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Applications of Large Eddy Simulation to Study Flow and Sediment Transport in Open Channel Flows

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APPLICATIONS OF LARGE EDDY SIMULATION TO STUDY FLOW AND
SEDIMENT TRANSPORT IN OPEN CHANNEL FLOWS

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Civil and Environmental Engineering

by

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Abstract

The motivation of this study is to extend applications of Large Eddy Simulation (LES) for typical open channel flows to elucidate the time dependent three dimensional flow and sediment transport features which are usually difficult to measure in experiments. Detailed investigations are performed on the unsteady features and, in particular, turbulent structures of the flow to demonstrate the great potential of eddy resolving methods.

The instantaneous flow and sediment transport fields are investigated together with the existence of coherent structures. These structures together with ejection events ($u' < 0, w' > 0$), are responsible for the vertical and lateral transport of suspended sediment from the near bed region. Stronger velocity perturbation vectors are also observed around the coherent structures, demonstrating that these areas are highly dynamic zones of flow and sediment transport. As a result of the enhanced viscosity, sediment induced stratification, and particle pressure effects, a reduction on the peak turbulence levels is shown for both the wall normal and Reynolds shear stress components in the sediment concentrated recirculation and near-bed regions. These phenomena can potentially decrease the vertical mixing and turbulent suspension of sediment particles in the flow field.

Three dimensional hydrodynamic simulations are also conducted for ∼10 meter section of the Expanded Small Scale Physical Model (ESSPM) of the Lower Mississippi River to gain insights on the effects of model distortion on various hydrodynamic variables. Analysis and comparisons are carried out at two distortion scales (i.e., 15, the design distortion and 7.5) using turbulence resolving simulations. Overall, the difference in horizontal mean velocity profiles and velocity fluctuations from the two distortion levels is small, supporting the ability of a distorted models to replicate bulk $1 - D$ sediment transport rates.

The work presented in this dissertation demonstrates that LES is advantageous for solving the complex flow and sediment transport dynamics by resolving the large scale eddies of the turbulent motion and that, when coupled with a sediment transport model, will provide valuable insights into three dimensional turbulence-sediment interactions.
Chapter 1
Introduction

This dissertation consists of six chapters. All chapters, except for the introduction (Chapter 1) and main conclusion (Chapter 6), are written based on papers that have been under review or are to be submitted to peer-reviewed journals, and are constructed using the journal paper format that is approved by the Graduate School of Louisiana State University. Therefore, each chapter is relatively independent, through some information of the reviews and references may be repeated in certain chapters for completeness and clarity. All chapters of the dissertation document the research work of the Ph.D. candidate under the guidance of the major advisor and committee members. This introductory chapter presents the general motivation, research objectives, and research questions of the study and the review of previous studies related to the dissertation topic. Detailed information can also be found in the subsequent chapters.

1.1 Background

Turbulence is one of the most important phenomena in the physics of fluids. In the simplest words, turbulence can be defined as a stochastic or irregular change of the fluid parameters, e.g. velocity, pressure, or as a process where chaotic movement of fluid takes place (Pope, 2000). Turbulence has governing influences on the details of the flow development, such as the velocity distribution, pressure variation, and the fluid forces on structures and sediment.

However, not all flows are turbulent - there are also laminar flows which are stable and without mixing between layers of fluid with different velocities. The Reynolds number (Re) which is the ratio of inertial to viscous forces (Reynolds, 1883) is commonly used to classify the flow regime. For a flow in an open channel of water depth \( H \) and bulk velocity \( U \), the flow is nearly always laminar and the viscous forces are dominating over the inertial ones when \( Re < 2000 \). If \( 2000 < Re < 4000 \) the flow can be be either laminar or smooth.
turbulent. In this range, transition from laminar to turbulent flow is possible if any flow instability occurs. For $Re > 5000$, flows are always assumed to become turbulent (Rott, 1990; Pope, 2000).

An increase in momentum transfer, caused by the fluctuations in turbulent motion, increases the friction on solid boundaries and causes a loss of energy in the flowing fluid. Therefore, turbulence plays a significant role in determining the flow rate and pressure drop in pipe flows and the water level in open channels. The fluctuating turbulent motion is also responsible for the spreading of jets, the entrainment of ambient fluid, and the dispersion of discharged pollutants (Rodi et al., 2013). Turbulence also enhances the erosion and deposition processes in river beds and banks due to ejection and sweep events and plays a major role in keeping sediment particles suspended in flowing water bodies such as rivers. Therefore, both bedload and suspended sediment transport rates are governed by the scales of turbulent motion.

1.2 Problem statement

Understanding the nature of flows through natural rivers and man-made hydraulic structures is critical for solving numerous hydraulic engineering problems, such as sediment transport, water diversion, hydropower development, and many environmental and ecological processes. Development and optimization of design solutions requires a good understanding of the flow physics is required. The development of computational tools to deal with the complexity related to turbulent open channel flows improves our understanding on the details of flow and sediment transport. A number of researchers have carried out both theoretical and numerical studies for flow and sediment transport in open channel flows (Nelson et al., 1995; Zedler and Street, 2006; Werf et al., 2008). Many investigations have focused on the relationship between flow and sediment transport based on the local boundary mean shear stress. However, McLean et al. (1994) argued that the nearbed turbulence statistics do not scale with the local mean shear velocity due to the spatial evolution of the turbulence field.
Near-bed turbulence exists over a wide spectrum from the large to small scales. Very fine meshes have to be used (with cell size smaller than the Kolmogorov scale), to perform numerical simulation of fluid motion by resolving all turbulent levels. For this type of solution, Direct Numerical Simulation (DNS) should be used (Moser et al., 1999). In Large Eddy Simulations (LES), only large scales (low frequency modes) are resolved and the small ones are modeled (Smagorinsky, 1963). This approach allows the use of coarser meshes (compared to DNS) and still provides information about the majority of turbulence. In Reynolds Averaged Navier Stokes (RANS), all turbulence scales are modeled. The RANS methodology is used when the averaged quantities are desired.

In many of the previous numerical studies for sediment transport, RANS equations are often employed (Johns et al., 1993; Hsu et al., 2003). However, evidences suggests that commonly used RANS models can not represent key turbulent quantities in unsteady boundary layers (Chang and Scotti, 2004). At the opposite end of the modeling spectrum, DNS has been successfully employed to simulate sediment transport in open channels and oscillating boundary layer studies (Moin and Manesh, 1998; Schmeeckle and Nelson, 2003; Penko et al., 2011). However, DNS simulations are severely limited by grid size and time step requirements.

