., 2013).

4.1.1.2 Pore-scale modelling methods

The validation pipeline in this study is applicable to CFD methods that can resolve pore-scale features; therefore, the details of such methods are examined next, and some representative works and reviews are highlighted for interested readers. The major pore-scale modelling methods include the lattice-Boltzmann method (LBM), conventional CFD methods, smoothed particle hydrodynamics (SPH) methods, and pore-network models (PNMs). The first three belong to the first class, as summarised by Yang et al. (2016), “that explicitly models the three-dimensional geometry of pore spaces”, while the second class consists of PNMs that “conceptualise the pore space as a topologically consistent set of stylized pore bodies and pore throats”.

LBMs evolved from lattice-gas models, a type of cellular automaton, which simulate how the fluid particles interact with each other while propagating through a regular lattice. The most popular collision rule is the single relaxation time Bhatnagar-Gross-Krook approximation.
LBM is advantageous because of its relative simplicity and suitability for parallelisation, but it is computationally inefficient. Modified LBM developed to tackle the broad pore size distribution challenge are highlighted by Bultreys et al. (2016). LBM is the earliest pore-scale CFD model and one of the first validated studies was Maier et al. (1998) using MRI propagator experiments in a random sphere packing. However, direct validation cannot be achieved by matching the aspect ratio and the porosity with the experiments. This challenge is addressed in the novel work by Manz et al. (1999), who conducted LBM on the same packing used in MRI experiments. A series of studies of three-dimensional (3D) LBM simulations in sphere packings was conducted by Hill et al. (Hill et al., 2001b, 2001a; Hill & Koch, 2002), who systematically examined the change of drag force with the increase in porosity and Reynolds number \((Re)\). Their studies also demonstrated the evolution of flow features with increased inertial effect. More recently, Rong et al. (2013, 2014) carried out systematic studies on the correlation of drag force with porosity for spheres of the same size and particle size distribution in random sphere packing.

Conventional CFD models, which numerically solve the Navier-Stokes equation via discretisation on a structured/unstructured mesh, are the most widely used for single-phase flow in porous media. The finite volume method is the most popular approach, which utilises the integral form of the governing equation that guarantees global conservation for an unstructured mesh. Mature commercial packages and open source solvers are readily available but the generation of high-quality meshes for packed beds, in particular at particle contact points, can be cumbersome. The mesh-related disadvantages can be addressed by the immersed-boundary/fictitious domain approaches, which solve the flow fields on a structured Cartesian grid that spans the entire region, including the solid and fluid phase. It was shown by Finn & Apte (2013) that the fictitious domain approach converged faster and achieved a better solution than finite volume method on an unstructured mesh. This method was further validated using PIV experiments in a random sphere packing (Patil et al., 2014; Wood et al., 2015).

SPH is a Lagrangian mesh-free particle-based method that does not require explicit interface tracking; thus, SPH is particularly suitable for applications with moving interfaces, such as multiphase flows. The complex geometry is easily modelled as in LBM, and SPH directly solves discretised forms of Navier-Stokes equations, like conventional CFD models. This method is computationally demanding (Bultreys et al., 2016), though the computing time can be alleviated by parallel computing (Tartakovsky et al., 2007). One challenge is that SPH becomes impractical for fluid with very low compressibility, but the moving-particle semi-
implicit (MPS) method could overcome the issue (Meakin & Tartakovsky, 2009). Tartakovsky et al. (2016) provided detailed descriptions of the SPH methods and reviewed the applications to pore-scale modelling.

Finally, PNM is an important class of mesoscale models that represent a complex pore space by a network of pore bodies and pore throats with idealised geometry and solve the flow equations on the network elements. The most popular PNM, the mixed-cell method, can be interpreted as a low-order, finite-volume method, where each pore is a homogeneous unit cell. Since the 1990s, extracting network models directly from 3D images has enabled more realistic network models and PNMs have been successfully applied to various complicated scenarios, including nonlinearly adsorbing solutes (Acharya et al., 2005) and multiphase flow (Blunt et al., 2013). Due to the coarse-grained geometry modelling strategy, PNM is computationally more efficient than other pore-scale models for large domain sizes. However, the simplifying assumptions vary between different geometries and the detailed flow field is not captured. Mehmani & Balhoff (2015) reviewed various PNMs, with the particular focus on transferring information from pore-scale models to continuum models.

### 4.1.2 Validation studies in porous media

<table>
<thead>
<tr>
<th>Study</th>
<th>CFD method</th>
<th>Re</th>
<th>Radial Porosity profile</th>
<th>Pressure drop</th>
<th>Radial axial velocity profile</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maier et al. (1998)</td>
<td>LBM</td>
<td>&lt;30</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Freund et al. (2003)</td>
<td>LBM</td>
<td>0.1-100</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Guardo et al. (2004)</td>
<td>FLUENT</td>
<td>Gas flow</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Atmakidis &amp; Kenig (2009)</td>
<td>ANSYS® CFX 10.0</td>
<td>&lt;100</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Eppinger et al. (2011)</td>
<td>STAR-CCM+</td>
<td>1, 100, and 1000</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Baker et al. (2011)</td>
<td>FLUENT</td>
<td>Gas flow</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Finn et al. (2012)</td>
<td>Finite volume in-house solver</td>
<td>10-200</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Boccardo et al. (2015)</td>
<td>OpenFOAM</td>
<td>0.01-110</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

A brief review of the validation methods will be provided, with particular focus on pixelwise validations. The scope is limited to hydrodynamic properties, such as the velocity distribution.

64
and pressure drop. For validation studies on the heat and mass transfer, interested readers are referred to the review by Dixon et al. (2006).

Due to limited availability of spatially resolved experimental results, the majority of the validations rely on macroscopic properties and empirical correlations, in particular, the pressure drop correlations. Because of the sensitivity of the flow properties to the detailed packing structure, considerable effort has been devoted to ensuring a good match between the simulated packing and the experimental one by matching the aspect ratio. The match is often validated via the azimuthally averaged porosity and velocity profile. A selected body of work on sphere packing is summarised in Table 4.1, in which $Re = \frac{U_{sf}D_p}{v}$, where $U_{sf}$ is the superficial velocity, $D_p$ is the particle diameter, and $v$ is the kinematic viscosity.

Another strategy of model validation is via a canonical model structure. One of the benchmark datasets used for sphere packing is the flow fields measured in the simple cubic packing (SCP) by Suekane et al. (2003). Several studies were conducted in a SCP unit cell with periodic boundary conditions to validate the CFD model, including the finite volume (Gunjal, Ranade, et al., 2005; Finn et al., 2012), fictitious domain (Finn & Apte, 2013), MPS (Ovaysi & Piri, 2010) methods, and LBM (Rong et al., 2013). The packing geometry shown in Fig 4.1 (b) was also used as a canonical model, where pixelwise validation using MRI velocimetry was conducted by Robbins et al. (2012); the complex backflow was predicted accurately up to $Re = 216$. However, there is a substantial difference between the regular and the periodic packing, even regarding macroscopic behaviour. For example, Atmakidis & Kenig (2009) studied a regular packing without periodic boundary condition at $N = 5.5$ and a random packing at $N = 5$. The authors found that the pressure drop in the regular packing agreed with the correlation by Carman (1937) but the random one agreed with the correlation by Reichelt (1972). Similarly, Finn et al. (2012) showed better agreements between SCP and the Ergun equation, while Eisfeld & Schnitzlein (2001) yielded a better fit for the pressure drop in the random packing. The difference between the pressure drop correlations is significant in numerical simulations. The contrast in pressure drop indicates that structured packing is insufficient to validate the flow field in the complex and tortuous random packing geometry. Next, we review the few studies that achieved validation on the same random packing.

The first study is by Manz et al. (1999), who applied LBM on the same flow domain captured by 3D MRI; the simulation results were validated using the velocity probability distribution function (PDF) measured by flow propagator experiments in the creeping flow regime. They
showed agreements between the experimental and simulation results and obtained valuable insight into the dispersion mechanism. Yang et al. (2013) conducted a validation study using 3D magnetic resonance velocimetry (MRV) in a high aspect ratio \( (N = 17.6, \text{aspect ratio is the ratio of the column diameter to the particle diameter}) \) column with 6864 spheres at \( Re_{\text{int}} = 0.26 \) (\( Re_{\text{int}} = \frac{U_{\text{int}} D_p}{v} \), where \( U_{\text{int}} \) is the interstitial velocity). The study validated two CFD solvers: one is an in-house code for a structured mesh and the other is a finite-volume method on an unstructured mesh implemented by the commercial software, STAR-CCM+. Moreover, the authors conducted a more detailed validation, including the pixelwise comparison and comparison of velocity PDFs. Another high-fidelity validation study is by Wood et al. (2015), who measured the flow fields using particle image velocimetry (PIV) and applied the fictitious domain method developed by Apte et al. (2009) on a structured mesh. The validation was only on a 2D slice at a single \( Re_{\text{int}} \) of 3.47. The size range of a representative elementary volume was proposed as a guideline for simulations in the random packing.

So far, few pixelwise validation studies exist and there is little comparison regarding the detailed flow structures. Furthermore, only the creeping flow regime has been investigated whilst no validation in the inertial regime has been reported.

### 4.1.3 Image-based meshing

This study focuses on the pixelwise comparison in the inertial regime and the crucial step is to reproduce the experimental geometry as an unstructured CFD meshing, often referred to as image-based meshing. Image-based meshing was originally developed in computational biomechanics, with the need to represent complex biological geometries, such as arteries or bronchial pathways, from medical scans (Plotkowiak et al., 2008). The primary techniques and relevant CFD validation studies are reviewed in this section.

#### 4.1.3.1 Geometry modelling

The first step of image-based meshing is to extract the geometry from 3D images, often acquired by 3D scanning techniques, such as MRI or micro-CT. The first strategy is to create the volume segmentation directly from the 3D data, as demonstrated by Tabor et al. (2008) on a porous foam using commercial software. Baker et al. (2011) created the CFD mesh based on an MRI scan of a packed bed of cylinders using the same method and demonstrated the ability of image-based meshing to deal with complex geometries and boundaries. The other possibility is to use...
the Marching Cube algorithm to create bounding surfaces separating the two phases, as demonstrated by Sains (2006). The principle of the two methods are the same.

The reverse of the above processes is to create a computational model of the domain and then reproduce the physical geometry using Additive Layer Manufacturing techniques (3D printing) (Baker et al., 2014). This approach would be particularly useful if the MRI or CT scan cannot achieve a certain required accuracy, e.g., due to a broad size distribution of particles, such as the volume-bidistributed bed studied by Baker et al. (2014).

The third approach is to identify the locations of the spheres. Yang et al. (2013) proposed an algorithm called “Sphere Loci extraction through Iterative Erosion (SLIE)” and generated the geometry by subtracting the spheres from a cylindrical bounding volume using the computer-aided design (CAD) tool in STAR-CCM+. Wood et al. (2014, 2015) obtained the 3D information by calculating the locations of the beads based on pairs of 2D PIV images. In this way, a more detailed geometry can be reconstructed, which is not restricted by the resolution of the original image, but this method has only been applied to monodisperse sphere packing and its scope of applicability is limited by the complexity of the geometry.

4.1.3.2 Marching Cube algorithm

The Marching Cube (MC) algorithm is often used to generate the bounding surface from 3D volume images. MC was first proposed by Lorensen & Cline (1987) to generate a 3D visualization of the volume of interest in order to achieve the full potential of medical imaging. MC uses a divide-and-conquer approach to locate the surface characterised by a contour value in a 3D space. The algorithm determines the surfaces in a logical cube, depending on the values at the vertices, and then marches to the next cube until all the cubes have been processed. Lorensen & Cline identified 15 variations, which can represent the 256 different configurations via rotation operations. Mid-points can be used in the triangulation while linear interpolation was suggested to achieve a smoother surface. An ambiguity problem was reported in the original segmentation methods. Configurations with four vertices greater and four vertices less than the contour value can lead to holes in the structure (Dürst, 1988), rendering the geometry invalid for further volume meshing and CFD modelling. A number of remedies have been suggested, including the asymptotic decider by Nielson & Hamann (1991), the Marching Tetrahedron algorithm, and case table refinement (Rajon & Bolch, 2003).
4.1.3.3 Volume meshing

The critical challenge for volume meshing is the treatment of contact points because either long-thin meshing elements are required, resulting in high error in CFD, or a large number of mesh elements are necessary. The conventional solution is under-sizing (Dixon & Nijemeisland, 2001; Bai et al., 2009; Augier et al., 2010) or over-sizing the spheres (Robbins, El-Bachir, et al., 2012). Dixon et al. (2013) studied the effect of meshing strategies systematically, including the established methods and another two meshing strategies, the Bridges and Caps techniques. The Bridges approach is to insert a cylinder between the contact points within a specified tolerance. The Caps approach is to flatten the particles near the contact points, which was also used by Eppinger et al. (2011). It was found by Dixon et al. (2013) that the Bridges and Caps methods yielded better predictions of the drag coefficient than the global enlarge/shrink methods, and Bridges approach was more promising for simulating heat transfer.

The contact point challenge can also be overcome by increasing the number of mesh elements. The mesh refinement strategy adopted by Boccardo et al. (2015) is to refine uniformly in the domain and subsequently near the particle surface. The key limiting factor is the resolution of the momentum boundary layer around each particle; the cell dimension used in bulk liquid was 80 µm and at the boundary layer was 40 µm for a random packing of spheres with an average diameter of 1.99 mm. Atmakidis & Kenig (2009) found that five layers of prismatic mesh elements were required to resolve the boundary condition at each particle surface.

4.1.4 Aims

With the advancement in experimental techniques, 3D imaging and velocity measurements have become more available, providing a rich library of data for validating numerical simulations of porous media flow. Such validations allow further innovations to address the deficiency in CFD exposed. Furthermore, the accurate prediction of flow characteristics is critical in determining the performance of the reactors. However, pixelwise validations of flow features have not been achieved for random sphere packings. Such studies are limited to the creeping regime and we lack the knowledge of the inertial regime. This chapter aims to address the above issues, and more specifically:

(1) To demonstrate a pipeline for pixelwise validation study using high-resolution MRI experimental data and commercial CFD software packages.
(2) To examine the accuracy of the CFD prediction in detail, especially the accurate prediction of the inertial flow characteristics.

4.2 Materials and Methods

4.2.1 Surface mesh

The surface meshing strategy is based on the MC algorithm. The full 255-case table can overcome the ambiguity problem and the implementation in the Visualization Toolkit (Preim & Bartz, 2007) was chosen for this work. A built-in smoothing method using a windowed sinc function interpolation kernel was applied afterwards to improve the cell shapes and distribute the vertices more evenly (Taubin et al., 1996). The current dataset is particularly challenging because the high resolution (67.6 pixels/$D_p$) gives rise to a large number of pixels that are partially filled with liquid. After attempting to step through a range of threshold values and apply automated error correction, a large number of pixels remained ambiguous. This ambiguity results in small holes at the contact points, where manual fix over millions of pixels is impractical. Therefore, a denoising method was applied with total variation regularisation to enhance the contrast between the two phases. The Rudin-Osher-Fatemi model (Rudin et al., 1992) was used for denoising and the optimization algorithm was the preconditioned alternating direction method of multipliers (Boyd et al., 2011). After denoising the 3D image, the threshold for a binary map was chosen to match the porosity evaluated on the original image, as described in §3.3.3. The binary map to generate the surface mesh using the MC algorithm, where a contour value of 0.5, was used.

The second meshing method is a modification of the SLIE algorithm described by Yang et al. (2013). First, the outer edge of the 3D binary structure (the same binary map used in the MC algorithm) was eroded iteratively with a cubic structured element using the ‘imerode’ function in MATLAB, such that the spheres would be separated from one another. The volume of connected components was calculated (two components are connected when the closest distance is less than 2). When the volume is small enough (less than 80% of the size of a sphere), the region is assigned to a single sphere, whose location is determined by the centre of mass of the region, and the connected volume was removed for further erosion. A total of 60 spheres was identified and high consistency was achieved for the axial slices number from 31 to 220 (out of a total of 256 slices). The two ends of the bed (slices < 31 and slices >220) were inaccurate due to the wrapping artefacts in the original intensity map.
Further optimisation of the locations of the sphere was conducted to improve the accuracy of sphere recognition and identify the slight difference in sizes. The edge of the sphere is characterised by the intermediate signal intensity level, $I_{th}$, as calculated in §3.3.3. For each sphere identified using SLIE, the difference between $I_{th}$ and the mean signal intensity of 10,000 points sampled on the surface of the recognized sphere was minimized with respect to the location and size of the sphere. The minimisation was implemented using the nonlinear least-squares solver in MATLAB®. To construct the model, the centre and size of the inner tube were determined using the MATLAB® function ‘imfindcircles’ at different axial slices and a slight tilt of the tube was identified. The surface mesh was then generated by subtracting the spheres from a cylindrical volume using the Autodesk Inventor® software.

4.2.2 Volume meshing

The volume meshing was performed using a commercial tool ICEM 16.0 provided by ANSYS Inc. because highly-specialised algorithms and compatibility with the commercial CFD solver are required. The meshing algorithms for generating unstructured tetrahedral meshing are broadly categorised as the (i) Octree, (ii) advancing front and (iii) Delaunay methods (Owen, 1998). The Octree technique was primarily developed by Mark Shephard and co-workers (Yerry & Shephard, 1984). The cubes containing the geometric model are recursively subdivided until the desired resolution is reached and the surface facets are formed wherever the internal octree structure intersects the boundary. The mechanism is demonstrated by its two-dimensional counterpart, the Quadtree method, shown in Fig 4.2. In advancing front algorithms, the tetrahedra are built progressively inward from the triangulated surface. In 3D, for each triangular facet on the front, an ideal location for a new fourth node is computed. The most popular meshing techniques are those utilising the Delaunay criterion, which states that any node must not be contained in the circumsphere of any tetrahedron. Similar to the advancing front algorithms, the Delaunay method is often implemented by inserting nodes with respect to an existing surface mesh while maintaining the Delaunay criterion.

Because of the irregular geometry of the random packing, a high-quality surface mesh could not be easily generated for the Delaunay and advancing front algorithms; thus, the more robust Octree algorithm has been chosen. Smoothing was applied to resolve the divergence problem of the numerical CFD solver, which was due to the low-quality meshing elements populated at the contact points. As a result, the number of elements at the contact points was reduced and the sharp features were smoothed out. The mesh was subject to several rounds of smoothing
until the numerical solver reached convergence. The summary of the mesh sizes is given by Table 4.2. Higher mesh resolution was not explored because of the limitation of the academic license of the software.

![Quadtree decomposition of a 2D object](image)

**Fig 4.2.** Quadtree decomposition of a 2D object (Owen, 1998).

**Table 4.2** Statistics of different mesh sizes used. The sizes are reported with respect to the MRI resolution ($\Delta x$).

<table>
<thead>
<tr>
<th></th>
<th>Number of elements</th>
<th>Number of nodes</th>
<th>Maximum edge size [$\Delta x^{-1}$]</th>
<th>Average area per triangle [$\Delta x^{-2}$]</th>
<th>Average volume per tetrahedron [$\Delta x^{-3}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse 2</td>
<td>575,961</td>
<td>102,982</td>
<td>3</td>
<td>2.78</td>
<td>1.91</td>
</tr>
<tr>
<td>Coarse</td>
<td>967,505</td>
<td>171,269</td>
<td>2.5</td>
<td>1.97</td>
<td>1.11</td>
</tr>
<tr>
<td>Reference</td>
<td>1,841,109</td>
<td>322,698</td>
<td>2</td>
<td>1.25</td>
<td>0.57</td>
</tr>
<tr>
<td>Fine</td>
<td>4,221,691</td>
<td>731,513</td>
<td>1.5</td>
<td>0.717</td>
<td>0.241</td>
</tr>
</tbody>
</table>

### 4.2.3 CFD solver

![Schematic of a control volume](image)

**Fig 4.3.** Schematic of a control volume, where the volume is denoted $\Omega$ and is bound by the surface $\partial \Omega$. The local velocity $\mathbf{v}$ is impinging on a surface element $dS$, which has an outward-pointing normal vector $\mathbf{n}$.

The governing equations are derived from the laws of conservation for mass, momentum, and energy over a control volume $\Omega$ (Fig 4.3). To derive a generic conservation law, we refer to the mass, momentum, and energy per unit volume as $\phi$. By balancing the convective, diffusive
flux, source and sink terms, the generalized integral form of the conservation law can be written as:

$$\frac{\partial}{\partial t} \int_\Omega \phi \, d\Omega + \oint_{\partial \Omega} \left\{ \phi (v \cdot n) - k \rho \left[ \nabla \left( \frac{\phi}{\rho} \right) \right] \right\} \, dS = \int_\Omega Q_v \, d\Omega + \oint_{\partial \Omega} (Q_s \cdot n) \, dS, \quad (4.1)$$

where $k$ is the rate of diffusion, $Q_v$ is the volumetric source, and $Q_s$ is the surface source. If $\phi$ is $\rho$, the specific form is the continuity equation. The momentum equation is when $\phi = \rho v = [\rho u, \rho v, \rho w]^T$ and the energy equation is derived by substituting $\phi$ with $\rho E = \rho (e + \frac{1}{2} |v|^2)$, where $e$ is the internal energy.

There are two main types of solvers: a pressure-based solver that solves the pressure Laplacian equation and a density-based solver, which uses a thermodynamic relationship $\rho = \rho(T, P)$. The density-based solver has difficulties in converging at low fluid velocity. One method to address this issue is to use a preconditioning matrix, as demonstrated by Robbins et al. (2012). In contrast, the pressure based algorithm is more widely-used and one popular algorithm is the semi-implicit method for pressure-linked equations (SIMPLE) algorithm for solving Navier-Stokes equations (Ferziger & Peric, 2001). FLUENT (Ansys Inc., 2015) is chosen for this work because it is one of the most powerful and widely used commercial packages and the more affordable academic license is used. In FLUENT, the SIMPLE algorithm was chosen and there was negligible difference between different pressure-based algorithms under the default settings. Constant flowrate was applied at the inlet and no-slip boundary condition was enforced at the walls. Second order discretization was used for pressure term and second-order upwind interpolation was applied for the momentum terms. Under-relaxation factors were left at the default settings in FLUENT to stabilize the convergence behaviour and the convergence criteria was the relative residual of the density, x-, y-, and z-velocity being less than $10^{-3}$. The residual, $R$, for the general variable $\phi$ is defined as

$$R^\phi = \sum_{cells P} \left| \sum_{nb} a_{nb} \phi_{nb} + b - a_p \phi_p \right|, \quad (4.2)$$

where $nb$ is the neighbouring cells of cell $P$, $a_p$ is the centre coefficient, $a_{nb}$ is the influence coefficient, and $b$ is the source term. The relative residual is used, given by

$$R_{\text{relative}}^\phi = \frac{R^\phi}{\sum_{cells P} |a_p \phi_p|}, \quad (4.3)$$
The solver had difficulty converging and the residual oscillated around a level higher than $10^{-3}$ for $Re = 115$ and 145 after 100 iterations. Moreover, decreasing the under-relaxation coefficients did not alleviate the problem. It could be due to an instability in the solver or the flow becoming unstable as $Re$ approaches the unsteady regime; therefore, the calculation was terminated at 500 iterations for $Re = 115$ and 145.

4.3 Results

4.3.1 Mesh comparison

The pixelwise error has been measured by the normalised root mean squared deviation ($NRMSD$), e.g., for the velocity in the y-direction, $v$, the expression is

$$NRMSD_v = \frac{\sqrt{\frac{\sum (v_{MRV} - v_{CFD})^2}{N}}}{v_{max} - v_{min}}, \quad (4.4)$$

where there are N pixels, and $v_{max}$ and $v_{min}$ are from the MRV measurements. The velocity in the x-direction is $u$, and the axial velocity is $w$.

The comparison of $NRMSD_w$ between the two meshing methods is shown in Fig 4.4(a); their trend and values are highly similar, but a smaller error is obtained using the MC algorithm. The SLIE mesh is expected to be more accurate as the contact points can be resolved beyond the resolution of the original image but the sharp features were eroded because of the smoothing applied to the volume mesh. Thus, the two meshes have comparable resolution. The inferior performance of SLIE stems from the error in the identification of centres and sizes of spheres.

Subsequent tests have been conducted using the surface mesh created by the MC algorithm. Fig 4.4(b) shows $NRMSD_w$ for different mesh sizes, and significant loss of accuracy is observed for the coarsest mesh. The difference between the coarse, reference and fine meshes is less significant, with the fine mesh producing slightly more accurate prediction as expected. The error is largest at the inlet because a uniform velocity was used as the inlet boundary condition due to the constraint in the commercial CFD solver. A larger discrepancy is also observed at the outlet, suggesting that the geometry downstream also affects the flow profiles.

$NRMSD$ for different velocity components using the reference mesh are shown in Fig 4.4(c) and the average errors are $6.5\pm1.2\%$, $6.3\pm1.1\%$, and $7.4\pm1.1\%$ for $u$, $v$, and $w$ respectively. Furthermore, there is little correlation between the errors in the three velocity components.
Fig 4.4. $NRMSD$ in the axial velocity at different axial positions (a) for the two meshing methods and (b) for different mesh sizes (Ref refers to the reference mesh), and (c) $NRMSD$ in the axial and transverse velocities for the reference mesh for $Re = 60$.

$NRMSD_w$ and $NRMSD_u$ for different $Re$ are shown in Fig 4.5. The entrance effect for $Re = 29$ is more significant in the axial direction, $w$, than the transverse direction, $u$, while the exit effect is less in both $w$ and $u$ compared with higher $Re$. From $Re = 29$ to 145, the error increases and the entrance effect in the axial direction becomes less significant. The decreased significance in the entrance effect with higher $Re$ is counter-intuitive because the entrance effect should
increase with flowrate (Kataoka et al., 1972). This could be due to the higher error associated with the increase in $Re$, which is more significant than the error due to entrance effect. Furthermore, a peak is seen around $Z = 0$ mm, which is due to the higher noise level at the centre of the bed in the MRV measurements.

**Fig 4.5.** $NRMSD$ in the (a) axial velocity $w$ and (b) transverse velocity $u$ at different axial positions for the reference mesh for $Re = 29, 60, 115,$ and $145$.

The global mass balance was estimated based on the axial flowrate across different slices, shown in Fig 4.6. The velocity has been interpolated from the unstructured CFD data at each node onto the MRV Cartesian grid. Although the mass balance was conserved in the CFD simulation, underprediction of flowrate was shown. The underprediction is worse for coarser meshes because a larger proportion of nodes are located at the solid, which has zero axial velocity due to the no-slip boundary condition. One coincidence is the variation of the flowrates at different slices between the MRV measurements and the interpolated CFD data. The coincidence suggests that the MRV measurement in each pixel is likely to be more representative as a point-wise estimate instead of an average velocity for the pixel. If the MRV
measurements are the average of each pixel, the flowrate should be constant due to mass balance. A large discrepancy from mass balance is expected where the axial velocity is highly heterogeneous if the MRV measures the point-wise velocity. Moreover, the deviation from mass balance measured by MRV is similar to the reference and coarse mesh, where the voxel size (the volume represented by each node) is similar to that of MRV (Table 4.2) while the fine mesh shows less deviation from the mean at different slices.

Fig 4.6. Slice-by-slice volumetric flux computed from the experimental and computational axial velocities for $Re = 60$ (CFD refers to the reference mesh). The dotted line is the volumetric flux measured using a graduated cylinder and a stopwatch.

4.3.2 Macroscopic flow behaviour

The intermediate sized mesh from the MC algorithm, i.e., the reference mesh, is chosen for further comparison and negligible difference is found using the fine mesh. The statistics are based on the data between $Z = -7$ and 10 mm to reduce the entrance and exit effects. It was identified by Yang et al. (2013) that the error in MRV has a substantial influence when comparing the PDF. To account for the broadening of the PDFs from experimental error, the PDF was convolved using a Gaussian point spread function (GPSF) with a variance of $\sigma^2 = \sigma_{MRV}^2/U_{st}^2$ ($\sigma_{MRV}$ of the corresponding velocity components and $Re$ are given in Table 3.2). The effect of the convolution is demonstrated in Fig 4.7; the transverse velocity $v$ is not shown because there is no qualitative difference from $u$. The convolved results match more closely with the experimental distribution than the raw CFD data, which suggests the stagnant region is underestimated and backflow area is overestimated in the MRV results due to the experimental noise.
Fig 4.7. PDFs from the MRV results, CFD data, and CFD data convolved with GPSF for the (a) transverse velocity $u$ and (b) axial velocity $w$ for $Re = 115$.

Fig 4.8. PDFs from the MRV results and CFD data convolved with GPSF for the transverse velocity $u$ (left column) and axial velocity $w$ (right column) for $Re = (a-b) 29$, (c-d) 60, (e-f) 115.
Fig 4.8 highlights the evolution of the PDFs with increasing $Re$; the PDFs at $Re = 145$ are the same as $Re = 115$, thus not shown. Overall, the PDFs from the experiments and simulations match very closely. The transverse velocity is underestimated at $Re = 60$ and 115 as shown by the narrower peak. For the axial velocity, the CFD overestimates the backflow at $Re = 29$ while underestimates it at $Re = 115$, which may be due to the limit of mesh sizes at higher $Re$ to resolve the detailed flow field. Another possible reason is the underestimation of experimental errors at higher flowrate because the error due to phase dispersion caused by shear stress was not considered.

![Fig 4.8](image)

Fig 4.9. Scatter plots for the transverse velocity $u$ (left column) and axial velocity $w$ (right column) from the CFD data (vertical axis) versus the MRV results (horizontal axis) for the complete dataset for $Re = (a-b) 29, (c-d) 60, (e-f) 115$. The 1:1 line is indicated by a solid black line; ± two standard deviations of the experimental error distribution are indicated with dashed black lines.
The PDFs depict the overall distribution, whereas a more detailed comparison is made pixelwise, as shown in Fig 4.9. The black solid line shows $y = x$, indicating the perfect match between the two and the two parallel dashed lines above and below the solid line represent two standard deviations of the experimental error. As observed in the $\text{NRMSD}_w$ for different $Re$ (Fig 4.5), the error increases with $Re$, which is characterised by the increased scattering from the $y = x$ line. If the discrepancy is only due to the experimental error, the probability density of the scatter plot should follow a Gaussian distribution that is symmetric with respect to the diagonal. However, the scatter plot is asymmetrical, in particular for $u$ and $v$, indicating systematic errors in the simulation. The higher population density with $|\nu_{\text{MRV}}| > |\nu_{\text{CFD}}|$ at high transverse velocity reinforces the conclusion drawn from PDFs that the large transverse velocity is underestimated in the simulation. Similarly, an underestimation of high axial velocity is also observed. The asymmetry in the axial velocity at $w_{\text{CFD}} < 0$ suggests that the prediction of the direction of backflow pixels is accurate although the magnitude is underestimated.

