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Entrainment of single particles in a turbulent open-channel flow: a numerical study

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ABSTRACT
This paper investigates erosion events in a turbulent open channel flow laden with monodisperse spherical particles. The data were generated in a previous study using direct numerical simulations with a phase-resolving immersed boundary method. The particles have a mobility below their nominal threshold of incipient motion and settle onto the rough bed that consists of a hexagonally packed layer of spheres with the same size. Conditioned averaging is employed to extract the characteristic features of an erosion event, defining a suitable criterion for detection and accounting for possible asymmetry of flow structures. The highly resolved dataset provides detailed insight into the key-mechanisms of erosion. The results show that a particle collision, together with a subsequent sweep event on time scales of several bulk units, is responsible for the erosion.

Keywords: direct numerical simulations; erosion processes; fluid–particle interactions; immersed boundary method; open-channel flow; particle entrainment; particle-laden flows

1 Introduction

Erosion and incipient motion of individual particles in a turbulent open channel flow is an important process for numerous industrial and environmental applications, such as sediment transport, pneumatic conveying, the mobilization of pollutants, etc. Despite the long history of research on this topic (Buffington & Montgomery, 1997), formulae that are based on mean quantities like the one proposed by Shields (1936) are of limited power to understand erosion events and incipient motion of inertial particles (Bathurst, 2007; Lajeunesse, Malverti, & Charru, 2010). On the other hand, a purely stochastic approach based on instantaneous extreme values of drag and lift as proposed by Einstein and El-Samni (1949) has not proven to be sufficient for the description of the relevant processes (Papanicolaou, Diplas, Evaggelopoulos, & Fotopoulos, 2002; Valyrakis, Diplas, & Dancey, 2011). This is due to the fact that unsteady and highly three-dimensional flow events are responsible for the mobilization of the particles (Keylock, Lane, & Richards, 2014; Shvidchenko & Pender, 2001). In the case of a turbulent flow over a rough wall, coherent structures account for the gross of the energy (Adrian, 2007), which then is available for sediment erosion. It has also been recognized that in addition to the magnitude of the forces acting on a particle the duration of large fluid stresses is of importance as well (Celik, Diplas, & Dancey, 2014; Diplas et al., 2008).

The fluid–particle interaction of coherent flow structures and particles with a size of the viscous length scale has been addressed in a number of studies both numerical and experimental (Lelouvetel, Bigillon, Doppler, Vinkovic, & Champagne, 2009; Niño, Lopez, & Garcia, 2003; Soldati & Marchioli, 2009; Vinkovic, Doppler, Lelouvetel, & Buffat, 2011). All of...
these studies have reported the consistent observation that ejections cause particles to move away from the wall or even make them become suspended. Experimental investigations of higher particle Reynolds numbers have been mostly limited to measurements of a fixed rough bed (Detert, Nikora, & Jirka, 2010; Dwivedi, Melville, Shamseldin, & Guha, 2011; Hofland, Battjes, & Booij, 2005). These studies have highlighted the importance of high-speed fluid events inducing large viscous stresses on the sediment bed over time scales of several bulk units, $H/U_b$, where $H$ is the water depth and $U_b$ is the bulk velocity of the flow. In addition, it has been shown in these studies that the pressure in the sediment bed decreases during high-speed events and a time lag between strong drag and lift forces exists. The interplay of strong drag and lift forces is believed to act as a destabilizing mechanism. A detailed understanding of the governing flow features actually responsible for particle erosion, however, is still lacking, which may partly be associated to the challenging task of experimentally measuring such phenomena with a proper resolution.

Indeed, the complex situation related to incipient motion raises the need for transient data with high resolution, in both space and time, to gain insight into the relevant mechanisms of particle erosion. Recently, sufficient computational power has become available to conduct phase-resolving numerical simulations. Pan and Banerjee (1997) were among the first to perform such a simulation, and since then computational resources have grown substantially. In particular, the immersed boundary method (IBM) (Uhlmann, 2005) has proven to be a powerful tool to generate such data on a scale relevant to a turbulent open-channel flow. Lee and Balachandar (2012) have carried out simulations of a fixed single particle on top of a rough bed being fully exposed to an idealized fluid flow to investigate drag and lift coefficients as a function of the particle Reynolds number. This idealized setup of a sediment bed was further developed in several studies employing direct numerical simulations. For example, Derksen and Larsen (2011) have investigated the forces onto a random assembly of wall-mounted particles in a laminar flow and Chan-Braun, Garcia-Villalba, and Uhlmann (2013) have addressed the force and torque on a fixed sediment bed with particles in a square arrangement. While all these studies provide highly resolved data, they do not address the actual process of incipient motion of the particles. Instead strong drag and lift forces were used as a surrogate for possible erosion events. Herwig, Kempe, and Fröhlich (2011) and Chan-Braun (2012) have recorded the forces on fixed particles and tried to link these events of strong forces to mobilization. In these studies, a critical Shields number was determined by releasing the particle in question with different particle densities in the same flow condition. Since this approach has turned out to be very costly, these studies had to be based on a small number of samples and the derivation of a more general picture of the typical velocity field of the fluid during entrainment was not possible.