To overcome the aforementioned limitations, it is necessary to develop, implement and test better tools for the prediction of flow, sediment transport, and turbulence in open channel flows. The improvement of numerical methods and computing power are providing the opportunity to develop more advanced models that can give solutions in a relatively short time with reasonably high accuracy. The use of LES can resolve a much larger range of smaller scales than Reynolds Averaged equations. Moreover, unsteady simulations using LES gives vital turbulent quantities which helps to understand particle and fluid motions over complex geometries.
1.3 Objectives and research questions

The main objective of this dissertation is to contribute to a better understanding of flow and sediment transport processes using detailed three dimensional numerical computation and LES. This approach handles complex geometries at a resolution sufficient enough to resolve turbulent flows at high Reynolds numbers. The main goals are (i) to assess the performance of different LES schemes with available experimental and DNS data; (ii) to extend an existing finite volume solver to simulate sediment transport processes; (iii) to demonstrate the new sediment transport solver by coupling with the flow and validating results with previously collected experimental data; and (iv) to use the new coupled flow and sediment transport solver to understand the detailed flow physics of open channel flows with complex geometries. Moreover, the following research questions will also be addressed by the end of the dissertation.

- **The range of applicability of different LES schemes for computation of turbulent flows over open channels:** The bed shear stress and the resolved turbulence fields are important for sediment transport processes in unsteady open channel flows. Before sediment transport calculations are attempted, the performance of various LES models in typical open channel flow conditions should be known. This question will be addressed in two steps. LES schemes are generally assumed to be good for moderate to high Reynolds numbers with an adequate mesh resolution in the near wall region. While this can be computationally expensive for engineering relevant flows, simulating the turbulent boundary layers can be reduced by using economical near-wall treatments such as wall functions. As a first step, the sensitivity of different LES results to grid resolution will be tested and the superiority of one LES scheme to the other will be justified by using a wall function. In the second step, comparisons of the resolved turbulence levels from various LES model results will be compared with DNS/experimental data. The results from this work will help guide the selection of a suitable scheme that can be applied for open channels flows with complex geometries.
• **The effect of topography on turbulence and sediment transport processes in open channel flows:** The near bed flow and shear stress distribution over bedforms is usually assumed to be nonuniform due to topographical changes in the bottom boundary layer. Moreover, the shape of the bed topography controls locations where sediment is eroded and deposited. Most importantly, the distribution of turbulent events and structures are also affected by the the shape of a bedform geometry. This part of the dissertation research will include detailed investigations of the spatial variations of flow, turbulence and sediment transport fields. Emphasis will be given to both two and three dimensional dunes and also using the bathymetry of the expanded small scale physical model of the Lower Mississippi River.

• **The role of near bed turbulence on sediment transport in unsteady non-uniform flows:** Due to changes in flow and turbulence fields, the initiation and motion of sediment particles from the bed up into the water column exhibits complex dynamics. Understanding the turbulence field behavior above the sediment bed will provide better insight for further understanding of 3D turbulence-sediment interactions leading to attain detailed sediment transport rate parameterizations. The existence of coherent structures as a means of vortex core identification will be used and the roles of these vortex structures for the ejection of sediment transport will be addressed.

• **The effect of hydraulic physical model distortion scales on various hydrodynamic variables:** The hydraulic similarity in the vertical direction is usually affected in distorted physical models. Deviations in the vertical direction may bring differences not only in the turbulence structures, but also in the scaled sediment transport rates. This issue will be examined by using a portion of the new Lower Mississippi River physical model. Three dimensional hydrodynamic simulations will be performed to understand the effect of distortion scales on the velocity, sediment transport, and turbulence fields.
An important parameter in the flow of suspended sediment transport is the Stokes number (St) that is defined as the ratio between the particle response time scale and the characteristic time scale of the flow. This non-dimensional parameter measures the inertial effect of the sediment particles in the flow. The particle response time is defined as, $\rho_s d^2/18 \mu_f$ (Ozdemir et al., 2010), where $\rho_s = 2650$ $kg/m^3$ is the particle density, $d$ is the particle diameter, and $\mu_f$ is the dynamic viscosity of water. Similarly, with a shear velocity, $u_\tau$ and flow depth, $h$, the flow characteristic time scale is defined as $h/u_\tau$ (Greimann and Holly Jr, 2001). As shown on Tab. 1.1, the Stokes numbers for the selected test cases in this dissertation are significantly smaller than unity. A one-way coupling Eulerian approach by neglecting particle-particle interactions and by assuming that sediment particles in water have small particle response time can be used (Ferry and Balachandar, 2001; Jha and Bombardelli, 2010; Ozdemir et al., 2010; Yu et al., 2014).

Table 1.1: Summary of flow characteristics for selected experimental data

<table>
<thead>
<tr>
<th>Reference</th>
<th>Test case</th>
<th>Depth (cm)</th>
<th>Grain size (mm)</th>
<th>Shear velocity (cm/s)</th>
<th>St ($x 10^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lyn (1987)</td>
<td>1565EQ</td>
<td>6.45</td>
<td>0.15</td>
<td>3.58</td>
<td>1.84</td>
</tr>
<tr>
<td>Lyn (1987)</td>
<td>1957EQ</td>
<td>5.72</td>
<td>0.19</td>
<td>3.95</td>
<td>3.67</td>
</tr>
<tr>
<td>Lyn (1987)</td>
<td>1965EQ</td>
<td>6.51</td>
<td>0.19</td>
<td>3.75</td>
<td>3.06</td>
</tr>
<tr>
<td>Lyn (1987)</td>
<td>2565EQ</td>
<td>6.54</td>
<td>0.24</td>
<td>4.25</td>
<td>5.51</td>
</tr>
<tr>
<td>Maddux et al. (2003)</td>
<td>T2</td>
<td>17.3</td>
<td>0.10</td>
<td>4.13</td>
<td>0.35</td>
</tr>
</tbody>
</table>

1.4 Large eddy simulation principles

The conservation equations of continuity and momentum in the Large Eddy Simulation (LES) framework for incompressible flows are obtained by filtering the Navier Stokes equations. As mentioned in the previous section, in LES the large scales are resolved and the small ones are modeled (Fig. 1.1). To separate the resolvable scales from the sub-grid scales, a filtering procedure has to be applied (Fureby et al., 1997). The filter cut-off should lie in the inertial range of the turbulence spectrum (Fig. 1.1).
\bar{f}(x) = \int_D f(x') G(x,x',\bar{\Delta}) \, dx \quad (1.1)

where D is the model domain, \bar{f}(x) is the resolved flow quantity, \(x'\) is the location where \(\bar{f}(x)\) is considered in the spatial integration, G is a filter function, and \(\bar{\Delta}\) is the filter width,
i.e., the wavelength of the smallest scale retained by the filtering operation. In this study, a top-hat filter, which is written in one dimension as Eq. 1.2 is used.

\[
G (x - x') = \begin{cases} 
\frac{1}{\Delta}, & \text{if } |x - x'| \leq \frac{\Delta}{2}, \\
0, & \text{otherwise}
\end{cases}
\] (1.2)

The filter function determines the size and structure of the small scales. The most common definition of a filter width is

\[
\Delta = (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}}
\] (1.3)

where \(\Delta_x, \Delta_y, \text{ and } \Delta_z\) refer to \(x, y\) and \(z\) directional grid spacing in 3D space.

