Hydrodynamic characteristics of flow past a square cylinder at moderate Reynolds numbers

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Abstract

Two-dimensional (2D) and three-dimensional (3D) hydrodynamic characteristics of flow past a square cylinder are investigated using direct numerical simulations. The variations of the hydrodynamic forces and wake flow characteristics with the Reynolds number (Re) are examined for $Re = 10$ to 400 with a high resolution in Re . Distinct features in the variation trends of the hydrodynamic forces with Re are examined and explained. In addition, for the 3D flows up to $Re = 400$, three critical conditions are observed at Re of approximately 165.7, 210 and 330. At the onset of the secondary wake instability of $Re = 165.7$, a sudden increase or decrease of the 3D flow property with respect to its 2D counterpart is observed, which is due to the sudden increase in the flow three-dimensionality at the mode A instability that is subcritical in nature. The second critical condition is because for $Re > 210$ the mode B flow structure becomes increasingly disordered and the wake flow becomes increasingly turbulent, such that the 3D flow property is increasingly deviated from its 2D counterpart. The third critical condition at $Re \sim 330$ is related to the disappearance and reappearance of the recirculation regions on the upper and lower sides of the cylinder. While the first two critical conditions are also observed for flow past a circular cylinder, the third one is not, since the geometry of a circular cylinder does not give rise to recirculation regions on the upper and lower sides of the cylinder.

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1. Introduction

Steady incoming flow past a nominally two-dimensional (2D) bluff body has been a classical problem in fluid mechanics owing to its fundamental and practical significance. Typical bluff bodies include circular and square cylinders. The scenario of steady incoming flow past a smooth circular/square cylinder (referred to as “flow past a circular/square cylinder” hereafter) is governed by a single dimensionless parameter, the Reynolds number $Re (= UD/\nu)$, which is defined based on the incoming flow velocity (U), the length scale of the cylinder perpendicular to the incoming flow (D), and the kinematic viscosity of the fluid (ν). Specifically, for a circular cylinder the length scale is the diameter of the cylinder, while for a square cylinder aligned with sides perpendicular and parallel to the incoming flow the length scale is the side length of the cylinder.

The wake transition regimes of flow past a circular cylinder have been well studied in the literature. With increasing Re a few flow regimes have been discovered (see, e.g., Williamson, 1996a):

- (i) Laminar steady regime ($Re < 47$). The flow is steady, with two recirculation regions formed symmetrical about the wake centreline.
- (ii) Laminar vortex shedding regime ($Re \sim 47$ to 190). At $Re = 47$, the primary wake instability develops as a result of a Hopf bifurcation. Periodic shedding of the Kármán vortices is observed in this regime.
- (iii) Three-dimensional (3D) wake transition regime ($Re \sim 190$ to 270). At $Re \sim 190$, the secondary wake instability develops (i.e. the flow transitions from 2D to 3D). The relatively large-scale mode A flow structure (with a spanwise wavelength of $\sim 4D$ and an out-of-phase sequence between the neighbouring streamwise vortices) with vortex dislocations is observed for $Re \sim 190$ to 230, while a gradual wake transition from mode A with dislocations to the finer-scale mode B flow structure (with a spanwise wavelength of $\sim 0.8D$ and an in-phase sequence between the neighbouring streamwise vortices) takes place at $Re \sim 230$ to 260.

- (iv) Wake transition to turbulence ($Re \sim 270$ to 1200). The mode B flow structure becomes increasingly disordered and the wake flow becomes increasingly turbulent. It is noted that the shear layer instability at $Re \gtrsim 1200$ is outside the scope of the present study.

For flow past a circular cylinder, the hydrodynamic forces and wake flow characteristics for each of the wake transition regimes have been quantified by a number of experimental and numerical studies. Through eliminating the “end effects” of the model cylinder that were commonly encountered in early experimental studies (see, e.g., Williamson, 1989), Williamson (1996b) made accurate measurements of the Strouhal–Reynolds number ($St-Re$) relationship for Re up to approximately 300. Previous experimental studies have also reported relationships between Re and a number of flow properties, such as the base pressure coefficient (Williamson and Roshko, 1990; Williamson, 1996a), the formation length L_f (Noca et al., 1998), the root-mean-square lift coefficient (Norberg, 2003), the separation angle (Wu et al., 2004), etc. On the other hand, based on direct numerical simulations (DNS), Henderson (1995) and Posdziech and Grundmann (2007) reported various 2D hydrodynamic characteristics for flow past a circular cylinder, while Jiang et al. (2016) and Jiang and Cheng (2017) reported 3D hydrodynamic characteristics. Excellent agreements of the experimental and numerical results have been reached for the $St-Re$ relationship reported in Williamson (1996b) and Jiang et al. (2016), and for the L_f-Re relationship reported in Noca et al. (1998) and Jiang and Cheng (2017).

Similarly, the wake transition regimes of flow past a square cylinder are summarized as follows:

- (i) Laminar steady regime ($Re \lesssim 46$).
- (ii) Laminar vortex shedding regime ($Re \sim 46$ to 166). The critical Re for the primary wake instability was identified at 47 ± 2 in Sohankar et al. (1997), 45 in Saha et al. (2000), 44.7 in Park and Yang (2016), and 46 in Jiang et al. (2018).
- (iii) Three-dimensional wake transition regime ($Re \sim 166$ to 210). The critical Re for the secondary wake instability (i.e. the mode A instability) was identified

at 164 in Sheard et al. (2009), 166.5 in Choi et al. (2012), 166.6 in Park and Yang (2016), and 165.7 in Jiang et al. (2018). Within the 3D wake transition regime, a gradual wake transition from mode A with dislocations to mode B takes place at $Re \sim 185$ to 210 (Jiang et al., 2018).