Statistically relevant studies, both numerical and experimental, addressing actual dislodgement of single particles (e.g. Amir, Nikora, & Witz, forthcoming; Fenton & Abbott, 1977; Papanicolaou et al., 2002) are still rare as the data are difficult to obtain and the conditions near the mobilization threshold lead to excessive waiting times for entrainment events. Another issue, which has received much less attention so far, is the role of mobile particles as a trigger for erosion events. Only recently, Frey and Church (2011) have pointed out the importance of particle–particle interaction as a key mechanism of sediment mobilization. Ancey and Heyman (2014) highlight the role of collective entrainment events as a nonlinear process possibly destabilizing a sediment bed, but such investigations are even more difficult to realize experimentally.

The present study addresses the gaps identified above and analyses in detail the characteristics of the flow field at the instant of an erosion event. The database was gained from a Direct Numerical Simulation (DNS) of a turbulent open channel flow first presented in Vowinckel, Kempe, and Fröhlich (2014) using the method proposed in Kempe and Fröhlich (2012a, 2012b) and Kempe, Vowinckel, and Fröhlich (2014). The computational domain employed is very large to resolve the relevant length scales typically encountered in turbulent flows over rough beds, which guarantees high realism and a sufficient amount of erosion events to gather proper statistics. The situation of thousands of mobile particles with a mobility well below their nominal threshold of incipient motion according to the Shields criterion addresses the role of particle–particle interaction. The actual dislodgement of particles out of the sediment bed allows the detection of erosion events and capture of the typical flow field by means of conditional averaging as first proposed by Blackwelder and Kaplan (1976) for coherent vortex structures in a single-phase flow. To the knowledge of the authors, the database for this purpose is larger than earlier studies conducted on this topic and can therefore provide insight into the relevant physical flow features with a better spatial resolution and a higher degree of statistical convergence.

2 Dataset investigated

2.1 Numerical method

The present study is based on a dataset previously presented by Vowinckel, Kempe, et al. (2014). The numerical method described in Kempe and Fröhlich (2012b) is briefly recalled here to keep the paper self-contained. The continuous phase was governed by the unsteady, three-dimensional Navier–Stokes equations for incompressible fluids. The spatial discretization was performed by a second-order finite-volume scheme on a staggered Cartesian grid. An Euler–Lagrange method with full resolution of the particle geometry and a coupling by an enhanced IBM was employed to represent mobile particles. When two particles approach, all interactions transmitted by the fluid were resolved as long as the particle surfaces are about two grid cells apart, since the geometry of the particles was fully represented. Once the particles came closer, the unresolved lubrication forces
were accounted for by an appropriate model. Upon direct contact, normal and tangential inter-particle forces were modelled by the adaptive collision model (ACM) with fairly high accuracy, as described in Kempe and Fröhlich (2012a). The actual particle–particle contact takes place on very small time scales. The idea of the ACM is to stretch this process in time to avoid a reduction of the time step of the fluid solver. Right before and after the contact, i.e. approach and rebound, lubrication forces act onto the particles diminishing their kinetic energy. For the actual contact phase, a restitution coefficient was imposed by adaptively calibrating stiffness and damping coefficients treating this process as a “dry” collision. In addition, tangential forces were adaptively calibrated to guarantee zero slip during rolling contact. The critical impact angle for distinction between rolling and sliding was chosen to be $\Psi_{\text{crit}} = 1$ and the coefficient of friction during sliding motion was chosen to be $\eta_f = 0.15$. These values were motivated by the measurements of Joseph and Hunt (2004) for glass beads. It has been shown in Kempe et al. (2014) that modelling lubrication forces and treating particle contact as dry collisions gives realistic results for simulations of bed-load transport phenomena. The model has already been employed in several studies of the present authors and produced results in good agreement with experimental evidence while exhibiting excellent numerical performance (e.g. Vowinckel, Kempe, Fröhlich, & Nikora, 2012; Vowinckel, Kempe, et al., 2014).

### 2.2 Computational set-up

A turbulent open-channel flow with periodic boundary conditions in streamwise and spanwise direction was considered featuring a free-slip condition on the top and a no-slip condition on the bottom wall and the particle surfaces. The sediment was constituted of a single layer of 13,500 fixed spheres with diameter $D$ in a hexagonal packing. The packing was arranged such that the fixed particles actually touch each other and that a straight line perpendicular to the streamwise direction can be drawn through their centre coordinates. The same amount of mobile particles with identical shape was released in the outer flow. This gave a total of $N_p = 27000$ particles. The restitution coefficient for collisions was set to $e = 0.97$ corresponding to the value of glass beads, which is close to the natural conditions of sand (Joseph, Zenit, Hunt, & Rosenwinkel, 2001). If all mobile particles settled regularly on top of the layer of fixed particles the first layer would be entirely covered and the sediment would have a total thickness of $H_{\text{sed}} = 1.82 \times D$. This configuration, termed the “clear-water case” in the following, is taken as a reference (Vowinckel, Kempe, et al., 2014). The origin of the vertical coordinate $y$ was set to the top of the upper layer, i.e. at $H_{\text{sed}}$ from the bottom of the domain. The friction velocity $u_t$ required as a reference for later normalization was taken from this flow by extrapolating the linear profile of total shear stress down to $y = 0$. The computational domain was $L_x \times L_y \times L_z = 24H \times (H + H_{\text{sed}}) \times 6H$ with a relative submergence of the particles of $H/D = 9$, where $H$ is the water depth from the top of the sediment bed to the upper boundary. The bulk Reynolds number $R_b = U_b H/\nu_f$ was 2941, where $\nu_f$ is the kinematic viscosity and $U_b$ the bulk velocity of the flow. The latter was kept constant during the simulation by an instantaneously adjusted and spatially constant volume force. The resulting particle Reynolds number $D^* = u_t D/\nu_f$ was 21.1 in the clear-water case. Each particle was resolved with 22.2 grid cells per diameter, which provided a resolution of $\Delta_x^* = u_t \Delta_x/\nu_f = 0.95$ in terms of wall units and resulted in a total of $n_{\text{tot}} = 1.4$ billion grid cells. To the knowledge of the authors, this simulation is one of the largest and best-resolved simulations of this phenomenon existing to date.