As noted earlier, various subgrid scale models have been developed. Most are eddy viscosity models based on the Boussinesq hypothesis to calculate eddy viscosity. In this study, detailed analysis and evaluation will be performed on four types of LES closure schemes namely, Smagorinsky Model (SM), Dynamic Smagorinsky Model (DSM), Dynamic Mixed Smagorinsky Model (DMM), and the SGS Kinetic Energy Model (SgsKEM). More detailed formulation and information on these LES schemes can be found in Chapter 2. Moreover, the predictive capabilities of each LES scheme is assessed for fully developed turbulent flow conditions over a wall bounded channel, a backward facing step, and a wavy wall.

### 1.5 Spatial discretization

Finite volume meshes represent elemental volumes where the governing equations are applied as volume integrals over each cell (Vreman et al., 1992). The divergence terms
of the transport equations are converted to surface integrals, using the Gauss divergence theorem. The surface integrals are then evaluated as fluxes through the surfaces of each finite volume. Fluxes are preserved between the volume elements; i.e., a flux leaving one cell directly enters another. Therefore, the finite volume discretization is a conservative scheme.

Each of the control volumes (CV) contains a computational point P at its centroid. The typical CV, an example of which is displayed on Fig. 1.2, is bounded by a set of convex faces of arbitrary shape resulting in polyhedral cells and an arbitrary unstructured mesh. In Fig. 1.2, d is the vector connecting adjacent cell centers P and N, and A is the face normal area vector for the face, f. While all main dependent variables u, p, etc. are defined at the cell centroid P resulting in a collocated arrangement, some derived properties may be defined at the cell face, f.

Figure 1.2: Finite volume discretization and face flux interpolation (OpenCFD, 2013)

The Finite Volume method requires that the Gauss theorem be satisfied over the control volume around the point P in the integral form,

\[
\int_v \nabla \cdot \vec{u} dV = \int_s \vec{u} \cdot n dS = 0 \tag{1.4}
\]

\[
\frac{\partial}{\partial t} \int_{V_p} \phi dV + \int_{V_p} \nabla \cdot (\vec{u} \phi) \ dV = \int_{V_p} \nabla \cdot (\Gamma \phi \nabla \phi) \ dV + \int_{V_p} S_\phi \left( \phi \right) \ dV \tag{1.5}
\]
Considering the variation of a flux \((\phi)\) around \(P\) (Fig. 1.2), we can find that,

\[
\int_{V_p} \phi(x) \, dV = \phi_p V_p \quad (1.6)
\]

Following Eq. 1.6, the convection term is a volume integral that contains the divergence operator, and it can be discretized using,

\[
\int_{V_p} \nabla \cdot (\bar{u} \phi) \, dV = \sum_f A_f (\bar{u}_f A) \phi_{f} = \sum_f F \phi_{f} \quad (1.7)
\]

where \(F\) is the the volume flux through the face and the values of \(\phi_{f}\) and \(\bar{u}_f\) are interpolated from the cell centers to cells faces using an interpolation scheme.

The upwind (UD) differencing scheme determines the face interpolant value \(\phi_{f}\) based on the direction of the flow through the face and it is defined according to the formulation,

\[
\phi_f = \begin{cases} 
\phi_P, & \text{if } F \geq 0, \\
\phi_N, & \text{otherwise}
\end{cases} \quad (1.8)
\]

The upwind scheme is guaranteed to provide a bounded solution, however, it is known to be only first order accurate with an excessive diffusivity due to the leading term truncation error (Peric, 1985).

The central differencing (CD) scheme, however, uses a weighted average of the cell values (Menon, 2011). Assuming a linear variation of \(\phi\) between \(P\) and \(N\) on Fig. 1.2, the face flux is calculated based on,
\[ \phi_f = f_x \phi_p + (1 - f_x) \phi_N \]  

(1.9)

In Eq. 1.9, the interpolation factor \( f_x \) is defined as the ratio of distances \( f_N \) and \( P_N \).

\[ f_x = \frac{f_N}{P_N} \]  

(1.10)

Although central differencing scheme introduces unphysical oscillations into the solution and does not preserve boundedness, mainly on convention dominated solutions, Ferziger and Perić (2002) showed that it is second order accurate even for non-uniform meshes.

Many approaches have been developed in the past to blend the schemes in ways that can guarantee both accuracy and solution boundedness, including higher order upwind (Leonard, 1979) and flux-limiting schemes (Harten, 1983; Sweby, 1984). The latter is an approach that results in a blended scheme which is higher than first order accurate, but without as many spurious oscillations as a second order accurate central differencing scheme. The concept of flux-limiting is used extensively in Total Variation Diminishing (TVD) schemes (Harten, 1983). The TVD schemes have a general form, suggested by Sweby (1984) with the following expression,

\[ \phi_f = (\phi)_{UD} + \Psi[(\phi)_{HO} - (\phi)_{UD}] \]  

(1.11)

where \((\phi)_{HO}\) is a selected higher order scheme and \(\Psi\) is a flux-limiter which is a function of downwind and upwind cells around the face \( f \). More details on different types TVD
schemes can be found in Van Leer (1974); Harten (1983); Darwish and Moukalled (1994). For this work, a Sweby flux-limiter (Sweby, 1984) was imposed for both momentum and sediment transport equations to avoid the spurious oscillations that would occur with the spatial discretization scheme due to shocks, discontinuities or sharp changes in the solution domain. More details about the implementation of TVD schemes for three dimensional computations in OpenFOAM can be found in Jasak et al. (1999).

The diffusion term is discretized in a similar manner as the convective term,

\[ \int_{V_p} \nabla \cdot (\Gamma \nabla \phi) \, dV = \sum_f S \cdot (\Gamma \nabla \phi)_f = \sum_f (\Gamma \phi)_f S \cdot (\nabla \phi)_f \]  

where the diffusion constant \((\Gamma \phi)_f\) can be calculated using an interpolation scheme.

Figure 1.3: Vector notation for non-orthogonal mesh (OpenCFD, 2013)

If the mesh is orthogonal, i.e. vectors \(d\) and \(S\) on Fig. 1.3 are parallel, it is possible to calculate the face gradient \(\phi\) using two values around the face (Eq. 1.13),

\[ S \cdot (\nabla \phi)_f = |S| \frac{\phi_N - \phi_P}{|d|} \]  

(1.13)
An alternative would be calculating the cell centered gradient for two cells sharing the face following,

\[
\left( \nabla \phi \right)_f = f_x (\nabla \phi)_p - (1 - f_x)(\nabla \phi)_N
\]  

(1.14)

Although both of the above described methods are second order accurate, Eqn. 1.13 uses a larger computational molecule (Jasak, 1996). The first term of the truncation error is larger than in the first method, which in turn cannot be used for non-orthogonal meshes.