(iv) Wake transition to turbulence ($Re \gtrsim 210$).

For flow past a square cylinder, the relationships between Re and the hydrodynamic forces have been reported by only a limited number of studies. Fig. 1 shows the variations of St and the time-averaged drag coefficient (the two most commonly-studied flow properties) with Re for a few studies available in the literature, together with the DNS results of the present study. In contrast to the aforementioned good agreement of different studies for a circular cylinder, considerable scatters are observed in Fig. 1 for a square cylinder, especially for the range of Re beyond the secondary wake instability, since the 3D flows are more difficult to be measured or simulated accurately. In light of this, the first aim of the present study is to establish a more accurate database of the hydrodynamic forces and wake flow characteristics for flow past a square cylinder.

Fig. 1. Variations of (a) the Strouhal number and (b) the time-averaged drag coefficient with Re for a few studies available in the literature.

In addition, the second aim of the present study is to explore the physical mechanisms responsible for the variations of the hydrodynamic forces and wake flow characteristics with Re . Different variation trends are expected for different wake transition regimes. For example, for flow past a circular cylinder, with increase in Re the formation length increases in the laminar steady regime, followed by a decrease in the laminar vortex shedding regime and an increase beyond the 3D wake transition regime (see, e.g., Williamson, 1996a), while a sudden increase is observed at the onset of the secondary wake instability (Jiang and Cheng, 2017). The critical Re values between the wake transition regimes (i.e. Re of approximately 47, 190 and 270 for the case of a circular cylinder) can be identified by the discontinuities in (i) the relationship between Re and some flow properties (such as the hydrodynamic forces on the cylinder and the flow characteristics in the wake), and (ii) the relationship between Re and the gradient of variation of some flow properties with Re . However, such discontinuities between the wake transition regimes for a square cylinder could hardly be identified by some previous results shown in Fig. 1, especially when relatively large intervals of Re were selected. High-quality data over the wake transition regimes would be necessary to shed light on the underlying physical mechanisms responsible for the flow behaviours.

2. Numerical model

2.1. Numerical method

OpenFOAM (www.openfoam.org) has been adopted in this study in solving the continuity and incompressible Navier–Stokes equations:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (2.1)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad (2.2)$$

where $(x_1, x_2, x_3) = (x, y, z)$ are Cartesian coordinates, u_i is the velocity component in the direction x_i , t is time, ρ is fluid density, p is pressure, and ν is kinematic viscosity.

The Finite Volume Method (FVM) and the Pressure Implicit with Splitting of Operators (PISO) algorithm (Issa, 1986) are used to solve the equations. The FVM, as implemented in OpenFOAM, is one of the preferred methods in computational fluid dynamics (CFD) owing to the following advantages (Moukalled et al., 2016): (i) inherent conservation, (ii) allowance of unstructured polygonal meshes, and (iii) easiness of implementing boundary conditions in a non-invasive manner (since the unknown variables are evaluated at the centroids of the volume elements rather than at their boundary faces). As pointed out in Versteeg and Malalasekera (1995), the PISO algorithm is an enhanced extension of the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm. In addition, Issa et al. (1986) showed with a benchmark laminar backward-facing step problem that by using PISO over SIMPLE the computational cost reduced significantly. For the Navier–Stokes equations, the advection, diffusion and time derivative terms are discretized, respectively, using a fourth-order cubic scheme, a second-order linear scheme, and a blended scheme consisting of the second-order Crank–Nicolson scheme and a first-order Euler-implicit scheme, respectively. Since the fully centred and second-order Crank–Nicolson scheme is often unstable for complex flows, it is necessary to “off-centre” the scheme to stabilize it while retaining greater temporal accuracy than the first-order Euler-implicit scheme (Seng et al., 2017; Pedersen et al., 2017; Vukčević et al., 2016). An off-centring coefficient of 0.5 (a value of 1.0 represents the Crank–Nicolson scheme while a value of 0 represents the Euler-implicit scheme) is adopted in this study as a compromise between accuracy and stability. The same numerical approach as outlined above has been successfully adopted in Jiang et al. (2016, 2018) for the simulations of wake transition of a circular and a square cylinder.

2.2. Computational mesh and boundary conditions

The computational mesh used in Jiang et al. (2018) for the simulations of flow past a square cylinder is adopted in the present study. As sketched in Fig. 2(a), the

computational domain size is $(L_x, L_y, L_z) = (60D, 60D, 15D)$, with L_x , L_y , and L_z being the domain sizes in the x -, y -, and z -directions, respectively. The boundary conditions for the computational domain are listed in Table 1, where $\partial/\partial\mathbf{n} = 0$ denotes a zero normal gradient condition. In particular, symmetry boundary conditions are applied at the top and bottom boundaries, while periodic boundary conditions are employed at the front and back boundaries that are perpendicular to the cylinder span. For the front and back boundaries, Jiang et al. (2017) demonstrated that the periodic boundary conditions are more suitable than the symmetry boundary conditions in simulating fully developed 3D flows. The periodic boundary conditions also follow the nature of the underlying instability modes which are spanwise-periodic (e.g. Henderson, 1997; Sheard et al., 2009).