The potential of a flow to erode a sediment bed is classically assessed by the Shields number (Shields, 1936):

$$Sh = \frac{u_t^2 \rho_f}{(\rho_p - \rho_f)gD} \quad (1)$$

in the sense that erosion is expected for $Sh$ being larger than some critical value $Sh_{\text{crit}}$, depending on the particle Reynolds number. Here, $g$ is the gravitational acceleration, $\rho_p$ the particle density, and $\rho_f$ the fluid density. To gather proper statistics of single-particle erosion events, a flow laden with particles heavy enough to settle onto the bottom but light enough to be eroded every now and then is needed. In the present simulation, this condition was met by choosing $(\rho_p - \rho_f)/\rho_f = 0.182$, resulting in a value 25% lower than the critical threshold of incipient motion, which is $Sh_{\text{crit}} = 0.034$ as extracted from Shields (1936) for the present conditions. The most important numerical and physical parameters of the simulation are assembled in Table 1.

### 2.3 Previous results

At the beginning of the simulation, here $t = 0$, the mobile particles were released at some elevation above the sediment bed and the simulation was run until $t_{\text{crit}} = 133H/U_b$, where erosion and deposition rates of the disperse phase were in equilibrium before averaging was started (Vowinckel, Kempe, & Fröhlich, 2013). Subsequently, the simulation was run for a total duration $T_{\text{aver}} = 435 H/U_b$ to detect erosion events. It was reported

<table>
<thead>
<tr>
<th>$H/D$</th>
<th>$L_x/H$</th>
<th>$L_y/H$</th>
<th>$L_z/H$</th>
<th>$R_b$</th>
<th>$D^*$</th>
<th>$D/\Delta_x$</th>
<th>$\Delta_x^*$</th>
<th>$n_{\text{tot}}$</th>
<th>$N_p$</th>
<th>$Sh/Sh_{\text{crit}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>24</td>
<td>1.2</td>
<td>6</td>
<td>2941</td>
<td>21.1</td>
<td>22.2</td>
<td>0.95</td>
<td>1.4-10$^9$</td>
<td>27000</td>
<td>0.75</td>
</tr>
</tbody>
</table>
in (Vowinckel, Kempe, et al., 2014) that during the simulation, most of the particles settled onto the bottom forming a closed sediment bed. Only about 3% of the mobile particles were travelling across a layer of temporally resting particles (Fig. 1), which is the desired situation for the present study. Since only few particles travelled above the sediment bed, the mean streamwise fluid velocity was almost the same as for the clear-water case. The same holds for the streamwise velocity fluctuations, $u'$. Their increase with respect to the clear-water case was about 50% to 100%. A detailed report of the conventionally averaged flow, as well as Reynolds stresses, two-point correlations, etc. is provided in Vowinckel, Kempe, et al. (2014) together with statistical information about the particle phase. Furthermore, these data are compared to other cases with bed-load transport in that reference.

3 Conditional averaging

3.1 Detection of erosion events

As mentioned above, almost all particles settled onto the bed composed of fixed particles forming a second layer of, in principal, movable but resting particles (white particles in Fig. 2). These resting particles reproduced the hexagonal ordering imposed by the fixed bed. The typical erosion event investigated then is the situation when a particle is lifted out of its pocket of the hexagonal packing, in which it has a relatively low exposure to the turbulent flow.

A convenient way to detect these erosion events is to record the wall-normal position of a particle centre, $y_p$, together with the particle velocity in streamwise direction, $u_p$. This is exemplified in Fig. 3. Particles embedded within the layer of resting sediment at the bottom of the channel have a wall-normal coordinate of $y_p = -0.5 D \approx -0.055 H$ and a velocity of $u_p \approx 0$ (situation A shown in Fig. 4a). An erosion event leads to a substantial increase of these two quantities well above zero. Here, the criterion to detect erosion events was chosen to be the simultaneous fulfilment of $y_p > 0$ and $u_p > u_t = 0.064 U_b$.

An example of an erosion event is illustrated by the evolution of these two quantities over time (Fig. 3) and three selected snapshots of the instantaneous flow field surrounding the particle in question (Fig. 4). In this particular case, the erosion event was triggered by a collision of an already eroded, mobile particle with the sediment bed in the vicinity of the particle in question, reflected by the spike in $u_p/U_b$ around $(t - t_{\text{init}}) = 203.2 H/U_b$ (situation B in Fig. 3b). The impact caused a slight dislocation off its initial position as shown by the curve of $y_p$. Once the particle was slightly lifted above the resting position, it protrudes into the flow so that fluid forces onto the particle were substantially enhanced (Fenton & Abbott, 1977). If the dislocation is large enough, the fluid forces can become sufficiently large to prevent the particle from falling back into its pocket, which indeed was observed in this case (situation C shown in Fig. 4c). The particle then starts to travel across the inactive bed with a saltating motion.