4.3.3 Inertial core

![Figure 4.10](image-url)

**Fig 4.10.** Contour maps of normalised axial velocity at the transverse planes from (a) MRV and (b) CFD at $Z = -0.4$ mm for $Re = 29$ to 145. The FOV is $16.6 \times 16.6$ mm$^2$. The FOV for all the figures are given in the horizontal ($x$) and vertical ($y$) axes of the figures as $x \times y$.

The primary advantage of the image-based meshing is the capability to validate detailed flow features. Representative results are shown with respect to the inertial core, backflow, and helical vortices. The axial velocity at $Z = -0.4$ mm is shown in Fig 4.10, where the results from MRV and CFD match closely with each other. The prominent flow channels are computed correctly,
including the details, such as the shape of the inertial core and the tear-drop shaped axial velocity profile near the wall. However, there is an underprediction of the maximum velocity, especially at the lower $Re$. Despite the underprediction of the maximum velocity, CFD captures the modulation of axial velocity at the bottom right of the black box.

![Fig 4.11](image)

Fig 4.11. Normalised axial velocity (colour scale) and transverse velocity vector (arrows) plots from (a) MRV and (b) CFD for $Re = 29$ to 145 at the edge of the inertial core at $Z = -0.4$ mm. The FOV is $3.1 \times 2.8$ mm$^2$.

It has already been emphasised that the interaction of vortices and inertial core induces change to the axial velocity profile in Chapter 3 and the region within the red rectangle in Fig 4.10 is examined in Fig 4.11 to observe if CFD predicts the same phenomenon. The transverse velocity from CFD features the closest resemblance at $Re = 29$. The two vortices are captured for all $Re$ and the movement of the dominant vortex towards the left is successfully reproduced. The major difference is the strong vortical motion at $Re = 115$, which is not shown in the CFD counterpart. The inaccuracy in the vortical profile prediction accounts for the smoother inertial core edge and this discrepancy is a recurring theme in this validation study.

The same pore used to demonstrate the evolution of inertial core in Chapter 3 is examined next. The transverse velocity is again underpredicted, as shown in Fig 4.12. The shape of the inertial core at different $Re$ is well captured and the velocity profiles become more top-hat shaped with increasing $Re$. The same trend of reduced channelling velocity has been predicted although the
maximum velocity is slightly underpredicted at $Re = 29$, as shown in Fig 4.13 (a). The major deviation is at the edge of the pore, at about $x = 4.2$ mm, especially for $Re = 145$.

![Fig 4.12. Normalised axial velocity (colour scale) and transverse velocity vector (arrows) plots from (a) MRV and (b) CFD for $Re = 29$ to 145 at $Z = 0.9$ mm. The FOV is $4.6 \times 4.2$ mm$^2$.](image)

![Fig 4.13. Normalised axial velocity profiles from MRV and CFD at the highlighted line in Fig 4.12 for $Re = (a) 29$, (b) 60, (c) 115 and (d) 145.](image)

**4.3.4 Recirculation and helical vortices**

The backflow features from CFD are shown in Fig 4.14 such that direct comparison can be made to Fig 3.19. For the small recirculation cell at the contact point in Fig 4.14(a), the vorticity continues to increase in MRV but there is a plateau of vorticity at $Re = 115$ in the CFD. The
vorticity is also underpredicted for $Re > 29$. There is more discrepancy in the large recirculation zone in Fig 4.14(b), especially the clockwise vortices. Although the CFD velocity profiles from $Re = 29$ to 60 are qualitatively similar to the MRV ones, the clockwise recirculation vortex is predicted to shrink in size with increasing $Re$, whereas the MRV shows it expands. The vorticity of both vortices is significantly lower than the MRV results.

![Fig 4.14](image)

**Fig 4.14.** Normalised vorticity (colour scale) and transverse velocity vector (arrows) plots for (a) a vortex at the contact point and (b) a large recirculation pore as examined in Fig 3.19(d) and (e). The FOV is (a) $2.5 \times 1.8 \text{ mm}^2$, and (b) $4.5 \times 3.7 \text{ mm}^2$.

The overall distribution of inertial cores and backflows are demonstrated in Fig 4.15 for $Re = 115$ and the other $Re$ show similar trends. The location and structure of the channelling region in the simulation agree with the experiment, despite the slight underestimation of the sizes of some flow channels. It is worth noting that a higher backflow threshold is chosen for MRV because, if the same threshold were used, the near stagnant regions would be speckled with backflow spots due to noise in the data. A higher threshold helps to visualise the recirculation region in the MRV data, which is consistent with the CFD prediction. Some of the recirculation zones are located around the contact points, as predicted by in the CFD study by Eppinger *et al.* (2011). In addition, the low aspect ratio in this study enables a clearer visualisation of the recirculation zone in the larger voids. Fig 4.15 (b) highlights that the large recirculation zones are present in the voids surrounded by high-velocity channels, which is reported for the first time. It is speculated that the recirculation vortices are induced by the high shear around the pore.
Fig 4.15. Isosurfaces of the axial velocity from (a) MRV and (b) CFD for the section of the bed from -5.3 to 7.3 mm for $Re = 115$. The blue represents backflow with $\frac{w}{U_{sf}} = -0.6$ for (a) MRV and $\frac{w}{U_{sf}} = -0.2$ for (b) CFD. The green represents channelling with $\frac{w}{U_{sf}} = 5$.

Fig 4.16. The streamlines for a helical vortex in a wall-bounded pore for $Re = 29$ to 145 from CFD. The streamlines are coloured by the velocity magnitude. The FOV is $3.7 \times 4.4 \times 5.1$ mm$^3$.

Equivalent plots for the helical vortices in a wall-bounded pore are examined in Fig 4.16, which can be directly compared to Fig 3.21. The velocity magnitude agrees well between CFD and MRV although the velocity at the pore entrance is higher in CFD. The key discrepancy is the lack of swirling motion at $Re = 115$ and 145. A more detailed validation can be done by comparing Fig 4.17 and Fig 3.23. There is qualitative similarity regarding the location of the helical vortex and its evolution pattern. For example, in Fig 4.17 (b), the reduced intensity of the side jet (at the bottom of the pore) along the axial direction agrees with the experimental observation. However, the jet velocity is underestimated by the CFD. Moreover, the vorticity is significantly lower in the simulated results, roughly than 50% less than the experimental
values. Since the swirling motion is due to the side jets, we can conclude that the low vorticity is due to underprediction of jet velocity.

Fig 4.17. Normalised vorticity (colour scale) and transverse velocity vector (arrows) plots for a wall-bounded helical vortex at different axial positions for (a) $Re = 60$ and (b) $Re = 115$. The FOV is $3.0 \times 2.4 \text{ mm}^2$.

4.4 Discussion

As the experimental data was examined in Chapter 3, only comments on the CFD results will be made in this section.

4.4.1 Macroscopic validation

In this section, we compare the macroscopic properties (§4.3.1-2) to the other two pixelwise validation studies of Yang et al. (2013) and Wood et al. (2015).

Wood et al. (2015) have reported that the errors in a certain slice for the axial and normal velocity components are 11.3% and 4.7% for a bed with $Re_p = 3.47$. In this work, the error at $Re = 29$ is about 5% in all three velocity components.

The flowrate is less consistent compared to Yang et al. (2013) and the main reason is due to the significant partial volume effect, as a result of the low aspect ratio in this study. It should be
noted that there is still about 1% fluctuation in the flowrates measured by MRV in Yang et al. (2013) and analysis based on the coincidence between CFD and MRV results in Fig 4.6 provides an explanation for the discrepancy. Although the agreement in flowrate is not as good as that from Yang et al. (2013), the PDFs of velocity from the CFD and MRV in this study are more consistent. Even after convolution with a GPSF, CFD underestimates the backflow and the faster velocities compared to MRV in Yang et al. (2013), while better agreement is shown in this study.

The better consistency in PDFs is also shown in the correct reproduction of the exponentially decaying population density in Fig 4.18. The match is the best at $Re = 29$ while there is an underestimation of high axial velocity at higher $Re$. The significance of the exponentially decaying pattern has been discussed in §3.5.1 and will not be repeated here.

![PDFs in log scale from MRV and CFD convolved with GPSF for (a) the transverse velocity $u$ and (b) the axial velocity $w$ for $Re = 29$.](image)

The scatter plot by Yang et al. (2013) at $Re = 0.26$ is shown in Fig 4.19 and the current study presents better pixelwise comparison. Both Yang et al. (2013) and this work underpredict the high axial velocity in CFD. Instead of underpredicted backflow in this study, zero backflow was observed in the CFD results by Yang et al. (2013). Similarly, no backflow was observed by Wood et al. (2015) in both CFD and PIV in the creeping flow regime. Yang et al. (2013) suggested that the backflow is likely to be due to the uncertainty in MRV measurements in the near stagnant regions. Conversely, in the inertial flow regime examined here, a better prediction of backflow has been made despite the error in MRV measurements, and the mechanisms of the backflow are revealed. The reasons for the lack of negative axial velocity in Yang et al. (2013) and Wood et al. (2015) is worth investigating.
4.4.2 Microscopic validation

In terms of channelling, the high-velocity channels are all correctly predicted, and the decrease in the maximum velocity is also captured by CFD. The slight discrepancies in the details are mainly due to the attenuated vortical motion compared to MRV. Underestimation of jet velocity was also reported by Yang et al. (2013), where the point velocity in the CFD was about 40% lower than MRV.

For all the flow features examined, the recurring theme is the lack of swirling motion although there is a reasonable qualitative agreement for the overall flow pattern. Some insight can be drawn from the detailed pictures of the helical vortex. As emphasized, the low vorticity is due to the underestimated jet velocity, which induces lower angular momentum. The plausible speculation of the cause of lower jet velocity is the unresolved features at the contact point. In order to guarantee convergence of the numerical solver, the mesh elements at the contact points were smoothed out, which can be seen in Fig 4.10. It is likely that the sharp corners are significant for the vortical motion but such geometrical features were not preserved in the volume mesh. The significance of the meshing at contact points was emphasised by Dixon et al. (2013) in a systematic study of the effect of meshing between two neighbouring spheres. It was found by Dixon et al. (2013) that the largest gap size gives rise to 40% higher axial velocity.
and the Bridges or Caps method can cause up to 10% over-estimation of drag coefficient. The sensitivity of the flow features to different contact point treatments suggests that the flow field is highly dependent on sharp features.

4.5 Conclusion

Pixelwise validation of CFD results on a random packing structure in the inertial flow regime has been achieved for the first time. The geometry of the sphere packing was reproduced via image-based meshing and the details of the processing pipeline, from denoising, threshold selection, surface and volume meshing, to CFD solver configurations, have been documented.

Both statistical and pixelwise validations were carried out in the developing inertial flow. The PDFs of different velocity components show good agreements when the uncertainty in the experimental data is taken into account. Underprediction of high transverse velocity is highlighted in both the PDFs and pixelwise comparisons.

Further insights are given by detailed comparison of the flow features with the MRV data. Channelling is captured with good fidelity and the velocity profiles of inertial cores match very well. The recirculation vortices and helical vortices in the CFD results show qualitative agreements, regarding their location, spatial and temporal evolution. The unsatisfactory features, including the shape and the low vorticity, are likely due to underpredicted transverse velocities, shown by the low vorticity in a helical vortex due to the underpredicted jet velocity. We propose that the reason for this underprediction is the over-smoothed contact points during volume meshing. This work further emphasizes the importance of the sharp geometric features to the accurate modelling of fluid flow.
Chapter 5 Unsteady flow in random packed beds of spheres

5.1 Introduction

In the last two chapters, the inertial effect was analysed and the accuracy of numerical simulations was evaluated. The unsteady flow in porous media has only been studied in recent years with the advancement of experimental techniques. In this chapter, we continue to investigate the flow in the same random packing with the focus on the transition to unsteady flow. In this section, we first review the experimental studies on the phenomenon. Then the prior understanding of the key unsteady flow features and the mechanism for the transition is summarised. The potential of using magnetic resonance velocimetry to study the transient phenomenon is discussed. In the end, the applications of proper orthogonal decomposition (POD) in studying fluid dynamics are reviewed.

5.1.1 Transition to unsteady flow in porous media

The earliest quantitative studies on the transition to turbulent flow are based on micro-electrode techniques, where measurements are taken from electrochemical probes embedded at the wall or the surface of the packing. The critical Reynolds numbers, \(Re_{\text{crit}} = \frac{U_{\text{str}} D_p}{v}\) of the microelectrode studies are summarised in Table 5.1. The range of \(Re_{\text{crit}} = 100 – 150\) is large because the transition is highly sensitive to the position of the probe and a number of authors have emphasised the heterogeneity of the unsteady behaviour. Rode et al. (1994) observed that the evolution of the unsteadiness with increasing \(Re\) based on different probes vary significantly within a local network embedded in the wall. A more detailed description is given by Seguin et al. (1998), who categorised the evolution of local velocity fluctuation into two types: a linear slope or a sharp slope increase depending on the location of probes. Seguin et al. (1998) and Yang et al. (2015) also reported that the wall probes transit at higher \(Re\) compared to internal ones. The dependency of the onset of unsteady flow on the local structure has been further illustrated in the study of different regular packings by Bu et al. (2015), who showed that a lower \(Re_{\text{crit}}\) was associated with the increase in tortuosity and complexity of the structure, from simple cubic packing (SCP), body-centered (BC) packing to face-centered cubic (FCC) packing. Seguin et al. (1998) reported a 40% relative standard deviation of the \(Re_{\text{crit}}\) of the
internal probes; the relative deviation from the seven wall probes measured by Yang et al. (2015) is approximately 30 – 50%. Besides the inhomogeneity in the transitional behaviour, the level of turbulence after the transition regime, quantified by the stabilisation of fluctuating rate of the current, also showed significant variation.

**Table 5.1** $Re_{\text{crit}}$ corresponding to the transition of flow regimes using micro-electrode technique in random sphere packing

<table>
<thead>
<tr>
<th>Study</th>
<th>Aspect ratio (N)</th>
<th>Mean porosity</th>
<th>Location of measurements</th>
<th>$Re$ at the onset of unsteady flow ($Re_{\text{crit}}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jolls &amp; Hanratty</td>
<td>12</td>
<td>0.41</td>
<td>Internal</td>
<td>110-150</td>
</tr>
<tr>
<td>Latifi et al. (1989)</td>
<td>10</td>
<td>0.39</td>
<td>Wall</td>
<td>110</td>
</tr>
<tr>
<td>Rode et al. (1994)</td>
<td>10</td>
<td>0.4</td>
<td>Wall</td>
<td>110-150</td>
</tr>
<tr>
<td>Seguin et al. (1998)</td>
<td>12, 7.5</td>
<td>0.36</td>
<td>Wall and internal</td>
<td>Wall: 132-139; Internal: 106-122.</td>
</tr>
<tr>
<td>Yang et al. (2015)</td>
<td>5.3, 8.1, 9.9, 12.5</td>
<td>-</td>
<td>Wall and internal</td>
<td>Wall: 95-126; Internal: 98-121.</td>
</tr>
<tr>
<td>Bu et al. (2015)</td>
<td>Simple cubic</td>
<td>0.48</td>
<td>Wall and internal</td>
<td>238-282</td>
</tr>
<tr>
<td></td>
<td>Body-centered cubic</td>
<td>0.32</td>
<td></td>
<td>103-148</td>
</tr>
<tr>
<td></td>
<td>Face-centered cubic</td>
<td>0.26</td>
<td></td>
<td>73</td>
</tr>
</tbody>
</table>

The heterogeneity of the transition has been demonstrated by micro-electrode studies; however, as a point-based measurement technique at the solid-liquid interface, a global characterisation is not available. Direct numerical simulation for the transitional regime in packed beds is computationally demanding; thus, it has been suggested that the flow properties can be estimated from laminar or temporally-averaged turbulent models (Dixon et al., 2006). Therefore, a global picture of the transition from steady to unsteady flow in porous media is critical for guiding the selection of numerical simulation methods.

The majority of the flow field measurements on unsteady flow in porous media are based on optical techniques on refractive index matched (RIM) systems. Particle imaging velocimetry (PIV) has gained popularity in recent years due to its high temporal and spatial resolution. The onset of turbulence in simple cubic packing (SCP) was studied by Horton & Pokrajac (2009) combining ultrasonic velocity profiler (UVP) and PIV. Blois et al. (2012) used endoscopic PIV where a camera and illumination endoscope are placed in an SCP packing to examine the velocity in a submerged packed bed driven by free-surface flow.
Patil & Liburdy (2012, 2013a, 2013b, 2015) studied the flow characteristics in porous media using PIV on a random packed bed of spheres with a low aspect ratio (N = 4.67). Detailed analysis of the turbulent statistics extracted from pore-scale flow fields was reported. The spatial variation of turbulence level was shown to be more uniform with increasing $Re$. The ratio of the longitudinal to lateral velocity fluctuation $v'/u'$ showed higher directional variation in pores with accelerated flow regions, including jet-like flow and recirculation regions. More recently, Khayamyan et al. (2016, 2017) conducted PIV experiments in a packing with a higher aspect ratio (N = 8) for a wide range of $Re$ from the creeping to turbulent regime. The level of fluctuation of the longitudinal velocity features a peak at $Re = 331$, after which the fluctuation slowly decreases and reaches a plateau at $Re = 621$ (Khayamyan et al., 2016). With all three velocity components measurement enabled by stereoscopic PIV, the fluctuation of the velocity magnitude has been presented (Khayamyan et al., 2017). Compared to the longitudinal velocity fluctuation, the asymptotic behaviour was less visible in the absolute velocity magnitude, which highlights the importance of the knowledge of all three velocity components.

5.1.2 Key flow features and their evolutions

Several key flow features, including the inertial core, backflow, and vortical structures, are widely observed in porous media flows, in both pore-scale experimental and numerical studies. The evolution of flow features during the transition can provide insight into the physical processes involved. Further, they exert a significant influence on the macroscopic behaviour, including the heat and mass transfer.

The development of the inertial core is a characteristic phenomenon during the transition from the creeping to inertial flow regime (Dybbbs & Edwards, 1984). Although the inertial cores cannot be fully represented by the longitudinal slices in the PIV visualisation, their behaviour can be inferred from the high longitudinal velocity regions, i.e., jet flow regions. Patil & Liburdy (2012) observed a lower channelling velocity and a more homogeneous velocity distribution from $Re = 184$ to 1744. The gradual reduction of the velocity gradient was explained by the increased momentum mixing due to turbulence. Similarly, the reduced area and lower magnitude of the high axial velocity region can be inferred from the mean velocity profiles reported in Khayamyan et al. (2016) for $Re = 50, 170, \text{ and } 484$. Khayamyan et al. (2017) further showed that the increase in homogeneity of the axial velocity resulted in a reduction in the longitudinal dispersion coefficient.
Backflow is another significant inertial flow feature, which occurs mainly due to the flow impingement and recirculation vortices. In Chapter 3, it was reported that the amount of counter-current flow was observed to increase from the creeping to inertial regime. Khayamyan et al. (2016) reported that the fraction of recirculation region increased sharply from $Re = 16$ to 33. No trend for the backflow area was shown from $Re = 33$ to 166 and the area decreased slowly afterwards. Patil & Liburdy (2012, 2013a) showed persistent recirculation bubbles in several pores, whose size and shape varied slightly in the unsteady regime. Furthermore, Patil & Liburdy (2013a) emphasised that the longitudinal dispersion is dominant by the longer retention time due to recirculation.

Besides the recirculation vortices, another important vortical flow feature in packed beds is the streamwise vortices featuring helical streamlines, often referred to as helical vortices. Helical vortices are widely observed in swirling flow (Syred, 2006) but there is very limited experimental evidence on helical vortices in packings. One such example is the four pairs of counter-rotating vortices observed in simple cubic packing (Suekane et al., 2003). Helical vortices are hypothesised to play a significant role in the development of turbulence. Finn et al. (2012) predicted that the major flow features in a random packing were helical vortices spiralling through the pore space in a corkscrew motion. They reported that the unsteady flow was characterised by the dynamic motion of the helical vortices, including the stretching of helical vortices and the translational movement of the helical core. In industries, helical vortices have been introduced in turbulent flow to enhance the heat transfer (Holloway et al., 2004), and the mechanisms were identified as (1) the higher heat flux due to the increase in the axial velocity near the wall and (2) the improved mixing associated with the high turbulence level by Chang & Dhir (1994, 1995).

### 5.1.3 Instability mechanism in packed beds

The critical transition point to the unsteady flow can be predicted theoretically by the linear stability theory, and the onset of unsteady flow frequently features unsteady vortical structures, such as the Kelvin-Helmholtz instability, Bernard cell, and von Karman vortex street. The onset of periodic instabilities and their further development via diverse routes to chaos is of fundamental interests in fluid dynamics (Drazin, 2002; Tritton, 2012). Wake instability characterised by vortex shedding in cylindrical packings has been observed although the frequencies are higher than that of an unbounded flow ($St \sim 0.2$) (Dybb & Edwards, 1984; Koch & Ladd, 1997). Lattice-Boltzmann method (LBM) simulations in the FCC packing
revealed that the transition occurs via a route from steady, periodic, quasi-periodic to chaotic regimes (Reynolds et al., 2000; Hill & Koch, 2002). Further, Hill & Koch (2002) identified a supercritical Hopf bifurcation that features periodic interactions of helical vortices. The periodic behaviour reported in unsteady flows in porous media and the dimensionless frequencies, the Strouhal numbers \( St = fD_p/U \), where \( f \) is the frequency and \( U \) is the characteristic velocity, are summarised in Table 5.2.

Hill & Koch (2002) predicted a quasi-periodic route in FCC, the same route as observed in the Taylor-Couette flow (Imomoh et al., 2010) and transition in a lid-driven cavity (Benson et al., 2011), but no such experimental evidence exist in sphere packings. Moreover, the experimental evidence on the periodic flow phenomena is scarce. Experimental characterisation of such periodicity is essential for validating the simulations and uncovering the transition process to turbulence.

Table 5.2 Summary of the periodic unsteady behaviour in packed bed reported in the experimental and numerical studies. \( Re_{\text{int}} = \frac{U_{\text{int}}D_p}{\nu} \), where \( U_{\text{int}} \) is the interstitial velocity.

<table>
<thead>
<tr>
<th>System</th>
<th>Methods</th>
<th>Periodic behaviour</th>
<th>( Re_{\text{int}} )</th>
<th>( St )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dybbs &amp; Edwards (1984)</td>
<td>Random complex rod bundle</td>
<td>Streakline visualisation</td>
<td>Travelling waves</td>
<td>100-300</td>
</tr>
<tr>
<td>Koch &amp; Ladd (1997)</td>
<td>Arrays of cylinder, area fraction = 0.2</td>
<td>2D LBM</td>
<td>Vortex shedding (flow is along the axis of symmetry)</td>
<td>120</td>
</tr>
<tr>
<td>Hill &amp; Koch (2002)</td>
<td>FCC, flow along (1,0,0) direction</td>
<td>3D LBM</td>
<td>Oscillating streamwise velocity</td>
<td>58, 91</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Torus bifurcation</td>
<td>98</td>
</tr>
<tr>
<td>Magnico (2009)</td>
<td>Random sphere packing (N = 5.96)</td>
<td>Finite volume method</td>
<td>Periodic</td>
<td>120</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Quasi-periodic</td>
<td>160</td>
</tr>
<tr>
<td>Horton &amp; Pokrajac (2009)</td>
<td>SCP</td>
<td>UVP</td>
<td>Periodic pulsing of inertial core</td>
<td>161*</td>
</tr>
<tr>
<td>Finn et al. (2012)</td>
<td>SCP</td>
<td>Finite volume method</td>
<td>Vortex shedding</td>
<td>600</td>
</tr>
<tr>
<td>Patil &amp; Liburdy (2013b)</td>
<td>Random sphere packing</td>
<td>PIV</td>
<td>Jet swaying back and forth</td>
<td>418</td>
</tr>
</tbody>
</table>

\* \( Re_{\text{int}} \) in Horton & Pokrajac (2009) is based on the mean velocity at the 5 mm diameter circular window in the pore centre and the characteristic length used is 5 mm.
5.1.4 Applications of MRI in the study of unsteady flow

Being a non-intrusive technique with relatively high spatial resolution and being capable to probe the fluid flow in opaque systems, MRI has furthered our understanding of the laminar flow in packed bed reactors (Sederman et al., 1998; Johns et al., 2000; Sederman & Gladden, 2001b). Ultra-fast MRI techniques have demonstrated great potential in studying unsteady flow, including Echo Planar Imaging (EPI) and spiral imaging. Kose (1991a) first applied EPI in studying the turbulent equilibrium puff by successive acquisitions of $32 \times 32$ images and demonstrated the evolution of vortices. The first quantitative flow measurements with three orthogonal velocity components using an EPI-based technique was conducted by Sederman et al. (2004). Full velocity profiles were measured by acquiring three $64 \times 32$ images within 60 ms. The study demonstrated several turbulent pipe flow features, including the formation of turbulent eddies and low $z$-velocity fingering. The same technique was applied by Mullin et al. (2009) in studying the bifurcation phenomena in a pipe with a 1:2 expansion, and intermittent bursting of the shear layer and oscillatory motions were observed.

As discussed in §2.5.1 spiral imaging is more robust to flow artefacts than EPI because it refocuses the first moment phase accuracy periodically. The robustness has been demonstrated numerically (Nishimura et al. 1995) and experimentally (Tayler et al., 2011). High temporal resolution velocity measurements using spiral imaging was first demonstrated by Tayler et al. (2011) with a 5.4 ms acquisition time for $32 \times 32$ images. The local oscillation and translating motion of wall instabilities in turbulent pipe flow were captured. The temporal resolution was further improved by combining subsampling spiral and compressed sensing reconstruction, enabling $64 \times 64$ three-velocity components velocity maps to be acquired at 47 Hz with an acquisition time of 5.3 ms per image (Tayler et al., 2012). With the unprecedented temporal resolution, the vortex shedding in the wake of a rising bubble was successfully characterised. Tayler et al. (2014) used compressed sensing based image reconstruction to measure a liquid-liquid two phase flow simultaneously and examined the motion of a rising oil droplet through stagnant water.

5.1.5 Proper orthogonal decomposition

POD was first introduced in fluid dynamics as a mathematical technique to extract coherent structures in turbulent flow fields (Berkooz et al., 1993) and has been applied in various unsteady systems, including turbulent jets (Bernero & Fiedler, 2000), jets in cross flow (Meyer et al., 2007), swirling jets in sudden expansion (Mak & Balabani, 2007), interaction of multiple
jets (Geers et al., 2005), backward-facing step configurations (Murray et al., 2009), turbulent boundary layer flows (Gurka et al., 2006), and turbulent wakes (Tang et al., 2015). POD will decompose a time series of fluctuating velocity fields into independent components (often referred to as POD modes), which are ranked by the turbulent kinetic energy (TKE) in each mode. In some cases, the coherent structures are directly represented by the POD modes, e.g., the vortex shedding (Tang et al., 2015) or shear-layer oscillations (Duwig & Iudiciani, 2010). More commonly the interpretation is enabled by superposition of the POD modes with the mean flow field (Graftieaux et al., 2001).

POD modes reveal significant insight into the turbulent dynamics; in particular, high energy periodic motion is often captured by two POD modes related by a certain symmetry, such as translational symmetry for vortex shedding (Tang et al., 2015). The advantage of POD over spectral analysis is that the frequencies of different coherent structures can be isolated by POD. For example, the frequencies of jet-flapping ($St = 0.02$) and shear-layer oscillation ($St = 0.02 - 0.1$) were separated based on different POD modes representing the corresponding coherent structures for both turbulent jets in counterflow and confined turbulent jets (Bernero & Fiedler, 2000; Semeraro et al., 2012). On the other hand, the interpretation of different frequencies in the spectral analysis is challenging.

It is noted that the maximum TKE is not directly associated with the dynamic importance of the mode. The extended POD (EPOD) has been proposed to overcome this limitation, especially when the crucial dynamic feature is not energetically dominant. EPOD was first demonstrated by Maurell et al. (2002) in the study of the interaction of flow structures in combustion engines where the key subject of interest, the large-scale vortex, accounts for only 3% of the total kinetic energy. Based on the POD analysis of the subdomain, the motion in the entire flow fields that is correlated with the vortex dynamics is decomposed into the corresponding EPOD modes. EPOD can be used to simplify computation; e.g., Podvin et al. (2006) showed that the 3D EPOD modes based on a 2D subsection matched the 3D POD analysis closely for an open cavity flow. EPOD has also been applied to different physical quantities such that the correlation between the fluid flow and the concentration, particle motion, or pressure variation can be extracted (Borée, 2003).

### 5.1.6 Aims

Recent advances in PIV have enabled acquisitions of important new flow images of the transition to turbulent flow in porous media. However, representative 2D flow features,
including the inertial core and helical vortices, cannot be effectively studied in longitudinal planes imaged by PIV. Furthermore, the fundamental physics, especially the mechanism of the transition, were not well understood. This chapter attempts to characterise the transition process and probe its mechanism using ultra-fast MRI techniques. The aims of this chapter are:

1. To quantify the transition to unsteady flow based on global measurements.
2. To characterise the dynamic behaviour of key flow features.
3. To demonstrate the capability of POD in extracting coherent structures from MRI flow visualisation.
4. To provide insight into the transition mechanism.

5.2 Experimental method

5.2.1 Packing material selection

![Visualisation of the susceptibility artefacts in the spiral imaging and the off-resonance frequency measured for different materials.](image)

The flow rig used was described in Chapter 3 and the selection of packing material will be discussed briefly. Since spiral imaging is very sensitive to the homogeneity of the magnetic field, the magnetic susceptibility difference between water and glass is too large for high-quality spiral imaging. Given the superiority of the susceptibility property of plastics (Wapler et al., 2014), four different plastic materials (acrylic, high-density polyethylene (HDPE), polypropylene, and polystyrene) were tested and their effects on the field homogeneity were quantified by examining the off-resonance frequency. An example is given in Fig 5.1, where the region with larger off-resonance frequency (Fig 5.1(b)) corresponds to significant distortion.
in the image (Fig 5.1(a)). Based on their magnetic susceptibility, acrylic and polystyrene qualify as potential packing material. In this work, 3/16 inch (4.76 mm) diameter polystyrene beads were purchased from the Precision Plastic Ball Co Ltd.

5.2.2 Spiral imaging

The details of spiral imaging technique were introduced in §2.5. The spiral trajectory was designed using the method described by Glover (1999) and the maximum gradient (70 G/cm) and the maximum slew rate (\(S_{\text{max}} = 1.2 \times 10^6 \text{ G/cm s}\)) were determined empirically. The pulse sequence for phase contrast spiral imaging was shown in Fig 2.11(a). To reduce the acquisition time, a 256 µs Gaussian excitation pulse was used to excite spins in a 1 mm slice at different axial positions. The tip angle for the excitation pulse was selected according to the Ernst angle to increase the signal-to-noise ratio.