Fig. 2. (a) Schematic model of the computational domain (not to scale), and (b) Close-up view of the 2D mesh near the cylinder.

Table 1. Boundary conditions for the computational domain.

Boundary	Velocity components	Pressure
Inlet	$u_x = U, u_y = u_z = 0$	$\partial p / \partial \mathbf{n} = 0$
Outlet	$\partial u_i / \partial \mathbf{n} = 0$	$p = 0$
Top and bottom	$\partial u_x / \partial \mathbf{n} = \partial u_z / \partial \mathbf{n} = 0, u_y = 0$	$\partial p / \partial \mathbf{n} = 0$
Front and back	$u_i(x, y, z = 0, t) = u_i(x, y, z = L_z, t),$ $\partial u_i / \partial z(x, y, z = 0, t) = \partial u_i / \partial z(x, y,$ $z = L_z, t)$	$p(x, y, z = 0, t) = p(x, y, z = L_z, t),$ $\partial p / \partial z(x, y, z = 0, t) = \partial p / \partial z(x, y, z$ $= L_z, t)$
Cylinder surface	$u_i = 0$	$\partial p / \partial \mathbf{n} = 0$

Some key parameters for the computational mesh are specified as follows. For the 2D mesh in the plane perpendicular to the cylinder axis (i.e. the x - y plane), the number of cells around the cylinder surface is 196. The smallest cell size at the leading edges of the cylinder is $0.005D \times 0.005D$. The cell expansion ratio in the whole domain is kept below 1.1. To capture detailed wake flow structures, a relatively high

mesh resolution is used in the near-wake by specifying a streamwise mesh size varying linearly from $0.05D$ at $x/D = 1$ to $0.1D$ at $x/D = 7$. A close-up view of the mesh near the cylinder is shown in Fig. 2(b). The 3D mesh is constructed by replicating the 2D mesh along the z -axis with a spanwise cell size of $0.125D$, which results in an identical mesh resolution in all planes perpendicular to the spanwise direction.

The time step size Δt is chosen based on a Courant–Friedrichs–Lewy (CFL) limit of less than 0.5, where the CFL number is defined as

$$\text{CFL} = \frac{|u| \Delta t}{\Delta l} \quad (2.3)$$

where $|u|$ is the magnitude of the velocity through a cell, and Δl is the cell size in the direction of the velocity. For $Re = 100$ and 400 , the time step sizes are 0.00187 and 0.00147 , respectively. The temporal convergence is checked based on the 2D cases at $Re = 50, 100, 200$ and 250 , because the fully developed 2D flows at $Re \leq 250$ are perfectly time-periodic (Sohankar et al., 1999) and are therefore unaffected by the choice of statistical data length (i.e. the number of vortex shedding cycles used for the statistics). For the 2D cases at $Re = 50, 100, 200$ and 250 , the temporal convergence is checked by re-calculating the cases with a halved time step size (i.e. with $\text{CFL} < 0.25$), and this results in variations of less than 0.1% for the Strouhal number and time-averaged drag coefficient, and less than 0.4% for the root-mean-square lift coefficient.

A 3D mesh convergence study has been reported separately in Jiang et al. (2018) with two variations to the above-mentioned reference mesh:

- (i) A mesh refined in the x - y plane. This mesh has a number of cells in both x - and y -directions 1.5 times that of the reference mesh. Specifically, the number of cells around the cylinder surface is increased by 1.5 times, while the height of the first layer of mesh next to the cylinder is reduced by 1.5 times. For this case, the time step size Δt is also reduced by 1.5 times so as to satisfy the same CFL limit, i.e. $\text{CFL} < 0.5$.
- (ii) A mesh refined in the z -direction. The spanwise cell size is reduced from $0.125D$

to $0.0625D$.

It has been shown in Jiang et al. (2018) that the hydrodynamic forces on the cylinder for $Re = 400$ (the largest Re adopted in this study) calculated with the two refined meshes are very close to those calculated with the reference mesh. Specifically, the relative differences are within 0.5% for the Strouhal number and time-averaged drag coefficient, and within 3.5% for the root-mean-square lift coefficient. In addition, for the critical Re values (Re_{cr}) of the modes A and B wake instabilities, the relative differences in Re_{cr} between those calculated with the two refined meshes and those calculated with the reference mesh are within 1%. The results calculated with the reference mesh, namely $Re_{cr} = 165.7$ for mode A and $Re_{cr} = 201.1$ for mode B, are very close to $Re_{cr} = 166.6$ for mode A and $Re_{cr} = 201.1$ for mode B reported in Park and Yang (2016), with relative differences of less than 1%. Therefore, the reference mesh is used in this study.

2.3. Data analysis methods

In the present study, the 2D simulations are performed for Re up to 265, since above which the vortex shedding process becomes irregular due to the restriction of a 2D computational domain (Sohankar et al., 1999). For $Re \geq 270$, it is found that the vortex shedding process no longer follows the Kármán vortex street pattern, and the time-averaged lift force is not zero. However, these features are not observed for the simulations with a 3D computational domain. The 3D simulations are therefore performed for Re up to 400.