During the course of the simulation, continuous recording of the particle trajectories was performed and a total number of $n_{\text{aver}} = 1486$ erosion events was detected. These events constituted the samples of the present statistical analysis to
Figure 3 Example of an erosion event. Three representative instants in time are marked with capital letters and correspond to the situations shown in Fig. 4. Note that instant B corresponds to the nominal start of the erosion \( t = t_e \). The dashed horizontal line indicates the respective criterion to detect incipient motion. (a) wall-normal particle coordinate; (b) instantaneous particle velocity

(a) (b) (c)

Figure 4 Zoom into the domain shown in Fig. 1, displaying the single erosion event considered in Fig. 3 with three marked instants in time. A: \( t - t_{\text{init}} = 200.5 \, H/U_b \); B: \( t - t_{\text{init}} = 203.2 \, H/U_b \); C: \( t - t_{\text{init}} = 204.0 \, H/U_b \). Contour plot and particle colouring as in Fig. 1. The particle being eroded is coloured in red and indicated with an arrow

compute the porosity:

\[
\phi_T = \frac{n_f}{n_{\text{aver}}}, \tag{2}
\]

where \( n_f \) is the number of events in which a grid cell is occupied by fluid. Furthermore, continuous recording of fluid data, albeit coarsened in space by a factor of five for the sake of limiting hard-disc storage, was carried out for the last 278 bulk units. Due to a modified sampling strategy during the course of the simulation, data were gathered for the streamwise velocity component \( u \) over the last 278 bulk units and over 249 bulk units for the wall-normal velocity component \( v \) and the spanwise velocity component \( w \), respectively. This yields a total of 1030 velocity fields for the streamwise component and 833 samples for the wall-normal and spanwise component of the fluid velocity vector. The sample sizes of the different physical quantities are summarized in Table 2. Note that the present analysis is a substantial improvement over experimental studies, such as e.g. Papanicolaou et al. (2002), who based their evaluations on a total of 26 erosion events for a dense packing. The present sample size allows for conditional averaging of quantities related to the disperse phase as well as to the continuous phase surrounding the particle being eroded.

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>( n_{\text{aver}} )</th>
<th>( T_{\text{aver}} ) [( H/U_b )]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \phi_T )</td>
<td>1460</td>
<td>435</td>
</tr>
<tr>
<td>( u )</td>
<td>1030</td>
<td>278</td>
</tr>
<tr>
<td>( v )</td>
<td>833</td>
<td>249</td>
</tr>
<tr>
<td>( w )</td>
<td>833</td>
<td>249</td>
</tr>
</tbody>
</table>

3.2 Transformation into local coordinates and interpolation

To investigate the characteristic flow features responsible for dislodging the particle out of its pocket in the sediment bed, conditionally averaged flow fields surrounding the particle were computed. Erosion events may occur at any location of the computational domain so that conditional averaging raises the need for a local coordinate system. It was defined with its origin at the centre coordinates of the considered particle at the start of the erosion event at \( x_e = x_p(t_e) \) and \( z_e = z_p(t_e) \). This yields the following coordinate transform between the global coordinates in space and time and the local coordinates:

\[
t_{\text{loc}} = t - t_e, \tag{3a}
\]

(b) (c)
\[ x_{\text{loc}} = x - x_c, \]  
\[ z_{\text{loc}} = z - z_c. \]  
\[ (3b) \]
\[ (3c) \]

No transform was performed for the wall-normal coordinate \( y \). The start of erosion at \( t = t_e \) (instant B in Fig. 3) was designated as the instant of time with the first local minimum of \( y \). The presen study focuses on the backward in time from the instant when the criteria of erosion are met. For each erosion event detected the transform according to Eq. (3) was performed and the spatio-temporal field was averaged over all events. The present study focuses on the instant \( t_{\text{loc}} = 0 \). The extent of the local averaging domain was chosen to be \(-2.2H < x_{\text{loc}} < 1H, -1H < z_{\text{loc}} < 1H, \) and \(-H_{\text{sed}} < y < 1H.\)

The particle centre is a Lagrangian point, it can be anywhere in a grid cell. The grid cells of the local domain constructed around the centre of the eroded particle, hence, do not in general coincide with the grid cells of the original domain. This issue was resolved by using linear interpolation to obtain the fluid information on a common grid in the local domain. As mentioned in Section 3.1, fluid data were stored on a spatial grid coarsened by a factor of five in all three directions. The resulting error was assessed by comparing interpolated coarsened datasets with a reference. For this purpose, selected datasets of the original numerical grid with fine resolution were interpolated using the above-mentioned transformation and interpolation. Afterwards, the Nash–Sutcliffe efficiency coefficient (Nash & Sutcliffe, 1970), which is a volume-averaged deviation of a target function from an expected value, was used as a measure to quantify the amount of information lost by the coarsening. Although the coarsening yielded a modified spatial resolution of 4.4 cells per diameter, it was found that more than 98% of the statistical information were retained for the streamwise velocity and 92% for the wall-normal and spanwise component, respectively. Since the study focuses on the conditional average of flow features much larger than the particle diameter, this procedure gave sufficient accuracy for the analysis presented in the following.