5.2.3 Velocity measurements

The timings of the velocity encoding gradients were minimized to increase the temporal resolution, giving a flow encoding time (\(\delta\)) of 212 µs and flow contrast time (\(\Delta\)) of 396 µs. With the timings fixed, the velocity encoding gradients (\(G_{\text{vel}}\)) were selected to optimise the sensitivity to velocity, i.e., maximizing the velocity dependent phase shift within a 2π window. 2D time-averaged measurements were taken at the axial position \(Z = 0\) mm for \(Re\) from 76 to 160 (the measurements at higher \(Re\) are inaccurate due to the unsteady flow). Based on linear interpolation, the maximum velocity was 40 cm/s in the axial direction and 18 cm/s in transverse directions at \(Re = 221\). Taking into account the inhomogeneity of flow field, the velocity encoding gradients were chosen such that the ranges of measurements were [−48, 48] cm/s and [−32, 32] cm/s for the axial velocity and transverse velocities, respectively. Reference phase maps were acquired with stationary liquid to correct the error in phase due to the image reconstruction, eddy-current, and \(B_0\) inhomogeneity.

To track the transient behaviour of the flow field, two types of measurements were conducted with successive excitations. The first type measures one velocity component by alternating the velocity encoding gradient in the direction of interest between \(−G_{\text{vel}}\) and \(G_{\text{vel}}\) while keeping the gradient in other directions zero. The second type measures all three velocity components in a group of four images with \(G_{\text{vel}}\) of (0, 0, 0), (0, 0, \(G_{\text{vel},z}\)), (0, \(G_{\text{vel},y}\), \(G_{\text{vel},z}\)), (\(G_{\text{vel},x}\), \(G_{\text{vel},y}\), \(G_{\text{vel},z}\)). Therefore, the velocity in the \(z\)-direction, \(w\), can be calculated based on the phase difference between images 2 and 1, while the velocity in the \(y\)-direction, \(v\), is the difference between
images 3 and 2 and the velocity in the x-direction, \( u \), between images 4 and 3. This design was intended to increase the accuracy by reducing the timing between the two acquisitions for each velocity encoding but the resulting measurements were subject to unsteady flow artefacts. The artefacts arise because the velocity in \( w \) is encoded in both the image 2 and 3; thus, the velocity fluctuations in \( w \) will affect the measurements of \( v \). The same applies to image 4 and the velocity fluctuations in \( w \) and \( v \) will affect \( u \). This artefact can be avoided by encoding only one velocity component in each image, using velocity encoding gradients of \((0, 0, 0)\), \((0, 0, G_{\text{vel},z})\), \((0, G_{\text{vel},y}, 0)\), and \((G_{\text{vel},x}, 0, 0)\). The experiments were repeated with a different packing using the new encoding method. In this work, the results are from the first measurements except for §5.4.5 because the artefacts were alleviated by subsampling and compressed sensing reconstruction.

### 5.2.4 Undersampling

Since reducing the acquisition time reduces the in-plane flow artefacts significantly, compressed sensing reconstruction of the undersampled data can provide more accurate measurements, especially at high \( Re \). A variable density trajectory with a Gaussian-weighted sampling density was used to preserve the high-power central \( k \)-space sampling in the spiral imaging acquisition. Imaging gradient trajectories were measured using the methods of Duyn \textit{et al.} (1998). The three different trajectories of 100\%, 50\% and 30\% of the fully-sampled rate (Fig 5.2) were used.

![Fig 5.2.](image)

**Fig 5.2.** The trajectories designed for the spiral imaging, sampling at 100\%, 50\%, and 30\% of the fully-sampled rate.

### 5.2.5 Summary of acquisition parameters

The temporal resolution is not only determined by the acquisition time but also subject to the limitation of the gradient units and writing speed of the computer. It is noted that the number
of corrupted data increases if the timing between successive acquisitions is too short. Therefore, the delay time used was slightly above the minimum time that satisfied the hardware limitations. Hence, the temporal resolution for $64 \times 64$ 2-dimensional one velocity component (2D1C) measurements was 72.3 Hz and, for three velocity components (2D3C), it was 21.1 Hz, given an acquisition time of 9.8 ms for fully sampled images. For 50% sampling, the acquisition time was 5.6 ms, and the corresponding sampling rates were 131 Hz (2D1C) and 32.7 Hz (2D3C). Because of the memory limitations, only 256 images could be recorded in a train of successive acquisitions, resulting in a maximum number of 255 2D1C and 64 2D3C velocity measurements. Given the negligible artefacts in the 2D1C measurements due to the velocity fluctuations, the statistical analysis of the flow instability was conducted using these datasets.

### 5.3 Data analysis

#### 5.3.1 Compressed sensing reconstruction

The algorithm for compressed sensing reconstruction was given in §2.6.3. The magnitude images were precomputed using the fully-sampled data, and the regularisation parameter, $\alpha$ was selected using the fully-sampled data as a reference. A number of $\alpha$ were tested for a sample of 64 images and the best $\alpha$ was chosen according to the variance level of the population that matched most closely with the fully-sampled data acquired at the same flowrate. Further visual inspection also confirmed that the best $\alpha$ achieves a balance between the denoising and smoothing.

#### 5.3.2 Pore segmentation

![Fig 5.3.](image)

Fig 5.3. Pore segmentation for the axial planes at (a) $Z = -2$ mm, (b) $Z = 0$ mm. The FOV is $18.0 \times 18.0$ mm$^2$. 
The flow maps at different axial positions have been segmented into various pores as shown in Fig 5.3. A first-pass segmentation was calculated based on a morphological thinning technique proposed by Baldwin et al. (1996), and some sections were merged manually to preserve the continuity of pore structure at different axial positions. The pores will be referred to by their number in the rest of this chapter.

5.3.3 Vortex identification

An effective vortex identification algorithm is needed to locate the position of the helical vortex and evaluate its strength. Although vorticity is high at the vortex core, vorticity alone does not distinguish between high shear region and the swirling motion. Effective and objective methods for vortex identification have been pursued by numerous studies, as vortical structure underpins the dynamics of the turbulent flow (Jeong & Hussain, 1995; Chakraborty et al., 2005; Kolář, 2007). The most widely-used methods based on local velocity gradient tensor, including the Δ criterion, Q criterion, \( \lambda_2 \) criterion, and the swirling strength are equivalent in 2D. Hence only the swirling strength was examined.

Fig 5.4. Schematic diagram for the calculation of \( \Gamma_2 \). The meaning of the symbols are given in the text.

One of the non-local criteria, \( \Gamma_2 \), proposed by Graftieaux et al. (2001) is based on the local velocity topology. This method evaluates a function around each point, \( P \), for the \( N \) points in the region \( S \) surrounding \( P \), as shown in Fig 5.4,

\[
\Gamma_2 = \frac{1}{N} \sum_{S} \frac{[PM \times (UM - UP)]}{\|PM\| \cdot \|UM - UP\|},
\]

(5.1)

where \( PM \) is the vector from \( P \) to \( M \), \( UM \) is the velocity at point \( M \), and \( UP \) is the mean velocity of all \( N \) points in the region \( S \), i.e., \( UP = \frac{1}{N} \sum_{S} UM \). \( \Gamma_2 \) differentiates whether the flow is locally dominated by strain or rotation and has been demonstrated to effectively identify the vortex
core of a Lamb-Oseen vortex with several different interrogation window sizes. This method was demonstrated by Morgan et al. (2009) to be more robust than using the vorticity and swirling strength.

The comparison between the vortex identification methods using the vorticity, swirling strength, and $\Gamma_2$ is demonstrated next. The data used for this test is the instantaneous 2D3C measurements in one of the pores at $Z = 0.5$ mm for $Re = 200$, and four such snapshots are shown in Fig 5.5(c), noted by their position in the 64 acquisitions. This example is challenging as the vortical motion and the bulk convective velocity are superposed. Moreover, the distorted vortex shape also contributes to the difficulty of vortex identification.

The disadvantage of using the vorticity is the ambiguity due to high shearing as demonstrated in Fig 5.5(a) for the 21st snapshot, where the vortex core includes the region with high shear at the bottom of the pore. Swirling strength and $\Gamma_2$ are consistent, while swirling strength is more sensitive to local velocity field, especially for highly skewed vortex, as seen in the 20th snapshot in Fig 5.5(b). Furthermore, the definition of the vortex core using swirling strength requires a threshold that depends on the velocity magnitude, while $\Gamma_2$ is a dimensionless quantity and the threshold can be chosen independent of the rotational speed.

Because of its non-local and dimensionless properties, $\Gamma_2$ was chosen for vortex identification in this application and was evaluated from an interpolated velocity field to increase the resolution to the vortex core. A threshold value of 0.6 was used and the vortex core was isolated by clustering the region above the threshold. The vortex centre was evaluated based on the
weighted average location of $\Gamma_2$ within the vortex core, and its strength was represented by the mean vorticity.

5.3.4 POD analysis

The aim of POD is to decompose a given ensemble of data into an optimal set of basis functions ($\phi$). Given a set of measurements of a scalar field $u(x, t_i)$, POD seeks the orthogonal basis functions ($\phi_k$) and their temporal coefficients ($a_k$),

$$u(x, t_i) = \sum_k a_k(t_i)\phi_k(x),$$

such that the following quantity is maximized:

$$\frac{\langle \|u, \phi\|_2^2 \rangle}{\langle \phi, \phi \rangle},$$

where $\langle \cdot \rangle$ represents ensemble average and $\langle \cdot, \cdot \rangle$ represents the inner product. By maximizing the inner product of the dataset and the basis functions, this procedure yields the optimal basis functions in the $L_2$-sense, i.e., the variance content is maximized. If $u(x, t_i)$ is a fluctuating velocity field, the reconstruction using the first N basis functions has the maximum TKE for any given number N. This problem is equivalent to finding the eigenfunctions ($\phi_k$) for the two-point correlation tensor $R(x, x') = \langle u(x)u(x') \rangle$, and the corresponding eigenvalues ($\lambda_k$) represent the variance fraction. The basis functions are often referred to as modes and are organised in a descending order according to their energy contents.

For $n$ measurements (snapshots) of the field at $m$ discrete locations, $u(x, t_i) = (u_1, u_2, \ldots, u_m)_{t_i}$, solving the eigenvalue problem for the $m \times m$ spatial correlation tensor matrix can be unfeasible given the rich spatial information from experimental and numerical studies, i.e., $m \gg n$. The Method of Snapshots transforms the problem into solving the eigenfunctions $\psi_i$ for the $n \times n$ temporal correlation tensor. Both can be realised using singular value decomposition, which is known for its robustness to round-off errors and can be easily implemented in MATLAB. The details of the method are given next.

The measurements with $n$ snapshots were organised as a $n \times m$ matrix $M$,

$$M = \begin{bmatrix} u_{1,t_1} & \cdots & u_{m,t_1} \\ \vdots & \ddots & \vdots \\ u_{1,t_n} & \cdots & u_{m,t_n} \end{bmatrix},$$

before applying singular value decomposition,
\[ M = \Psi \Sigma \Phi^T. \] (5.5)

The mode \( k, \phi_k \), is the \( k \)th vector in \( \Phi \), corresponding to the eigenvector of the spatial correlation tensor, and the eigenvalue \( \lambda_k \) is related to the singular value, \( \lambda_k = \sigma_k^2 \). The temporal coefficients of the mode \( k, a_k(t_i) = \sqrt{\lambda_k} \psi_k \), where \( \psi_k \) is the \( k \)th vector in \( \Psi \).

For 2D3C snapshots, given the additional velocity measurements of \((v_1, v_2, ..., v_m)_{t_i}\) and \((w_1, w_2, ..., w_m)_{t_i}\), each column of the corresponding data matrix is a concatenation of all three velocity vectors, i.e., \((u_1, u_2, ..., u_m, v_1, v_2, ..., v_m, w_1, w_2, ..., w_m)_{t_i}\). Therefore, the POD of the \( n \times 3m \) matrix \( M \) yields modes that optimise the TKE.

### 5.3.5 Extended POD

EPOD is an extension of POD and finds correlation between two datasets. For simplicity, the domains of the two datasets are assumed to be the same while the same procedure can be applied to different domains as demonstrated by Maurell et al. (2002). Given POD of \( u, u(x, t_i) = \sum_k a_k(t_i) \phi_k(x) \), where \( u \) is acquired at the same time \((t_1, t_2, ..., t_n)\) as \( v \). The EPOD modes, \( \phi'_k(x) \), for \( v \) is

\[ \phi'_k(x) = \frac{1}{\lambda'_k} \sum_{i=1}^n a_k(t_i) v(x, t_i). \] (5.6)

Therefore, the data \( v \) can be decomposed into the correlated and uncorrelated part, \( v_C \) and \( v_D \),

\[ v(x, t_i) = v_C(x, t_i) + v_D(x, t_i) = \sum_k a_k(t_i) \phi'_k(x) + v_D(x, t_i). \] (5.7)

It can be shown that the \( k \)th EPOD mode \( \phi'_k(x) \) represents the part of \( v \) that is correlated with the \( k \)th mode of \( u \), and EPOD modes capture the energy in the correlated part of \( v \),

\[ \langle (v(x), v(x)) \rangle = \sum_k \lambda'_k \langle (\phi'_k(x), \phi'_k(x)) \rangle + \langle (v_D(x), v_D(x)) \rangle. \] (5.8)

In summary, EPOD is useful in studying the correlated events while the extended modes are generally neither orthogonal nor optimal.

### 5.3.6 Number of snapshots

The results of POD depend on the number of snapshots since the components may not be well represented in a small population. Insufficient data size is manifested by the asymmetry of modes, especially with higher mode number, and convergence test on the number of snapshots...
needed is often conducted using a subsample of the population (Bernero & Fiedler, 2000; Meyer et al., 2007). The similarity index and the energy fraction of the modes were examined on cyclic combustion engine flow by Chen et al. (2012) and the first mode was demonstrated to be robust for a sample size larger than 20 when compared to the full population of 200. The effect of sample size is examined qualitatively on the unsteady inertial core in pore 1 at Z = -0.5 mm; Fig 5.6 shows the first three POD modes extracted from 64 random samples from a population of 255 measurements at $Re = 211$. Skewed patterns of the second modes are observed and the third modes do not resemble each other.

**Fig 5.6.** The mean axial velocity and the first three POD modes for 6 different samples with 64 snapshots from 255 2D1C $w$ snapshots for $Re = 211$ at $Z = 0$ mm. The FOV is $4.5 \times 3.7$ mm$^2$.

![Image](image.png)

**Fig 5.7.** The (a) similarity metric, (b) error in the energy fraction, and (c) relative variation of the energy fraction in the first three POD modes for different sample sizes from 255 2D1C $w$ snapshots for $Re = 211$ at $Z = 0$ mm.

The statistics extracted from 32 different subsampled populations with varying sample sizes are shown in Fig 5.7, and similar trends are observed for other $Re$ and flow features. The similarity metric is defined as the normalised inner product of $\phi_i$ of the subsampled and full population. As expected, the similarity index (Fig 5.7(a)) is much lower for the third mode while that for the first mode is larger than 0.9 using more than 48 snapshots, indicating its dynamic significance. The energy fraction of the modes (Fig 5.7(b)) is less affected by the number of modes while an over-estimation of 1-2% is often observed at the sample size of 64. The
variation (Fig 5.7(c)) evaluated are less than 15% for all three modes. In conclusion, a 10% error due to the small sample size is expected for the first two modes and the third mode may not be representative. To further address the challenge of small sample size, consistency of the POD modes between different Re and at different axial positions is used to confirm the reproducibility of the coherent structures.

**5.3.7 Spectral analysis**

The power spectrum of a time series signal, $x(t)$, describes the distribution of power with respect to the frequency components of the signal and has been widely used to characterise the strength of the periodic velocity fluctuations in unsteady flow. The power spectral density, $S_{xx}$, refers to the spectral energy distribution at a specific frequency, defined by

$$S_{xx}(f) = \lim_{T \to \infty} \left\{ \frac{1}{2T} \left| \int_{-T}^{T} x(t)e^{-i2\pi ft} dt \right|^2 \right\} \quad (5.9)$$

For $N$ discrete measurements with time increment $\Delta t$, the following discrete estimate of the integration in Eq. 5.9 is used:

$$S_{xx}(f) = \frac{1}{T} \left\{ \sum_{n=1}^{N} x(n\Delta t)e^{-i2\pi ft}\Delta t \right\}^2 \quad (5.10)$$

The spectral analysis has been implemented in MATLAB using the ‘periodogram’ function with a rectangular window.

**5.4 Results**

The results are based on the CS reconstruction of the 2D1C and 2D3C experiments using 50% subsampled acquisitions unless otherwise stated. As mentioned in §5.2.3 the same study was repeated on two different packings and the results from the first packing are reported (except for §5.4.5) because the same conclusions can be drawn from both.

**5.4.1 Global features of the onset of unsteady flow**

The transition and the level of fluctuation is first examined statistically and the normalised TKE\(^1\), $k/U_{sf}^2 = (u'^2 + v'^2 + w'^2)/2U_{sf}^2$, has been used to represent the level of unsteadiness. The normalised variance, $u'^2/U_{sf}^2$, will be referred to as the variance in the following text. In

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\(^1\) TKE is a concept from the study of turbulence. Here the same definition is used but the flow is not yet turbulent.
Fig 5.8(a-c), the area-averaged variance \( \langle (u'^2)/(U_{sf}^2) \rangle \) is shown for three different axial slices and the onset of unsteady flow is observed at \( Re = 143 \) (the other slices show very similar trend). An approximately linear increase is observed in the level of fluctuation within the slice from \( Re = 169 \); the increase rate is slower from \( Re = 143 \) to 169.

**Fig 5.8.** The area-averaged normalised variance in three velocity components for \( Z = -1.0, 0.0 \) and 1.0 mm: (a) \( u \), (b) \( v \) and (c) \( w \).

The onset of unsteady flow in packed beds is characterised by the localised development of flow instability. The localised development is shown in Fig 5.9, where the unsteady flow is only present in pores 2 and 8, while TKE is nearly zero in pore 1 at \( Re = 143 \). The area-averaged variance in the three pores shown in Fig 5.10(a-c) suggests that pore 1 remains steady until \( Re = 169 \). The ratio of the unsteady area within each pore, demarcated by the noise threshold, depicts the evolution of instability. Within a range of \( Re \) of 20-30, the unsteady area increases sharply from zero to more than 80% in the majority of the pores (Fig 5.10(d-f)), indicating that once instability starts to develop, it spreads rapidly to the entire pore. Although pores 1 and 2 are connected at \( Z = 0 \) mm, there is little fluctuation in pore 1 when the majority of pore 2 has become unsteady. In contrast, the same pore at different axial positions features the same \( Re_{crit} \).
and a similar trend of evolution, suggesting that the flow instability translates mainly longitudinally.

**Fig 5.10.** The area-averaged normalised variance in the three velocity components \((u, v, \text{and} w)\) for pore (a) 1, (b) 2, and (c) 8 at \(Z = 0\) mm, and the ratio of unsteady area at \(Z = -1.0, 0.0\) and \(1.0\) mm for pore (d) 1, (e) 2, and (f) 8 for \(Re = 113\) to 221.

The global evolution of the unsteady area is shown in Fig 5.11. The first instability within the packed bed is observed at \(Re_{crit} = 143\), which is consistent with the increase in mean TKE (Fig 5.8). Rapid expansion is observed from \(Re = 157\) to 191, after which 80% of the area has become unsteady and the rest of the steady region slowly shrinks until \(Re = 221\).

The level of fluctuation also shows significant heterogeneity. On the local level, the area-averaged variance in pore 8 is approximately two to three times that of pore 1 (Fig 5.10(a,c)); on the global scale, it is reflected by the percentage of TKE within the 10% and 20% most unstable area. It can be seen from Fig 5.11 that the 10% most unstable region accounts for about 26% to 30% of the total TKE, and the TKE in the 20% of the area can reach 50%. Furthermore, the ratios reach a maximum around \(Re = 170\) to 180, which corresponds to the late-stage of the expansion of unsteady region. The heterogeneity decreases with further development of unsteady flow.
Fig 5.11. (a,b) The ratio of unsteady area, (c,d) the percentage of TKE for the 10% most unstable area, and (e,f) the percentage of TKE for the 20% most unstable area at six different slices (a,c,e for $Z = -2, -1, -0.5$ mm and b,d,f at $Z = 0, 0.5, 1$ mm) for $Re = 113$ to 221. The most unstable area consists of pixels with the highest TKE.

The ratio of the longitudinal to lateral velocity fluctuation measures the directional variation of unsteadiness and is calculated as $\frac{w'}{V'}$, where $V = \sqrt{u'^2 + v'^2}$ represents the transverse velocity magnitude. A steady increase in the global anisotropy is observed from $Re = 132$ to 200 (Fig 5.12), and the distribution remains stable at $Re > 200$. Higher directional variation has been associated with regions that contain a large degree of accelerated flow, e.g., jet-like regions (Patil & Liburdy, 2013b). From the spatially resolved distribution in Fig 5.12(b), coherent regions with higher axial and lateral variations are observed. Moreover, by comparing Fig 5.12(b) and Fig 5.12(c), the spatial positions with higher lateral variation (negative $\log(w'/V')$) correspond to regions with higher vorticity, i.e., higher acceleration in transverse directions.
5.4.2 The unsteady behaviour of different flow features

In this section, the unsteady behaviour of different flow features is examined, including the inertial core, backflow and helical vortices, using 2-3 examples each. For each feature, a qualitative description is first given, based on the mean and individual velocity profiles. The quantitative analysis results are then presented to show the evolution of flow features with increasing $Re$.

5.4.2.1 Inertial core

Pores 1 and 2 have been chosen for studying the inertial core characteristics. The mean axial velocity profiles and the fluctuating velocity variance for pore 1 are shown at $Z = -1$, 0, and 1 mm in Fig 5.13(a,b). The contour and vector plots in this chapter are based on the mean velocity profile unless otherwise stated. The axial velocity starts fluctuating at $Re = 157$. The high variance region initiates at the edge of the inertial core and gradually spreads inwards. A coherent variance pattern is observed across the channel at different axial positions, supporting the longitudinal transport of flow instability.
It is seen from Fig 5.13(c) that the variations of the individual profiles are most significant at the edge of the vortex core, where the instability initiates. Furthermore, similar to the mean velocity profiles, the peak axial velocity decreases with $Re$.

![Contour maps](image)

**Fig 5.13.** Contour maps of (a) normalised axial velocity and (b) normalised fluctuating axial velocity variance for pore 1 for $Re = 143$ to 191 at $Z = -1.0$, 0.0, and 1.0 mm. (c) Contour maps of normalised axial velocity for pore 1 for the mean profile and four instantaneous snapshots for $Re = 143$, 191, and 221 at $Z = 1.0$ mm. The red plus sign represents the centre of the inertial core. The locations of the pores are shown in Fig 5.3. The FOV is $5.3 \times 5.1$ mm$^2$. 
Further analysis of the 255 axial velocity profiles at different \( Re \) has been conducted to quantify the unsteady behaviour and heterogeneity of inertial cores. A threshold of 3 \( U_{sf} \) has been used to define the boundary of the inertial core and its location \( (r) \) is the weighted average position based on the axial velocity, as demonstrated in Fig 5.13(c), where \( \Delta r \) is the average deviation from the mean location. The peak velocity has been calculated using the mean velocity of the 10% fastest flowing area to reduce the effect of noise. Fig 5.14 shows that the variations in the locations of the inertial cores increase for both pores follow the same trend as the variance. The heterogeneity of the inertial core, quantified by the standard deviation (std) of the axial velocity, decreases steadily with \( Re \) (Fig 5.15(a,c)). A more homogeneous inertial core is also characterised by a lower peak velocity (Fig 5.15(b,d)), and the two metrics (std and peak velocity) follow nearly the same trend. It is worth noting that the decrease begins when the flow is still steady at \( Re = 122 \), suggesting that the increasing homogeneity can arise from both the increased inertial force and velocity fluctuation. A comparison between the homogeneity due to inertial force only and the overall effect confirms that the velocity fluctuation also contributes to the increased homogeneity in the mean flow field in pore 2 (the results for this comparison is not shown here).

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**Fig 5.14.** The average deviation from the mean location and the area-averaged fluctuating axial velocity variance of the inertial core for pores (a,b) 1 and (c,d) 2 for \( Re = 122 \) to 221 and at \( Z = -1.0, 0.0, \) and 1.0 mm.
Fig 5.15. The average deviation from the mean location and the area-averaged fluctuating axial velocity variance of the inertial core for pores (a,b) 1 and (c,d) 2 for $Re = 122$ to 221 and at $Z = -1.0, 0.0,$ and 1.0 mm.

5.4.3 Backflow

Fig 5.16. Normalised axial velocity contour plots for $Re = 191$ at (a) $Z = 0.0$ mm and (b) $Z = 1.0$ mm with the backflow region highlighted. The three regions in $Z = 1$ mm are region 1 (blue), 2 (red), and 3 (black). The FOV is $18.0 \times 18.0$ mm$^2$.

Two backflow examples to be examined in detail are highlighted in Fig 5.16: one is the large recirculation cell located at $Z = -0.5$ and 0 mm, and the other consists of three pore necks surrounding a flow channel at $Z = 1$ mm. Based on Fig 5.17(a), the backflow region is persistent while the mean backflow velocity decreases with increasing $Re$. The variance profiles shown in Fig 5.17(b) indicate that the onset of unsteadiness initiates at the shear layer around the

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backflow region. With increasing $Re$, the area of the stable region shrinks, and the variance is lower at the backflow region compared to the channelling region. In Chapter 3, we concluded that the recirculation vortices form in restricted regions due to the high shear stress from the adjacent inertial core; in addition, it is observed in Fig 5.17(b) that the variance initiates at the shear layer of the adjacent inertial core. These two pieces of evidence suggest that the fluctuating inertial core is the driving force for the unsteady behaviour of backflow region.

Further quantitative analysis was conducted regarding the developing instability and change in flow characteristics. For both recirculation regions, the variation of the locations shares the same trend as the variance in the fluctuating axial velocity, as shown in Fig 5.18. For the three pore throats, the level of fluctuation is the largest for region 3 (Fig 5.19), where the variances of the adjacent inertial cores are much higher than the other two pore throats (Fig 5.17(b)), which also supports that the instability is due to the fluctuating inertial core.

Fig 5.17. Contour maps of (a) normalised axial velocity and (b) normalised fluctuating axial velocity variance for pore 1 for $Re = 143$ to 191 at $Z = 0.0$ mm (first row) and the three pore necks at $Z = 1.0$ mm (second row). The FOV is $5.9 \times 6.2$ mm$^2$ for pore 1 and $9.0 \times 8.7$ mm$^2$ for the three pore necks.
Fig 5.18. The average deviation from the mean location and the area-averaged fluctuating axial velocity variance for (a,b) the large recirculating cell at $Z = -0.5, 0.0$ mm and (c,d) the three pore necks at $Z = 1.0$ mm for $Re = 113$ to 221.

Fig 5.19. The percentage of backflow volumetric flowrate and the mean area for (a,b) the large recirculating cell at $Z = -0.5, 0.0$ mm and (c,d) the three pore necks at $Z = 1.0$ mm for $Re = 113$ to 221.
Fig 5.20 compares the level of unsteadiness in the backflow, inertial core, and the other regions. The same trend is observed for the three axial positions: velocity fluctuation is lower at the backflow region and a slightly higher fluctuation is observed in the inertial core region. Therefore, the heterogeneity of velocity fluctuation at the onset of flow instability is strongly correlated with different flow features.

Fig 5.20. The area-averaged normalised fluctuating axial velocity variance for the backflow, inertial core, and other regions for \( Re = 122 \) to 221 and for \( Z = (a) -0.5, (b) 0.0, \) and \( (c) 1.0 \) mm.

5.4.3.1 Helical vortices

Helical vortices play an important role in the transition to turbulence; Such phenomena have not been captured by PIV studies because they can only be effectively identified in the axial plane while PIV visualisations have only been conducted in the longitudinal planes. Three helical vortices in pore 6, 9, and 10 being investigated are located along a pore formed by two adjacent spheres and the wall (Fig 5.21).

Fig 5.21. Normalised vorticity (colour scale) and velocity vector (arrows) plots for \( Re = 191 \) at \( Z = 0.0 \) mm with the helical vortices highlighted pore 6 (blue), 9 (red), and 10 (black). The vector plot is the normalised transverse velocity and is dimensionless. The FOV is \( 18.0 \times 18.0 \) mm\(^2\).
Fig 5.22. Normalised vorticity (colour scale) and velocity vector (arrows) plots for pore 6, 9, and 10 at four axial positions for \( Re = 143 \) and \( Re = 221 \). The FOV are \( 5.6 \times 3.4 \text{ mm}^2 \) for pore 6 and \( 4.5 \times 2.5 \text{ mm}^2 \) for pore 9, and \( 3.7 \times 4.2 \text{ mm}^2 \) for pore 10.

As the axis of the helical vortex is along the axial direction, the vorticity based on transverse velocities can be used to quantify its rotational speed, which is twice the angular velocity (s\(^{-1}\)). Fig 5.22 demonstrates the evolution of velocity profiles along the axial direction. The size of the vortex core for a converging pore (pore 6) decreases while that for a diverging pore (pore 9 and 10) increases. Furthermore, the size and strength of the vortex core are substantially different between \( Re = 143 \) and 221.

The instability of helical vortices is demonstrated by the difference of individual velocity profiles and vorticity distribution in Fig 5.23. Compared to the stable vortices at \( Re = 143 \), there is a slight variation in the rotational speed at \( Re = 191 \). At \( Re = 221 \), the shape and location of the individual vortex core deviate from the mean profiles, especially for pore 6. Further, a higher rotational speed and smaller vortex core are observed with increasing \( Re \).
Fig 5.23. Normalised vorticity (colour scale) and velocity vector (arrows) plots for the mean profile and four instantaneous snapshots for $Re = 143, 191, \text{and } 221$ for (a) pore 6 and (b) pore 10 at $Z = 0.0 \text{ mm}$. The FOV are the same as Fig 5.22.