All variables of the original equation (Eq. 1.5) that cannot be written as convection, diffusion or temporal contributions are treated as sources. The source term \( S_\phi(\phi) \) can be a function of \( \phi \) and other variables that need to be linearized (Eqn. 1.15) in the solution matrix (de Villiers, 2006).

\[
S_\phi \phi = S_c + S_p \phi
\]  

(1.15)

where \( S_c \) and \( S_p \) can also depend on \( \phi \). Following Eqn. 1.5, the volume integral is formulated as,

\[
\int_{V_p} S_\phi (\phi) \, dV = S_c V_p + S_p V_p \phi
\]  

(1.16)
1.6 Temporal discretization

In contrast to RANS, the unsteadiness of the motion is of great importance in LES and hence higher order time discretization schemes and small timesteps $\Delta t$ are desirable. In theory, all time discretization methods produce stable solutions if $\Delta t$ is sufficiently small. However, explicit temporal methods are subject to rigorous stability conditions which are generally known as the CFL condition (Courant et al., 1928). For a stable solution, the CFL ($U \Delta t / \Delta x$) should be less than one in most of the discretization schemes.

In addition to the spatial discretization, a temporal scheme is required for the governing equations. In Eq. 1.5, every term must be integrated over a time step $\Delta t$,

\[
\int_t^{t+\Delta t} \left[ \frac{\partial}{\partial t} \int_{V_p} \phi \, dV + \int_{V_p} \nabla \cdot (\bar{u}\phi) \, dV \right] \, dt = \int_t^{t+\Delta t} \left[ \int_{V_p} \nabla \cdot (\Gamma \nabla \phi) \, dV + \int_{V_p} S_\phi (\phi) \, dV \right] \, dt
\]

(1.17)

If the spatial discretization are given as $Z(\phi)$, the governing equation becomes,

\[
\frac{\partial \phi}{\partial t} = Z(\phi)
\]

(1.18)

It should be noted that the accuracy of the temporal discretization in Eq. 1.17 need not be the same as the temporal discretization of the spatial terms (convection, diffusion and sources). As long as the individual terms are second order accurate, the overall accuracy will also be second order.

**The Crank Nicholson scheme:** This temporal discretization scheme is second order accurate in time and requires the face and cell-centred values of $\phi$ and $\Delta \phi$ along with the convective and diffusive fluxes for both the current and new time levels.
\[
\frac{\phi_p^n - \phi_p^{n-1}}{\Delta t} V_p = \frac{1}{2} \left[ Z(\phi)^{n-1} + Z(\phi)^n \right]
\]  
(1.19)

where \( \phi^n = \phi(t + \Delta t) \) and \( \phi^{n-1} = \phi(t) \) represent the value of the dependent variable at the new and previous times respectively. Eq. 1.19 provides the temporal derivative at a centered time between times \( n-1 \) and \( n \).

Since the flux and non-orthogonal component of the diffusion term have to be evaluated using variables at the new time, the Crank-Nicholson scheme requires inner-iterations during each time step. This scheme uses more memory due to the large number of stored variables, thus making it expensive. The Crank-Nicholson method of temporal discretization is unconditionally stable (Jasak, 1996), but does not guarantee boundedness of the solution.

**Second order backward scheme:** This is a temporal scheme that is second-order accurate in time and still neglects the temporal variation of the face values. In order to achieve this, each individual term of Eq. 1.17 needs to be discretised to second order accuracy. Since the variation of \( \phi \) in time is assumed to be linear, Eq. 1.17 provides a second order accurate representation of the time derivative at \( t + \frac{1}{2} \Delta t \) only. Assuming the same value for the derivative at time \( t \) or \( t + \Delta t \) reduces the accuracy to first order. However, as indicated before, if the temporal derivative is discretised to second order, the whole discretization of the transport equation will be second order without the need to center the spatial terms in time.

\[
\frac{3}{2} \phi_p^n - 2\phi_p^{n-1} + \frac{1}{2} \phi_p^{n-2} \over \Delta t V_p = Z(\phi)^n
\]  
(1.20)
Although the backward differencing method is cheaper and considerably easier to implement than the Crank-Nicholson method, the truncation error is larger (de Villiers, 2006). This is due to the assumed lack of temporal variation in face fluxes and derivatives. This error manifests itself as an added diffusion similar to that produced by upwind differencing of the convection term. As mentioned previously, this added diffusion is not recommended in LES where the sub-grid diffusion may be very small and could be easily affected by the added error.

1.7 Boundary and initial conditions

Large Eddy Simulations are usually carried out in finite size computational domains chosen by the user. Solution of the governing differential equations requires that boundary conditions must be specified at all boundaries of the domain as well as initialization of all of the dependent variables within the entire domain at the start of the simulation.

The specification of boundary conditions depends on the numerical procedure employed. In finite volume methods, conditions must be provided that allow evaluations of convective and diffusive fluxes at the faces of the numerical control volumes coinciding with boundaries in the discretised filtered Navier Stokes equations. This requires the specification of either the fluxes or the values of the dependent variables at the boundaries, or a means to express them as a function of the interior cell values. Specifying values at boundaries, e.g. the sediment concentration or the velocity components, is called a Dirichlet condition. The specification of fluxes generally involving gradients, such as at the outflow or at walls, is known as a Neumann condition.

**Inlet boundary condition:** The flow field at the inlet is prescribed and, for consistency, the boundary condition on pressure is zero gradient.

**Outlet boundary condition:** The outlet boundary condition should be specified in such a way that the overall mass balance for the computational domain is satisfied. The velocity distribution for the boundary is projected from the inside of the domain (first row of cells next to the boundary). These velocities are scaled to satisfy overall continuity. The
fixed value boundary condition is used for the pressure, with the zero gradient boundary condition on velocity. Overall mass conservation is guaranteed by the pressure equation.

**Symmetry plane boundary:** The symmetry plane boundary condition implies that the component of the gradient normal to the boundary should be fixed to zero. The components parallel to the boundary are projected to the face from the inside of the domain.

**No-slip walls:** The velocity of the fluid on the wall is equal to that of the wall itself, so the fixed value boundary conditions prevail. As the flux through the solid wall is known to be zero, the pressure gradient condition is zero gradient.

**Periodic boundary conditions:** Periodic conditions can be used at artificial boundaries when the flow is statistically homogenous in a certain direction or the geometry is periodic in one or two directions. Periodicity in the streamwise direction prevails as the distribution of the statistical quantities over the cross section is the same at each section. In wide open channels in the absence of secondary motions, the flow is commonly homogenous in the spanwise direction and hence periodicity can also be used.