The hydrodynamic forces on the cylinder, including the drag coefficient (C_D), the lift coefficient (C_L), and the Strouhal number (St), are defined as:

$$C_D = \frac{F_D}{\frac{1}{2}\rho U^2 D L_z} \quad (2.4)$$

$$C_L = \frac{F_L}{\frac{1}{2}\rho U^2 D L_z} \quad (2.5)$$

$$St = \frac{f_L D}{U} \quad (2.6)$$

where F_D and F_L are the drag force and lift force integrated over the entire cylinder surface, respectively, and f_L is the frequency of the fluctuating lift force. The time-averaged drag and lift coefficients are denoted as $\overline{C_D}$ and $\overline{C_L}$, respectively.

The root-mean-square lift coefficient C_L' is defined as:

$$C_L' = \sqrt{\frac{1}{N} \sum_{i=1}^N (C_{L,i} - \overline{C_L})^2} \quad (2.7)$$

where N is the number of values in the time-history.

In addition, the time-averaged pressure coefficient (C_p) at a specific point on the cylinder surface is defined as:

$$C_p = \frac{p_{cyl} - p_\infty}{\frac{1}{2} \rho U^2} \quad (2.8)$$

where p_{cyl} is the time-averaged pressure at this point, and p_∞ is the reference pressure at the inlet of the domain. The base pressure coefficient (C_{pb}) is defined as:

$$C_{pb} = \frac{p_b - p_\infty}{\frac{1}{2} \rho U^2} \quad (2.9)$$

where p_b is the time-averaged pressure at the rear stagnation point of the cylinder, namely $(x/D, y/D) = (0.5, 0)$.

Prior to the onset of vortex shedding of $Re = 46$, the $\overline{C_D}$ and C_p values are obtained from the fully developed steady flow, while the fluctuations of the hydrodynamic forces are equal to zero. For $Re = 46 - 265$, since the fully developed 2D flows are time-periodic, the hydrodynamic forces are calculated based on the time-histories of a complete vortex shedding cycle. Beyond the onset of the secondary wake instability of $Re = 165.7$, the fully developed 3D flows become irregular. For each 3D case, the simulation is run for at least 1000 non-dimensional time units (defined as $t^* = tU/D$) to ensure that the flow has become fully developed. After that, at least 800 non-dimensional time units (~ 120 vortex shedding cycles) of the fully developed flow are used to calculate the statistical stationary hydrodynamic forces on the cylinder. For 3D flows, f_L is determined as the peak frequency derived from the fast Fourier transform (FFT) of the time-history of C_L .

In addition to the hydrodynamic forces on the cylinder, the flow field around the cylinder will also be examined. The time-averaged streamwise, transverse and spanwise velocities are denoted as $\overline{u_x}$, $\overline{u_y}$ and $\overline{u_z}$, respectively, while the root-mean-square streamwise, transverse and spanwise velocities are calculated as:

$$u_x' = \sqrt{\frac{1}{N} \sum_{i=1}^N (u_{x,i} - \overline{u_x})^2} \quad (2.10)$$

$$u_y' = \sqrt{\frac{1}{N} \sum_{i=1}^N (u_{y,i} - \overline{u_y})^2} \quad (2.11)$$

$$u_z' = \sqrt{\frac{1}{N} \sum_{i=1}^N (u_{z,i} - \overline{u_z})^2} \quad (2.12)$$

For a 3D flow, at least 800 non-dimensional time units of the fully developed flow are used to calculate the time-averaged and root-mean-square 3D flow fields.

Ideally, for a 3D flow the hydrodynamic forces at different spanwise locations would be identical when the statistical period is sufficiently long. When a finite statistical period is used (even for more than 120 vortex shedding cycles), the 3D hydrodynamic forces at different spanwise locations may be slightly different, and the span-averaged values can be used to improve the accuracy. Hence equations (2.4) – (2.7) give the span-averaged hydrodynamic forces. By using equations (2.4) – (2.7), the hydrodynamic forces for the 3D flow at $Re = 400$ calculated with the statistical data range of at least 800 non-dimensional time units are very close to those calculated with the second half of the data range (of at least 400 non-dimensional time units), with relative differences of less than 0.3% for St and $\overline{C_D}$, and less than 2% for C_L' (Jiang et al., 2018).

Similarly, for a 3D flow the wake flow characteristics (such as the formation length and the wake width) at different spanwise locations may be slightly different when using a finite statistical period. To approximate to the ideal results, the time-averaged/root-mean-square 3D flow field is further averaged over the spanwise direction to form a time-averaged/root-mean-square 2D flow field (called span-averaged 3D flow hereafter). Such a 2D flow field can be used to determine the

span-averaged flow characteristics of the corresponding 3D flow.

Comparisons of the flow characteristics of flow past a square cylinder and a circular cylinder are also included in some of the analyses. For the DNS results of flow past a circular cylinder reported in this study, the computational meshes used in Jiang et al. (2016) and Jiang and Cheng (2017) are adopted. Convergence checks of the meshes for a circular cylinder have been reported separately in Jiang et al. (2016) with $Re = 220$ and 300 and in Jiang and Cheng (2017) with $Re = 400$ and 1000.