The observed unsteady features are quantified accordingly, including the moving vortex centre ($\Delta r$), the fluctuation in the strength ($\omega'_z/\overline{\omega_z}$), and varying size ($A'/\overline{A}$). The trend of unsteadiness is measured by TKE in Fig 5.24(d) and is consistent with the unsteady features of the helical vortex (Fig 5.24(a-c)). $\Delta r$ and $A'/\overline{A}$ become significant after $Re = 160$, corresponding to the onset of the velocity fluctuation. It is shown in Fig 5.24(e,f) that, with increasing $Re$, the size of the vortex core decreases nearly linearly and the rotational velocity increases in general. Additionally, the relative variation of the vortex strength and size (Fig 5.24(b,c)) are consistent at different axial locations while the mean vorticity and area of the helical vortex vary significantly along its axis. In pores 6 and 9, the unsteady characteristics of the vortices are also consistent axially, suggesting that the unsteady behaviour is coherent along a helical vortex despite the changing pore geometry.
Fig 5.24. (a) The average deviation from the mean location, (b) the percentage of fluctuation of the mean vorticity and (c) the relative standard deviation of the area of the vortex core, (d) the area-averaged normalised TKE, (e) the average normalised mean vorticity and (f) the average area for the helical vortex in pore 10 at four different axial positions for $Re = 122$ to 221.

A more detailed examination of the velocity profiles in radial coordinates for the same helical vortex was conducted. Fig 5.25 demonstrates the instability features resolved in polar coordinates, where $u_x$, $u_r$, and $u_\theta$ are the axial, radial, and angular velocity, respectively. One prominent feature is the significantly lower velocity fluctuation at the vortex core, which is consistent at all $Re$ (except for the axial velocity at the highest $Re$). Local maxima are observed in $u_\theta^2$ and $u_r^2$ at $r\approx0.25D_p$, which correspond to the high velocity variance near the pore wall, as shown in Fig 5.25(b,c). Significantly higher $u_r^2$ is observed at the bottom of the vortex where there is entrainment due to the in-plane jets and the high shear stress at the edge of the vortex. Besides the inhomogeneity, the instability also features anisotropy: the axial velocity
fluctuation $u'_z$ is about half of $u'_\theta$ and $u'_r$ (Fig 5.25) while the mean value of $u_z$ is twice as high (not shown).

Fig 5.25. (a) Normalised fluctuating axial, tangential, and radial velocity variance (colour scale) and velocity vector (arrows) plots from $Re = 169$ to 221. The FOV is $3.7 \times 4.2 \text{ mm}^2$. (b-d) The radial distribution of azimuthally averaged normalised fluctuating axial, tangential, and radial velocity variance at $Z = 0.0$ mm for pore 10.

5.4.4 Coherent structures in unsteady flow

The coherent structures identified from the POD modes include the flapping jet, unstable inertial core, unsteady vortex, and vortex shedding. In this section, the capability of POD in extracting the coherent structure is demonstrated first. Then the application of extended POD is discussed.

5.4.4.1 Flapping jet

Jet flapping has been identified and captured by POD. The flapping jet is represented by the first POD mode shown in Fig 5.26. The representative snapshots are the snapshots that have the highest positive and negative mode 1 coefficients. The positive mode 1 corresponds to a high-speed jet in the axial direction and the negative mode 1 captures the jet tilting towards the top of the pore. Fig 5.27 shows the first POD modes for different $Re$ and the increasing axial
velocity magnitude from \( Re = 157 \) to 180 in the first mode suggests that the flapping jet motion becomes more dominant in terms of TKE. Moreover, highly consistent first POD modes are extracted from 64 2D3C snapshots from \( Re = 180 \) to 221.

**Fig 5.26.** The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the first POD mode (first column) and the representative snapshots (second to fourth columns) in pore 3 for \( Re = 200 \) at \( Z = -0.5 \) mm. The FOV is \( 3.1 \times 5.1 \) mm\(^2\).

**Fig 5.27.** The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the mean velocity and the first POD mode in pore 3 for \( Re = 157 - 221 \) at \( Z = -0.5 \) mm. The FOV is \( 3.1 \times 5.1 \) mm\(^2\).
5.4.4.2 Inertial core

**Fig 5.28.** The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the first two POD mode (first column) and the representative snapshots (second to fourth columns) in pore 1 for $Re = 200$ at $Z = -0.5$ mm. The FOV is $4.5 \times 3.7$ mm$^2$.

The dynamic behaviour of an inertial core is showcased to demonstrate coherent structures in transverse velocity fluctuations. The first two POD modes and representative snapshots are shown in Fig 5.28 for $Re = 200$. The snapshots with positive mode 1 coefficients feature an elongated inertial core and the central jet is directed towards the left in the negative mode 1 snapshots. The variation in the transverse velocity at the bottom left of the pore is highlighted by mode 2. In the positive mode 2 snapshots, the inertial core is directed towards the top left, while for the negative mode 2, the bottom left of the inertial core features a vortical structure, which is likely to represent a shear layer vortex. Similar results are shown at other $Re$.

5.4.4.3 Unsteady vortex

In pore 8, the first POD mode reveals an unsteady vortex. Fig 5.29 shows that the unsteady vortex is present at different axial positions. A clockwise vortex can be seen in the representative positive mode 1 snapshots, whereas, for those dominant by negative mode 1, there is no such structure. It is likely an unsteady helical vortex formed when the fluctuating centrifugal force exceeds a critical value. The unsteady vortex is also persistent for different $Re$, and Fig 5.30 shows the first two POD modes at $Z = -0.5$ mm. It is worth noting that the vortex structure is in mode 2 for $Re = 180$, indicating that it is not the most energetic structure. Furthermore, the flow profiles for the first mode are substantially different for the higher $Re$ and it might be due to mode mixing as the flow becomes more chaotic.
Fig 5.29. The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the mean profiles and representative snapshots in pore 8 for Re = 211 from Z = -1.0 to 1.0 mm. The FOV is 3.9 × 4.2 mm².

Fig 5.30. The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the mean profiles and the first two POD modes in pore 8 for Re = 157 - 221 at Z = -0.5 mm. The FOV is 3.9 × 4.2 mm².

The lack of consistency at different Re due to mode mixing can be addressed by applying the extended POD. As shown in Fig 5.31, the first EPOD modes based on $u'$ all correspond to the vortical feature and there is better consistency than Fig 5.30. The effectiveness of EPOD in extracting the coherent structure implies that the unsteady vortices correlate highly with $u'$ but may not be the most energetic feature at all Re. The other possible reason is the limited number of snapshots. Because only 64 snapshots are available, some modes that occur intermittently can mix with the mode of interest, i.e., the unsteady vortex mode.
Periodic vortex shedding

The application of POD to characterise periodic features is demonstrated in this section and its implication in the instability mechanism is interpreted from the characteristic frequencies. In one of the pores, the local flow topology changes significantly at the onset of unsteady flow, as shown in Fig 5.32. A Hopf bifurcation represented by vortex shedding is identified at $Re = 158$ and Fig 5.33 shows the cross sections of the von Karman vortex street within two cycles. At $Re = 168$, the quasi-periodic behaviour is observed at higher frequencies. The unsteady feature is the emerging counter-rotating vortex, which travels towards the top left and merges with the stronger vortex. Three cycles are shown in Fig 5.34 with the unsteady vortex highlighted. The vorticity of the stronger stationary vortex increases after the vortex shedding (0.18, 0.32, and 0.5 s in Fig 5.34), which can be explained by the increase in angular momentum when two equal-signed vortices merge. Overall, by comparing the corresponding instantaneous profiles with the mean velocity profiles in Fig 5.32, the dominant flow feature evolves from a stable clockwise vortex ($Re = 148$) to an unstable counter-clockwise vortex ($Re > 158$). The flow profiles oscillate between the two via vortex shedding at $Re = 158$. Similar transition and periodic features are also observed at $Z = -0.5$ mm.
Fig 5.32. The normalised axial velocity (colour scale) and velocity vector (arrows) plots at \(Z = -0.5\) and 0.5 mm for \(Re = 148\) to 178. The FOV is \(3.1 \times 3.6\) mm\(^2\).

Fig 5.33. The normalised vorticity (colour scale) and velocity vector (arrows) plots for 24 snapshots of the vortex shedding region for \(Re = 158\) at \(Z = 0.5\) mm. The FOV is \(2.3 \times 2.5\) mm\(^2\).

Fig 5.34. The normalised vorticity (colour scale) and velocity vector (arrows) plots for 15 snapshots of the vortex shedding region for \(Re = 168\) at \(Z = 0.5\) mm. The counter-rotating vortex highlighted with the red box. The FOV is \(4.2 \times 4.2\) mm\(^2\).

The periodic behaviour can be better quantified by the POD. Two symmetrical POD modes are observed at \(Re = 158\) and their temporal coefficients, shown in Fig 5.35(a), characterise the periodic motion. The snapshots at the beginning and middle of each cycle in Fig 5.35(c) demonstrate that the two POD modes have the capability of representing periodic dynamics. At \(Re = 168\), the first mode captures the shedding of the unsteady counter-clockwise vortex (Fig 5.35(d)) and the irregularity in the periodic motion is seen from the variation of temporal
coefficients in Fig 5.35(b). The irregularity is also observed in the loss of symmetry and the increased disparity of the energy content in the first two modes, similar to that observed by Van Oudheusden et al. (2005) for vortex shedding with different incidence angles in the wake of a square-section cylinder.

**Fig 5.35.** The temporal coefficients for the first two POD modes for (a) $Re = 158$ and (b) $Re = 168$ at $Z = 0.5$ mm. The normalised axial velocity (colour scale) and velocity vector (arrows) plots of the vortex shedding region at the time points highlighted in (a) and (b) are shown in (c) and (d), respectively. The corresponding vorticity pattern can be found in Fig 5.33 and Fig 5.34. The FOV is $3.1 \times 3.6$ mm$^2$.

Based on 255 2D1C consecutive measurements of $u$ at $Z = -0.5$ mm, the power spectral density for different $Re$ of the temporal coefficients of the first POD mode is shown in Fig 5.36. Although the TKE within the pore at $Re = 148$ is below the noise threshold and the first mode accounts for only 12% of TKE compared to 42% at $Re = 158$, the dominant frequency, $f_1 = 2.2$ Hz is distinguished. This may be due to weak oscillation of the stationary eddy before vortex shedding commences at $Re = 158$ at the same frequency. At $Re = 168$, the peak at 2.2 Hz is much weaker and the second mode of instability at $f_2 = 5.2$ Hz initiates. A peak at $f_1 + f_2 = 7.4$ Hz can be seen from $Re = 168$ to 208. The broadband of frequencies in the spectra at $Re > 208$, as shown by the spectrum at $Re = 217$ in Fig 5.36, indicates the onset to the chaotic regime. From $Re = 168$-208, the PSD shows quasi-periodic characteristics whilst further evidence is required to determine whether there is a torus bifurcation as predicted by Hill & Koch (2002).
Fig 5.36. The power spectral density for the temporal coefficients of mode 1 at $Z = -0.5$ mm for $Re = 148, 158, 168, \text{and} 217$.

5.5 Discussion

5.5.1 Global features of the onset of unsteady flow

The statistical analysis of the global behaviour of the onset of unsteady flow adds further insight to the results reported in the literature. First, the variation of the $Re_{\text{crit}}$ in the micro-electrode studies can be explained by the heterogeneous initiation of flow instability. The expansion of the unsteady area occurring within a narrow range of $Re$ ($Re = 157-191$) is consistent with the difference between the upper and lower bound of $Re_{\text{crit}}$ by point measurements, as summarised in Table 5.1. Moreover, the initiation of unsteady flow being limited by the pore space is demonstrated for the first time, which provides corroborating evidence for the underlying assumption in most turbulent models in porous media that turbulence is limited by the pore-scale (Nield, 2001; Jin et al., 2015; Jin & Kuznetsov, 2017).

One contradictory piece of evidence is reported by Khayamian et al. (2017), who attributed the sharp increase in velocity fluctuation from $Re = 16$ to 33 to the onset of instability. On the contrary, Patil & Liburdy (2012) reported that the flow was steady at $Re = 25$. Furthermore, the onset of instability in various regular packings are also much higher than this regime (Table 5.2), and there is no other experimental evidence of the instability at the low $Re$ range (16-33).
Therefore, we conclude that the transition from steady to unsteady laminar regime is likely to be in the range $Re = 100 – 150$ depending on the bed structure.

### 5.5.2 The unsteady behaviour of different flow features

For all the flow features observed, different unsteady characteristics, including both the macroscopic and microscopic features, demonstrate highly consistent trends. The macroscopic characteristics include the location, size, and strength of the pore-scale features, while the microscopic feature is the local velocity fluctuation. By examining their characteristics along the axial direction within the pore space, the longitudinal coherence of the instability is seen for the inertial core, recirculation, and helical vortices. Furthermore, the heterogeneity in the level of fluctuation is related to the flow features; e.g., Fig 5.20 emphasised that the velocity fluctuation is lower in the recirculation region, same as that observed by Patil & Liburdy (2013a).

The relationship between the helical vortices and swirling flow is now discussed. The formation of the helical vortices in the packed bed, as a result of the converging pore, resembles the tangential injector (Alekseenko et al., 1999; Zhang & Hugo, 2006) and swirl generator (Grundmann et al., 2012), which are widely used to create swirling flow in pipes or combustion engines. The mean velocity profiles and unsteady features are similar to the swirling flow reported in the literature (Kitoh, 1991; Chang & Dhir, 1994; Rocklage-Marliani et al., 2003; Zhang & Hugo, 2006). For example, the low variance at the vortex core was explained by the stabilising centrifugal force in the vortex core by Kitoh (1991) and Chang & Dhir (1994). In addition, the higher velocity fluctuation at the pore wall is consistent with the dominant turbulence production due to wall boundary layer, as shown by several experimental studies (Kitoh, 1991; Chang & Dhir, 1994; Rocklage-Marliani et al., 2003).

Regarding the unsteady features, the temporal variation of the vortex core centre is also widely observed in swirling flows, often referred to as the precessing vortex core. The phenomenon has been studied extensively as a major mode of vortex breakdown in combustion engines and is characterised by the periodic oscillation of the forced vortex region (Syred & Beér, 1974; Syred, 2006). On the other hand, the helical vortices in the packed bed are much weaker and the unsteady motion lacks periodicity. The difference is due to the low swirl number in the packing, defined as the ratio of the momentum flux of tangential velocity to the momentum flux of axial velocity across the transverse plane.
In practice, helical vortices are often introduced in heat exchangers to improve heat transfer (Chang & Dhir, 1995). Therefore, a particular configuration of sphere packings or a specific packing structure can be implemented to promote the formation of helical vortices for heat transfer enhancement. Moreover, the heterogeneous and anisotropic velocity fluctuation in packed beds result in local variations of transport properties. To summarise, the presence and influence of the helical vortices on the local heat and mass transfer are of interest to the design and optimisation of packed bed reactors.

5.5.3 Periodic behaviour in random packing

Scarce experimental evidence exists for periodic unsteady flow behaviour in porous media, especially in random structures, thus the comparison can only be made with relevant flow features in other configurations. The dimensionless frequency of a flapping jet reported experimentally in the literature is $St = 0.02 - 0.03$ (Bernero & Fiedler, 2000; Semeraro et al., 2012). In this study, the flapping jet mode (§5.4.4) shows a dominant frequency at $Re = 180$ being 0.9 Hz. Using the sphere diameter as the characteristic length and the mean velocity of the jet ($3U_{st}$) as the characteristic velocity, $St$ in this study is 0.036, similar to the range in the literature. However, at higher $Re$, no dominant frequency is identified.

The vortex shedding in the unbounded flow at the wake of a sphere has been widely studied and the dimensionless frequency, $St$, was reported to be in the range 0.15-0.17 at $Re_{int} = 300-420$ (Sakamoto & Haniu, 1990). In this work, the equivalent phenomenon occurs at $Re = 158$, i.e., $Re_{int} = 343$, and $St = 0.15$, which is similar to literature values. However, $St$ of further bifurcation at $f_2$ and $f_3$ are 0.32 ($Re = 168$) and 0.36 ($Re = 198$), much higher than the expected range. Similarly, for the vortex shedding observed in a complex rod bundle (Dybbs & Edwards, 1984) and predicted by 2D LBM simulation in a cylinder array, where $St = 0.8$ (Koch & Ladd, 1997), the frequencies are at $St = 0.8-1.5$ and $St = 0.8$, respectively, which are higher than the unbounded flow ($St = 0.12$ to 0.18) (Sakamoto & Haniu, 1990). Koch & Ladd (1997) hypothesized that the phenomenon arises from the smaller vortex size, compared to the unbounded flow, due to the confinement of the adjacent cylinders. The flow instability in the flow through FCC packing was predicted by Hill & Koch (2002) to initiate via a supercritical Hopf bifurcation at $Re_{int} = 120$, and a torus bifurcation with three incommensurate oscillations is seen at $Re_{int} = 198$, which evolves to a chaotic dynamic at $Re_{int} = 205.2$. The experimental evidence in this work supports the numerical predictions in structured packings that the transition to turbulence develops from steady to periodic, quasi-periodic, and chaotic regimes.
5.6 Conclusion

The characteristics and mechanism of the onset of unsteady flow in a randomly packed bed of spheres were studied experimentally using spiral imaging. The packing material was susceptibility matched to minimize off-resonance artefacts. Combined with sparse acquisition data sampling and compressed sensing reconstruction, 2D3C velocity maps were acquired at 33 Hz and 2D1C measured at 131 Hz when subsampling at 50% of the Nyquist rate. The analysis targets the four aims and the corresponding concluding remarks are the following:

1) A global $Re_{\text{crit}}$ was identified for the transition and is consistent with the range of $Re_{\text{crit}} = 100-150$ in the literature. The onset of unsteady flow is highly heterogeneous due to the asynchronous instability initiation in different pores. The heterogeneity of the velocity fluctuation reaches a maximum at $Re = 170-180$ when approximately half of the area transits to the unsteady regime. During the transition, the unstable region expands rapidly within each pore. It is the first time that this process has been revealed.

2) The characteristics of the key flow features, including inertial cores, recirculation regions, and helical vortices, were examined. With increasing $Re$, the inertial effect results in more homogeneous velocity profiles and lower peak velocity for the inertial cores. The unsteady features of helical vortices include the moving vortex centre and the fluctuating vortex core strength and size. Based on the radial inhomogeneity of unsteady helical vortices, the stabilising effect in the vortex core and the instability due to wall shear layer are identified. For all the flow features, a comparison across different axial slices indicates that the instability translates in the longitudinal direction.

3) Proper orthogonal decomposition (POD) analysis has been conducted to reveal the coherent structures in unsteady flow, including the flapping jet, inertial core fluctuation, unsteady vortex, and vortex shedding. Extended POD was demonstrated to be useful in extracting coherent structures with small sample size.

4) The characteristics of the vortex shedding provide the first experimental evidence that the evolution of flow instability occurs via a periodic, quasi-periodic to chaotic route. Further evidence and a more detailed picture are presented in the next chapter via the investigation in a structured packing.
Chapter 6 Onset of flow instability in simple cubic packing

6.1 Introduction

There are two unsteady flow regimes in porous media: the unsteady laminar and turbulent regimes. Due to the complexity of the physical phenomena, the nature of the unsteady flow in porous media has been a standing question. Recently, several studies have focused on the transition to turbulence in porous media (Horton & Pokrajac, 2009; Patil & Liburdy, 2012; Khayamyan et al., 2016), but little is known regarding the onset of unsteady flow. In this chapter, we focus on the instability mechanism and the characteristics of the early unsteady regime in a regular porous medium. We chose to focus on simple cubic packing (SCP) because of the availability of previous experimental studies. In this section, we first inspect the previous work related to the mechanism of flow instability in packed beds, then we review the canonical wake instability and some recent theoretical and numerical findings on instability mechanism. Finally, the dynamic mode decomposition (DMD) is introduced.

6.1.1 Instability mechanism in packed bed

The earliest experimental observation of unsteady laminar regime is from Dybbs & Edwards (1984), who reported laminar wake oscillations in the form of travelling waves of different periods, amplitudes, and growth rates in a complex cylinder packing. By analysing movies of streaklines using dye injection, the frequencies of the wake oscillations were obtained at several Reynolds numbers \( Re = \frac{U_{\text{int}} D_p}{\nu} \), where \( U_{\text{int}} \) is the interstitial velocity, \( D_p \) is the particle diameter, and \( \nu \) is the kinematic viscosity). At \( Re \) from 200 to 250, the dimensionless frequency, Strouhal number, \( St = \frac{f D}{U_{\text{int}}} \) (\( f \) is the frequency) decreased from 1.5 to 1.3, whilst at \( Re > 250 \), \( St \) oscillated at about 0.9. The formation of vortices from \( Re = 250 \) was shown clearly, but the vortex shedding frequencies were not obtained. The authors suggested that the transition to unsteady flow in the rod bundle geometry was due to a laminar, wake instability. Wake instability was also observed in aligned cylinder arrays using lattice-Boltzmann methods (LBM) simulations by Koch & Ladd (1997), and the frequency of the characteristic vortex shedding was shown to be higher than that of an unbounded flow. The
authors proposed that this was due to the confinement of the flow by neighbouring cylinders, which gave rise to smaller vortices that were shed more frequently.

Two representative studies examining the transition in a face-centered cubic (FCC) packing using LBM are Reynolds et al. (2000) with flow along (1,1,1) direction and Hill & Koch (2002) along the (1,0,0) direction. The critical Re at the onset of different unsteady flow regimes are shown in Table 6.1.

Table 6.1 Critical Re corresponding to the transition of flow regimes using LBM in FCC for flow at different directions.

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<td>Periodic fluctuations in the stream-wise direction</td>
<td>56</td>
<td>~120</td>
</tr>
<tr>
<td>Periodic fluctuations in the all directions</td>
<td>~80</td>
<td>~180</td>
</tr>
<tr>
<td>Quasi-periodic fluctuations</td>
<td>88</td>
<td>198</td>
</tr>
<tr>
<td>Chaotic flow</td>
<td>~160</td>
<td>205.2</td>
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Fig 6.1. A schematic diagram of the periodic velocity fluctuations in FCC. The plus and minus signs indicate the direction of rotation within the vortices identified by the circle (Hill & Koch, 2002).

Hill & Koch (2002) predicted that the first bifurcation was a Hopf bifurcation characterised by the interaction of vortices, which is illustrated in Fig 6.1. The schematic diagram describes the
vortical motion in the transverse plane with the maximum cross-sectional area (CSA). The steady state flow consisted of four pairs of counter-rotating vortices, as shown in Fig 6.1(a). When the flow was perturbed with a net rotation in the axial direction, the vortices of the opposite rotation were attracted to the centre (Fig 6.1(b,c)). After the coalescing of the attracted vortices, the net rotation was reversed (Fig 6.1(d)). A torus bifurcation was predicted at $Re = 98$, which was different from the period-doubling route to chaos in arrays of aligned cylinders (Koch & Ladd, 1997). The quasi-periodic regime exists in a narrow $Re$ range, as the chaotic behaviour commenced at $Re = 102.6$. Furthermore, the symmetry, broken in the quasi-periodic regime, was regained in the chaotic regime.

In the periodic regime, the amplitude of the fluctuating axial velocity grew with $(Re - Re_{crit})^{1/2}$; thus, the authors suggested that this was a supercritical Hopf bifurcation. The amplitude then decreased after the onset of chaotic flow at $Re \sim 100$ before increasing again at $Re \sim 140$. The strengths of the axial and transverse velocities were comparable in magnitude from the onset of chaotic motion.

Periodic motion was also predicted in the numerical study using the finite volume method by Finn et al. (2012) in an SCP. At the steady regime ($Re = 230$), there were four recirculation regions with multi-lobed vortex ring structures in each pore (the axis-symmetrical recirculation vortex is often referred to as a vortex ring). In the unsteady laminar regime ($Re = 600$), there were two lobes in each pore, and the location of the two lobes alternated in neighbouring pores. Vortex shedding of the vortex ring occurred at $St = 1.02$. This periodic motion is similar to the vortex shedding in the wake of a single sphere, especially the one-sided shedding (see §6.1.2).

To summarise, the periodic behaviour has been predicted numerically in sphere packings in several studies; however, currently there is no experimental validation.

### 6.1.2 Wake instability

Based on the studies in packings, a resemblance of the instability in porous media to bluff body wake instability is suggested. This led us to examine the characteristics of wake instability behind spheres.

The wake structure and dynamics of flow past a single sphere have been widely studied due to its significant theoretical importance and wide application in industrially relevant flows, such as the particle-laden fluid. The instability mechanism and vortex structures are reviewed by Kiya et al. (2001). The $Re$ is determined by the free-stream velocity and the sphere diameter.
The steady state flow topology is characterised by an axisymmetric torus-shaped vortex ring, as a result of boundary layer separation, and the size of the recirculation region increases with $Re$ (Taneda, 1956). Symmetry breaking bifurcation has been observed experimentally and numerically at the wake behind a sphere at $Re = 210$ (Sakamoto & Haniu, 1990; T. A. Johnson & Patel, 1999). This bifurcation corresponds to a transition from steady axisymmetric wake to steady non-axisymmetric, double-thread wake with plane symmetry (T. A. Johnson & Patel, 1999).

At $Re = 270-350$, a second bifurcation occurs, where one-sided hairpin shaped vortices begin to shed periodically, whilst preserving the reflectional symmetry. Further instability causes a loss of planar symmetry when the orientations of the hairpin vortices begin changing from cycle to cycle. Another transition occurs with increasing irregularity in the vortex shedding, where the vortex shedding location and orientation start varying. The flow is entirely laminar until $Re = 650$ when the hairpin vortices transit from laminar to turbulent. Kelvin-Helmholtz instability at the separated shear layer starts to develop at $Re = 800$ and was at a higher frequency than the vortex-shedding.

Given the brief review, we then compare the difference from the transition in packings to wake flow behind a single sphere. First, the transition in FCC (§6.1.1) is different in two aspects: (i) the range of $Re$ of the periodic regime is narrower in FCC, and (ii) $Re$ is lower for the transition to the chaotic flow in FCC (Hill & Koch, 2002). In the cylinder bundle the characteristic frequencies did not increase monotonically with $Re$ (Dybbs & Edwards, 1984), whereas a monotonic increase in the frequency is observed in the wake of a single cylinder (Sakamoto & Haniu, 1990). Moreover, a wide spectrum of frequency in the random sphere packing was predicted by the CFD study by Finn et al. (2012). Such higher dimensional dynamical behaviour is likely a result of complicated interactions of the wake of multiple spheres. Yoon & Yang (2009) conducted a numerical study by systematically varying the relative positions of two spheres. Ten distinct flow patterns were reported with $St$ from 0.09 to 0.15 for the dominant vortex shedding, and multiple dominant frequencies arised from the mutual interference of the wakes. Even with the simpler system of two adjacent cylinders, complicated wake interaction and numerous vortex shedding patterns were shown experimentally, as reviewed by Sumner (2010). In conclusion, there are similarities and differences compared to the wake instability; however, further experimental evidence on the unsteady flow in porous media is required to address the discrepancies.
6.1.3 Travelling waves in a square duct

A brief review of travelling wave (TW) solutions in a square duct will be given as similar characteristics are found in this experimental study. Recent advances have been made in studying turbulent flow via a dynamical system approach and the invariant solutions to the full Navier-Stokes equation are not only significant for understanding the transition to turbulence but also provide insight into the fully turbulent flow (Kawahara et al., 2011). TW solution is one of the invariant solutions and has been found in many wall-bounded flows, such as plane Couette, plane Poiseuille, Hagen-Poiseuille, and square-duct systems. The most significant structural features of TWs include the streamwise vortices and streaks (Waleffe, 1998).

More recently, TW solutions have been found in pipe flows (Wedin & Kerswell, 2004), which were first confirmed experimentally by Hof et al. (2004) using stereoscopic high-speed particle image velocimetry (PIV). Although the observed states did not sustain a full periodic cycle in the turbulent puffs, the symmetrical high-velocity streaks at the wall and the streamwise vortices showed a striking similarity to the theoretical solutions. Such structures were also found in fully-developed turbulent pipe flow (Dennis & Sogaro, 2014; Hellström & Smits, 2014).

Some of the TW solutions in a square duct are shown in Fig 6.2. Uhlmann et al. (2007) conducted a DNS study on the marginal turbulent states in a square duct, and two symmetrical marginal states with four coherent vortices were revealed at the onset of turbulence. The authors conjectured that the secondary flow is the statistical average of the two symmetrical coherent structures. The two coherent structures consist of a pair of counter-rotating vortices and a low-velocity streak at the centre of the two facing walls (i.e., ‘active’ wall). The TW solution was further pursued by Biau et al. (2008) by applying optimal perturbation to a steady laminar solution. The four-vortex structure was isolated in a TW solution by Wedin et al. (2009), as shown in Fig 6.2(a,b). The instantaneous snapshots of the edge states identified by Biau & Bottaro (2009) (Fig 6.2(c)) were asymmetrical, where there were two pairs of vortices at the ‘active’ wall, similar to the edge states in pipe flow (Pringle & Kerswell, 2007).

Uhlmann et al.(2010) found a TW solution (Fig 6.2 (d,e)) with simultaneous presence of streamwise vortices and streaks at each wall. They emphasized the similarity between the TW solution and with the secondary flow features in the turbulent flow in square duct. Furthermore, based on the recent experimental study using laser Doppler velocimetry (Owolabi et al., 2016) at even higher $Re$, it can be speculated that additional TW solutions with distinct vortex patterns
(4, 6, 8, ... vortices and 5, 7, 9, ... high- and low-speed streaks per edge) progressively occur with increasing $Re$.

**Fig 6.2.** The instantaneous disturbance velocity field at (a) the turning point and (b) mean flow with contours representing the streamwise velocity fluctuation of the TW at $Re = 598.2$ (Wedin et al., 2009). (c) Instantaneous secondary flows of the solution on the edge by Biau & Bottaro (2009). (d) The isosurfaces of the streamwise velocity ($0.55 u_{max}$) and streamwise vorticity ($0.55 \omega_{max}$) and (e) the mean primary flow of the lower branch solution at $Re \sim 1400$ by Uhlmann et al. (2010).
6.1.4 Dynamic mode decomposition

Modal analysis is a class of techniques to extract energetically and dynamically important features from fluid flow. POD is the most widely used data-based modal analysis methods, and yields orthogonal modes that capture the maximum variance in the data with the least number of modes. However, the POD modes that maximise the variance might not be significant dynamically. DMD, which can overcome this challenge, has gained popularity in the past ten years. It was first proposed by Rowley et al. (2009) and Schmid (2010) based on spectral analysis of a linear operator, known as the Koopman operator, which approximates any nonlinear system with an infinite number of linear operators. DMD is a data-based approach for estimating Koopman eigenvalues and modes, which are often referred to as DMD eigenvalues and DMD modes. DMD aims at decomposing the time series data into oscillatory components: the DMD modes are spatial fields corresponding to the coherent structures, and the associated eigenvalues represent the growth/decay rate and oscillation frequency. In addition to the temporal periodicity, Schmid (2010) also demonstrated that DMD is capable of extracting spatially oscillatory patterns from PIV measurements.