The numerical treatment of periodic boundaries is such that on both ends of the simulation domain so-called ghost cells are added to the domain and the variables at one side of the domain are copied after every computed time step into the ghost cells of the other side and the vice versa.

### 1.8 Scope/applications of the dissertation

Flow and sediment transport processes in open channel flows are among the most complex and least understood processes in nature. It is very difficult to find analytical solutions for most problems in hydraulics and it is also not easy to obtain three dimensional numerical solutions without high speed computers. With the recent advancements in computational power, numerical models have been greatly improved and widely used to solve problems in open channel flows that have great practical importance. This dissertation presents applications of Large Eddy Simulation to understand and answer a range of flow and sediment transport processes in open channel flows. Detail investigations are performed on the un-
steady features and, in particular, turbulent structures of the flow to demonstrate the great potential of eddy resolving methods for situations where these features play an important role.

1.9 Organization of dissertation

This dissertation is organized into six chapters following journal style format recommended by LSU Graduate School. The main part of the dissertation is comprised of four chapters (two-five) that are based on four peer-reviewed journal manuscripts either already submitted or in preparation. Since each chapter is prepared as a stand-alone journal paper, some information may be repeated in certain chapters for clarity and completeness.

In Chapter 2, the predictive capabilities of various Large Eddy Simulation (LES) schemes for fully developed turbulent flow conditions are assessed over a wall bounded channel, a backward facing step, and a wavy wall. The sensitivity of different LES schemes to grid resolution are tested and the superiority of one LES scheme to the other is also justified using a wall bounded turbulent open channel flow and the LES results are compared to available DNS data. In the second step, the resolved turbulence levels from various LES model results are compared with DNS/experimental data for flow conditions which are commonly found in geophysical applications. The term “geophysical” in this dissertation refers to typical open channel flows without Coriolis effects due to the small spatial and time scales.

In Chapter 3, LES is applied over flat-bed turbulent channel flows to understand the instantaneous flow, bed shear stress, and turbulent fields and to elucidate the role of vortex coherent structures on the entrainment of suspended sediment transport from the bottom boundary layer. Flow and suspended sediment transport in fully developed turbulent open channel flows are investigated using a three-dimensional, non-hydrostatic model, Open-FOAM.

In Chapter 4, LES is demonstrated for fully developed turbulent flows over two and three dimensional dunes which can help to further understand the influence of these bed-
forms on the temporal and spatial variations of the flow and sediment transport field. The instantaneous flow fields are investigated together with the occurrence of coherent structures which are identified by a Q-criterion (Hunt et al., 1988). The coupled solver accounts for fluid-sediment and sediment-sediment interactions.

In Chapter 5, three dimensional hydrodynamic simulations are performed using the geometry and flow conditions of a ∼10 meter section of the Expanded Small Scale Physical Model (ESSPM) of the Lower Mississippi River to understand the effect of vertical distortion on various hydrodynamic variables. This chapter first focuses on a description of the similarity laws that were used in the ESSPM design and what limitations are expected due to the use of a distorted scale. Analysis and comparisons are carried out at two distortion scales (i.e., 15, the design distortion and 7.5) using turbulence resolving simulations.

Finally, Chapter 6 summarizes and concludes the major findings of the whole dissertation. Possible future research directions for detailed three dimensional flow and sediment modeling are also addressed.

1.10 References


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Chapter 2
Evaluation of large eddy simulation closures for fully developed turbulent flows

2.1 Introduction

Numerical simulation of turbulent flows has become popular in the past decades for different applications which use the principles of fluid motion. In recent years, Computational Fluid Dynamics (CFD) is widely applied in a broad spectrum of engineering and environmental flows, ranging from geophysical to cardiovascular. Numerical simulations are more flexible and cost effective than experimental methods. Numerical results have the advantage that any flow quantity can be sampled at high space-time resolutions to gain a detailed insight into the turbulent flow dynamics. Even though simulation techniques are well established as a means of studying turbulent flows, the numerical results are commonly presented together with experimental investigations to confirm validity and applicability.

The most straightforward approach to the solution of turbulence is direct numerical simulation (DNS), in which all scales of motion are resolved (Pope, 2000). With no explicit modeling involved, expected errors are only due to the numerical discretisations and the imposed initial and boundary conditions. Therefore, numerical simulations using DNS can provide an accurate flow field with all scales of turbulence (Kim et al., 1987). However, the computational cost and time step requirement is highly dependent on the Reynolds number (Re). The ratio between the energetic and dissipative length scales increases with the Reynolds number and the complexity of the flow geometry (Moin and Manesh, 1998). If the numerical time step is assumed to be proportional to the grid size, then the total computational cost is expected to be in the order of $Re^{9/4}$ (Rogallo and Moin, 1984).

The large eddy simulation (LES) technique is a highly promising approach which can be used to predict practically relevant flows at a reasonable computational cost (Rodi et al.,
2013). In LES, the flow variables are decomposed into resolved (large) scales and subgrid (small) scales (Piomelli, 1999). LES directly resolves the large scale motions and the small scales, usually with lengths smaller than the computational grid size, are modeled with closure schemes. The large scales are responsible for most of the momentum and energy transport while, the small scales are much weaker and also have a much more homogeneous and isotropic structure (Ghosal and Moin, 1995). Hence, it is reasonable to directly compute the energy carrying large scales and to model the dissipative small scales. The desired flow statistics can be obtained directly from the computed flow fields in the production range, as well as from the ones which are entering into the inertial subrange where the energy cascade takes place (Moin et al., 1991). On the other hand, an unclosed subgrid scale stress (SGS) term has to be approximated by a model (Germano et al., 1991; Mason, 1994; Smagorinsky, 1963). LES is expected to be more robust than Reynolds Average Navier Stokes equations (RANS) predictions, where all scales of motion are modeled. RANS methods often have limitations when they are applied to complex flows with large scale flow separation, reattachment, and vortex shedding (Chang and Scotti, 2004).