3. Numerical results

3.1. Variations of flow properties with Re

Fig. 3 shows the variations of some flow properties with Re , including the time-averaged drag coefficient, the root-mean-square lift coefficient, the base pressure coefficient, the maximum 2D Reynolds stress $u_x'u_y'$ in the flow field, the formation length, and the Strouhal number. The formation length is calculated as the streamwise distance between the rear surface of the cylinder and the wake stagnation point, as sketched in Fig. 4.

Fig. 3. Variations of flow properties with Re : (a) the time-averaged drag coefficient, (b) the root-mean-square lift coefficient, (c) the base pressure coefficient, (d) the maximum $u'_x u'_y$ in the flow field, (e) the formation length, and (f) the Strouhal number. The vertical dashed lines mark the critical points at $Re = 46, 165.7, 210$ and 330 .

Fig. 4. A sketch of the definition of the formation length L_f . The blue lines represent the streamlines of the time-averaged flow, where two recirculation regions are observed in the near wake of the cylinder.

The variations of flow properties with Re shown in Fig. 3 reveal four critical points for Re up to 400, as marked by the vertical dashed lines in Fig. 3. The first two critical points at $Re = 46$ and 165.7 are induced by the primary and secondary wake instabilities, respectively. It is not surprising that significant changes in the flow pattern, such as the onset of vortex shedding and the onset of three-dimensionality, would result in sudden variations in the values of the flow properties. Fig. 5 shows some instantaneous vorticity fields for Re in different wake transition regimes. The onset of three-dimensionality is evidenced by the emergence of streamwise vortices for $Re > 165.7$. Beyond the secondary wake instability, two more critical points are observed at Re of approximately 210 and 330. These two critical points are hardly identified in previous studies (see Fig. 1b).

Fig. 5. Instantaneous vorticity fields in the near wake of a square cylinder for (a) $Re = 165$ (with only spanwise vortices), (b) $Re = 170$ (with mode A streamwise vortices and vortex dislocations), (c) $Re = 220$ (with relatively ordered mode B streamwise vortices), and (d) $Re = 330$ (with disordered mode B streamwise vortices). The translucent iso-surfaces represent spanwise vortices with $\omega_z = \pm 1.0$, while the opaque iso-surfaces represent streamwise vortices with $\omega_x = \pm 0.5$. Dark grey and light yellow denote positive and negative vorticity values, respectively. The flow is from left to right past the cylinder on the left.

Some variation features observed in Fig. 3 are summarised below, and some of which will be further investigated in sections 3.2 – 3.4.

- (i) Similar variation trends are observed for the base pressure coefficient shown in Fig. 3(c) and the maximum 2D Reynolds stress shown in Fig. 3(d). This feature is a result of the balance of forces from pressure and shear stress in the recirculation region, as is also observed for the case of a circular cylinder (Williamson, 1996a). In addition, the variation trends for the formation length shown in Fig. 3(e) are opposite to those of the base pressure coefficient and maximum 2D Reynolds stress, which suggests that an increase in the forces in the recirculation region would lead to a reduction in the size of the recirculation region, and vice versa.
- (ii) At the onset of the primary wake instability of $Re = 46$, a discontinuity in the gradient of variation with Re is observed for each of the flow properties shown in Fig. 3. For $Re \geq 46$, a monotonic increase or decrease is observed for each of the 2D flow properties shown in Fig. 3(b–e). However, for the time-averaged drag coefficient shown in Fig. 3(a) a local minimum is observed at $Re = 144$, while for the Strouhal number shown in Fig. 3(f) a local maximum is observed at $Re = 168$. The physical mechanisms for these two extreme values are investigated in sections 3.2 and 3.3, respectively.
- (iii) The two critical points beyond the secondary wake instability (at $Re \sim 210$ and 330) are observed for all the flow properties shown in Fig. 3 except for the Strouhal number shown in Fig. 3(f). The different behaviour for the 3D $St-Re$ relationship is investigated in section 3.4.

3.2. The drag coefficient

To further examine the variation of the time-averaged drag coefficient with Re shown in Fig. 3(a), the total drag is separated into the pressure and viscous components in Fig. 6(a). To facilitate comparison, the pressure and viscous drag coefficients for a circular cylinder are shown in Fig. 6(b). It is seen in Fig. 6(b) that the coefficients calculated with the present 2D DNS are in good agreement with the results reported in Henderson (1995). As stated in Henderson (1995), as Re exceeds the onset of the primary wake instability, the pressure drag coefficient starts to

increase while the viscous drag coefficient continues to decrease (Fig. 6b). The local minimum in the total drag coefficient at $Re \sim 150$ is due to combined effects of the pressure and viscous components. Similar variation trends are also observed in Fig. 6(a) for flow past a square cylinder, which explains the local minimum in the total drag at $Re = 144$.

For the case of flow past a square cylinder, an interesting feature observed in Fig. 6(a) is that the viscous drag coefficient decreases to negative values for $Re \geq 154$, and consequently the total drag coefficient is smaller than the pressure drag coefficient. The reason for the negative viscous drag is that the sizes of the recirculation regions on the upper and lower sides of the square cylinder expand with increasing Re , such that the upper and lower surfaces of the cylinder are increasingly covered with backward flow rather than forward flow. For $Re > 150$ the backward flow covers almost entirely the upper and lower surfaces of the cylinder. In contrast, for flow past a circular cylinder the flow separates at the downstream half of the cylinder surface (Wu et al., 2004), and the forward flow prior to the separation point is stronger than the backward flow after separation, such that the viscous drag integrated over the cylinder surface is positive (Fig. 6b).