Over the past decades, DMD has been applied to numerous flow systems on both numerical simulations, particularly DNS and large eddy simulation, and experimental results, from Schlieren to PIV snapshots. Rowley & Dawson (2017) summarised a non-exhaustive list of the applications and selected examples will be briefly discussed here. When the flow behaves as a periodic oscillator, POD and DMD may yield similar results. For TWs, a phase difference of $\pi/2$ is present in the two associated POD modes, and they resemble the real and imaginary parts of the single DMD mode. This relationship was shown in the vortex shedding (K. K. Chen et al., 2012), jet between two cylinders (Schmid, 2010), and transitional water jet (Schmid et al., 2012). DMD identifies the frequency and growth rate of the oscillator, thus generating dynamically more coherent information than POD. For example, in the turbulent confined jet, oblique structures originating from the wall were present in the DMD modes representing the jet flapping motion, which were significant to the dynamics of the boundary layer, while such structures were absent from the POD modes (Semeraro et al., 2012).

The relationships between DMD and other modal decomposition methods have been discussed in literature. In addition to the direct link of DMD with Koopman operator theory, Tu et al. (2014) also established its connection with eigensystem realisation algorithm and linear inverse modelling. K. K. Chen et al. (2012) demonstrated that DMD is equivalent to the temporal
discrete Fourier transform when the mean of the data is subtracted. Furthermore, DMD is capable of yielding meaningful information beyond the Nyquist frequency constraint (Semeraro et al., 2012; Tu, Rowley, Kutz, et al., 2014; Brunton et al., 2015).

The DMD algorithm has been thoroughly explored by several authors, and numerous variants were proposed to address specific shortcomings or extend the capabilities of DMD. A tractable and robust realisation of DMD, as a variant of the Arnoldi algorithm, often consists of projecting the linear operator onto a POD basis to overcome the rank-deficiency in the data (Rowley et al., 2009; Schmid, 2010). However, the rank of the data is ambiguous; the variants of DMD algorithm to overcome this challenge include optimal mode decomposition (Wynn et al., 2013), optimised DMD (K. K. Chen et al., 2012), and sparsity-promoting DMD (Jovanović et al., 2014). Furthermore, the effect of noise was quantified empirically (Duke et al., 2012), and Dawson et al. (2016) and Hemati et al. (2017) explained this effect theoretically and proposed modifications to the algorithms to improve its robustness to noisy data.

6.1.5 Aims

The understanding of the origin and development of instability is of fundamental importance, both theoretically and practically. One of the biggest hurdles is the lack of experimental evidence. Therefore, a representative packing, SCP, is chosen to investigate this transition process and explore the connections with the latest dynamical system theory. The experimental results of the onset and development of unsteady flow in an SCP flow channel will be presented in this chapter to address the following targets:

(1) To investigate the route to chaos and identify the critical Re during the transition.
(2) To characterise the dynamic features and validate the observations found in numerical studies.
(3) To extract the coherent structures and investigate the transition mechanism.

6.2 Experimental method

A schematic of the experimental set-up is shown in Fig 6.3 (a), where gravity-driven flow with constant pressure head was established through an SCP flow cell; the pressure head was from 4-23 kPa for different flowrates. The complex structure is enabled by the state-of-the-art 3D printing technology and was printed by Projet 3500 HDMax at the highest resolution of 16 µm using the specially engineered VisiJet® M3 material. The computer-aided design (CAD) model
is demonstrated in Fig 6.3 (b) and it consists of 10 unit cells, as shown in Fig 6.3 (c). The imaging region was located at the 7th and 8th unit cell to avoid the entrance effect, which persisted in the first 4-5 layers in the turbulent gas flow (Van der Merwe & Gauvin, 1971).

The experiments in SCP followed the same procedure as described in Chapter 5. The 4 images for the three velocity components measurements were acquired at $G_{vel}$ of (0, 0, 0), (0, 0, $G_{vel,z}$), (0, $G_{vel,y}$, 0), and ($G_{vel,x}$, 0, 0). The timing of the experiments was minimised under the hardware constraints. The excitation pulse was 256 µs, giving rise to a flow encoding time of 212 µs and flow contrast time of 396 µs. The delay between consecutive experiments was 1-2 ms, depending on the image acquisition time.

There are two modifications on the experimental method in Chapter 5. First, in order to increase the sensitivity to weak velocity fluctuations, phase-wrapping was used to improve the signal-to-noise ratio (SNR) in the velocity measurements. The velocity encoding gradients were selected such that each continuous $2\pi$ phase window spanned at least three pixels. The other major difference was the acquisition of axial images, which was enabled by (1) the improved SNR due to the high porosity and (2) a novel slice selection method to avoid regions with high magnetic inhomogeneity. To achieve the optimised slice selection, images at different angle from the XZ-plane (from 0 to $\pi$ with an increment of $\pi/8$) were acquired by changing the directions of the slice selection gradient and spiral imaging gradients simultaneously. The angle

Fig 6.3. (a) The schematic diagram of experimental setup of the flow loop for magnetic resonance velocimetry (MRV). (b) Half of the SCP CAD model. (c) Schematic of a unit cell of the simple cubic packing flow channel.
of the image with the best quality was selected, and then the SCP cell was repositioned such that the imaging plane aligned the optimal angle. Although the SNR was reasonable for imaging axial planes, the noise was still higher than the transverse plane and spiral artefacts were more prominent in axial planes.

The FOV of the transverse images \((x \times y)\) ranged from \(12 \times 12\) to \(18 \times 18\) mm\(^2\) and the FOV of the axial plane \((x \times z)\) was \(18 \times 30\) mm\(^2\) with 1 mm slice thick. The total acquisition time was 12.1 ms for fully sampled images, achieving a temporal resolution of 70 Hz for \(64 \times 64\) two-dimensional one velocity component (2D1C) measurements and 17 Hz for the three velocity components (2D3C) acquisitions. For 50\% sampling, the acquisition time was 7.9 ms, and the sampling rates were 117 Hz (2D1C) and 28 Hz (2D3C). In this thesis, two transverse planes were examined at: (i) \(Z = -2.67\) mm with FOV = \(18 \times 18\) mm\(^2\) and resolution = 0.281 mm/pixel, and (ii) \(Z = 4.33\) mm with FOV = \(12 \times 12\) mm\(^2\) and resolution= 0.188 mm/pixel. The spatial resolutions in the axial plane were 0.281 and 0.469 mm/pixel for \(x\) and \(z\), respectively. The data in Chapter 7 was acquired with the same data acquisition procedures, at the same spatial resolution. There are slight variations in the temporal resolutions because of the adjustment in velocity encoding time and delay time (within 1 ms).

6.3 Data analysis

6.3.1 Phase unwrapping

Unwrapping the phase maps was a challenging task, especially for the high shear regions, despite the careful selection of velocity encoding gradients during the data acquisition. After applying the least-squares based method proposed by Ghiglia & Romero (1994), smooth phase distribution was obtained, but the highest velocity was always underestimated given the phase correction was not multiples of \(2\pi\). The path-following method described in Goldstein et al. (1988) avoided the previous shortcoming but failed in the high shear regions. The best performance was achieved using the path-following method proposed by Herráez et al. (2002) that uses the second difference to assess the reliability of each pixel and conducts unwrapping following a noncontinuous path. The implementation in the python package Scikit-image was adopted for the unwrapping task (van der Walt et al., 2014).
6.3.2 Dynamic mode decomposition

In this work, the de-biased DMD algorithm proposed by Hemati et al. (2017) was implemented. Given the velocity data from \( m \) snapshots with a fixed temporal difference, the flow field at time \( i \) is first structured as a vector \( x_i \) then organised into matrices \( X \) and \( Y \):

\[
X \triangleq [x_0 \ldots x_{m-1}], Y \triangleq [x_1 \ldots x_m]. \tag{6.1}
\]

The commonly adopted exact DMD algorithm computes the least-square approximation of the mapping matrix, \( A \), which is equivalent to the following optimisation problem,

\[
\min_A \|\varepsilon\|_F \text{ s.t. } Y + \varepsilon = AX, \tag{6.2}
\]

where \( \|\cdot\|_F \) denotes the Frobenius norm of a matrix, and \( E_Y \) is the error in \( Y \). However, the results are biased when \( X \) is noisy as well, with error \( E_X \). The de-biased DMD algorithm reformulated the problem as a total least squares regression:

\[
\min_A \|\varepsilon\|_F \text{ s.t. } Y + \varepsilon = A(X + x_X), \text{ where } \varepsilon = \begin{bmatrix} E_X \\ E_Y \end{bmatrix}. \tag{6.3}
\]

The DMD algorithm used in this work takes the following steps:

1. Construct the augmented snapshot matrix \( Z \) based on \( X \) and \( Y \), \( Z \coloneqq [X \ Y] \), and compute the singular value decomposition (SVD) of \( Z \).
2. Construct the projection matrix \( Q \) using the first \( r \) right singular vectors.
3. Project the snapshot matrices, \( \hat{X} = XQ \) and \( \hat{Y} = YQ \).
4. Compute the singular value decomposition (SVD) of \( \hat{X} \):
   \[
   \hat{X} = U\Sigma V^* \tag{6.4}
   \]
5. Truncate the SVD by the first \( r \) columns of \( U \) and \( V \) and the first \( r \) singular values as \( U_r, V_r, \) and \( \Sigma_r \).
6. Compute projected operator \( \hat{A} \), i.e., the projection of \( A \) onto the POD space:
   \[
   \hat{A} = \Upsilon_r^*AU_r = U_r^*\hat{Y}V_r\Sigma_r^{-1}. \tag{6.5}
   \]
7. Compute the eigendecomposition of \( \hat{A} \):
   \[
   \hat{A}w_i = \lambda_i w_i. \tag{6.6}
   \]
8. Compute the DMD modes:
   \[
   \psi_i = YV_r\Sigma_r^{-1}w_i. \tag{6.7}
   \]
6.3.3 Optimising the DMD implementation

During the periodic regime, the system exhibits low-dimensional dynamics and a truncation of the POD space before computing the projected operator, $\tilde{A}$, is desirable, which also improves the robustness of the algorithm to noise (Dawson et al., 2016). However, the truncation number, $r$, needs optimising; thus, the tests were done to assess the optimal truncation and the robustness. The loss function that evaluates the reconstruction error is defined as

$$
\text{Loss} = \frac{\|X - \Psi D_\alpha V_{\text{and}}\|_F}{\|X\|_F},
$$

(6.8)

where $\Psi$ is the DMD mode matrix constructed by $\psi_l$, $D_\alpha$ is a diagonal matrix consisting of the amplitudes of the DMD modes ($\alpha_l$) in the first snapshot, and $V_{\text{and}}$ is the Vandermonde matrix constructed from the DMD eigenvalues. The loss function was used to examine the effect of the truncation level and 10 different subsamples, with 200 snapshots each, were used. Fig 6.4 (a) suggests an optimal number of 13 modes for $Re = 599$. On the other hand, there is little improvement in increasing the number of modes for $Re = 772$ (Fig 6.4 (b)) and the performance is even worse with more modes, indicating that low-dimensional dynamics is unlikely to be present.

![Fig 6.4](image)

Fig 6.4. Loss function at different truncation levels based on 10 subsamples of 200 snapshots for $Re = (a) 599$ and (b) 772 for the out-of-plane velocity in the axial plane. The lines are to guide the eye.

Furthermore, the reproducibility of the DMD modes was assessed by comparing the similarity between the equivalent modes with 10 subsamples. The difference between each subsample and a base-case scenario using 250 snapshots was used. To evaluate the similarity between mode shapes, we use the structural similarity (SSIM) index. SSIM measures the similarity between two images (Z. Wang et al., 2004) regarding three characteristics: luminance, contrast, and structure, and yields a number from 0 to 1 (1 for two identical images). The function ‘ssim’ in MATLAB was used for the task and the parameters were left as the default ones. We selected
the optimal SSIM between two modes within an allowed axial offset \(< \frac{D_p}{2}\) of the mode from the subsample as two modes corresponding to the same wave structure may exhibit a phase shift, resulting in underestimated SSIM.

The reproducibility of mode shapes and frequency is shown in Fig 6.5(a) and (b), respectively, and the mean and standard deviation of the mode amplitude \(|\alpha_i|\) and decay rate \(|\lambda_i|\) are given in Fig 6.5(c,d). It can be seen that the mode shapes are highly reproducible except for the result at 1 Hz. The mode amplitude for the DMD mode at approximately 4.9 Hz is high, as shown in Fig 6.5(c), but there are larger variations in the frequency and growth rate. Therefore, this mode is dynamically important but not reproducible. Based on this sensitivity analysis, the two modes at 3.9 and 5.2 Hz are the most stable, and the DMD mode at 5.2 Hz is more energetic, as shown by its highest mode amplitude.

**Fig 6.5.** (a) The similarity index, (b) the frequency deviation from the mean, (c) the mode amplitude, and (d) the mode growth rate of the 7 DMD modes based on 10 subsamples of 200 snapshots for \(Re = 599\) with truncation level = 13 for the out-of-plane velocity in the axial plane.

In summary, optimal truncation was used based on the loss function, and further sensitivity analysis was conducted to select the modes based on their dynamical importance and reproducibility.

### 6.4 Results

All the results used are the fully sampled phase-unwrapped data acquired at 70 Hz (2D1C) and 17 Hz (2D3C). Phase wrapping was only implemented in the fully sampled measurements
because the compressed sensing reconstruction cannot handle the phase wrapping. In terms of
the notation of the three velocity components, for transverse planes, the positive directions of
\( u, v, \) and \( w \), are left-to-right, bottom-to-top, and out-of-plane with respect to the plots. For the
axial plane, positive \( u, v, \) and \( w \) are out-of-plane, left-to-right, and top-to-bottom. Therefore,
\( w \) always refers to axial velocity and is positive when aligned with gravity; \( u \) and \( v \) are
transverse velocities. It should be noted that \( u \) and \( v \) are along the same direction for all
transverse planes but are different between the axial and transverse planes. The FOV for all the
figures are given in the horizontal (\( x \)) and vertical (\( y \)) axes of the figures as \( x \times y \). In this
chapter, the white pixels in contour/colour plots represent the solid phase.

6.4.1 Mean velocity profiles at the onset of instability

The contour plots in Fig 6.6 are the mean velocity profiles for the steady flow at \( Re < 451 \), and
the onset of unsteady flow at \( Re = 451 \) and 537. All the velocities are normalised with respect
to the interstitial velocity, computed using \( U_{\text{int}} = \frac{u_{\text{sf}}}{\varepsilon} = \frac{Q/D^2}{1-\pi/6} \), where \( Q \) is the volumetric flow
rate. The recirculation zones can be identified between two connected unit cells (Fig 6.6(a-d))
due to the separation of the boundary layer and there are four regions with higher recirculation
velocity in the void surrounded by four spheres. The recirculation profiles and the four pairs of
symmetrical counter-rotating helical vortices were also observed experimentally (Suekane et al., 2003)
and numerically (Gunjal, Kashid, et al., 2005; Finn et al., 2012). Furthermore, there
is a shear layer at the edge of the central high-velocity channel, characterised by the close
adjacency of the contour lines, i.e., high shear stress, and the channel is referred to as the jet or
central jet.

With the onset of unsteady flow from \( Re = 451 \), the symmetry of the flow field varies
significantly. At steady flow (\( Re < 451 \)), there is approximately 90° rotational symmetry but
slight asymmetry is present at the edge of the recirculation zone (\( Z = -2.67 \) mm) and the four
corners of the shear layer (\( Z = 4.33 \) mm). At the onset of unsteady flow, the centre of the jet
shifts downwards, accompanied by increased recirculation at the bottom, and the streamwise
vortices become asymmetrical. The central jet is approximately symmetrical along the bisecting
plane from top right to bottom left. Although this mirror symmetry does not apply to the
recirculation cells, it is significant for the unsteady vortical motion at higher \( Re \), which will be
demonstrated in §6.4.3.
Fig 6.6. Normalised axial velocity (colour scale) and velocity vector (arrows) plots at $Z = -2.67$ mm for $Re = (a) 321$, (b) 355, (c) 451, and (d) 537 and at $Z = 4.33$ mm for $Re = (e) 321$, (f) 355, (g) 451, and (h) 537. Contour values from 0.5 with 0.5 increments are shown with black solid lines and from 0 with -0.1 increments with white dash-dot lines. The FOV are (a-d) $16.6 \times 16.6$ mm$^2$ and (e-h) $8.8 \times 8.8$ mm$^2$.

6.4.2 Periodic motion of the shear layer

Fig 6.7. Normalised axial velocity (colour scale) and velocity vector (arrows) plots for $Re = 537$ for the transverse planes at (a) $Z = -2.67$ mm and (b) $Z = 4.33$ mm and (c) the axial plane with the maximum CSA. The FOV are (a) $16.6 \times 16.6$ mm$^2$ and (b) $10.7 \times 10.7$ mm$^2$ and (c) $14.1 \times 22.3$ mm$^2$.

Periodic motion is identified for the onset of unsteady flow in SCP, and weak periodic velocity fluctuation is first observed at $Re = 451$. The periodic feature is demonstrated by the velocity fluctuation in the highlighted sections at two transverse planes and one axial plane in Fig 6.7 at $Re = 537$. The axial plane is the plane with maximum CSA and the white pixels at the top-left
and top-right corners and in the middle are assigned as solid phase because of the partial volume effect, where the spheres touch.

**Fig 6.8.** Contour maps of normalised fluctuating axial velocity for $Re = 537$ at (a) $Z = -2.67$ mm, (b) $Z = 4.33$ mm and (c) the axial plane corresponding to the highlighted regions in Fig 6.7. The FOV are (a) $8.2 \times 8.2$ mm$^2$ and (b) $5.4 \times 5.4$ mm$^2$ and (c) $5.6 \times 13.9$ mm$^2$.

Periodic shear layer oscillation is seen in Fig 6.8(a,b) and the strength of the velocity fluctuation is the strongest at the bottom left, where the most significant distortion of the shear layer was shown in Fig 6.6. We refer to the spatially coherent variation in streamwise velocity as streaks (Waleffe, 2001; Hof *et al.*, 2004). The positive and negative streaks denote whether they are travelling faster or slower than the temporally averaged mean velocity. As visualised in the axial plane in Fig 6.8(c), the temporally periodic oscillation of the shear layer is manifested as a spatially periodic pattern translating downstream. The fluctuating axial velocity for $Re < 757$ features similar patterns, whereas there is significant irregularity at $Re = 757$.  

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Fig 6.9. (a) The temporal evolution of the fractional volumetric flowrate within the positive and negative streaks (absolute value), and (b) the time difference between the maximum fluctuations of neighbouring streaks for Re = 537 at the bottom left at Z = -2.67 mm, as highlighted in Fig 6.8(a). (c,d) are the equivalent plots for Re = 599 and (e,f) are for Re = 675.
The region at the bottom left of the widest plane, as highlighted in Fig 6.8(a), is selected to further examine the characteristics of the streak. The velocity fluctuation was integrated within the region highlighted and then normalised by total volumetric flowrate, which yields the fluctuation of fractional volumetric flowrate, $\Delta Q/Q_{\text{tot}}$, due to the streak. Fig 6.9(a,c,e) shows $\Delta Q/Q_{\text{tot}}$ due to the passing positive and negative streaks. The amplitude of the streak, indicated by $\Delta Q/Q_{\text{tot}}$, increases with $Re$. The corresponding half periods in Fig 6.9(b,d,f) were calculated as the time difference between the neighbouring peak positive and negative velocity fluctuations (noted by the markers). The periodic variation of the flowrate for $Re = 599$ is the most regular compared to other $Re$. The irregularities include the intermittency at $Re = 451$ (not shown) and missing negative streaks are missing between adjacent positive streaks at $Re = 537$ and 675 shown in Fig 6.9.

![Fig 6.10.](image)

**Fig 6.10.** (a) The maximum fractional volumetric flowrate for the positive and negative streaks, and (b) the time between adjacent opposite sign streaks (i.e., approximately half of the period $T$) for $Re = 451$ to 757 at the bottom left at $Z = -2.67$ mm. The lines are to guide the eye. The maximum fractional volumetric flowrate (in log scale) for the (c) positive and (d) negative streaks and the dotted line is the least-square fit with the first four points.

As is summarised in Fig 6.10, the increase in velocity fluctuation with $Re$ follows an exponential trend. The regularity of the periodic motion, quantified by the error bar in the half period, increases from $Re = 451$ to 599 and decreases at higher flowrates. The strength of the streaks is plotted on the log scale in Fig 6.10(c,d) and the linear fit confirms the exponential growth at $Re < 757$. At $Re = 757$, the wave amplitudes deviate from the exponential trend as
the streaks are observed to expand beyond the region of interest. This deviation might indicate the saturation of the periodic motion.

6.4.3 Periodic motion of streamwise vortices

Synchronised velocity fluctuation in the transverse velocity components is present, manifested by the periodic vortical motion in the transverse planes. The normalised axial vorticity contours and the transverse velocity vectors for approximately half a period are shown in Fig 6.11. The dominant unsteady feature is the strong counter-rotating vortex pair at the bottom left while the other six weaker vortices only slightly oscillate. The vortical structure is shown more clearly in Fig 6.12 and the relevant vortices are denoted by alphabets. The pair of counter-clockwise vortices, A and B, grows stronger for the first half of the cycle until 0.1 s and then becomes weaker. The other pair with the opposite sign, C and D, exhibits similar behaviour, whereas it is located closer to the edge compared to pair AB. From 0.1 s to 0.17 s, C and D become stronger and, at about 0.2 s, and merge with the vortices of the same sign, C₀ and D₀, which are C and D from the previous cycle. In the next cycle, from 0.2 s, the vortices pair, A₂ and B₂, appears and follows the same growth and motion as A and B.

![Fig 6.11. Normalised vorticity (colour scale) and velocity vector (arrows) plots of four consecutive instantaneous velocity profiles for Re = 599 at Z = -2.67 mm. The FOV is 12.9×12.9 mm².](image)
Fig 6.12. Vorticity contour plots of eight consecutive snapshots for $Re = 599$ at $Z = -2.67$ mm. Contour values from 1 with 0.5 increments are shown with black solid lines and from -1 with -0.5 increments with white dash-dot lines. The FOV is 12.9×12.9 mm$^2$.

The vortical motion becomes stronger with increasing $Re$, as demonstrated in Fig 6.13 for $Re = 675$. The periodic motions are the same compared with $Re = 599$ but the spanwise movement is more prominent. For instance, the vortices A and B move further apart at 0.1 s than the maximum distance previously viewed (0.14 s in Fig 6.12). Fig 6.14 shows the periodic motion.

Fig 6.13. Vorticity contour plots of six consecutive snapshots for $Re = 675$ at $Z = -2.67$ mm. Contour values from 1.5 with 1.5 increments are shown with black solid lines and from -1.5 with -1.5 increments with white dash-dot lines. The FOV is 12.9×12.9 mm$^2$. 

The vortical motion becomes stronger with increasing $Re$, as demonstrated in Fig 6.13 for $Re = 675$. The periodic motions are the same compared with $Re = 599$ but the spanwise movement is more prominent. For instance, the vortices A and B move further apart at 0.1 s than the maximum distance previously viewed (0.14 s in Fig 6.12). Fig 6.14 shows the periodic motion.
in about one cycle for $Re = 757$. Consistent patterns can be seen as before, but the periodic motion is less regular, especially the location of the characteristic vortex pairs and their movement. In particular, the vortex pair AB drifted further apart during their growth and vortex A moves further upwards and interacts strongly with the vortex of the same sign at the top. In addition, there are other strong streamwise vortices in addition to the two vortex pairs (AB and CD).

**Fig 6.14.** Vorticity contour plots of six consecutive snapshots for $Re = 757$ at $Z = -2.67$ mm. Contour values from 2.5 with 2.5 increments are shown with black solid lines and from -2.5 with -2.5 increments with white dash-dot lines. The FOV is $12.9 \times 12.9$ mm$^2$.

The interaction of the streamwise vortices and streaks will be analysed next. Fig 6.15 shows the 3D reconstruction of the flow features based on instantaneous snapshots for $Re = 599$. Reconstruction of the 3D structure by tracing the temporal evolution of the measurement at a fixed position is routinely done, using Taylor’s frozen turbulence hypothesis (Hof et al., 2005; Lemoult et al., 2014). Taylor’s hypothesis states that the spatial structure can be reconstructed from the temporally resolved measurements by multiplying with the mean advection speed of the flow structures (De Lozar et al., 2012). The challenge in this geometry is that the spatial structure will vary in the axial direction because of the varying channel cross section. Two pieces of evidences justify the validity of the 3D reconstruction in Fig 6.15: (i) the two transverse planes demonstrate that the spatial structures are coherent; (ii) the reconstructed 3D patterns are consistent with flow characteristics in the axial plane, which represents the spatial
structure. In the 3D structure, the most distinct features are the pairs of counter-rotating vortices, represented by the yellow and blue isosurfaces. The modulation of the streamwise velocity in Fig 6.15(b,d) indicates that the unsteady low-velocity streak is in synchronized motions with the vortices. To highlight the details, the left corner of the whole structure at \( Z = D_p/2 \) is shown in Fig 6.15(e), which is rotated to the front. The low-velocity streak undergoes periodic modulation and is flanked by pairs of counter-rotating quasi-streamwise vortices.

**Fig 6.15.** (a) Isosurfaces of streamwise vorticity at \( Z = -2.67 \) mm within 0.31 s for \( Re = 599 \). The blue and yellow represents negative and positive vorticity isosurfaces \((\omega/|\omega| = \pm 2.5)\), respectively. (b) Isosurfaces of axial velocity in cyan \((w/U_{int} = 2.3)\). The grey surfaces represent the solid boundary. (c) and (d) are the equivalents at \( Z = -4.33 \) mm, and the threshold for vorticity is \( \omega/|\omega| = \pm 2.8 \). (e) Isosurfaces of streamwise vorticity superposed isosurfaces of axial velocity within 0.39 s for \( Re = 599 \). The region is at the left-most corner shown in (c,d) rotated to the front-facing direction, and the meaning of the colours are the same as (c,d). The temporal direction is scaled arbitrarily.

The equivalent plots for higher \( Re \) at \( Z = -2.67 \) mm are shown in Fig 6.16. The vortical features for \( Re = 675 \) are similar to \( Re = 599 \) whilst the spatial scale of the vortices and streaks are larger. The regularity in the vortical motion and shear layer structure for \( Re = 757 \) are lost compared to lower \( Re \), although the dominant pairs of vortices at the front can still be recognised.
6.4.4 Recirculation vortices

Recirculation bubbles are widely observed in backwards-facing steps and bluff body wakes. The shedding of the vortices is the most prominent feature of the unsteady wake motion (Williamson, 1996; Kiya et al., 2001), and this feature is visualised in Fig 6.17. At $Re = 675$, the vortices on both sides shed off simultaneously at 0.06 s and 0.17 s, and the mirror symmetry is emphasized by the vorticity contour. It is worth noting that there are two vertical bands of high vorticity region at the shear layer on each side. The inner vorticity band is due to the shear layer, and the outer one is due to the recirculation bubble. The vorticity pattern $Re = 675$ suggests that the periodic shear layer oscillation and vortex shedding are synchronised. At $Re = 757$, the vortex expands, and the mirror symmetry is lost. As a result, the vortex on the left sheds off at 0.12 s while the vortex on the right at 0.17 s. Neither vortex shedding nor the two vorticity bands is observed at lower $Re$, and only slight variation of the recirculation bubble shape is seen at $Re = 599$ (not shown).
Fig 6.17. Normalised vorticity (colour scale) and velocity vector (arrows) plots of four consecutive instantaneous velocity profiles for (a) $Re = 675$ and (b) $Re = 757$ at the axial plane. The FOV is $16.3 \times 15.8 \text{ mm}^2$.

6.4.5 Onset of the chaotic regime

The onset of the chaotic regime was identified between $Re = 757$ and 772. Fig 6.18 shows the area-averaged velocity variance for all three velocity components and the transition corresponds to a sudden decrease. A similar decrease in velocity fluctuation was reported for the axial velocity at the onset of chaotic flow in FCC (Hill & Koch, 2002). Spatially resolved mean velocity and velocity fluctuation are shown in Fig 6.19. The mean velocity distribution undergoes significant variation from $Re = 599$ to 757, but high-velocity fluctuation is observed in the same region, suggesting that the underlying dynamic remains the same. At $Re > 757$, significant changes in the velocity fluctuation profiles can be observed, indicating a transition in the underlying dynamic. After this critical point, the transverse velocity variance features mirror symmetry, and the axial velocity variance features a $90^\circ$ rotational symmetry.

Fig 6.18. Velocity fluctuation for all three velocity components at $Z = -2.67 \text{ mm}$ for $Re = 321$ to 968. The lines are to guide the eye.
Fig 6.19. Contour maps of normalised velocity (top row) and fluctuating velocity variance (bottom row) for (a,b) $u$, (c,d) $v$, and (e,f) $w$ for $Re = 599$ to 968 at $Z = -2.67$ mm (within the highlighted region in Fig 6.7(a)). Note that the fluctuating velocity variance for $Re = 599$ is displayed is 5 times the actual value. The FOV is $8.2\times8.2$ mm$^2$.

Fig 6.20 demonstrates the transition in the mean velocity profiles at $Z = -2.67$ mm. Compared with the eight symmetrical vortices at lower $Re$ (Fig 6.6(a)), only six vortices are seen at $Re = 599$; at the left and right corners, there is one dominant vortex instead of a pair of vortices due to the unsteady streamwise vortical motion. As the in-plane velocity undergoes significant variation, the mean velocity profile becomes less smooth at $Re = 675$ and 757. Beyond the second bifurcation, the mean velocity profile restores symmetry and resembles the steady-state profiles, but each instantaneous snapshot deviates significantly from the mean velocity profile.
Fig 6.20. Normalised axial velocity (colour scale) and velocity vector (arrows) plots at $Z = -2.67$ mm for $Re = (a) 599$, (b) 675, (c) 757 and (d) 799. The FOV is $16.6 \times 16.6 \text{ mm}^2$.

6.4.6 Spectral analysis

Fig 6.21. PSD of the velocity fluctuation all three velocity components (a) $Z = -2.67$ mm for $Re = 451$ to 772.

The periodicity of the velocity fluctuation is further analysed using the power spectral density (PSD) based on the velocity fluctuation at $Z = 4.33$ mm. In Fig 6.21, the dominant peak at 11 Hz for $Re = 451$ is due to the high-frequency measurement noise while the weak oscillation is at 3.5 Hz. Two dominant frequencies at 3.5 and 5.8 Hz are present at $Re = 537$ in the transverse velocity fluctuations while the two peaks are at 4.3 and 5.8 Hz for the axial velocity. Strong periodic oscillation at 5.1 and 6.1 Hz are observed for at $Re = 599$ and 675, respectively. The dominant frequencies in the transverse velocity components decrease to 5.6 Hz at $Re = 757$, while there is a second dominant frequency in the streamwise velocity at 7.4 Hz. $St$ follows a linear trend with increasing $Re$, using the frequencies $f_1$ highlighted by the red circle (Fig 6.22). The PSD after the second bifurcation features multiple peaks that represent a more broadband distribution of frequency.
6.4.7 DMD modes

Spatially periodic modes with different frequencies and wavelengths in the axial plane are successfully separated by DMD, and the corresponding DMD modes are shown for $Re = 451$ and 537 in Fig 6.23. A correlation between the frequency and the wavelength can be observed. The two lower frequencies for both $Re$ are at a ratio of about 2:3, approximately inversely proportional to the wavelength. Similarly, for $Re = 537$, the wavelength of the mode at 5.9 Hz is nearly half of that at 2.7 Hz.