3.3 Averaging operators

After the transform of the coordinates and the interpolation of the data onto a local grid, any conditionally averaged scalar quantity \( \theta \) defined in the fluid was determined from:

\[ \langle \theta \rangle^c(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}) = \frac{1}{n_\text{er}} \sum_{i=1}^{n_\text{er}} \gamma_i(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}) \theta_i(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}). \]  
\[ (4) \]

Here, the index \( i \) denotes the \( i \)th erosion event and \( y \) is a clipping function being one in the fluid and zero otherwise. The integer \( n_\text{er} = \sum_{i=1}^{n_\text{er}} \gamma_i(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}) \) is the number of instants in the collected fields a given point was occupied by fluid. The superscript \( c \) in Eq. (4) denotes conditioned quantities to distinguish them from the classical global averaging operator:

\[ \langle \theta \rangle(y) = \frac{1}{T_H L_x L_z} \int_{t_{\text{start}}}^{t_{\text{end}}} \int_{L_x} \int_{L_z} \gamma(x, y, z, t) \theta(x, y, z, t) \, dz \, dx \, dt \]  
\[ (5) \]

as employed, for example, in Nikora, Ballio, Coleman, and Pokrajac (2013) and Vowinckel, Kempe, et al. (2014), which is the average over the total simulation time and the entire horizontal plane. The globally averaged profiles were used to define the fluctuation of the conditional averages as:

\[ \langle \theta \rangle^c(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}) = \frac{1}{n_\text{er}} \sum_{i=1}^{n_\text{er}} \gamma_i(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}) \times [\langle \theta \rangle(x_{\text{loc}}, y, z_{\text{loc}}, t_{\text{loc}}) - \langle \theta \rangle(y)]. \]  
\[ (6) \]

This allowed applying the theory of coherent structures as defined by Robinson (1991) or Adrian (2007) based on the investigation of low-speed and high-speed fluid. In what follows, the conditional averages of all quantities will be evaluated at the instant of erosion as defined above, i.e. for \( t_{\text{loc}} = 0 \), except if specified otherwise.

4 Results

4.1 Particle configuration at instant of entrainment

The typical ensemble-averaged particle configuration of the closed bed is addressed by the porosity \( \phi_T \) according to Eq. (2), i.e. the probability of a cell to be occupied by fluid. Vice versa, the quantity \( 1 - \phi_T \) is the probability of a cell to be occupied by a particle at the time of erosion \( t_{\text{loc}} = 0 \). Figure 5 shows the iso-surface of \( \phi_T \) for two different thresholds near the eroded particle (coloured in red) in a close-up of the averaging domain. As expected, the porosity reflects the very regular pattern imposed by the hexagonal geometry of the fixed bed. Three principle types of events seem to be possible: erosion from the plane bed without involvement of another particle, collision with a mobile particle triggering the erosion event, and erosion in the presence of a gap, as illustrated in Fig. 5a. A low threshold of \( \phi_T = 0.1 \), indicating a high probability of a particle resting in a pocket of the hexagonal packing, reveals a gap in the upstream front of the eroded particle (blue circles in Fig. 5a). This means that, with some probability, the upstream positions are unoccupied, resulting in an enhanced exposure of the particle to the mean flow, which increases the probability for mobilization (Fenton & Abbott, 1977). It should be mentioned that the quantity \( \phi_T \) is an integral average over all events. Thus, the two blue circles indicate two particles missing in the hexagonal ordering, which actually means that three particle configurations are possible: (i) one particle missing at \( z_{\text{loc}} < 0 \); (ii) one particle missing at \( z_{\text{loc}} > 0 \); and (iii) two particles missing. The probability of these options will be analysed further below by means
of the surface occupancy. If the threshold of the iso-surface is increased to $\phi_T > 0.2$ the gap is not present anymore (not shown here). Hence, the probability of encountering this configuration during an erosion event is small. The threshold $\phi_T = 0.5$ reveals that there is a high probability of finding a particle on top of the eroded one at the instant of erosion (Fig. 5b). This particle was fully exposed to the mean flow and travels across the closed bed. Its mean velocity $\langle u_p \rangle$ is $0.3 U_b$, which is about half the mean fluid velocity at the elevation of the particle centre $y_p \approx 0.5 D$ for this situation (Vowinckel, Kempe, et al., 2014). Moving particles collide very frequently with the underlying sediment in the present regime, thus transferring kinetic energy to the particles resting in the closed bed as witnessed by Fig. 3b. This feature increases the probability for entrainment.

To elucidate the importance of the configuration of the layer of resting particles on the erosion process, a surface occupancy was defined along the lines of Derksen and Larsen (2011):

$$\sigma = \frac{A_{\text{par}}}{A_{\text{tot}}} = \frac{\pi/2(3 + n/3)}{3\sqrt{3}},$$

where $A_{\text{par}}$ is the projected area occupied by particles and $A_{\text{tot}}$ is the total projected area. In the present case, this ratio is determined by the representative hexagonal element in the horizontal plane depicted in Fig. 6a, with the particle being eroded in its centre. The total projected area hence is the area of the hexagon while the area covered by particles depends on the number $n$ of particles occupying adjacent positions of the lattice, resulting in the second equality in Eq. (7). The surface occupancy gives a measure to determine the area of this self-similar cell occupied by surrounding particles in order to determine the local exposure of the eroded particle to the flow. A complete hexagonal packing with $n = 6$ yields a surface occupancy of $\sigma = 90.7\%$, for example.