Fig. 6. Variations of the pressure and viscous drag coefficients with Re for (a) flow past a square cylinder, and (b) flow past a circular cylinder.

It is also seen in Fig. 6 that the pressure drag coefficient for a square cylinder is

larger than that for a circular cylinder. This is mainly because the front surface of the square cylinder is perpendicular to the incoming flow, such that the streamwise velocity at the front of the cylinder (except for the areas very close to the edges) reduces to almost zero. A comparison of the time-averaged pressure coefficient on a square cylinder and a circular cylinder for $Re = 100$ is shown in Fig. 7(a,b). To reveal better the pressure drag in the streamwise direction, the streamwise component of the pressure coefficient is shown in Fig. 7(c,d). As shown in Fig. 7(c), the majority of the front surface of the square cylinder (except for the areas very close to the edges) is covered with a positive pressure, which is due to a sudden changeover of the velocity from the streamwise direction to the transverse direction. In contrast, for a circular cylinder the positive pressure is observed only within approximately $\pm 39^\circ$ from the front point of the cylinder (Fig. 7d), within which a sudden changeover of the direction of the velocity takes place.

Fig. 7. Time-averaged pressure coefficient on the cylinder for $Re = 100$ for (a) flow

past a square cylinder, and (b) flow past a circular cylinder. In addition, (c) and (d) show the streamwise component of the pressure coefficient for a square and a circular cylinder, respectively. The cylinder surface is shown in black while the pressure coefficient is plotted in blue. The flow is from left to right.

3.3. The 2D $St-Re$ relationship

For the 2D $St-Re$ relationship, a major difference between a circular cylinder and a square cylinder is that for a circular cylinder St increases monotonically with increase in Re up to at least $Re = 1000$ (see, e.g., Henderson, 1997), whereas for a square cylinder the $St-Re$ curve peaks at $Re = 168$ (Fig. 3f).

The physical reason is analysed below. Roshko (1955) suggested that the Strouhal number of a bluff body would scale better on the velocity at separation (U_s) and the wake width (D'), rather than simply on U and D . The Strouhal number based on such a definition was called the wake Strouhal number (St^*) in Roshko (1955), i.e.

$$St^* = f_L \frac{D'}{U_s} = St \frac{U}{U_s} \frac{D'}{D} \quad (3.1)$$

In the present study, the U_s and D' values for a square cylinder are determined based on the spanwise vorticity contours of the time-averaged flow field. The spanwise vorticity ω_z is defined in a non-dimensional form:

$$\omega_z = \left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right) \frac{D}{U} \quad (3.2)$$

As illustrated in Fig. 8, D' is chosen as the largest vertical distance between the positive and negative ω_z peaks. This is because such a distance reveals directly the cross-flow extent for the vortices to roll up to trigger vortex shedding (Jiang and Cheng, 2017). On the other hand, U_s , which serves as a representative of the regional flow rate prior to the rolling up of the vortices, is chosen as the mean streamwise velocity along the velocity profile shown by the solid vertical line located at $x/D = 0.465$ (Fig. 8). The streamwise location is chosen at $x/D = 0.465$ because it is very close to the saddle point between the recirculation regions on the upper/lower side of

the cylinder and in the wake region, which will be further explained later on in this section. The length of each vertical line is twice the distance between the peak point of ω_z at $x/D = 0.465$ (marked by a solid dot on the vertical line in Fig. 8) and the cylinder surface. The U_s-Re and $D'-Re$ relationships based on the present method are shown in Fig. 9(a) and Fig. 9(b), respectively. The corresponding St^*-Re relationship is shown in Fig. 10(a).

Fig. 8. Determinations of U_s and D' based on the spanwise vorticity contours of the time-averaged 2D flow field at $Re = 168$. Positive and negative contours are marked by solid and dashed lines, respectively.

Fig. 9. (a) The U_s – Re relationship, and (b) the D' – Re relationship, determined based on the spanwise vorticity contours of the time-averaged flow field.

Fig. 10. (a) The 2D and 3D St^* – Re relationships over the laminar and 3D wake transition regimes. (b) Comparison of the uniformness of the St and St^* values, shown by the relative differences of the St values with respect to the 2D St value at $Re = 168$, and the relative differences of the St^* values with respect to the 2D St^* value at $Re = 168$.

To examine the uniformity of the St and St^* values over the range of Re , Fig. 10(b) shows (i) the relative differences of the St values with respect to the 2D St value at $Re = 168$, and (ii) the relative differences of the St^* values with respect to the 2D St^* value at $Re = 168$. It is seen in Fig. 10(b) that the 2D St^* values (with relative

differences smaller than 10%) are indeed more uniform than the 2D St values (with relative differences up to 29%). This suggests that the vortex shedding frequency scales better on U_s and D' rather than on U and D . The inconsistency of the 2D St^* values may be due to some secondary factors such as the selection criterion for U_s in representing the regional flow prior to vortex shedding, and the redistribution of the velocity profile before the rolling up of the vortices.