The relationship between the wavelength and the frequency can also be observed for the out-of-plane velocity, and the most reproducible modes with wavelengths of about 1, 0.8, and 0.4 $D_p$ are shown in the left, centre, and right in Fig 6.24. The modes share similar structures at
different $Re$ although the mirror symmetry with respect to the central $z$-axis is absent at $Re = 757$ (Fig 6.24 (c)). The asymmetrical pattern is observed across all the modes and is also consistent with the asynchronous vortex shedding on the two sides shown in Fig 6.17. It may be that a fixed phase difference is present azimuthally, resulting in the observed pattern.

**Fig 6.24.** The DMD modes of out-of-plane velocity for $Re =$ (a) 599, (b) 675, and (c) 757. The FOV is $12.1 \times 19.6$ mm$^2$.

**Fig 6.25.** $St$ as a function of $Re$ based on the frequency of the DMD modes with similar wavelengths. The dashed lines are to guide the eyes.
St for the corresponding wavelengths increases with Re, as shown in Fig 6.25. The trend is consistent with that based on PSD (Fig 6.22). Deviation from the linear trend is seen at Re = 451 because the wavelength is less than 0.8 D_p.

![Fig 6.25](image)

**Fig 6.26.** (a) Normalised vorticity (colour scale) and velocity vector (arrows) plots of five consecutive instantaneous velocity profiles for Re = 675 at Z = -2.67 mm. The first row is the original data, and the second row is the DMD reconstruction. (b) The corresponding plots for Re = 757. The FOV is 16.6 × 16.6 mm^2.

The capability of DMD to extract periodic features and its potential in lower-order modelling is demonstrated using the streamwise vortical motion. DMD was applied to the 64 snapshots of 2D3C measurements at 28 Hz with 50% sampling. Fig 6.26 compares the original data and the corresponding snapshots reconstructed using the dominant DMD mode; the similarity between the two are remarkable. Moreover, the motion of the alternating streamwise vortices is the same as highlighted in Fig 6.14. Even when there is increased chaotic motion at Re = 757, the key dynamics are reproduced in Fig 6.26(b). Furthermore, the primary unsteady characteristic at Re = 757 is seen more clearly in the reconstructed motion, i.e., the streamwise vortices move further apart during the periodic motion. The difference between the original data and the DMD reconstruction with the dominant mode indicates that multiple modes are present at Re = 757.
Such features are consistent with the unsteady flow in the wake of a cylinder at $Re > 260$: there is increasing disorder in the fine-scale three dimensionalities manifested by the increase in streamwise vortex structures (Williamson, 1996).

6.5 Discussion

6.5.1 Transition process

We first compare the transition process with the related prior work. The MRV results have shown that the route to chaos in SCP consists of the following three stages: periodic, quasi-periodic, and chaotic. One question that needs further investigation is whether there is symmetry-breaking bifurcation before the transition to the periodic flow, as in the wake flow behind a single sphere. The slight asymmetry of the mean velocity profiles (Fig 6.6) might be a symmetry breaking bifurcation, but may be due to the imperfect experimental setup or the onset of the periodic regime. The other ambiguity is at which $Re$ the transition from the periodic to quasi-periodic regime happens. As multiple reproducible wavelengths are revealed by DMD at $Re \geq 451$, we can confirm the presence of a quasi-periodic regime. However, there is not enough evidence to determine the $Re_{crit}$ demarcating the periodic and quasi-periodic regimes because of the low temporal resolution and low SNR.

A periodic motion was also predicted in the CFD study by Finn et al. (2012) in SCP at $Re = 600$. In the CFD study, there were two lobes of vortex ring in a single pore and they shed off periodically. The half ring was located in opposite sides in consecutive pores, and the vortices were always located in the same quadrant during the shedding. In this study, the unsteady motion is dominated by one counter-rotating vortex pair in the same quadrant, which alters its rotational direction within each cycle (Fig 6.14). Furthermore, the four pairs of helical vortices were not reported by Finn et al. (2012), but they are still present in MRV flow visualisation, albeit much weaker in strength compared with the unsteady vortices. The difference may be due to the different boundary condition since there is only one row of SCP unit cells in this study, compared to the infinite 3D arrays of SCP cells in the CFD work.

During the periodic regime, the alternating dominance of vortices of the opposite rotational direction is consistent with the characteristic of the periodic vortical motion, predicted at the onset of unsteady flow in FCC (Hill & Koch, 2002). Whether the torus bifurcation identified by Hill & Koch (2002) is present is unclear. Further, the simulation results in Hill & Koch
(2002) also showed a local maximum of the velocity variance observed right before the second bifurcation, which is qualitatively the same as shown in Fig 6.18 for SCP.

### 6.5.2 TW solutions

The connection with dynamical system theory will be discussed in this section, in particular, the similarity to the TW solution in a square duct.

The characteristic of the streaks and streamwise vortices are demonstrated in §6.4.2 and §6.4.3 respectively. It is shown in Fig 6.15 that the low-velocity streak is flanked by pairs of counter-rotating quasi-streamwise vortices. Such configuration resembles the TW solutions in plane Couette flow (Hamilton et al., 1995), as well as experimental observations in pipe flow (Hof et al., 2005) and in the turbulent spot in channel flow (Lemoult et al., 2012). Moreover, the counter-rotating vortices and low velocity streaks between the vortex pairs at an edge of the shear layer show striking similarity to the TW at each wall of the square duct, e.g. the TW solution found by Uhlmann et al. (2010) at $Re = 1042$, as shown in Fig 6.2(d). The dominant motion is also similar to the TW solution found numerically by Wedin et al. (2009) and Okino et al. (2010) via homotopy approaches.

The streaks and streamwise vortices are strongest at one edge, and this asymmetry is similar to the numerical solution of the marginal turbulent states by Biau & Bottaro (2009), who found isolated TW at a single edge (Fig 6.2(c)). Another distinct phenomenon of the TW in SCP is the rotational direction of the streamwise vortices. The majority of TW solutions in a square duct feature a counter-rotating pair and a single low velocity streak at the centre of the wall, and the pair has the same direction as the vortex pair AB in SCP. However, in the second half of the periodic motion in SCP, the vortex pair CD corresponds to a high velocity streak at the centre.

In the turbulent regime, the flow in a square duct features a secondary flow with four pairs of counter-rotating vortices (Uhlmann et al., 2007), as was seen in the mean velocity profiles in the chaotic regime in SCP, shown in Fig 6.20. This similarity suggests that the same unsteady mode may remain active after the onset of the chaotic regime. It was suggested by Uhlmann et al. (2007, 2010) that “the occurrence of secondary motion is a statistical footprint of the preferential location of coherent structures”. This explains the observation by MRV that instantaneous velocity profiles at the chaotic regime being strikingly different from the symmetrical vortices in the mean profile.
Given the qualitative similarity, we then attempt to establish the quantitative relationship. The ‘square duct’ embedded in the SCP channel is determined by the narrowest area, and the height of the square duct is approximately \((\sqrt{2}-1)D_p\). Using the definition of \(Re_b = \frac{U_{in}h}{v}\) in the square duct, where \(h\) is half of the channel height, we can convert the \(Re\) that demarcates the onset of a periodic motion in SCP, \(Re = 451\), to \(Re_b = 544\). This value is consistent with \(Re_b = 598\) and 644 in Wedin et al. (2009) and Okino et al. (2010), whereas it is slightly higher than the minimum \(Re_b = 471\) found by Uhlmann et al. (2010). Besides the initiation of the unsteady flow, the critical \(Re\) for the onset of chaos (equivalent to \(Re_b = 932\)) is consistent with critical \(Re_b \approx 1000\), for the sustaining turbulent flow, in the DNS study by Uhlmann et al. (2007).

Despite the similarity, TW solutions found numerically are unstable and TWs observed experimentally are transient (Hof et al., 2004, 2005; De Lozar et al., 2012; Lemoult et al., 2012). The periodic phenomenon in SCP is likely a supercritical Hopf bifurcation and whether it corresponds to TWs will be further discussed in the next chapter.

### 6.5.3 Wavelengths of periodic modes

The difference from a TW solution in a square channel arises from the periodically converging-diverging channel. We speculate that the wavelengths in SCP are determined by the periodic sphere packing structure.

The preferred wavelength of 0.8 \(D_p\) can be related to the critical wavelength in self-sustained oscillations of impinging shear layers (Rockwell & Naudasher, 1979). The ratio of the impingement length to the wavelength between vortices in the impinging shear layer was deduced to be \((n+1/4)\) in the semi-empirical theory by Curle (1955), based on the smoke visualisation study by Brown (1937). In the SCP structure, the impingement length can be approximated by the sphere diameter \(D_p\); therefore, the wavelength of \(4/5D_p\) corresponds to the first harmonic with \(n = 1\), i.e. \(D_p = (1 + 1/4)\lambda\). The most stable and energetic mode at \(Re = 599\) is \(\lambda = 4/5D_p\) and both are dynamically important at \(Re = 675\). However, at \(Re = 757\), the most reproducible and energetic mode is the one with \(\lambda = D_p\) at 5.6 Hz, corresponding to the peak in \(u\) and \(v\) in the PSD (Fig 6.21). It could be that there is a shift in the dominance of dynamic between the two wavelengths.

Based on the analysis and comparison with different systems, the following interpretation of the evolution of instability in SCP is proposed. The onset of instability, first observed at \(Re = 451\), is dominated by two pairs of opposite sign counter-rotating vortices and synchronised
shear layer oscillations, characterised by streaks. The two pairs of vortices alternate within each cycle. The preferred longitudinal wavelength results from the packing geometry, which may be interpreted as self-sustained oscillations of an impinging shear layer. An exponential growth of the strength of the streaks is observed and while the growth is possibly hindered by the pore structure. The periodic motion becomes irregular with multiple dominant modes at $Re = 757$ and chaotic flow is observed from $Re = 772$ onwards.

### 6.6 Conclusion

In this work, the transition to the unsteady flow regime in SCP was characterised and analysed. The analysis focused on three aspects: (1) the route to chaos, (2) characteristics of the unsteady motion, and (3) the transition mechanism.

The first bifurcation is the appearance of periodic motion at $Re = 451$, and the transition from quasi-periodic to chaotic motion was identified between $Re = 757$ and 772. This confirms the Hopf bifurcation observed in the LBM simulations by Reynolds et al. (2000) and Hill & Koch (2002). The transition from the periodic to the quasi-periodic regime is subject to further investigation.

The (quasi-)periodic regime is characterised by the streamwise vortices and the streaks, and three-dimensional reconstruction was shown. In addition, the shedding of recirculation vortices was also revealed. The similarity and difference to the numerical prediction of the periodic motion in SCP and other sphere packings were discussed.

The periodic mode resembles the TW solution in shear flows and a comparison was made with a square duct. The secondary flow in the chaotic regime also resembles that in a square duct. Moreover, the periodic modes with multiple wavelengths were extracted by DMD and the dominant wavelength is consistent with the self-sustained oscillation of an impinging shear layer.
Chapter 7 Transition to turbulence in simple cubic packing

7.1 Introduction

The evolution of flow during the onset of unsteady flow in simple cubic packing (SCP) was analysed in detail in the last chapter, whereas the transition to the turbulent flow has not yet been examined. The focus of this chapter is on the statistical analysis of experimental velocity data, which reveals salient characteristics in the transition to turbulence. A brief overview of the theories and modelling methods will be given at the beginning to put the experimental results into context and address the synergy between this work and the greater porous media community. Then the literature on the critical Reynolds number \( \textit{Re}_{\text{crit}} \) and the flow characteristics will be reviewed. Finally, previous studies using SCP will be introduced in more detail.

7.1.1 Turbulence modelling in porous media

The earliest models of turbulent flows in porous media are based on simplifying assumptions to account for the effect of complex pore geometry and turbulence. Often, the models require parameters derived from phenomenological models. The macroscopic model known as Reynolds averaged Navier-Stokes (RANS) is the cornerstone for industrial turbulence modelling. The major approaches to adapting RANS for flows in porous media include time averaging the volume-averaged equations (Antohe & Lage, 1997) and volume averaging the time-averaged equations (Masuoka & Takatsu, 1996). The latter enables one to take into account the effects of turbulence inside the pores, i.e., microscopic turbulence in porous media. It was suggested by Nield (2006) that true macroscopic turbulence is impossible, for the size of turbulent eddies is limited by the length scale of pore structures (Hlushkou & Tallarek, 2006).

With the advancement of computing power, temporally and spatially resolved model, represented by large-eddy simulation and direct numerical simulation (DNS) have gained popularity. DNS has become especially popular because it is able to simulate turbulent flows down to the smallest length scale, i.e., the Kolmogorov scale (S. B. Pope, 2001). Jin et al. (2015; 2017) have verified the previous hypothesis, that the eddy size is generally limited by the pore size, using DNS in generic porous matrices with a relatively high porosity (up to 0.8).
RANS is still the dominant approach for modelling turbulence in porous media thanks to the low computational cost associated with RANS. The spatial and temporal scales inherent to the underlying flow are crucial for the correct closure relationship in RANS. For example, the integral length scale is critical in the observed enhanced mixing and is frequently used for the closure of the Reynolds stress terms. Therefore, experimental observations with a high spatial and temporal resolution can shed light on the modelling of turbulent flows in porous media.

7.1.2 The onset of turbulence in packed bed

The first quantitative technique used to study the transition to turbulence in porous media was the microelectrode method, which uses electrochemical probes embedded in the wall or the surface of the packing. Jolls & Hanratty (1966) reported the onset of turbulent flow at $Re_{sf} = \frac{U_{sf}D_p}{v} = 300$, where $U_{sf}$ is the superficial velocity, $D_p$ is the particle diameter, and $v$ is the kinematic viscosity. In their experiments, the transition to turbulence featured highly irregular patterns of the micro-electrode signal and vigorous motion of the streamlines. More accurate quantification of the transition to turbulence can be obtained by the calculation of the power spectral density (PSD) of the high-frequency signal. The procedure is as follows: first, the PSD of diffusional current fluctuations, $W_{ti}(f)$ is computed; second, the PSD of velocity gradient fluctuations, $W_{ss}(f)$ is calculated based on $W_{ti}(f)$ (Deslouis et al., 1983; Nakoryakov et al., 1984); lastly, the average fluctuating rate of the velocity gradient, $F.R_s$, is calculated by integrating $W_{ss}(f)$ (Latifi et al., 1989; Rode et al., 1994). Rode et al. (1994) observed the stabilisation of $F.R_s$ on most of the electrodes at $Re = \frac{U_{int}D_p}{v} > 875$ ($U_{int} = U_{sf}/\varepsilon$ is the interstitial velocity). The most comprehensive examination was conducted by Seguin et al. (1998) on plate packings and porous foams, in addition to the sphere packings. The stabilisation of $F.R_s$ for more than 90% of the probes was used as the demarcation of the onset of turbulence, and $Re_{crit}$ in random sphere packings was found to be 1480; a similar method was used to identify $Re_{crit}$ by Bu et al. (2014, 2015) and Yang et al. (2015). The experimental details and $Re_{crit}$ from relevant studies are summarised in Table 7.1.

Similar to the onset of unsteady flow in porous media, as discussed in §5.1.1, the onset of turbulence is also highly inhomogeneous. The inhomogeneity was emphasised by the difference in $Re_{crit}$ between the wall and the internal probes in Bu et al. (2015). The relative standard deviation of $Re_{crit}$ is about 16 – 50% among the internal probes and 34 – 50% among the wall probes within a single packing (Bu et al., 2015). The inhomogeneity results from the difference
in local structure within the random packing and is evidenced by the variation of $Re_{\text{crit}}$ in different packing structures shown by Seguin et al. (1998); in particular, no fully turbulent regime was observed in the synthetic foam until $Re = 1245$.

**Table 7.1** Reynolds numbers corresponding to the onset of turbulence in random sphere packings.

<table>
<thead>
<tr>
<th>Study</th>
<th>Aspect ratio (N)</th>
<th>porosity</th>
<th>Location of measurements</th>
<th>Onset of turbulence ($Re_{\text{crit}}$)</th>
<th>Criterion for flow regime characterization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jolls &amp; Hanratty (1966)</td>
<td>12</td>
<td>0.41</td>
<td>Internal</td>
<td>732</td>
<td>Visualization of turbulent streamlines</td>
</tr>
<tr>
<td>Latifi et al. (1989)</td>
<td>10</td>
<td>0.39</td>
<td>Wall</td>
<td>949</td>
<td>$W_{\text{t}}(f)$ and friction factor evolution</td>
</tr>
<tr>
<td>Rode et al. (1994)</td>
<td>10</td>
<td>0.4</td>
<td>Wall</td>
<td>1200</td>
<td>$W_{\text{s}}(f)$ evolution; Liquid aggregate sizes</td>
</tr>
<tr>
<td>Seguin et al. (1998)</td>
<td>12, 7.5</td>
<td>0.36</td>
<td>Wall and internal</td>
<td>1480</td>
<td>The stabilisation of $F.R_s$ for 90% of the probes</td>
</tr>
<tr>
<td>Bu et al. (2014)</td>
<td>10.5</td>
<td>0.39</td>
<td>Internal</td>
<td>1023</td>
<td>The stabilisation of fluctuating rate of limiting current for 90% of the probes</td>
</tr>
<tr>
<td></td>
<td>10.8</td>
<td>0.40</td>
<td></td>
<td>875</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>0.38</td>
<td></td>
<td>797</td>
<td></td>
</tr>
<tr>
<td>Bu et al. (2015)</td>
<td>SC</td>
<td>0.48</td>
<td>Wall and internal</td>
<td>979 and 840</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BCC</td>
<td>0.32</td>
<td></td>
<td>1813 and 1094</td>
<td></td>
</tr>
<tr>
<td></td>
<td>FCC</td>
<td>0.26</td>
<td></td>
<td>1115 and 958</td>
<td></td>
</tr>
<tr>
<td>Yang et al. (2015)</td>
<td>5.3, 8.1, 9.9, 12.5</td>
<td>-</td>
<td>Wall and internal</td>
<td>($Re_{\text{af}}$) 398 and 328.</td>
<td>Mean stabilisation $Re$ defined as Bu et al.</td>
</tr>
</tbody>
</table>

Although consistent results have been obtained from different studies in Table 7.1 on a wide range of packings, the microelectrode method, as a point-based method, has limited capabilities to study the transition process in porous media. The major challenge is that the probes are only located on the surface of packing structures, whilst the true isotropic turbulence is likely to happen in the pore centre. The more advanced particle imaging velocimetry (PIV), with the capabilities to measure spatially resolved velocity fields at a high frequency, can overcome this challenge. Patil & Liburdy (2012, 2013a, 2013b) conducted a study using PIV on an index-matched random packing of spheres up to $Re \approx 5000$. Measurements of in-plane velocity distributions with high spatial and temporal resolutions were acquired in axial planes. The onset of turbulence was characterised by the asymptotic behaviour of various statistical quantities. They found that the integral length and time scales reached asymptotic limits at $Re = 1666$ and 2326, while the local turbulent characteristics, e.g., the area-averaged velocity variance, converged only at $Re \sim 3666$. Patil & Liburdy (2013b) explained that the macroscopic quantities
represented the interaction of the turbulence with the mean velocity field, which reached an asymptote before the smaller scales of turbulence fully develops. In contrast to the large variations of the $Re_{crit}$ based on different electrochemical probes, the asymptotic behaviour of the turbulent characteristics in Patil & Liburdy (2013b) was reasonably consistent across different pores.

7.1.3 Turbulent characteristics

7.1.3.1 Velocity fluctuation

The transition to different flow regimes is frequently examined through the investigation of the evolution of the turbulent kinetic energy (TKE) and the variance of each fluctuating velocity component. In microelectrode studies, the fluctuating rate of the velocity gradient, $F.R_e$, follows the general trend as that shown in Fig 7.1(a). A slow or sharp increase is observed at the onset of unsteady flow and its stabilisation represents the onset of turbulent flow, as discussed in §7.1.2. Seguin et al. (1998) reported that the fluctuating rate of the velocity gradient stabilised at 15-25% in the sphere packings. This value underestimates the overall fluctuation since the unsteady motion in the centre of the pore is often more energetic. For example, in the study of turbulent air flow using hot-wire anemometry (HWA), the relative turbulence intensity ($\sigma(u)/\bar{u}$, where $\sigma(u)$ is the standard deviation and $\bar{u}$ is the time-averaged velocity) is 40-55% in the void centre and 15% in the constricted area in a rhombohedral packing $Re \approx 1.8 \times 10^4 - 2.7 \times 10^4$ (Mickley et al., 1965).

Fig 7.1. (a) The evolution of the average fluctuating rate of the velocity gradient by Seguin et al. (1998). (b) Distributions of normalised axial velocity fluctuation variance at different $Re$ from the PIV study by Patil & Liburdy (2013b).
Fig 7.1 (b) shows the probability distribution of velocity fluctuation within a pore presented by Patil & Liburdy (2013b), where the velocity fluctuation attains the maximum value during the transition regime. By averaging the variance within different pores, they reported that the mean axial velocity fluctuation peaked with a value of 0.13-0.17 at about $Re = 1000-1500$ and later converged to 0.1-0.14. The asymptotic value corresponds to a relative turbulent intensity of about 30%. The stereoscopic PIV (sPIV) results obtained by Khayamyan et al. (2017) showed significantly different $Re$ for the peak velocity fluctuation, where a decrease of mean TKE from $Re = 400$ was observed at various locations. They suggested that this decrease demarcates the onset of turbulence.

### 7.1.3.2 Integral length scale

The integral length scale ($L$) is often evaluated from the spatial autocorrelation function of velocity fields, though it can also be interpreted from the integral time scale based on the temporal fluctuation in the point-based measurements. The maximum size of the turbulent eddies was assumed to be proportional to the macroscopic time scale, which is the time of the first annulment of the temporal autocorrelation function; the average size of the eddy was evaluated based on the integral time scale, i.e., the integration of the autocorrelation function up to the macroscopic time scale (Latifi et al., 1989; Seguin, Montillet, Comiti, et al., 1998). Rode et al. (1994) reported that from $Re = 500-2400$, the average eddy size remained constant at about half of the pore size. On the other hand, the maximum eddy size was close to the average pore size but it decreased with $Re$. In the sphere packing examined by Seguin et al. (1998), in a fully turbulent flow, the mean eddy size is about 30 to 80% of the pore size, which was calculated based on the capillary model proposed by Comiti & Renaud (1989). In the turbulent air flow through a rhombohedral structured packing, the longitudinal integral length scale (integration of the entire autocorrelation function) is 30% of the pore diameter at $Re = 2.7 \times 10^4$ (Mickley et al., 1965).

The above results based on the temporal fluctuation are greater than the asymptotic value assessed directly from the spatial correlation function using two-dimensional (2D) PIV measurements (Patil & Liburdy, 2013b). By estimating the pore scale $dx = \frac{4Ve}{s} = \frac{e}{1-\varepsilon} \frac{2}{3} D_p = 0.55D_p$, the integral length scale is about 18% that of the pore size. The discrepancy suggests that the approximation method from a point-based measurement is not applicable for the flow in porous media.
7.1.3.3 Coherent structure

The integral length scale is a statistical feature determined by the dominant coherent structures, which is largely unexplored in porous media. The identification of coherent structures plays a critical role in understanding the turbulent transport processes. Horton & Pokrajac (2009) examined the velocity fluctuation using PIV at two connected pores in the SCP and demonstrated that the coherent structures at $Re_{wvp} = 340$ are highly consistent in neighbouring pores. Although spatially resolved information is made available by PIV, no coherent structure has been shown for porous media flow.

The advances in DNS simulations have revealed interesting coherent structures in various configurations, including recent studies in porous media (Jin et al., 2015; Uth et al., 2016; Jin & Kuznetsov, 2017). Their numerical simulations in designed generic porous matrices, from square and circular cylinders to staggered sphere packings, demonstrate that the size of turbulent structures is restricted by the pore scale. Their work is critical in clarifying the difference between pore-scale and macroscale turbulence in porous media; however, it calls for further experimental validations.

7.1.4 Turbulence in the SCP

Previous studies on the turbulent flow in SCPs will be reviewed in more detail in this section.

One of the earliest studies was conducted by Van der Merwe et al. (Van der Merwe & Gauvin, 1971; Van der Merwe et al., 1971) on turbulent airflow from $Re = 5 \times 10^3$ to $5 \times 10^4$ on 10 layers of spheres. Each layer was a square region with sides equal to $4D_p$, which consisted of 9 whole spheres in the centre and half and quarter spheres at the edge and corners. At $Re = 5.7 \times 10^4$, the mean pressure drag coefficients for the central spheres of the first layer was 35.5 times the drag coefficient of a single sphere at the same $Re$, and the pressure drop ratio decreased significantly in the second layer and then increased gradually to an asymptotic value at ~21 after five layers (Van der Merwe & Gauvin, 1971). Based on the pressure distribution, they inferred that the boundary layer on the second and subsequent spheres was turbulent, which separates at an angle (measured from the front stagnation point) of about $130^\circ$; however, on the first layer, the separation occurs at about $90^\circ$. Moreover, vortex shedding only occurred behind the first bank at $Re \approx 5000$. The integral length scale close to the boundary layer increased from 9% to 30% from $Re = 5 \times 10^3$ to $5 \times 10^4$ and the integral length scale in the pore centre was about 50% higher.
Yevseyev et al. (1991) examined the mean and temporal fluctuations for all three velocity components of the turbulent liquid flow using laser Doppler anemometry (LDA). Flow separation behind the wake contact points (between adjacent spheres aligned longitudinally) and reverse flow near the lateral contact points were identified. At $Re = 5000$, the flow in the central channel resembled a turbulent jet but the maximum axial velocity in the jet was slightly off the centreline. Given that the turbulence intensity in the axial velocity attained its maximum value in the mixing layer between the jet and separation area, they suggested that the turbulence was generated primarily by the interaction of jets and separation area. A linear decreasing trend was observed in frequency spectra.

It should be noted that the previous studies all focused on the fully developed turbulent flow whereas the onset of turbulence in an SCP has only been investigated by Horton & Pokrajac (2009); the experimental techniques used are ultrasonic velocity profiler (UVP) and PIV. The definition of $Re$ is unconventional and will be referred to as $Re_{uvp}$, covering the range from $67 < Re_{uvp} < 436$. The authors reported that UVP measured the mean velocity for a circular region of 5 mm with 0.74 mm resolution at 30 Hz across the channel of an SCP packing with 12 mm diameter spheres.

Different flow regimes were identified from the temporal correlation of the velocity measurements at distances of $D_p$, $2D_p$, $3D_p$ and $4D_p$ apart as shown in Fig 7.2. At $Re_{uvp} = 67$ (test 1), the flow fluctuated with a period of 0.2 s and was speculated to be a pulsating motion of the inertial core. From $Re_{uvp}$ of 110 (test 2), a transition flow regime was identified and the peaks were interpreted as regular disturbances translating downstream. The equal time lags between adjacent peaks in Fig 7.2 indicated a constant translation speed of the disturbances; the shorter time lag with increasing $Re_{uvp}$ suggested faster motion. After $Re_{uvp} = 440$ (test 9), the peaks became Gaussian, which was interpreted as coherent structures at a range of scales and thus the onset of turbulence. Spatially resolved velocity profiles were measured using PIV at $Re_{uvp} = 340$ with the same spatial resolution at 500 Hz. At $Re_{uvp} = 340$, a time lag of 0.15 s was identified from the temporal correlation plots in the UVP results. The PIV results showed consistent features as strong velocity fluctuation profiles were coherent between the upstream pore and its adjacent downstream pore with a 0.15 s delay. Further details of the UVP study will be disclosed in the discussion section when comparing with magnetic resonance velocimetry (MRV) measurements.
Fig 7.2. Two point temporal correlations with the separation of 12 mm (dashed black line), 24 mm (dashed grey line), 36 mm (solid black line), and 48 mm (solid grey) from Horton & Pokrajac (2009). Test 1-10 refer to data acquired at different $Re_{exp}$ (from 67 to 436 in the ascending order).

7.1.5 Aims

The challenges of studying turbulence in porous media stem from the complex pore geometry and the resulting flow heterogeneity, in both $Re_{crit}$ and the turbulence intensity. Investigation of the flow in random packings is desirable since random packings have a wide range of industrial applications. However, the interpretation is obscured by the complexity of the structure in random packings and may be of limited benefits for theoretical studies. Furthermore, it is challenging to reproduce the same flow features in a random packing geometry using numerical methods. Therefore, a representative packing structure SCP has been chosen to advance the understanding of the transition to turbulence and to motivate future numerical simulations of flow in porous materials. The aims of this chapter include:

1. To extract the characteristics of the unsteady flow in the SCP.
2. To study the transition to turbulence regarding both microscopic and macroscopic statistics.
3. To extract the coherent structures and discover their significance in turbulent flow.
7.2 Data analysis

7.2.1 Data summary

The experimental methods were introduced in Chapter 6. A summary of the number of snapshots of different types and positions of measurements are given in Table 7.2, where 2D1C is the two-dimensional, one-velocity component measurement and 2D3C refers to the three-velocity component measurement.