The first step in applying the LES concept is to decompose the turbulent motion by spatial filtering (Germano, 1992) into large eddies to be resolved and small scales that require a subgrid scale model. Several modeling approaches for the small scales have been proposed in the past decades, where most of them are eddy viscosity models, which follow the Boussinesq hypothesis. The eddy viscosity describes the proportionality between the subgrid scales and the large scale strain rate tensor. The determination of the eddy viscosity is purely based on an algebraic relation, and the value of the eddy viscosity can vary both in space and time depending on the local flow structure and levels of turbulence (Wan et al., 2007). The first subgrid scale model, equivalent to Prandtl's mixing length theory (Vreman et al., 1994), was proposed by Smagorinsky (1963). The fundamental difference between the two is in the determination of the characteristic length scale. The Smagorinsky Model (SM) approach uses a model coefficient ($C_s$) and a filter width to calculate the subgrid
length scale for the calculation of turbulent eddy viscosity, whereas the mixing length theory assumes the energy transfer within a newtonian fluid boundary layer is similar to a molecular movement in a low density gas (Bardina et al., 1983; Bradshaw, 1974). In order to take into account the reduction of the subgrid scale length in the vicinity of a wall, SGS eddy viscosity can be adjusted with a damping function (Van Driest, 1956). The SM is only valid under equilibrium assumptions. However, non-equilibrium conditions can occur in many practical flows such as, free shear layers, separating and reattaching flows, and wall bounded turbulent flows (Ghosal and Moin, 1995; de Villiers, 2006; Vuorinen et al., 2015). The SGS Kinetic Energy Model (SgsKEM) of Yoshizawa and Horiuti (1985) addresses this problem by including a temporal history effect with the transport equation of the subgrid turbulence through its kinetic energy.

Despite the Smagorinsky model being extremely simple, it has several disadvantages. First of all, the value for the model coefficient is not uniquely defined. Secondly, the process of energy backscatter (energy transfer from small to large scales) is not allowed. According to Rodi et al. (2013), the SM is also found to be dissipative for the resolved motions in the near-wall region due to an excessive eddy viscosity arising from high velocity gradients (mean shear) close to solid walls. To overcome some of the shortcomings, a dynamic procedure for computing the model coefficient was first proposed by Germano et al. (1991), where the local flow characteristics are used during parameterization. The Dynamic Smagorinsky Model (DSM) calculates the model coefficient by using information available from the smallest resolved scales (Lilly, 1992). The detailed formulation of this model can be found in Fureby et al. (1997b); Piomelli (1999); Pope (2000); Gullbrand and Chow (2003); Rodi et al. (2013). The Dynamic Mixed Model (DMM) combines the Scale Similarity Model of Bardina et al. (1980) without the eddy viscosity concept. This model assumes that the smallest resolved scales are similar to the largest unresolved scales corresponding to different filter widths. For the formulation for the SGS stresses, it uses the information from the two filter levels (Vreman et al., 1994; Fureby et al., 1997b; Gullbrand
and Chow, 2003; Ciardi et al., 2005). For example, the DMM model proposed by Zang et al. (1993) combines the scale similarity concept of Bardina et al. (1980) with the original Smagorinky model. Different types of dynamic SGS models were also proposed by Moin et al. (1991); Vreman et al. (1994); Ghosal et al. (1995); Salvetti and Banerjee (1995); Meneveau et al. (1996).

Recent studies showed that the instantaneous bed shear stress and the resolved turbulence fields are important for sediment transport processes in unsteady open channel flows (McLean et al., 1994; Nelson et al., 1995; Maddux et al., 2003; Zedler and Street, 2006; Niroshinie et al., 2013). Before sediment transport calculations are attempted, the merits and limitations of various turbulence resolving models at typical flow conditions should be known. The motivation of this work is to assess the predictive capabilities of various Large Eddy Simulation schemes for fully developed turbulent flow conditions. Our ultimate goal is to choose an optimal LES scheme which can be applied to investigate the interactions between flow and sediment transport processes at relatively high Reynolds numbers which is typically found in geophysical flows. In this paper, we will address this question in two steps. LES schemes are generally assumed to be good for moderate to high Reynolds numbers with an adequate mesh resolution in the near wall region. Because this can be computationally expensive for engineering relevant flows, simulating the turbulent boundary layer can be reduced by using economical near-wall treatments such as a wall function. Therefore, at the first step, the sensitivity of different LES schemes to grid resolution will be tested and the superiority of one LES scheme to the other will also be justified using a wall bounded turbulent open channel flow and the LES results will be compared to available DNS data (Moser et al., 1999) of a similar computational setup. In the second step, comparisons of the resolved turbulence levels from various LES model results will be compared with DNS/experimental data for flow conditions which are commonly found in geophysical applications. The results from this work will help to guide the selection of a suitable method that can be applied for open channel flows with complex geometries.
where flow separation and reattachment commonly occurs and it is critical for initiation of sediment transport, bedform evolution, contaminant transport, and many others.

2.2 Mathematical formulation

The software used in this study is OpenFOAM, Open Field Operation and Manipulation (Weller et al., 1998). This model is three-dimensional, non-hydrostatic and freely available. It is organized with a flexible set of C++ written modules that are used to build solvers to simulate specific problems in engineering and fluid mechanics (Jasak and Weller, 2000). Utilities to perform pre- and post-processing tasks and libraries to create toolboxes are accessible to the solvers/utilities, such as libraries for turbulence models, combustion, and mesh transformation. The model is free, both in terms of source code and in its structure and hierarchical design. This makes the solvers, utilities and libraries fully extensible. OpenFOAM employs finite volume numerics to solve systems of partial differential equations on either structured or unstructured meshes. The fundamental equations are developed within a robust, implicit, pressure-velocity, iterative solution framework. OpenFoam uses a domain decomposition method in which the geometry and other fields are divided and allocated to separate processors for computation of the Navier Stokes equations or any other partial differential equations.

The governing equations for incompressible unsteady fluid flow are,

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{2.1}
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu_{eff} \frac{\partial u_i}{\partial x_j} \right] + f_i \tag{2.2}
\]

where \( u \) is velocity vector field, \( p \) is the pressure field, \( f \) is a body force, \( x_1, x_2, \) and \( x_3 \) are the streamwise, spanwise, and wall-normal directions, also referred to as \( x, y, \) and \( z. \nu_{eff} \) is the total viscosity of the flow which is the sum of molecular and turbulent viscosities.
To solve the conservation equations in a finite volume scheme, the values of the flow variables are required at the face centers. A second order linear central differencing scheme was applied in this study. A standard second order finite volume discretization of a Gaussian integration scheme (Gauss linear) was used for the gradient terms such as $\nabla p$. For finite volume discretisation, surface normal gradients are evaluated at the cell faces (de Villiers, 2006). A cell face connects two cells where the gradient is taken from the values at the centers of these two cells. The surface normal gradient is then the gradient component which is normal to the cell faces. For this study an explicit non-orthogonal correction scheme is used (Jasak, 1996). The implicit, second order backward scheme is applied for the temporal derivatives. The Gauss scheme is the only available scheme for the laplacian terms such as $\int_V \nabla^2 (\nu_{eff} \bar{u}) dV$. More details about the available numerical schemes can be found in Jasak (1996); de Villiers (2006).