In addition, it was investigated whether the erosion process of the particle in question was triggered by a collision. For this purpose, a critical spherical area surrounding the particle in question with a shell of thickness $D/2$ was defined. If a fast moving particle travelling across the sediment bed is within a distance less than or equal to $D$ from the centre of the eroded particle at the time of erosion, a collision must have taken place at the time of the erosion event, which could serve as a trigger. This is visualized by the grey shaded area in Fig. 6b showing a side view of the sediment around the particle being eroded.

The results obtained are assembled in Table 3. This analysis confirms the hypothesis made above that several types of erosion events were encountered. With a probability of 59.3\%, the most frequent configuration was a complete hexagonal packing of resting spheres. About 31.1\% of the erosion events happened with one particle missing in the hexagon; the likelihood of an erosion event with a gap of two particles was 6.7\% and
only 2.8% with three or less neighbouring particles being absent. These data allow further understanding of Fig. 5a showing that the pattern depicted only partly results from two neighbours missing but mainly from the added probability of only one missing neighbour upstream of the particle being eroded.

The analysis presented in Table 3 also illustrates that 96.5% of the events were triggered by a collision. In this case, two different scenarios of mobilization are possible. In the first one, kinetic energy transferred during the collision pushes the particle out of its position. This is in line with the data in Table 2 (Vowinckel, Jain, Kempe, & Fröhlich, 2014). The magnitude of the variance remains very low especially in the vicinity of the particle, i.e., within a spherical radius of 3D from the origin of the local coordinate system. It is, hence, well justified to use all samples available regardless of the configuration of the sediment bed to compute a conditionally averaged velocity field.

There is, however, a particular issue to be addressed. The present configuration exhibits geometrical symmetry in spanwise direction. As a result, individual events breaking this symmetry have the same probability for both orientations, so that statistical data inherit the spanwise symmetry. Fig. 5a is an illustrative example for this issue. Erosion with one neighbouring particle missing occurred in 31.1% of the events, with two particles only in 6.7%. Nevertheless, Fig. 5a shows a symmetric picture since the configuration with one missing neighbour is equally probable, be it the right or the left one. The conditionally averaged velocity field \( \langle u \rangle \) as defined by Eq. (4), hence, should also exhibit symmetry with respect to the plane \( z_{\text{sym}} = 0 \). This was indeed observed in first results (Vowinckel, Jain, et al., 2014). This symmetry, however, only results from the large-scale symmetry of the set-up and from the averaging procedure, i.e., the symmetry does not need to be a feature of the individual events.

To address the issue of asymmetric fluid structures, a measure to quantify the degree of symmetry was introduced. The quantity:

\[
S = \int_{-0.5H}^{0.5H} \int_{0}^{H} u(x_{\text{loc}} = 0, y, z_{\text{loc}}) z_{\text{loc}} dy \, dz
\]

(8)

constitutes the first moment of the transformed velocity field in \( z_{\text{loc}} \) and can be used to determine if a high-speed fluid event has its centroid at \( z_{\text{loc}} > 0 \) or \( z_{\text{loc}} < 0 \). For the latter, \( S \) becomes negative. To apply the averaging operator Eq. (4) to the present ensemble of erosion events without losing a potential asymmetry of the typical coherent fluid structure, yet another coordinate transform was performed for the spanwise coordinate:

\[
z_{\text{sym}} = \begin{cases} 
  z_{\text{loc}} & \text{if } S \geq 0 \\
  -z_{\text{loc}} & \text{if } S < 0 
\end{cases}
\]

(9)
before averaged values were computed according to Eq. (4). In addition, this symmetry transform requires conversion of the spanwise velocity before averaging assigning:

$$w_{\text{sym}} = \begin{cases} w & \text{if } S \geq 0 \\ -w & \text{if } S < 0 \end{cases}$$

(10)

while the streamwise and wall-normal velocity components remain unchanged. Using Eqs (9) and (10) in combination with the averaging operator Eq. (4) allowed a proper description of the conditionally averaged fluid field at the instant of erosion, which accounts for possible asymmetry. This procedure has also been performed in Vowinckel, Jain, Kempe, and Fröhlich (2016), albeit with a smaller dataset than used below.

### 4.3 Results for the conditionally averaged streamwise fluid velocity

The three velocity components of the conditionally averaged flow field at the instant of an erosion event are shown in Figs 8–10 respectively. Each of these figures shows three slices cutting through the local domain used for the conditional average, the centre plane cutting through $z_{\text{sym}} = 0$, the cross plane cutting through $x_{\text{loc}} = 0$, and a top-view cutting through the near-wall region at $y = 0.038 H = 0.038 D$.

For the streamwise component, a large fluid structure of high-speed fluid becomes evident, extending far into the outer flow (Fig. 8a and b). It reaches more than $1.0 H$ in the positive and more than $1.5 H$ in the negative streamwise direction (Fig. 8a). Furthermore, Fig. 8b reveals that the fluid structure is not symmetric in the cross-plane. High positive values are reported for the streamwise velocity fluctuations for $-0.2 H < z_{\text{sym}} < 0.3 H$ and small negative values for $-0.7 H < z_{\text{sym}} < -0.2 H$. The negative values were induced by a low-speed streak of similar size as the high-speed streak at $z_{\text{sym}} \approx 0$. Looking from the top (Fig. 8c), the high-speed fluid streak shows a high degree of symmetry in the spanwise direction up to about $x_{\text{loc}} \approx -1.5 H$, which was not expected a priori, especially after accounting for possible asymmetry via Eq. (8).