<table>
<thead>
<tr>
<th>Re</th>
<th>Location and Type</th>
<th>No. of snapshots</th>
</tr>
</thead>
<tbody>
<tr>
<td>675, 939, 1180, 1444, and 1658</td>
<td>Transverse, 2D1C</td>
<td>765</td>
</tr>
<tr>
<td></td>
<td>Axial, 2D1C</td>
<td>1275</td>
</tr>
<tr>
<td></td>
<td>Transverse, 2D3C, 50% sampling</td>
<td>320</td>
</tr>
<tr>
<td>599, 757, 772, 799, and 969</td>
<td>Both locations, 2D1C</td>
<td>255</td>
</tr>
<tr>
<td></td>
<td>Both locations, 2D3C</td>
<td>128</td>
</tr>
</tbody>
</table>

7.2.2 Higher order velocity statistics

The skewness, S, and flatness, F, for the fluctuating transverse velocity, $u'$, are calculated using the following equations

$$S(u') = \frac{\overline{u'^3}}{\sigma_u^3} \quad \text{and} $$

$$F(u') = \frac{\overline{u'^4}}{\sigma_u^4} \quad (7.1)$$

where $\sigma_u$ is the standard deviation of $u$. S and F are useful as they characterise the details of the probability density distribution of the velocity fluctuation, especially the non-Gaussian behaviour of turbulent fluctuations. Invalid data due to noise results in over-estimated skewness and flatness in the stagnant regions, as demonstrated in Fig 7.3(a). To remove the outliers is challenging because the velocity fluctuation is also spiky because of the intermittency of the turbulence, such as the one in Fig 7.3(b). Despike algorithms from Goring & Nikora (2002) were tested, including the thresholding based on the standard deviation, RC filters, Tukey 53H, and a new algorithm proposed by Goring & Nikora (2002). Tukey 53H is most suitable for the spiky data in this study as it distinguishes the spikes according to the deviation from the smoothed signal. A slight modification in smoothing the sequence $u_i$ was made to suit the current dataset and the preprocessing procedures used were the following:

1. Construct the Hanning smoothing filter: $u_i^s = \frac{1}{4}(u_{i-1} + 2u_i + u_{i+1})$;
2. Construct the sequence $\Delta_k = |u_i - u'_i|$ and reject the points with $\Delta_i > k\sigma$, where $\sigma$ is the standard deviation of $u_i$ and $k$ is a threshold to discriminate the two types of spikes.

3. Replaced the spike by the average of the two adjacent points.

The outcome of this algorithm is demonstrated in Fig 7.3(a,c) and the threshold used has been optimised for the effective removal of spikes in the stagnant region. The high skewness and flatness at the edge due to noise are remedied with the proposed algorithm.

![Fig 7.3](image)

Fig 7.3. (a) The spatially-resolved skewness and flatness of the axial velocity fluctuation before and after the despike process. The FOV is $16.6 \times 16.6$ mm$^2$. In this chapter, the white pixels in similar plots represent the solid phase. The FOV for all the figures are given in the horizontal ($x$) and vertical ($y$) axes of the figures as $x \times y$. Demonstration of the despike algorithm for the noisy time-series data obtained (b) at the shear layer and (c) at the stagnant region. The signal is shown by the solid line and the upper and lower bounds are shown by dashed lines. The spike is marked by a triangle.

### 7.2.3 Quadrant analysis

Quadrant analysis is a useful turbulence data-processing technique, especially in turbulent shear flow, and is widely applied to analyse the ejection and sweep in the turbulent boundary layer (Kim et al., 1987; R. Adrian & Moin, 1988; Nolan et al., 2010; Loucks & Wallace, 2012; Wallace, 2016). The technique was proposed by Wallace et al. (1972) in the analysis of turbulent boundary layer flow. The analysis divides the velocity fluctuations into four quadrants of the Reynolds shear stress plane, $Q_1 (w' > 0, u' > 0)$, $Q_2 (w' < 0, u' > 0)$, $Q_3 (w' < 0, u' < 0)$, and $Q_4 (w' > 0, u' < 0)$, where $w'$ is streamwise velocity fluctuation and $u'$ is the wall normal velocity fluctuation. The Reynolds shear stress plane is often represented by the joint probability distribution function (PDF) of $w'$ and $u'$. In the four quadrants, $Q_2$ and $Q_4$ are related to the dominant turbulent events in turbulent boundary layers. The $Q_2$ events or
Ejections refer to the intermittent eruption of low-momentum streaks at the shear layer, with decreasing the streamwise velocity \((w' < 0)\) and increasing the wall-normal velocity \((u' > 0)\). Ejections are often followed by large-scale connected motion towards the wall, called sweeps or Q4 events, since the motion \((w' > 0, u' < 0)\) corresponds to the 4th quadrant. The ejection and sweep quadrants, Q2 and Q4, usually make the largest contributions to the Reynolds shear stress in boundary layer flow. In this work, we evaluated the contribution from each quadrant using the total probability density.

### 7.3 Results

**7.3.1 Mean velocity profiles and velocity fluctuation**

![Fig 7.4. Contour maps of normalised velocity (top row) and fluctuating velocity variance (bottom row) for (a,b) \(u\), (c,d) \(v\), and (e,f) \(w\) for \(Re = 675\text{-}1648\) at \(Z = -2.67\) mm. The FOV is 16.6 × 16.6 mm\(^2\).](image-url)
The mean velocity at the maximum pore cross section area (CSA) is shown in Fig 7.4 and the velocity profiles remain the same after the second bifurcation \((Re > 757)\) until the highest \(Re\) measured. The mean transverse velocities \((u \text{ and } v)\) become larger with increasing \(Re\). The velocity fluctuations in all three components (Fig 7.4) are dominant in the shear layer and each velocity component features a distinct symmetry since the second bifurcation. Fig 7.5 compares the spatially averaged velocity fluctuations of different components at two axial positions. In the chaotic regime, there is a consistent increasing trend from \(Re = 939\) to 1180 and the increase is slower afterwards. The velocity fluctuation may have reached an asymptote but further experiments are required to confirm this. The velocity fluctuations in the axial velocities are approximately 2.5 to 3 times higher than the transverse velocity at the same \(Re\).

**Fig 7.5.** Velocity fluctuation for the transverse velocity components for \(Re = 675\)-1648 at (a) \(Z = -2.67\) mm and (b) \(Z = 4.33\) mm. The lines are to guide the eye in the rest of the chapter unless otherwise stated.

**Fig 7.6.** Contour maps of (a) normalised velocity and (b) fluctuating velocity variance for \(w\) for \(Re = 675\)-1648 at the axial plane. The FOV is \(13.8 \times 20.4\) mm\(^2\).
Fig 7.7. The axial velocity distribution as highlighted in Fig 7.6 at (a) the horizontal line and two vertical lines at (b) the centre and (c) the shear layer.

The axial velocity profiles are shown in Fig 7.6 for the axial plane. The velocity distributions, taken along the two highlighted vertical lines and the single highlighted horizontal line, are plotted in Fig 7.7. There is a central jet with an approximately parabolic profile, surrounded by near stagnant and recirculation region, as demonstrated by Fig 7.7(a). The velocity profiles in the centre given in Fig 7.7(b) match that described by Horton & Pokrajac (2009). The central channel consists of a relatively long diverging section and a shorter converging part. The diverging section commences from the point of boundary layer separation and ends at the point of reattachment. The axial velocity decreases slowly at the diverging section and then increases to a maximum at the converging section, and the maximum velocity is about 5-6% higher than the minimum. The maximum velocity at the centre occurs slightly downstream of the pore neck; see Fig 7.7(b), due to the inertial effect analogous to the vena contracta. The minimum velocity
at the shear layer (Fig 7.7(c)) occurs further upstream than the centre. The velocity distribution is very similar with increasing \( Re \) up to 968 except that there is a slight decrease in the centre-line velocity from \( Re = 799 \) to 968 accompanied by the gradual broadening of the central jet. Furthermore, the velocity distribution converges from \( Re = 968 \) onwards (not shown).

The velocity fluctuations corresponding to the horizontal line and the vertical line at the shear layer are examined in Fig 7.8. The turbulence production in the shear layer shown in Fig 7.4 and Fig 7.6 is further emphasised. The distribution across the pore in Fig 7.8(a) demonstrates that maximum velocity fluctuation occurs at the shear layer. In contrast, there is negligible fluctuation at the centre and the stagnation region. Along the axial direction, the maximum fluctuation corresponds to the minimum axial velocity at the shear layer (Fig 7.8(b)). From \( y = -2 \) to 6 mm, the decreased velocity fluctuation is accompanied by an increased axial velocity.

![Graphs](image)

**Fig 7.8.** The axial velocity fluctuation distribution as highlighted in Fig 7.6 at (a) the horizontal line and two vertical lines at (b) the shear layer.

### 7.3.2 Higher order statistics

The spatially resolved skewness and flatness provide further insight into the mechanism of turbulent production. The data at the transverse plane with the maximum CSA for all three velocity components are shown in Fig 7.9. The higher order statistics at \( Re = 675 \) is determined by the periodic velocity fluctuation and the patterns at \( Re \geq 939 \) are determined by the dynamics
of chaotic motions. The following analysis will focus on the chaotic regime. First, a distinct and similar pattern is present at all $Re$ for each velocity component. Mirror symmetry is present in the skewness and flatness in the streamwise velocities $u$ and $v$, and the pattern for the axial velocity features the same 90° rotational symmetry, just as the velocity fluctuation does. The deviations of skewness from 0 and flatness from 3 indicate the non-Gaussian behaviour of the velocity fluctuations, which is most significant at the shear layer. Overall, the flatness and skewness decrease with higher $Re$.

**Fig 7.9.** Contour maps of the skewness (top row) and flatness (bottom row) of the velocity fluctuations for (a,b) $u$, (c,d) $v$ and (e,f) $w$ for $Re = 675$-$1648$ at $Z = -2.67$ mm. The FOV is $16.6 \times 16.6$ mm$^2$.

The more detailed pictures are shown in Fig 7.10. As observed in Fig 7.9, the maximum skewness and flatness decrease with increasing $Re$, whereas there is little difference at the jet.
region in the centre. Furthermore, the peaks of maximum skewness and flatness become wider and move radially outwards.

The PDFs of axial velocity fluctuations in the representative positive skewness region noted in Fig 7.9(e) at $Re = 1180$, is shown in Fig 7.11(a). As expected for positive skewness, the probability at high positive axial velocity fluctuation is higher than the negative counterparts. The high flatness in this region indicates that the large positive $w'$ events occur intermittently. Similarly, the PDF in the negative skewness region shown in Fig 7.11(b) suggests that the axial velocity fluctuation exhibits large negative spikes within the jet region. Note that the rest of the positive and negative skewness regions have similar distributions to the two examples.

**Fig 7.10.** The distribution of the (a) skewness and (b) flatness of the axial velocity for $Re = 939$-$1648$ at the blackline highlighted in Fig 7.9.

**Fig 7.11.** The probability distributions of axial velocity fluctuations at (a) the positive skewness region and (b) the negative skewness region for $Re = 939$-$1648$. The two regions are highlighted in Fig 7.9(e) at $Re = 1180$ and 1444 respectively.
The deviation from Gaussian behaviour in the higher-order statistics is often explained by the characteristic events, so quadrant analysis is conducted. The vertical stripe with high skewness highlighted in Fig 7.9 (e) at $Re = 1648$ is chosen because, in this region, $u$ is equivalent to the wall normal velocity in the turbulent shear layer. The joint PDF of $w$ and $u$ are shown in Fig 7.12. There are dominant Q2 events ($2^{nd}$ quadrant: $w' < 0, u' > 0$) and the probability of Q4 events ($4^{th}$ quadrant: $w' > 0, u' < 0$) is also higher than average within the region. The quadrant analysis suggests a consistent picture with the skewness data. During the ejections (Q2), the entrainment of fluid from the shear layer into the central jet region causes the PDF to bias towards the $w' < 0$ and results in negative skewness in Fig 7.11(b). Similarly, the positive skewness (Fig 7.11(a)) corresponds to the sweeps (Q4) that transport high-speed fluid from the jet towards the shear layer ($w' > 0$). The observed wider peak in the skewness at higher $Re$ indicates that the ejection/sweeps occur in a broader region than they do at lower $Re$. The simultaneously decreasing flatness implies that such events occur at reduced intermittency with increasing $Re$.

![Fig 7.12](image)

**Fig 7.12.** The joint probability distribution of the axial velocity and horizontal velocity for (a) $Re = 939$ and (b) $Re = 1648$. The data is from the highlighted region in Fig 7.9(e) at $Re = 1648$. The title denotes the total probability density within the $2^{nd}$ and $4^{th}$ quadrants.

### 7.3.3 Spatial correlation and integral length scale

The spatial correlations ($R$) are now examined for the velocity fields in the axial plane and the relevant regions are defined in Fig 7.13(a). Fig 7.14 shows $R$ in the axial plane for all three components, e.g., $R_{ww}$ is the spatial correlation in $w'$. Overall, the decaying patterns are similar at different $Re$. The correlation function decays faster at higher $Re$, indicating a decreasing length scale of turbulent eddies. The patterns for all three velocity components are also similar, though an exception to this is the axial velocity at the centre (Fig 7.14(b)), where there is no
anti-correlation peak. This is also observed in the quasi-periodic regime at \( Re = 675 \) (not shown). Here we refer to \( Re \geq 537 \) as the quasi-periodic regime based on the PSD in Chapter 6. In the quasi-periodic regime, \( R_{ww} \) at the centre decays slowly without periodic fluctuation while \( R_{ww} \) at the shear layer has a decaying periodic form because of the shear layer oscillation.

**Fig 7.13.** Mean axial velocity distribution in the axial plane with highlighted regions for correlations: (a) the shear layer and the centre region for spatial correlation and (b-c) the relevant regions for temporal correlation. The FOV is 14.1 × 22.3 mm\(^2\).

**Fig 7.14.** The spatial correlation function for all three velocity components at (a) the shear layer and (b) the centre of the axial plane for \( Re = 772, 939 \) and 1648. The two regions are highlighted in Fig 7.13(a).

The integral length scale, \( L \), has been evaluated by integrating the spatial autocorrelation function until its first zero-crossing and Fig 7.15 shows the results. The notation \( L_x(u') \) represents the integral length scale of \( u' \) in the x-direction. A steep increase in \( L_x \) can be seen at the onset of chaotic flow. After the second bifurcation (\( Re \geq 799 \)), \( L \) decreases gradually with increasing \( Re \) before reaching a plateau. The integral scale along the direction of the velocity is
the largest, i.e., $L_x(u')$, $L_y(v')$, and $L_z(w')$, compared to the other two velocity components, which are very similar in scale. There is a difference in $L_x(u')$ and $L_z(v')$ at the shear layer in the axial plane with maximum CSA as in Fig 7.15(a) as the two directions are not isotropic. In the symmetrical axial plane, $L_x(u')$ and $L_z(v')$ are comparable, as shown in Fig 7.15(b). The integral scales in the transverse planes are much smaller (Fig 7.15(c,d)), indicating that the scale of coherent structures in the transverse directions is smaller than the axial direction. On average, at $Re > 1180$, $L_z$ is about 0.1-0.12 $D_p$, and $L_x$ and $L_y$ are about 0.04-0.06 $D_p$.

![Fig 7.15.](image)

**7.3.4 Temporal correlation**

A similar analysis to Horton & Pokrajac (2009) using a temporal correlation at two different locations was conducted. Fig 7.16 shows the temporal correlation function evaluated for the velocity fluctuation at two positions separated by 0.5 $D_p$, as highlighted in Fig 7.13(b). At the centre, the periodic pattern is most distinct in the velocity fluctuation for the out-of-plane velocity, $u$, but the periodicity is also captured by the peak at $t = 0.07$ s in $v$ and $w$. After the onset of the chaotic regime, there is no long-range correlation and only a single peak remains. The peak width and height decrease steadily with increasing $Re$ except for $R_{pp}$ at $Re = 1444$. 

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Fig 7.16. The temporal correlation functions for all three velocity components at the shear layer of the axial plane between two regions separated by 0.5$D_p$ (highlighted in Fig 7.13(b)) for (a) $Re = 675$-$968$ and (b) $Re = 1180$-$1648$.

The time lag, $t_{\text{lag}}$, is defined by the time of the maximum correlation for two regions at $D_p$ apart and is used to calculate the convection velocity $u_c = D_p/t_{\text{lag}}$. The convective velocity (Fig 7.17) at both the shear layer and the centre is very similar to mean velocity at the shear layer ($\sim 2U_{\text{int}}$), even though the bulk velocity at the centre is about 3.6$U_{\text{int}}$, which suggests that the shear layer underpins the turbulent dynamics.

Fig 7.17. The convection velocities at (a) the shear layer and (b) the centre of the axial plane between two regions separated by $D_p$ (highlighted in Fig 7.13(c)) for $Re = 675$ to 1648.

7.3.5 Coherent structure

The coherent structures and their evolution during the transition to turbulence will be analysed in this section. The coherent structures were extracted using proper orthogonal decomposition (POD), and the number of snapshots are given in Table 7.2. Dynamic mode decomposition (DMD) is not applicable in the chaotic regime as there are no dominant frequencies.
Fig 7.18 shows the first four POD modes of the axial velocity, where the dominant feature is the stripe located at the shear layer. At $Re = 675$, the first and second modes are related by a phase shift of $\pi/2$, which is the signature of a spatially periodic mode. There is a loss of symmetry in the first two POD modes at $Re = 757$, but the mode shapes are similar to $Re = 675$. The transition to chaotic regime at $Re = 772$ is manifested by the significant difference of the POD modes and the first two modes feature a one-sided streak at opposite sides. From $Re = 939$ to 1444, the first two modes represent the spatial correlation of streaks on two sides of the channel. At $Re = 1648$, the first four modes represent isolated streaks at the four corners, indicating their spatiotemporal independence.

It can be speculated that the symmetry of the shear layer oscillation is broken after the initiation of chaotic flow when the other unsteady modes become active. However, there is still a spatial correlation at $Re < 1648$, both horizontally and vertically. The streaks on the two sides of the channel, at $Re = 939$-1444, indicate a preference of either a symmetrical or anti-symmetrical configuration. The lack of spatial coherence on the two sides at $Re = 1648$ suggests that a loss of coherence azimuthally may be a characteristic of turbulent flow.

**Fig 7.18.** The mean axial velocity and the first four POD modes extracted from 2D1C $w$ snapshots for $Re = 675$-1648 at the axial plane. The FOV is $12.1\times19.6$ mm$^2$. 
The (a,c) energy and (b,d) cumulative energy in the first 20 POD modes from the 2D1C w snapshots for Re = 675-1648 at the axial plane. The cumulative energy in the first (e) 1, 2, 3, and 4 modes and (f) 10, 20, 30, and 50 modes from the 2D1C w snapshots for Re = 675-1648.

The energy distribution of the POD modes, given in Fig 7.19, provides further insight into the transition process. As is seen in Fig 7.19(a, b), at Re = 675, the first four POD modes capture 80% of the energy and it is likely that they represent the two most energetic wavelengths. From Re = 757, the drop in the energy content of the first four modes is prominent, indicating that the periodic modes are no longer dominant. There is a significant contrast between Re = 939 and 1180 and the mode energy distributions are highly similar for Re ≥ 1180, as demonstrated in Fig 7.19(c,d). This convergence of energy is further emphasised in Fig 7.19(e,f), which shows good convergence for the first four modes at Re ≥ 1180. On the other hand, the slight decrease in the cumulative energy at a high mode number for Re ≥ 1180 suggests that the energy is
distributed into more modes, which might correspond to an increase in small-scale uncorrelated coherent structures.

The streamwise vortices are synchronised with the shear layer oscillation in the quasi-periodic regime and will be examined next based on the 2D3C snapshots from the compressed-sensing reconstruction of 50% subsampled experiments. At the quasi-periodic regime, the first two POD modes represent the periodic streamwise vortical motion; see Fig 7.20. The analysis in §6.4.3 shows that the periodic motions are qualitatively the same while the range of motion expands from $Re = 599$ to 757. The same trend is present in the POD modes, showing the coherent motion extends to a higher spanwise range with increasing $Re$. Mode 1 also highlights the streak between the two vortices, which is consistent with the 3D reconstruction in Chapter 6.

![Fig 7.20.](image)

**Fig 7.20.** The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the mean velocity and the first two POD modes extracted from 2D3C snapshots for $Re = 599$-$757$ at $Z = -2.67$ mm. The FOV is $12.9 \times 12.9$ mm$^2$.

At the beginning of the chaotic regime, from $Re = 772$ to 939, the dominant POD modes capture streamwise vortical structures with coherent axial velocity motion, as shown in Fig 7.21. The transverse flow is directed outwards where there is axial acceleration, and the radially inwards flow is present in the region with decelerated axial velocity. The former is consistent with the Q4 events, and the latter corresponds to the Q2 events at the shear layer. Additionally, the velocity vectors demonstrate that the coherent in-plane flow is related by a streamwise vortex. The dominant mode resembles the first mode in the quasi-periodic regime, featuring streaks
and vortices, and we refer to this mode as a travelling wave (TW) given its similarity to the TW solution. It might be that the Q2 and Q4 events are triggered by the TW.

Furthermore, the dominant modes are related by symmetry, as has been demonstrated in the axial plane previously. For example, the 1st and 2nd modes at \( Re = 772 \) feature a 180° rotational symmetry and the 1st and 2nd modes at \( Re = 799 \) are related by a 90° rotation. The similarity between the dominant modes at \( Re = 772-939 \) and the modes in the quasi-periodic regime (Fig 7.20) suggests that the streamwise vortices are due to the TWs occurring at various locations azimuthally.

Coherence and symmetry are not observed in the data at \( Re \geq 1180 \). At \( Re = 1444 \) and 1648, there is much less streamwise vortical motion in the POD modes compared to the lower \( Re \). The lack of TW features can be due to the increasing number of energetic small-scale coherent structures. Although coherent streak and vortical dynamics are not seen, the POD modes still coincide with the Q2 and Q4 events. Moreover, the dominant motions are located closer to the walls than lower \( Re \).

![Fig 7.21. The normalised axial velocity (colour scale) and velocity vector (arrows) plots for the mean velocity and the first three POD modes extracted from 2D3C snapshots for \( Re = 772-1648 \) at \( Z = -2.67 \) mm. The FOV is 12.9 x 12.9 mm².](image)

The energy distributions of the POD modes in Fig 7.22 show some similarity and difference from the mode energy in the axial plane. The general trend is similar; however, at \( Re = 675 \), there are only two dominant modes in the transverse plane, instead of four in the axial plane.
The two periodic modes have different wavelengths streamwise but the spanwise motions are the same, and thus not differentiable by POD in the transverse plane. The energy content of the first two modes at $Re = 757$ is much higher than in the axial plane, indicating that the streamwise vortex pair is still dominant energetically at $Re = 757$. The second bifurcation is more apparent in terms of mode energy than in the axial plane (Fig 7.19). A gradual decrease in the cumulative energy is observed from $Re = 772$ to 1444. The energy distributions are identical at $Re = 1444$ and 1648, suggesting that the dynamic has reached an asymptote.

![Graph 1](image1.png)

**Fig 7.22.** The (a) energy and (b) cumulative energy in the first 20 POD modes from the 2D3C snapshots for $Re = 675$-$1444$ at $Z = -2.67$ mm.

![Graph 2](image2.png)

**Fig 7.23.** Contour maps for the mean axial velocity and the first four POD modes extracted from 2D1C $w$ snapshots for $Re = 675$-$1648$ at the recirculation region in the axial plane. The FOV is $3.4 \times 9.2$ mm$^2$. 

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The oscillation of recirculation vortices and vortex shedding, observed in the axial plane, are characteristic coherent structures in the periodic regime (§6.4.4). However, their presence is not obvious in the POD modes due to their low energy levels. By conducting POD on the recirculation region only, such dynamic behaviour can be revealed. The mean axial velocity profile and the first two POD modes for the recirculation bubble are shown in Fig 7.23. The velocity amplitude in the recirculation region increases from \( Re = 675 \) to 939, and the dominant dynamical motion resembles one another for \( Re \geq 939 \), as shown by the POD modes.

The POD modes can be interpreted from the reconstructed snapshots (Fig 7.24), which are constructed via the superposition of the mean velocity profiles and the POD modes. Fig 7.24(b) and (c) demonstrate the effect of the positive and negative first modes, which corresponds to the shrunk and enlarged recirculation bubbles, respectively. In other words, the radial motion of the shear layer is captured by the first mode. The positive second mode reconstruction (Fig 7.24(d)) depicts an elongation of the recirculation bubble, while the negative counter-part in Fig 7.24(e) represents an upward movement of the backflow region with the reattachment position shifting slightly upstream.

**Fig 7.24.** (a) The mean axial velocity and (b-e) the reconstruction using the first two POD modes for \( Re = 1648 \) at the recirculation region in the axial plane. The FOV is 3.4×9.2 mm².

### 7.4 Discussion

Prior to discussing the comparisons with the previous experimental studies, the differences in experimental configurations that can result in discrepancies will be listed below and the particular reasons will be further examined where relevant.

It was emphasised in §0 that the major drawbacks in the microelectrode studies are the limitation of the probe location and flawed application of Taylor’s ‘frozen’ turbulence hypothesis. The experiments using HWA by Van der Merwe *et al.* in the SCP used gas. Moreover, both the HWA study and the LDA study by Yevseyev *et al.* (1991) in the SCP are

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for $Re$ ranging from $5 \times 10^3$ to $5 \times 10^4$, higher than the MRV measurements. The studies with the closest range of $Re$ and temporal/spatial resolution to this work are the ones using PIV (Patil & Liburdy 2012, 2013a, 2013b), although these studies were conducted in random packings.

The most similar study is Horton & Pokrajac (2009) and the following issues are worth addressing beforehand. First and foremost, their definition of $Re$ is unconventional. $Re_{uvp}$ is defined using the temporally and spatially averaged velocity from the UVP measurements and the characteristic length scale of the imaging region, i.e., 5 mm. However, this definition contradicts their PIV results. The UVP measurement at $Re_{uvp} = 340$ is approximately the same as the maximum velocity measured by PIV. By their definition, the UVP measurement should be the same as, instead of 30% higher than, the averaged PIV velocity in the 5 mm diameter circular region. It is more plausible that UVP technique measured the maximum velocity, implying that the equivalent $Re$ can be calculated as $Re \approx 0.69 Re_{uvp}$. Second, assuming that the results from UVP are the mean axial velocity in the circular region, the same statistical tests were conducted by coarse-graining the MRV results; however, the discrepancies in the further discussion cannot be resolved. Lastly, the authors commented that there were defects in the pore geometry, manifested by the poor agreement in the transverse velocity profiles between the upstream and downstream pores in their PIV data.

![Fig 7.25. Demonstration of the SCP 2D array: (a) The experimental apparatus used by Horton & Pokrajac (2009) and (b) the SCP geometry used in the numerical study by Finn et al. (2012).](image-url)

One limitation of the MRV dataset is the unconventional geometry, using a single row of unit cells (Fig 6.3(b)), instead of a number of unit cells stacked in a 2D array, such as the apparatus in Fig 7.25(a). That being said, some evidence from previous work exists to suggest that a single row is sufficient. In the laminar regime, the MRV measurements by Suekane et al. (2003) in a single row are the same as numerical results in the array configuration, as predicted by Gunjal & Ranade (2007) and Finn et al. (2012). Finn et al. (2012) also applied periodic boundary
conditions to the geometry shown in Fig 7.25(b). Although the MRV data agree well with the majority of the results, some variation may be due to the single row geometry.

### 7.4.1 Mean velocity profiles and velocity fluctuation

The MRV mean axial velocity profile in the chaotic regime, reported in this thesis, is consistent with that observed in the fully-developed turbulent flow measured by LDA (Yevseyev et al., 1991). However, the small dip at the jet centre in the plane with maximum CSA is absent in this study as well as in the turbulent gas flow measured by HWA (Van der Merwe et al., 1971). Furthermore, the location and axial span of the recirculation region revealed by MRV also match well with the LDA study. The reattachment of the separated boundary layer occurs at about 40° in this work, the same as that in a study of turbulent gas flow study by Van der Merwe & Gauvin (1971).

The location of the maximum axial velocity fluctuation aligns with previous studies and this evidence supports the statement by Yevseyev et al. (1991) that turbulence is generated mainly in the shear layer between the central jet and the recirculation region. The standard deviation of the velocity fluctuation at the shear layer is about 18% of the maximum axial velocity in MRV, comparable to the 24% measured by LDA. The underestimation of the velocity fluctuation in MRV may be due to the limited spatial resolution or the higher Re (Re ≈ 5000) in the LDA study.

A discrepancy is present in the transverse velocity fluctuations when compared to those reported by Yevseyev et al. (1991), who reported that the velocity fluctuation profiles in all three components are the same. In this study, the maximum streamwise fluctuation is about twice of that in the transverse directions. On the other hand, the ratio observed in the present work is similar to that measured by PIV by Horton & Pokrajac (2009). Moreover, the anisotropy is predicted by the numerical study and the turbulence level in the axial direction is about 50% higher than that in the transverse direction at relatively low Re (Jin & Kuznetsov, 2017).

The MRV turbulent intensity profiles do not match the profiles in Horton & Pokrajac (2009). First, in their study, the local maxima in the turbulent intensities, evaluated from the PIV data, in both axial and transverse velocities are not located at the shear layer. Another difference is that the maximum fluctuation in axial velocity evaluated by MRV is located at the widest CSA; this is further upstream than the maximum in the UVP results. The probable explanation is that the mean velocity measured by UVP is not sensitive to the fluctuation close to the recirculation
zone, and thus underestimates the fluctuation in the plane with maximum CSA. The reduced velocity fluctuation downstream of this plane, which was also observed in the LDA study, can be explained by the contraction of the channel suppressing the production of turbulence.

Regarding the evolution of turbulence intensity with increasing $Re$, some difference compared to studies of flow in the random porous media has been identified. A decreasing trend was reported in the area-averaged variance in different pores, except for that of the recirculation region (Patil & Liburdy, 2013a). The decrease is also shown at different axial slices by Khayamyan et al. (2017). The mean variance reached an asymptote at $Re = 2860$ in the former study and at $Re = 2000$ in most slices in the latter. In this work, after reaching the local maximum of at the end of the periodic regime, the velocity fluctuation decreases from $Re = 757$ to 799; then a mild increase was observed. Based on Chapter 6, the peak turbulence intensity in SCP corresponds to the end of the quasi-periodic regime, which is dominated by periodic large-scale unsteady motion. The MRV data indicates that the turbulent intensity drops at the onset of the chaotic flow, similar to the prediction by LBM in FCC (Hill & Koch, 2002). Thus, we can speculate that the trend in the random packing is a superposition of instabilities at various scales located in different pores.

### 7.4.2 Higher order statistics

The skewness quantifies the asymmetry of PDF and flatness is a measure of the level of intermittency. The high skewness and flatness are typical for turbulent jets and boundary layers, which are quantitatively similar to the turbulent flow in SCP based on the MRV results. As shown in Fig 7.10, the skewness increases from the centre to the shear layer, from -0.5 to 1.5, which is consistent with the rise from -0.5 to 1 for a turbulent jet (S. B. Pope, 2001). Similarly, the skewness moves from -0.5 to 0.85 in the turbulent shear layer (Kim et al., 1987) and the near wall region of pipe flow (Durst et al., 1995). The skewness of -0.5 in the jet region suggests that the jet in the SCP exhibits fully-developed turbulent flow (Kim et al., 1987; S. B. Pope, 2001). In the SCP shear layer, the flatness rises simultaneously with the skewness, indicating that the turbulent events are intermittent, with the values being consistent with the literature. Further, the more significant intermittency at lower $Re$ observed in this work is the same as that reported in a turbulent jet (Abdel-Rahman et al., 1996), which was explained by the competing effect of the viscous stress hindering the development of turbulence.