2.2.1 Large eddy simulation closures

The conservation equations of continuity and momentum in the Large Eddy Simulation (LES) framework for incompressible flows are obtained by filtering the Navier Stokes equations. As mentioned in the previous section, in LES the large scales are resolved and the small ones are modeled. To separate the resolvable scales from the sub-grid scales, a filtering procedure has to be applied (Fureby et al., 1997a) and the filter cut-off should lie in the inertial range of the turbulence spectrum.

\[
\bar{f}(x) = \int_D f(x') G(x, x', \bar{\Delta}) dx
\]  

(2.3)

where D is the model domain, $\bar{f}(x)$ is the resolved flow quantity, $x'$ is the location where $\bar{f}(x)$ is considered in the spatial integration, G is a filter function, and $\bar{\Delta}$ is the filter width, i.e., the wavelength of the smallest scale retained by the filtering operation.
\( G(x - x') = \begin{cases} \frac{1}{\Delta}, & \text{if } |x - x'| \leq \frac{\Delta}{2}, \\ 0, & \text{otherwise} \end{cases} \) \hspace{1cm} (2.4)

The filter function determines the size and structure of the small scales. The most common definition of a filter width is

\[ \tilde{\Delta} = (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}} \] \hspace{1cm} (2.5)

where \( \Delta_x, \Delta_y, \) and \( \Delta_z \) refer to \( x, y \) and \( z \) directional grid spacing in 3D space.

As noted earlier, various subgrid scale models have been developed. Most are eddy viscosity models based on the Boussinesq hypothesis to calculate eddy viscosity. In this study, detailed analysis and evaluation will be performed on four types of LES closure schemes namely, Smagorinsky Model (SM), Dynamic Smagorinsky Model (DSM), the Dynamic Mixed Model (DMM), and the SGS Kinetic Energy Model (SgsKEM).

- **Smagorinsky Model (SM)**

The SGS stress tensor aids in providing model closure for the LES and is modelled through an eddy viscosity model (Smagorinsky, 1963). In the SM, the SGS tensor \( \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \) is related to the resolved strain rate, \( \bar{S}_{ij} \) through a turbulent eddy viscosity and it can be written as:

\[ \tau_{ij} = 2\nu_t \bar{S}_{ij} + \frac{1}{3} \delta_{ij} \tau_{kk}^R \] \hspace{1cm} (2.6)
where \( \frac{1}{3} \delta_{ij} \tau_{kk} \) is the normal stress which is twice the subgrid scale kinetic energy, and \( \bar{S}_{ij} \) is defined as:

\[
\bar{S}_{ij} = \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]

and the eddy viscosity of the residual turbulent motion, \( \nu_t \), is defined as:

\[
\nu_t = (C_s \Delta)^2 \sqrt{2 \bar{S}_{ij} \bar{S}_{ij}}
\]

where \( C_s \) is the Smagorinsky constant. This is the only adjustable parameter in this scheme and lies in the approximate range 0.094 to 0.2. In the presence of a mean shear layer, Deardorff (1971) found that a higher value of this parameter causes excessive damping of the large scale motions and recommended the values in the lower range such as, \( C_s = 0.094 \). For isotropic turbulence, Lilly (1992) estimated a \( C_s \) value of 0.17 assuming local equilibrium in the inertial subrange.

- **Dynamic Smagorinsky Model (DSM)**

Germano et al. (1991) and Lilly (1992) developed a procedure where the constant coefficient model becomes a dynamic coefficient; i.e., the Smagorinsky constant is no longer taken as constant but allowed to vary in both space and time. The formulation of the dynamic coefficient model (or simply dynamic model) requires the sequential application of two well-characterized filters on the Navier-Stokes equations, namely the primary and test filters. The width of the test filter is typically twice that of the primary filter. The test filter generates another unknown residual stress tensor denoted as,
\[ T_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \] (2.9)

The bar hat notation denotes the application of a filter (of width \( \hat{\Delta} \)) resulting from a sequential applications of the primary (grid) filter and the test filter. The Germano identity between the grid and the test filtered fields, \( L_{ij} = T_{ij} - \hat{\tau}_{ij} \) is used to dynamically determine \((C_s \Delta)^2\) in the Smagorinsky Model. The importance of the tensor \( L_{ij} \) lies in that it can be expressed in terms of the filtered or resolved velocity \( \bar{u}_i \) as well as the terms in the Smagorinsky model. In terms of the resolved velocity, the Germano identity (Leonard stress), \( L_{ij} \) becomes,

\[ L_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \] (2.10)

Based on the Smagorinsky model, the deviatoric portion of \( L_{ij} \) can be expressed by test filtering (Eq. 2.6).

\[ \hat{\tau}_{ij} = 2(C_s \hat{\Delta})^2 |S| \hat{S}_{ij} \] (2.11)

and by modeling the deviatoric portion of the subtest scale stress as,

\[ T_{ij}^R = 2(C_s \hat{\Delta})^2 |\hat{S}| \hat{S}_{ij} \] (2.12)
In Eq. 2.12, the strain rate tensor, $\hat{S}_{ij}$, and its norm, $|\hat{S}|$, are based on the double filtered velocity $\hat{u}_i$. The model coefficient $(C_s \Delta)^2$ is dynamically computed by minimizing the square of the difference $Q_{ij}Q_{ij}$ (Eq. 2.13) between the modeled, and the resolved $T_{ij}^R$ (Lilly, 1992), where the difference is given as,

$$Q_{ij} = T_{ij}^R - 2(C_s \Delta)^2 M_{ij}$$

(2.13)

and

$$M_{ij} = |\hat{S}|\hat{S}_{ij} - \beta |\hat{S}| \hat{S}_{ij}$$

(2.14)

where $\beta = \left(\frac{\bar{\Delta}}{\hat{\Delta}}\right)^2$ is the square of the filter width ratio. From the minimization procedure, the dynamic model coefficient becomes,

$$(C_s \Delta)^2 = \frac{1}{2} \frac{L_{ij}}{M_{ij}} \frac{M_{ij}}{M_{ij}}$$

(2.15)

The model coefficient from Eq. 2.15 can give either positive or negative in contrast to a constant coefficient in the Smagorinsky model.

- **Dynamic Mixed Model (DMM)**

Zang et al. (1993) modified the DSM of Germano et al. (1991) by employing a scale similarity model based on Bardina et al. (1983). The DMM explicitly calculates the mod-
ified Leonard term and only models the cross term, and the SGS Reynolds stress. Due to the scale similarity model, the DMM is expected to reduce the excessive backscatter represented by the model coefficient that may cause numerical instability. Compared to the DSM, the DMM also undertakes less modeling due to the explicit calculation of the modified Leonard term and the requirement only to model the residual stresses.

\[
\hat{\tau}_{ij}^R = (\bar{u}_i \bar{u}_j - \hat{u}_i \hat{u}_j) - 2(C_s \hat{\Delta})^2 |\hat{S}| \hat{S}_{ij}
\]  

(2.16)

The first term on the right hand side is the similarity model, whereas the second part represents the unresolved residual stress, adopting the smagorinsky eddy viscosity formulation. Similar to Germano et al. (1991), Zang et al. (1993) calculated the deviatoric portion of the subtest scale stress for the DMM as,

\[
T_{ij}^R = (\hat{\bar{u}_i \bar{u}_j} - \hat{\hat{u}_i \hat{u}_j}) - 2(C_s \hat{\Delta})^2 |\hat{S}| \hat{S}_{ij}
\]  

(2.17)

Using Eq. 2.16 and Eq. 2.17 for the Germano identity for the anisotropic part gives,

\[
L_{ij} = 2(C_s \hat{\Delta})^2 M_{ij} + H_{ij}
\]  

(2.18)

where \( M_{ij} \) and \( L_{ij} \) are similar to the previously formulated quantities in DSM.