To provide a comparison of the globally averaged velocity profile Eq. (5) to the present conditionally averaged fluid field, the wall-normal profile at $x_{\text{loc}} = 0$, $z_{\text{loc}} = 0$ is plotted against the ensemble-averaged data computed with Eq. (4) in Fig. 8d. This comparison shows that the fluctuations were strongest in the near-wall region at $y \approx 0.1 H = 1 D$. This is exactly the region in which the large-scale fluid structure carries the triggering particle shown in Figs 5b and 8a. It has been shown in (Vowinckel, 2015) that particles in this region are moving with a velocity close to the fluid velocity across the bed of resting particles and have a wake with a streamwise extent of approximately two particle diameters in the downstream direction. After the triggering particle has loosened up the packing, the high-speed streak flowed across the eroded particle inducing high viscous stresses on the phase boundary.

### 4.4 Results for the conditionally averaged wall-normal fluid velocity

The same conditional average was computed for the wall-normal component of the fluid velocity fluctuations (Fig. 9). These data reveal that in addition to the high-speed streamwise velocity, strong negative values of the wall-normal velocity

![Figure 8](image-url)
were present in the same region just upstream of the eroded particle transporting the triggering particle (Fig. 9b). Hence, this region can be characterized as a strong sweep event (Bialik, 2013; Dwivedi et al., 2011; Robinson, 1991). It reaches far into the outer flow of the channel (Fig. 9a) and is strongest in the near-wall region at \(-0.5 H < x_{\text{loc}} < 0\) and \(-0.1 H < z_{\text{sym}} < 0.1 H\) (Fig. 9c). The fluid, hence, flowed into the pocket of the eroded particle after the triggering collision takes place. In addition, two more characteristic regions become evident. A region of positive wall-normal velocity occurs in the region \(x_{\text{loc}} \approx 0\) that extends over \(-0.5 H < z_{\text{sym}} < 0.5 H\) as visualized in Fig. 9b. Hence, the upward-pointing fluid motion is not a local feature introduced by the wake of the triggering particle simply because the fluid has to flow around it, but the large spanwise extent proves this a relevant feature in the far field of the fluid surrounding the eroded particle. This location also coincides with the region of negative fluctuations of the streamwise velocity component discussed above with Fig. 8c. The streamwise fluctuations and the wall-normal fluctuations being negative and positive, respectively, this region can be identified as an outward ejection. In addition, yet another sweep event in the downstream region at \(x_{\text{loc}} \approx 0.25 H\) is visible, albeit with lower intensity than the one located upstream. This pattern also explains the time lag in the correlation between extreme values
of the streamwise velocity component and the resulting drag force on the particle described, e.g. by Dwivedi et al. (2011).

4.5 Results for the conditionally averaged spanwise fluid velocity

The ensemble averaged spanwise component of the fluid velocity vector shown in Fig. 10a, b and c reveals diverging fluid in the vicinity of the eroded particle. This was expected, because as soon as the sweep event discussed above hits a wall, energy transfer from the vertical component to the tangential ones must take place due to continuity of mass (Nezu & Nakagawa, 1993). This even amplifies the effect of the loosened packing and illustrates that the spanwise coordinate of the core of the high-speed fluid structure must be close to the spanwise centre coordinate of the eroded particle to have an effective attacking point. Combining the information of the Figs 9b and 10b reveals a large-scale vortex in the interval \(-0.5 H < z_{sym} < 0.5 H\) with high values of the wall-normal and spanwise fluid velocity components in the near-wall region at \(y/H < 0.4\) transporting momentum from the outer flow towards the sediment bed. The values of the two velocity components show magnitudes up to 5% of the bulk velocity, which is comparable to the magnitude of well-developed secondary currents in rough-bed channel flows (e.g. Nezu & Nakagawa, 1993). Further away from the particle at \(|z_{sym}| > \pm 0.5 H\), two more neighbouring cells can be identified by the changing sign of the spanwise velocity component at \(y/H < 0.4\), albeit with lower magnitude. This type of fluid structure resembles two parallel hair-pin like vortices that create a region of fast downward rushing fluid with a strong erosive potential at the location, where the two neighbouring legs of the vortices intersect. This flow feature is similar to the one reported by Best (2005), who found these vortices to be characteristic downstream of a dune-like roughness feature.

4.6 Coherent fluid structures

To address the regions of sweep events in more detail, a quadrant analysis along the lines of Robinson (1991) was conducted for the 833 erosion events with data for both the streamwise and wall-normal velocity components (Table 2). Sweeps are defined by streamwise fluctuations being positive and wall-normal fluctuations being negative, respectively, and are, hence, located in the fourth quadrant. Ejections, on the other hand, show negative streamwise fluctuations and positive wall-normal fluctuations, hence located in the second quadrant according to the numbering in Fig. 11a. The coordinates of the analysis were chosen to be \(P_1 = (-1.8 D, 0.36 D, 0)\), i.e. within the region of the largest values of \(\langle u' \rangle^c\) and \(-\langle v' \rangle^c\). A decorrelated distribution would correspond to 25% of the samples per quadrant. For the location investigated, the turbulence structure for most of the events shows a sweep-like behaviour (Fig. 11a). Of the 833 samples, 82% of the events are located in the fourth quadrant. This is also confirmed by the coherent structure visualized by iso-surfaces of the vorticity \(\omega_x\) describing regions of fluid rotating around the streamwise axis (Fig. 11b). Two regions of counter rotating fluid can be identified near the eroded particle sweeping high speed fluid from the outer flow towards the wall.