As shown in Fig. 9, the peak of the $St-Re$ curve at $Re = 168$ (Fig. 3f) is due to the peak of the U_s-Re curve and the corresponding trough of the $D'-Re$ curve (a larger U_s leads to a thinner shear layer and thus a smaller D') at Re very close to 168. Based on flow visualization, it is found that the decrease in U_s for $Re > 168$ (Fig. 9a) is due to the emergence of a reverse flow from the wake recirculation region to the upper and lower sides of the cylinder past the two trailing edges of the cylinder, as illustrated with the streamlines of the time-averaged 2D flow field in Fig. 11. The reverse flow is not observed at $Re = 166$ (Fig. 11a) but emerges for $Re \geq 167$ (e.g. Fig. 11b). It is also noticed that the streamlines shown in Fig. 11 may slightly dive through the corner of the square cross-section, since the streamlines are drawn based on the time-averaged flow field rather than an instantaneous flow field. Nevertheless, the time-averaged velocity near the ends of the streamlines is well below $0.01U$.

Fig. 11. Streamlines of the time-averaged 2D flow field for (a) $Re = 166$, and (b) $Re = 175$. The streamlines are shown at near the lower right corner of the square cylinder, as marked by a rectangular frame in the inset. The saddle point is marked by a cross.

It is noted that the streamwise location for the calculation of U_s is chosen at $x/D = 0.465$ (which is very close to the saddle point shown in Fig. 11) so as to properly consider the reverse flow in the calculation of U_s . It is also worth noting that the U_s

value for a square cylinder is chosen as the mean streamwise velocity along a certain vertical range at $x/D = 0.465$, rather than the velocity at a particular point. This is because the velocity profile still redistributes as the flow travels from the separation point to the point where vortices start to roll up. The use of the mean streamwise velocity for U_s allows the reverse flow to be considered. For the case of a circular cylinder, however, the peak value along the streamwise velocity profile has been used to represent U_s (Williamson and Brown, 1998; Jiang and Cheng, 2017), since there is no reverse flow prior to the wake recirculation region. For the case of a square cylinder, if the peak value along the streamwise velocity profile is used to represent U_s , the reverse flow would be overlooked, since such a U_s value increases monotonically with increasing Re (also shown in Fig. 9(a)).

3.4. The 3D St - Re relationship

The St^* values for the (span-averaged) 3D flows are also examined. The U_s - Re , D' - Re and St^* - Re relationships for the 3D flows are plotted in Fig. 9 and Fig. 10(a). Fig. 10(b) shows (i) the relative differences of the 3D St values with respect to the 2D St value at $Re = 168$, and (ii) the relative differences of the 3D St^* values with respect to the 2D St^* value at $Re = 168$.

At the onset of the secondary wake instability of $Re = 165.7$, the relative difference between the 3D and 2D St values is approximately 6%, while the relative difference between the normalised 3D and 2D St^* values reduces to less than 1%. This suggests that the sudden drop of the 3D St from its 2D counterpart at $Re = 165.7$ is due to the sudden decrease in the separating velocity (Fig. 9a) and the sudden increase in the wake width (Fig. 9b) at the onset of the secondary wake instability.

The 3D St^* values are relatively uniform for $Re = 165.7 - 210$, followed by an obvious increase starting at Re of approximately 210 to 220 and a sharp decrease starting at Re of approximately 320 to 330 (Fig. 10b). Compared with the original 3D St - Re relationship, after normalisation the 3D St^* - Re relationship reveals better the two critical conditions of $Re \sim 210$ and 330 that have been identified in Fig. 3(a-e).

However, the two critical conditions in Fig. 10(b) are less distinct than those shown in Fig. 3(a–e), since the separating velocity U_s used in the normalisation of St is an approximation of the regional flow rate immediately prior to the rolling up of the vortices.

As an analogy to the case of a circular cylinder reported in Jiang and Cheng (2017), the increase in the 3D St^* as Re exceeds 210 for a square cylinder is because the flow becomes increasingly turbulent with increasing Re , and for turbulent flows the vortex shedding frequency no longer scales on U_s and D' . Specifically, the cross-flow distance for the vortex from one side of the cylinder to roll up to trigger the shedding of the vortex on the opposite side becomes increasingly smaller than D' . In other words, the vortex shedding frequency scales on a length which is increasingly smaller than D' . When D' is used to normalise the vortex shedding frequency, the 3D St^* value would be over-estimated.

Fig. 12 shows instantaneous ω_z contours of the span-averaged 3D flows for different Re values, at the time instant that the streamwise velocity u_x on the lower side of the cylinder is about to increase (i.e. u_x is the smallest at this time instant) and the lower shear layer is about to roll up to form a new vortex (which is indicated by an arrow in Fig. 12). As Re increases from 210 to 330, vortex shedding occurs when the negative vortex is further away from the positive vortex being shed (Fig. 12a,b). As Re increases from 330 to 400, the opposite trend happens (Fig. 12b,c), such that the 3D St^* (which is normalised based on D') decreases.

Fig. 12. Instantaneous ω_z contours of the span-averaged 3D flows for (a) $Re = 210$, (b) $Re = 330$, and (c) $Re = 375$. The wake width is obtained from the ω_z contours of the time- and span-averaged flow. The arrow on the lower shear layer marks the location where the lower shear layer is about to roll up to form a new vortex.