This non-Gaussian behaviour was also observed in the gas flow in the SCP, where the flatness was particularly high in the shear layer and in the recirculating flows (Van der Merwe et al.,
1971). Similarly, Horton & Pokrajac (2009) reported that the skewness was about -0.8 and the flatness was 3.5-4 in the jet centre at the early unsteady regime. Moreover, they reported that the skewness and flatness converge to a Gaussian distribution at higher $Re_{uvp}$ and suggested that this demarcates the onset of turbulent flow. In contrast to this finding, such a sudden transition is not seen in the MRV results. Given the evidence in turbulent boundary layers and jets, we speculate that their argument that the transition to turbulent flow characterised by the Gaussian behaviour is unsound.

### 7.4.3 Integral length scale

The faster decay of the spatial correlation function with increasing $Re$ shown in Fig 7.14 contradicts the observation by Horton & Pokrajac (2009), who reported a much slower decay at $Re_{uvp} = 440$, which the authors assigned to be representative of the fully turbulent flow. The slower decay in the UVP data was not reproduced by coarse-graining the MRV data and the reason for this discrepancy needs further investigation.

By scaling the integral length scale, $L$, with respect to the pore diameter calculated from the capillary model (Comiti & Renaud, 1989), $dx = 0.61 D_p$, $L$ in the longitudinal direction converges at 16-20% $dx$ in this work, which is similar to the 18% $dx$ in the random packing measured by PIV (Patil & Liburdy, 2013b). In transverse directions, $L$ ranges from 7% to 10% $dx$, half of that in the longitudinal direction. Moreover, $L$ is smaller than the minimum cross section length scale (44% $dx$), which supports the hypothesis that the size of turbulent structure is restricted by the pore scale in the porous media.

Regarding $L$ with increasing flowrates, the trend shown here is also consistent with the PIV data, where there was a decreasing trend before plateauing in most pores (Patil & Liburdy, 2013b). The decrease of $L$ from the onset of turbulence implies the establishment of the energy cascade with an increasing number of small-scale eddies. The plateauing can be related to fully-developed turbulence. However, this trend is not universal. Rode et al. (1994) observed that the average aggregate size in a random packing is independent of $Re$ up to 2000, similar to that seen in a rhombohedral packing up to $Re = 2.7 \times 10^4$ by Mickley et al. (1965). On the other hand, a 3-fold increase was reported from $Re = 5 \times 10^3$ to $5 \times 10^4$ in the SCP by Van der Merwe & Gauvin (1971).
7.4.4 Temporal correlation

Regarding the spatiotemporal correlation shown in Fig 7.16, a lack of long-range correlation was also reported by Horton & Pokrajac (2009) and the authors suggested that the single peak was due to the intermittent large-scale fluctuation translating downstream. However, the peak height decreases in this work instead of increasing, as in the UVP results. Moreover, the broadening of the peak seen at Re_{uvp} = 440 is not observed in the MRV data.

The convective velocity estimated from the temporal correlation in this work is slower than that reported by Horton & Pokrajac (2009), which was more than the maximum axial velocity, at about 4.7 U_{int}. In the PIV study in a random packing (Patil & Liburdy, 2013a), the convective velocity of the eddies, based on large eddy scale (LES) filtering, was about 0.8 U_{int} in the tortuous channel region, substantially slower than the maximum velocity, 2.4 U_{int}. This evidence supports the conclusion drawn from the MRV results that the convective velocity is determined by the axial velocity in the shear layer.

7.4.5 Coherent structure

The coherent structures found in this work can justify the integral length scale and provide further evidence on the turbulent mechanism. The coherent structures in the axial plane shown in Fig 7.18 have an elongated shape, which accounts for the larger L_{z}(w') than L_{x}(w') in Fig 7.15(a). Moreover, the streamwise vortices revealed in the axial plane have approximately twice the size in the dominant flow direction compared to the perpendicular direction (e.g., Re = 772 in Fig 7.21); this explains the statistics L_{x}(u') > L_{x}(v') and L_{y}(v') > L_{y}(u'). Furthermore, the continuous decrease in integral length scales L_{x} and L_{y} from Re = 772 to 1180 might be due to the decreasing number of streamwise vortices, as shown by the POD modes at Re ≥ 1180.

Although the dynamics in the quasi-periodic regime resembles the TW solutions, they differ in their stability. In the early chaotic regime, the most energetic POD modes also show similar characteristics. As they are unstable, they may correspond to TW solutions. The TWs have also been extracted by POD from the turbulent pipe flow (Hellström & Smits, 2014; Hellström et al., 2016), and the dominant modes feature 60/90/120° rotational symmetry, which match the analytical solution by Wedin & Kerswell (2004). These structures, featuring streamwise vortices and streaks in the cross-section, are similar to the POD modes in this study but they are absent in the two highest Re. We may draw some insight from the studies of square duct flow regarding the absence at high Re. Based on the DNS results from Pinelli et al. (2010) and
the recent LDA study by Owolabi et al. (2016) in the square duct, it was speculated that additional TW solutions with increasing number of streaks and vortices emerge progressively with increasing \(Re\). For instance, it was reported by Pinelli et al. (2010) that the number of streaks grow from 3 to 5 per edge from \(Re_b = 1753\) to \(2205\) (\(Re_b\) is defined by the half height of the square duct). With more TW solutions coming into play, each individual mode would become less energetic, explaining their absence in the POD modes at the highest \(Re\) (\(Re_b=1989\), for the justification of the \(Re\) conversion, see §6.5.2). To summarise, the transient features revealed by POD resembles the periodic modes in the quasi-periodic regime; their similarity to the TW solutions in a square duct suggests that they may be TWs. Further numerical or experimental studies with higher temporal resolution is required to verify whether such coherent structures correspond to TWs in shear flow.

In the recirculation region, the two POD modes are very similar to the modes in a backward-facing step, which are related to the flapping and the undulating motion of the shear layer (Schrijer et al., 2014). The flapping motion, represented by the first mode, was attributed to momentum ejection when a vortical structure with greater forward motion escapes the recirculation zone. The coherent structure depicted by the second mode, the undulating motion, is due to momentum injection upstream from the separation bubble and momentum ejection downstream. The flapping motion described by Schrijer et al. (2014) corresponds to a vortex shedding event, which is also the most energetic mode in this work. However, there is no dominant frequency in the PSD. Similarly, Van der Merwe et al. (1971) claimed that there is no periodic vortex shedding in the fully developed SCP flow. Given the evidence, we can speculate that there is irregular vortex shedding, whose mechanism and characteristics are worth further investigation.

### 7.5 Conclusions

The characteristics of the unsteady flow were extracted and analysed, including the mean velocity profiles, other various velocity fluctuation statistics (variance, skewness and flatness), the spatial and temporal correlations, and coherent structures. The analysis was focused on their dependency on the pore structure and the evolution with \(Re\), and comparisons were made with previous experimental studies using micro-electrodes, LDA, UVP, and PIV. The conclusions are organised regarding the three questions (§7.1.5) on (1) flow characteristics, (2) transition to turbulence, and (3) coherent structures.
The key features of the transition to turbulence are the heterogeneity and the pore-limited integral scale. Not only is the turbulent intensity heterogeneous, it was suggested that the turbulence is fully developed first in the jet region before spreading to the stagnant regions. The evidence from the integral length scale and the coherent structures both support the hypothesis that the turbulent is restricted by the pore space, and thus macroscopic turbulence is unlikely to be present in porous media.

The velocity distribution, turbulent intensity profile, major turbulent-producing dynamics, and the shape of correlation functions were qualitatively the same after the onset of the chaotic regime from \( Re \geq 772 \). The convergence of integral scale was seen at \( Re > 1180 \) but the small-scale features (the skewness and flatness pattern, POD mode shapes, and POD mode energy) were still evolving at \( Re > 1180 \). The POD mode structures and energy spectrum in the transverse plane converged at \( Re > 1444 \), but further exploration is needed to confirm the microscopic asymptote. Overall, the results agrees with the conclusions of Patil & Liburdy (2013b) regarding the difference in the transitions to turbulence between macroscopic and microscopic statistics.

The extraction of coherent structures has been done for the chaotic regime in porous media for the first time. The dominant characteristics are the longitudinal streaks and streamwise vortices, which is similar to the TWs in shear flow. The coherent structures, along with the Quadrant analysis, revealed the importance of ejections and sweeps in porous media. The energy distribution of the POD modes provides further evidence of the developing small-scale eddies.

In summary, the spatial and temporal resolution velocity measurements, enabled by the ultra-fast MRV experiments, has provided significant insight into the transition to turbulence in porous media flow.
Chapter 8 Conclusions and future work

8.1 Conclusions

I will organise the conclusions into three sections: (i) the technique development, (ii) contributions towards flow in porous media, and (iii) insights into fluid dynamics in general.

8.1.1 Technique development

The entire work centres around the magnetic resonance imaging (MRI) techniques, and the major advantages are the applicability of MRI to opaque and inhomogeneous systems and its non-invasiveness. The principles of other experimental methods used in porous media flow were introduced in Chapter 1. To acquire high-resolution time-averaged three-dimensional (3D) flow fields, an optimal 3D magnetic resonance velocimetry (MRV) pulse sequence was selected among several implementations; the acquisition and post-processing procedures were given in Chapter 3. Similarly, after comparing the major fast MRI techniques in Chapter 2, the most promising one, spiral imaging, was chosen to study the transient flow behaviour. Compared to the second best, echo planar imaging (EPI), spiral imaging is more robust to shear, which is necessary for imaging flow in porous media. The challenge of susceptibility difference was addressed by optimising the material for the packing structure (see Chapter 5).

Moreover, spiral imaging showed approximately 2- to 3-fold acceleration with subsampling acquisition and compressed sensing (CS) reconstruction. One of the innovations in this thesis is the combination of CS advancements and spiral imaging protocol, using the variable-density spiral sampling pattern for subsampling. MRV encodes the velocity in the phase of the complex image matrix, and this phase variation is particularly challenging for CS reconstruction. A novel CS technique was applied to address this challenge. The algorithm was given in §2.6.3 and was used in Chapter 5 and 7 for reconstructing flow fields.

8.1.2 Flow in porous media

By adopting and optimising the techniques, a series of experimental studies was conducted to investigate the transition between flow regimes in porous media. In Chapters 3 and 4, the focus was on the inertial effect in the steady flow regime in a random sphere packing, and detailed analysis of the principal flow characteristics was provided, including the inertial core, backflow, and helical vortices. Chapter 3 described the experimental setup and analysed the data, which
was then used in the computational fluid dynamics (CFD) validation study in Chapter 4. The pipeline to reproduce of the experimental geometry for CFD, known as image-based meshing, was documented. Image-based meshing enabled a pixel-wise comparison. This is the first validation study in the inertial regime, and the accuracy of the simulation was comparable to the similar studies in the creeping flow. Moreover, one of the primary sources of errors, the meshing of the contact points (Dixon et al., 2013), was identified to be the primary cause of the discrepancies.

Regarding the transition to unsteady regimes, the transient flow fields in both the random and structured packings were acquired using spiral imaging. Despite decades of investigation of the onset of unsteady flow in random packings, the heterogeneity of the process has been confirmed for the first time. Similar to the transition to the inertial regime (Johns et al., 2000), MRV revealed that flow instability also initiated asynchronously in different pores. In addition, the unsteady area spread across the pore quickly with increasing Reynolds number (Re). The evolution of unsteady flow was characterised according to the flow features. The coherent structures, i.e., recurring unsteady flow patterns, were extracted using proper orthogonal decomposition (POD). Further analysis of the temporal features based on the POD modes revealed frequency signatures of the unsteady vortical motion, which suggests a route to chaos from steady, periodic, quasi-periodic, to chaotic.

The last two results chapters summarised the study in a simple cubic packing (SCP). The instability occurred first as periodic oscillation of the shear layer and synchronised streamwise vortices, which then became quasi-periodic before chaotic flow commenced. The wavelengths were extracted by the dynamic mode decomposition, and the dominant wavelength was determined by the characteristic length of the packing. The final stage of the transition in porous media is towards the turbulent flow. The convergence of the macroscopic features (normalised turbulent kinetic energy, integral length scale) occurred at lower Re than the microscopic features (skewness, flatness, and POD modes). This trend agrees well with a pioneering study in a random packing (Patil & Liburdy, 2013a). Moreover, the integral length scale and the coherent structures are constrained by the pore size, which justifies a fundamental assumption in the turbulent simulation of flow in porous media.

8.1.3 Fluid dynamics research

In this thesis, the synergy between the three approaches to fluid dynamics research, i.e., the experimental, theoretical and numerical techniques, was highlighted.
First, the collaboration between experimental and numerical approaches was demonstrated. In Chapter 4, the image-based meshing protocols are applicable to other complex structures and provide a framework to fully leverage the growing repository of spatially resolved data, both experimentally and numerically, via pixel-wise validation. Phenomenon predicted by numerical studies were observed for the first time in packing structures, e.g., helical vortices, vortex shedding and travelling waves (Chapters 3-7). Moreover, the pore-scale flow fields are crucial for validating the trending direct numerical simulations. We conclude that spatially-resolved flow experiments will make significant contributions to accurate CFD modelling.

Second, the experimental data also contributes to theories. The spatial-temporal structures in the SCP in chapters 6 and 7 were remarkably similar to the travelling wave solutions of Navier-Stokes equations. Such structure underpins the self-sustaining process, which is speculated as the building block for turbulent flow.

### 8.2 Suggestions for future work

#### 8.2.1 Future work on experimental studies

First, we suggest some fruitful experimental studies that arise from the work presented in this thesis. We propose to apply the same experimental techniques and analytical tools to a face-centered cubic (FCC) packing. Because the onset of unsteady flow in the FCC packing was characterised in detail by Hill & Koch (2002) using Lattice-Boltzmann method (LBM) simulations, the results from this experiment can be used to validate the route to chaos directly. In particular, the new results can verify the presence of torus bifurcation, which was not clearly shown in the unsteady flow in SCP. It would be interesting to explore the bifurcations in SCP in more detail, which can be discovered by conducting experiments at smaller incremental steps of flowrate, from the maximum $Re$ of the steady flow to $Re$ at the onset of the chaotic regime, revealed by this work. Towards the transition to turbulence, the evidence regarding the asymptotic behaviour of the microscopic properties was not strong because only two $Re$ showed convergence. To determine the transition without ambiguity, the maximum $Re$ for experimental measurements should be higher. For an accurate quantification of the critical $Re$, the resolution of $Re$ in the future experiments needs increasing.

Next, we can apply the same technique to similar problems. In this work, only the packings with sphere particles were examined, due to the ubiquitous observations and predictions in sphere packings. In contrast, the particles used in industrial settings are in a variety of different
shapes, including cylinders, raschig rings, and trilobes. The experimental techniques (3D MRV and ultra-fast imaging) and the analysis approaches (flow characteristics, POD, etc.) can be used to investigate how the particle shapes affect the flow fields and the transition phenomena. Moreover, the aspect ratio of catalytic reactors is higher than this work; thus, a systematic examination of the influence of the aspect ratio of a packed bed is desirable. Besides packed bed reactors, MRV is suited to other porous media; e.g., in biomaterials, MRV was used to measure the local hydrodynamics, including flow fields, pressure, shear, and fluid permeability fields (Mack et al., 2013; Youssef et al., 2017).

8.2.2 Technique development for MRV

Substantial efforts have been made to reduce acquisition time in clinical MRI applications and the techniques can be used to further accelerate MRV. The first group of acceleration methods is parallel MRI, using spatially varying information of multiple coils. Pruessmann et al. (1999) proposed a technique based on different sensitivity of the receiver coils, called SENSitivity Encoding (SENSE). The other popular technique is the Generalized Autocalibrating Partially Parallel Acquisitions (GRAPPA), which reduces the computational demand for reconstruction compared to SENSE (Heidemann et al., 2006). Further acceleration can be achieved by utilising the temporal correlation in the $k$-$t$ space, such as $k$-$t$ BLAST (Broad-use Linear Acquisition Speed-up Technique), $k$ -$t$ SENSE (Tsao et al., 2003), and $k$ -$t$ FOCUSS (FOCal Underdetermined System Solver) (Jung et al., 2007). $k$-$t$ BLAST was first applied to acquire time-resolved 3D phase-contrast MRV, i.e., four-dimensional (4D) flow MRI, for pulsatile fluid flow by Marshall (2006), who achieved acceptable results with an acceleration factor of 12 (i.e., 1/12 of the fully-sampled data). Similar techniques were used to measure flow in aortic valve stenosis (Thunberg et al., 2012), intracranial aneurysm (Van Ooij et al., 2013), and in the brain (Sekine et al., 2014).

The second group of acceleration approaches relies on iterative reconstruction and CS techniques, which are often combined with parallel MRI. For example, by combining GRAPPA and CS, Lustig & Pauly (2010) proposed the iterative self-consistent parallel imaging technique. Similarly, Hutter et al. (2015) introduced the Multi-Dimensional Flow-preserving Compressed Sensing algorithm by exploiting the spatial-temporal correlations in 4D flow MRI. This approach achieved an acceleration factor of 8 in the in vivo study, acquiring three 2D three-components velocity maps of size $224 \times 224$ in 56 s. Given the prolific applications in
medical imaging, the combination of multiple coils and advanced compressed sensing algorithms can be applied to study highly transient flows.

8.2.3 Future numerical and theoretical work

The image-based meshing provided valuable information regarding the CFD simulation in the steady flow regime, and the same workflow can be applied to the unsteady regime in the future. One of the most promising CFD studies is to investigate the unsteady flow in SCP, given the detailed data provided by this work. The additional benefits of conducting this numerical study include the accessibility of 3D instantaneous flow fields, thus allowing a direct comparison of the travelling waves between SCP and the closely-related square ducts. Besides conventional CFD methods, it is likely that numerical methods for finding the invariant solutions may be more suitable, e.g., the continuation procedure (Kerswell, 2005) and Newton-Krylov iteration (Kawahara et al., 2011). Such information can fill the gaps in the theoretical work on the dynamical systems approach to turbulence, regarding more complex flow configurations.
Bibliography


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Youssef, K., Jarenwattananon, N. N., Archer, B. J., Mack, J., Iruela-Arispe, M. L., & Bouchard,


## Nomenclature

### Roman symbols

<table>
<thead>
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<th>Symbol</th>
<th>Description</th>
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<td>$\alpha$</td>
<td>Acceleration</td>
<td>[m/s$^2$]</td>
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<td>Area</td>
<td>[m$^2$]</td>
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<td>[m]</td>
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<tr>
<td>$D_p$</td>
<td>Particle diameter</td>
<td>[m]</td>
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<td>$D_\alpha$</td>
<td>a diagonal matrix consisting of the magnitudes of the DMD modes</td>
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<tr>
<td>$E$</td>
<td>Energy</td>
<td>[J]</td>
</tr>
<tr>
<td>$f$</td>
<td>Frequency</td>
<td>[Hz]</td>
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<tr>
<td>$F$</td>
<td>Subsampled Fourier transform operator</td>
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<tr>
<td>$G$</td>
<td>Gradient in magnetic field</td>
<td>[Tesla/m]</td>
</tr>
<tr>
<td>$h$</td>
<td>Planck’s constant</td>
<td>[J s]</td>
</tr>
<tr>
<td>$I$</td>
<td>Nuclear spin quantum number</td>
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<td>$I$</td>
<td>Signal intensity</td>
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<tr>
<td>$I_{\text{lim}}$</td>
<td>Limiting current</td>
<td>[A]</td>
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<td>$J$</td>
<td>Regulariser</td>
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<tr>
<td>$k$</td>
<td>Reciprocal space vector</td>
<td>[m$^{-1}$]</td>
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<td>$k$</td>
<td>Turbulent kinetic energy</td>
<td>[m$^2$/s$^2$]</td>
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<td>$k_B$</td>
<td>Boltzmann constant</td>
<td>[J/K]</td>
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<td>wave vector of the scattered and incident light</td>
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<tr>
<td>$M$</td>
<td>Magnetization vector</td>
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<td>$n$</td>
<td>Number of repetitions</td>
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<tr>
<td>$N$</td>
<td>Column-to-diameter ratio</td>
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<tr>
<td>$N$</td>
<td>Spin population</td>
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<td>$P_s$</td>
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<td>$q$</td>
<td>Dynamic reciprocal space vector</td>
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<td>$Q$</td>
<td>Volumetric flowrate</td>
<td>[m$^3$/s]</td>
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<td>$r$</td>
<td>Position vector</td>
<td>[m]</td>
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<td>$r$</td>
<td>Radial position</td>
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<td>$R$</td>
<td>Displacement vector</td>
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<td>$Re$</td>
<td>Reynolds number</td>
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<td>$Re_b$</td>
<td>Reynolds number in square ducts</td>
<td>[-]</td>
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<tr>
<td>$Re_{\text{crit}}$</td>
<td>Critical superficial Reynolds number</td>
<td>[-]</td>
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<tr>
<td>$Re_p$</td>
<td>Pore Reynolds number</td>
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<td>Unit</td>
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<tr>
<td>$Re_{sf}$</td>
<td>Superficial Reynolds number</td>
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<td>$S$</td>
<td>Signal</td>
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<td>Maximum slew rate</td>
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<td>Velocity gradient in the microelectrode measurements</td>
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<td>Power spectral density</td>
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<tr>
<td>$St$</td>
<td>Strouhal number</td>
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<td>$t$</td>
<td>Time</td>
<td>$[\text{s}]$</td>
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<td>$t_p$</td>
<td>Phase encoding time</td>
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<tr>
<td>$T$</td>
<td>Temperature</td>
<td>$[\text{K}]$</td>
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<tr>
<td>$T_1$</td>
<td>Spin-lattice relaxation time constant</td>
<td>$[\text{s}]$</td>
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<td>$T_2$</td>
<td>Spin-spin relaxation time constant</td>
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<td>$T_2^*$</td>
<td>Apparant spin-spin relaxation time constant</td>
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<tr>
<td>$T_2'$</td>
<td>Irreversible spin-spin relaxation time constant</td>
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<tr>
<td>$T_R$</td>
<td>Recycle time</td>
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<tr>
<td>$TR$</td>
<td>Recycle time</td>
<td>$[\text{s}]$</td>
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<tr>
<td>$u$</td>
<td>Magnitude of reconstructed image/fluid velocity</td>
<td>$[-]/[\text{m/s}]$</td>
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<td>$u_\theta$</td>
<td>Angular velocity in radial coordinate</td>
<td>$[\text{m/s}]$</td>
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<tr>
<td>$u_r$</td>
<td>Radial velocity in radial coordinate</td>
<td>$[\text{m/s}]$</td>
</tr>
<tr>
<td>$u_z$</td>
<td>Axial velocity in radial coordinate</td>
<td>$[\text{m/s}]$</td>
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<td>$\mathbf{u}$</td>
<td>Fluid velocity vector</td>
<td>$[\text{m/s}]$</td>
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<tr>
<td>$U_{int}$</td>
<td>Interstitial velocity</td>
<td>$[\text{m/s}]$</td>
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<td>$U_{sf}$</td>
<td>Superficial velocity</td>
<td>$[\text{m/s}]$</td>
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<tr>
<td>$v$</td>
<td>Fluid velocity</td>
<td>$[\text{m/s}]$</td>
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<td>$V$</td>
<td>Transverse velocity magnitude</td>
<td>$[\text{m/s}]$</td>
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<td>$V_{and}$</td>
<td>Vandermonde matrix</td>
<td>[-]</td>
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<tr>
<td>$V$</td>
<td>Volume</td>
<td>$[\text{m}^3]$</td>
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<tr>
<td>$w$</td>
<td>Fluid velocity</td>
<td>$[\text{m/s}]$</td>
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<tr>
<td>$x$</td>
<td>Fully sampled signal</td>
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<tr>
<td>$y$</td>
<td>Subsampled signal</td>
<td>[-]</td>
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<tr>
<td>$z_0$</td>
<td>Distance of the source of signal from the gradient isocentre</td>
<td>$[\text{m}]$</td>
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<tr>
<td>$Z$</td>
<td>Axial location</td>
<td>$[\text{mm}]$</td>
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**Greek symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
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<th>Unit</th>
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<tr>
<td>$\alpha$</td>
<td>Regularisation parameter</td>
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<tr>
<td>$\alpha_t$</td>
<td>DMD mode amplitude</td>
<td>$[\text{m/s}]$</td>
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<tr>
<td>$\gamma$</td>
<td>Gyromagnetic ratio</td>
<td>$[\text{rad/(Tesla s)}]$</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Tip angle or phase offset</td>
<td>[rad]</td>
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<tr>
<td>Symbol</td>
<td>Definition</td>
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<tr>
<td>$\delta$</td>
<td>Pulse length of a flow-encoding gradient pulse [s]</td>
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<tr>
<td>$\Delta$</td>
<td>Time between two flow-encoding pulses [s]</td>
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<tr>
<td>$\epsilon$</td>
<td>Porosity [-]</td>
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<tr>
<td>$\zeta$</td>
<td>Phase change due to applied magnetic gradient(s) [rad]</td>
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<tr>
<td>$\lambda_i$</td>
<td>DMD mode decay rate [s$^{-1}$]</td>
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<tr>
<td>$\lambda_k$</td>
<td>Eigenvalue of the $k^{th}$ eigenvector [-]</td>
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<tr>
<td>$\Gamma_2$</td>
<td>Criteria for vortex identification proposed by Graftieaux et al. (2001) [-]</td>
<td></td>
</tr>
<tr>
<td>$\mu$</td>
<td>Coherence or mean of normal distributions [-]</td>
<td></td>
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<tr>
<td>$\nu$</td>
<td>Kinematic viscosity [m$^2$/s]</td>
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</tr>
<tr>
<td>$\rho$</td>
<td>Mass density or spin density [kg/m$^3$ or m$^{-3}$]</td>
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<tr>
<td>$\sigma$</td>
<td>Standard deviation of normally distributions [-]</td>
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<tr>
<td>$\sigma_k$</td>
<td>Singular value of the $k^{th}$ eigenvector [-]</td>
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<tr>
<td>$\tau$</td>
<td>Time delay [s]</td>
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<tr>
<td>$\varphi$</td>
<td>Basis vector of the sparsifying transform matrix [-]</td>
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<table>
<thead>
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<th>Definition</th>
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<tr>
<td>$\phi$</td>
<td>POD spatial basis function [-]</td>
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<td>$\phi_i$</td>
<td>Basis vector of the measurement matrix [-]</td>
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<td>$\Phi$</td>
<td>Measurement matrix in Chapter 2; Matrix with right singular-vectors in Chapter 5 [-]</td>
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<tr>
<td>$\psi$</td>
<td>POD temporal basis function [-]</td>
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<tr>
<td>$\Psi$</td>
<td>Sparsifying transform matrix in Chapter 2; Matrix with left singular-vectors in Chapter 5; Matrix with DMD modes in Chapter 6 [-]</td>
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<td>$\omega$</td>
<td>Angular frequency or vorticity [rad/s]</td>
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<td>$\Omega$</td>
<td>Volume of the control volume [m$^3$]</td>
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**Abbreviations**

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<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>2D</td>
<td>Two-dimensional parameter space</td>
</tr>
<tr>
<td>2D1C</td>
<td>Two-dimensional one component velocity measurement</td>
</tr>
<tr>
<td>2D3C</td>
<td>Two-dimensional three components velocity measurement</td>
</tr>
<tr>
<td>3D</td>
<td>Three-dimensional parameter space</td>
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<td>BFS</td>
<td>Backward-facing step</td>
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<td>BLAST</td>
<td>Broad-use linear acquisition speed-up technique</td>
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<tr>
<td>CAD</td>
<td>Computer-aided design</td>
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<td>CFD</td>
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<td>CPMG</td>
<td>Carr-Purcell-Meiboom-Gill</td>
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<td>CSA</td>
<td>Cross-sectional areas</td>
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<td>CT</td>
<td>Computed tomography</td>
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<td>DMD</td>
<td>Dynamic mode decomposition</td>
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<td>Acronym</td>
<td>Description</td>
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<td>---------</td>
<td>-------------</td>
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<td>DNS</td>
<td>Direct numerical simulations</td>
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<tr>
<td>EPI</td>
<td>Echo planar imaging</td>
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<tr>
<td>EPOD</td>
<td>Extended proper orthogonal decomposition</td>
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<td>FCC</td>
<td>Face-centred cubic</td>
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<td>FFT</td>
<td>Fast Fourier transform</td>
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<tr>
<td>FLASH</td>
<td>Fast low angle shot</td>
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<tr>
<td>FLIESSEN</td>
<td>Flow imaging employing single-shot encoding</td>
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<tr>
<td>FOV</td>
<td>Field-of-view</td>
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<td>FOCUSS</td>
<td>Focal underdetermined system solver</td>
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<td>FWHM</td>
<td>Full width at half maximum</td>
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<td>GARPPA</td>
<td>Generalized autocalibrating partially parallel acquisitions</td>
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<td>GPSF</td>
<td>Gaussian point spread function</td>
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<td>HCP</td>
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<td>HWA</td>
<td>Hot-wire anemometry</td>
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<td>Laser-Doppler anemometry</td>
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<td>LDV</td>
<td>Laser-Doppler velocimetry</td>
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<td>Marching Cube</td>
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<td>MRI</td>
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<td>MRV</td>
<td>Magnetic resonance velocimetry</td>
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<td>MPS</td>
<td>moving-particle semi-implicit</td>
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<td>NMR</td>
<td>Nuclear magnetic resonance</td>
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<td>NRMSD</td>
<td>Normalised root mean squared deviation</td>
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<td>Non-uniform fast Fourier transform</td>
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<td>Probability distribution function</td>
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<td>PFG</td>
<td>Pulsed field gradient</td>
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<td>pore-network models</td>
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<td>Proper orthogonal decomposition</td>
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<td>r.f.</td>
<td>Radial frequency</td>
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<td>Root-mean-square</td>
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<td>RARE</td>
<td>Rapid acquisition with relaxation enhancement</td>
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<td>REV</td>
<td>Representative elementary volume</td>
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<td>RIP</td>
<td>Restricted isometry property</td>
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<td>sPIV</td>
<td>Stereoscopic particle imaging velocimetry</td>
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<td>Sensitivity Encoding</td>
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<td>SIMPLE</td>
<td>Semi-implicit method for pressure-linked equations</td>
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<td>SLIE</td>
<td>Sphere Loci extraction through Iterative Erosion</td>
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<tr>
<td>SNR</td>
<td>Signal-to-noise-ratio</td>
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<td>SPH</td>
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<td>SSIM</td>
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<td>Turbulent kinetic energy</td>
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<td>TV</td>
<td>Total variation</td>
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<td>Travelling wave</td>
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<td>Ultrasonic velocity profiler</td>
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<td>VDS</td>
<td>Variable density spiral</td>
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