The present results in Figs 8–11 strongly suggest that the flow structures responsible for the erosion of particles in the transitionally rough regime have a very distinct shape, which is in contrast to observations made for simulations of point particles like Vinkovic et al. (2011) and Soldati and Marchioli (2009). While it was reported in these studies that a single ejection can have the power to suspend small particles, the present analysis of erosion events in the transitionally rough regime suggest a mechanism that is more differentiated. It was shown for the present dataset that sweeps with a considerable duration together with a triggering particle is needed to obtain erosion events. Similar observations were made by
Chan-Braun et al. (2013), who investigated an open channel flow over a fixed bed of square arrangement in the transitionally rough regime. In this study, strong drag and lift forces were used as an indication for possible erosion events. For such events, fluid structures elongated in streamwise direction were reported, which supports the present results. The discussed temporal and spatial scales are also in line with the findings of Detert et al. (2010). For a fixed bed in the fully rough regime these authors observe that high speed events with a duration of up to 3.5 bulk units cause pressure drops destabilizing the sediment.

5 Summary and conclusions

Direct numerical simulations of bed-load transport using the IBM for the representation of the fluid–particle interaction were carried out. The physical parameters of the particles were chosen such that they form a closed sediment bed of resting particles with only a small percentage of the mobile particles travelling across this particle packing. On the other hand, the mobility allowed the erosion of single particles every now and then to generate a multitude of independent erosion events. The events were analysed by conditional averaging to elucidate quantitatively the relevant physical quantities such as porosity and mean fluid velocity fluctuations so as to identify the most important mechanisms for particle entrainment.

For the present scenario, it was found that collision with already eroded particles is a very important trigger mechanism for a resting particle to be eroded. The collision causes a slight displacement of the particle loosening the packing of the sediment bed. Subsequently, a characteristic fluid structure is needed in order to dislodge a particle out of its pocket. This fluid structure is characterized by a strong sweep event penetrating into the sediment bed. This mechanism is responsible for pushing the particle out of its pocket. The erosion process takes place on time scales of several bulk units, which is consistent with experimental studies carried out at fully rough conditions. The erosion mechanisms can be enhanced by a gap in the packing upstream of the particle in question, since this feature increases the exposure to the turbulent flow, but this was not found to be a prerequisite for erosion events of single particles.

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Notation

\begin{align*}
A_{\text{par}} &= \text{area of } A_{\text{tot}} \text{ occupied by particles (m}^2) \\
A_{\text{tot}} &= \text{hexagon built by seven particles in a hexagonal packing (m}^2) \\
D &= \text{particle diameter (m)} \\
D^+ &= \text{particle Reynolds number (–)} \\
e &= \text{restitution coefficient (–)} \\
g &= \text{gravity acceleration (m s}^{-2}) \\
H &= \text{water depth} \\
H_{\text{sed}} &= \text{height of sediment bed} \\
L_x &= \text{streamwise extent of the computational domain (m)} \\
L_y &= \text{wall-normal extent of the computational domain (m)} \\
L_z &= \text{spanwise extent of the computational domain (m)} \\
N_p &= \text{total number of particles (–)} \\
N_{\text{aver}} &= \text{total number of samples (–)} \\
N_t &= \text{number of samples a cell was occupied by fluid (–)} \\
N_{\text{tot}} &= \text{total number of grid cells (–)} \\
R_b &= \text{bulk Reynolds number (–)} \\
Sh &= \text{Shields number (–)} \\
Sh_{\text{crit}} &= \text{critical Shields number (–)} \\
t &= \text{time (s)} \\
t_{\text{init}} &= \text{initialisation time (s)} \\
T_{\text{aver}} &= \text{averaging time interval (s)} \\
U_b &= \text{mean bulk velocity (m s}^{-1}) \\
u_f &= \text{friction velocity (m s}^{-1}) \\
U_p &= \text{streamwise component of particle velocity vector (m s}^{-1}) \\
x &= \text{streamwise/longitudinal coordinate (m)} \\
x_p &= \text{streamwise particle coordinate (m)} \\
y &= \text{wall-normal coordinate (m)} \\
y_p &= \text{wall-normal particle coordinate (m)} \\
z &= \text{spanwise/transverse coordinate (m)} \\
z_p &= \text{spanwise particle coordinate (m)} \\
\Delta_x &= \text{grid cell size (m)} \\
\gamma &= \text{clipping function} \\
\theta &= \text{fluid quantity} \\
\theta_p &= \text{particle quantity} \\
\nu_f &= \text{kinematic viscosity of the fluid (m}^2 \text{ s}^{-1}) \\
\rho_f &= \text{fluid density (kg m}^{-3}) \\
\rho_p &= \text{particle density (kg m}^{-3}) \\
\sigma &= \text{surface occupancy (–)} \\
\phi_T &= \text{porosity} \\
< \ldots > &= \text{averaging operator} \\
\ldots^c &= \text{superscript indicating conditioned variables} \\
\ldots_{\text{loc}} &= \text{subscript indicating transformed local coordinates} \\
\ldots_{\text{sym}} &= \text{subscript indicating transformed local coordinates accounting for asymmetry}
\end{align*}
References