3.5. Critical conditions for the 3D flows

At the onset of the secondary wake instability of $Re = 165.7$, a sudden increase or decrease of the 3D value with respect to its 2D counterpart is observed for each of the flow properties shown in Fig. 3 as well as the viscous and pressure drag coefficients shown in Fig. 6(a). This is due to the sudden increase in the flow three-dimensionality at the mode A instability that is subcritical in nature (Jiang et al., 2018).

For the 3D flows beyond the secondary wake instability, two critical conditions are observed at Re of approximately 210 and 330. The critical condition at $Re \sim 210$ is due to the development of increasingly disordered mode B flow structures (i.e. increasingly turbulent wake flow) at $Re \geq 210$ (Fig. 5(c,d)), such that the deviations between the 3D and 2D hydrodynamic forces increase with increasing Re values (Fig. 3(a–d)). The critical point of $Re \sim 210$ is slightly ($\Delta Re \sim 10$) above the global instability of mode B (e.g. $Re = 198$ in Sheard et al. (2009) and $Re = 201$ in Choi et al. (2012), Park and Yang (2016) and Jiang et al. (2018)). We found that this conclusion is also valid for the case of flow past a circular cylinder, for which a similar critical condition is observed at $Re \sim 270$ (Williamson, 1996a), while the global instability of mode B occurs at $Re = 259$ (Barkley and Henderson, 1996), again showing a difference of $\Delta Re \sim 10$.

The critical condition at $Re \sim 330$ is related to the disappearance and reappearance of the recirculation regions on the upper and lower sides of the cylinder. Fig. 13 plots the recirculation regions for a few Re values obtained with the time- and span-averaged 3D flow. In addition, the evolution of the size of the recirculation region with Re is indicated in Fig. 13 by the left and right ends of the recirculation region. It is noted that the right end is the saddle point illustrated in Fig. 11. As Re increases from 167 (the onset of flow reversal) to 330, the amount of flow travelling from the wake to the upper and lower sides of the cylinder increases monotonically (Fig. 14), such that the recirculation region is diverted away from the cylinder, and the size of the recirculation region is squeezed by the reverse flow from the lower, left

and upper sides (see Fig. 13). At $Re = 330$, the recirculation region almost disappears, which leads to a critical condition. Unlike the critical conditions at the onset of the secondary wake instability (of $Re = 165.7$) and at the point where the wake flow becomes increasingly turbulent (of $Re \sim 210$), such a critical condition at $Re \sim 330$ for a square cylinder is not observed for a circular cylinder, since the geometry of a circular cylinder does not give rise to such a flow reversal.

Fig. 13. The recirculation region on the upper side of the cylinder obtained with the time- and span-averaged 3D flow. Different horizontal and vertical scales are used to allow for a better visualization of the recirculation region.

Fig. 14. Flow rate of the reverse flow in the time- and span-averaged 3D flow field. The flow rate is integrated vertically from the right end of the upper recirculation region (i.e. the saddle point) down to the cylinder surface.

4. Conclusions

This paper presents a DNS study of the 2D and 3D hydrodynamic forces and wake flow characteristics for flow past a square cylinder. The hydrodynamic forces and wake flow characteristics are presented for a range of Re from 10 to 400, with a high resolution in Re to capture all the variation trends.

Distinct features in the variation trends of the hydrodynamic forces with Re are examined. A local minimum in the time-averaged drag coefficient is observed at $Re = 144$, which is due to combined contributions of the pressure drag and viscous drag. It is also found that the viscous drag decreases to negative values for $Re \geq 154$, which is due to the increasing coverage of backward flow on the upper and lower surfaces of the cylinder. For the 2D $St-Re$ relationship, a local maximum is observed at $Re = 168$. This is because the separating velocity is the largest and correspondingly the wake width is the smallest at Re very close to 168. The decrease in the separating velocity for $Re > 168$ is due to the flow entrainment from the wake recirculation region to the upper and lower sides of the cylinder. For the 3D $St-Re$ relationship, a sudden drop of

the 3D St value from its 2D counterpart is observed at the onset of the secondary wake instability, which is due to the sudden decrease in the separating velocity and the sudden increase in the wake width at this point.

For the 3D flows, three critical conditions are observed at Re of approximately 165.7, 210 and 330. At the onset of the secondary wake instability of $Re = 165.7$, a sudden increase or decrease of the 3D flow property with respect to its 2D counterpart is observed, which is due to the sudden increase in the flow three-dimensionality at the mode A instability that is subcritical in nature. The second critical condition happens at $Re \sim 210$. As Re exceeds 210, the 3D flow properties are increasingly deviated from their 2D counterparts, which is because for $Re > 210$ the mode B flow structure becomes increasingly disordered and the wake flow becomes increasingly turbulent. The critical point of $Re \sim 210$ is slightly ($\Delta Re \sim 10$) above the global instability of mode B of $Re \sim 201$. This conclusion is also applicable to a circular cylinder. The third critical condition occurs at $Re \sim 330$, which is related to the disappearance and reappearance of the recirculation regions on the upper and lower sides of the cylinder. This critical condition is not observed for the case of a circular cylinder, since the geometry of a circular cylinder does not give rise to recirculation regions on the upper and lower sides of the cylinder.

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