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\[ H_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j - \left( \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \right) = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \] (2.19)

Finally, the model coefficient is calculated dynamically based on the following formulation.

\[ (C_s \Delta)^2 = \frac{1}{2} \frac{(L_{ij} - H_{ij}) M_{ij}}{M_{ij} M_{ij}} \] (2.20)

- **SGS Kinetic Energy Model (SgsKEM)**

In this model, the SGS Reynolds stress is written in terms of a generalized SGS eddy viscosity representation, which is expressed using the SGS kinetic energy and characteristic grid width (Yoshizawa and Horiuti, 1985). The turbulent SGS viscosity \( \nu_t \) is calculated from a transport equation for the SGS kinetic energy, which is assumed to be isotropic (de Villiers, 2006).

\[
\frac{\partial K}{\partial t} + \nabla . (\bar{u} K) - \nabla . (\nu_{eff} \nabla \bar{K}) = G - \epsilon
\] (2.21)

where \( K \) is the subgrid kinetic energy, \( \bar{u} \) is the resolved velocity field, \( \epsilon \) is the turbulent dissipation at the smallest scales, \( \nu_{eff} \) is the effective viscosity of the fluid which is the sum of molecular and turbulent viscosities, and \( G \) represents the decay of turbulence from through the energy cascade to the resolved scales to the subgrid scales. Furthermore, the dissipation rate and decay of turbulence are calculated from the subgrid scale kinetic energy.
\[ \epsilon = C_e K^{3/2} / \Delta \]  
(2.22)

\[ G = C_k \sqrt{K} \Delta |\bar{S}|^2 \]  
(2.23)

\[ \nu_t = C_k K^{1/2} \Delta \]  
(2.24)

where \( C_e \) and \( C_k \) are the energy dissipation and decay of turbulence coefficients, respectively. Modified versions of the dynamic SGS models were also proposed by (Moin et al., 1991; Vreman et al., 1994; Ghosal et al., 1995).

According to Ghosal et al. (1995), an SGS model based on subgrid kinetic energy reduces the stability issues which are common in dynamic and dynamic mixed models. However, Fureby et al. (1997b) found that these types of models are limited due to the discrepancy between the principal axes of the SGS stress and the rate of strain tensor.

2.3 Computational domain setup

2.3.1 Fully developed wall bounded channel flow

The direct numerical simulation setup of Moser et al. (1999) was chosen to evaluate the mean flow and turbulence profiles from Large Eddy Simulations. The Reynolds number (\( \text{Re}_r \)) is 590 based on the friction velocity (\( u_r \)) and channel half height (h). The channel geometry is defined in (Fig. 2.1) with x, y, and z aligned with the streamline, wall normal, and spanwise directions respectively. No-slip boundary conditions are applied to the top and bottom walls, and periodic boundary conditions are used on both the stream & spanwise directions. The computation was carried out with three different grid resolutions to study the scale dependency of eddy structures. The simulation setups were chosen based on the non-dimensional wall distance (\( Y^+ = u_r y/\nu \)). The grids considered are, 150 × 202 × 100 (303000 finite volume grids with \( Y^+_{\text{min}} \approx 0.74 \)), 100 × 50 × 75 (375000 finite volume grids with \( Y^+_{\text{min}} \approx 2.95 \)), and 60 × 40 × 45 (108000 finite volume grids with
$Y^+ \approx 14.7$ on the streamwise, wall normal, and spanwise directions, respectively. For all the three computational setups, the cells are stretched out with a ratio of 1:10 in the wall normal direction. Moreover, two types of simulations were carried out for the third grid with $Y^+_{min} \approx 14.7$, one considering smooth walls, and the other by applying a Spalding’s wall function (Spalding, 1961) to understand the advantages and limitations of the wall function.

![Figure 2.1: Coordinate system of the model setup](image)

During the numerical computation, it was found that the flow gets a false steady solution, unless it is provoked with an initial condition that produces vorticity. According to de Villiers (2006), the near-wall turbulence cycle is naturally initiated through a process of transition, that comes as a result of the growth of small initial perturbations or imperfections on the wall boundary. Near-wall parallel streaks were given to the parabolic velocity profile. The parabolic profile was found to be effective to generate free shear and shedding than an initial logarithmic profile. The solution of the plane channel rapidly became turbulent as the sinuous streaks induce vortex formation and further instability. During the computation at each time step, flow was forced with a pressure gradient ($\partial p/\partial x = u_x^2/h$), which yields a depth integrated streamwise velocity ($U_b$) of the DNS data. After the
pressure-velocity corrector step, the streamwise velocity was adjusted for a constant mass flow rate by comparing the depth integrated streamwise velocities. Here we assumed that the variation of depth integrated mass flux in the wall normal and spanwise directions are negligible. Therefore, mass flux adjustment was only applied on the streamwise direction.

LES computations were performed using four different types of SGS schemes including the Smagorinsky Model (SM), SGS Kinetic Energy Model (SgsKEM), Dynamic Smagorinsky Model (DSM), and Dynamic Mixed Model (DMM). The performance of each SGS scheme was analyzed by comparing with the DNS results of (Moser et al., 1999), considering the mean flow and Reynolds stress profiles. For the given computational domain, the simulations required nearly 200 flowthrough times ($L_x/U_b$) or nearly 9200 seconds before a statistically-steady state flow. Flow fields were collected for about additional 100 flowthrough times and temporal averaging followed by spatial averaging were performed. First we are going to present the results for the two computational setups which have near wall $Y^+$ values in the laminar region and next the results from the third computational grid will be addressed.

Figure 2.2: Mean streamwise velocity profiles for $Y^+ \approx 0.74$ (left) and $Y^+ \approx 2.95$ (right)
### Table 2.1: Shear velocity ($u_\tau$) values from different models

<table>
<thead>
<tr>
<th>$Y_{min}^+$</th>
<th>Value (m/s)</th>
<th>DNS</th>
<th>SgsKEM</th>
<th>SM</th>
<th>DSM</th>
<th>DMM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.74</td>
<td>0.0117</td>
<td>0.0113</td>
<td>0.0113</td>
<td>0.0111</td>
<td>0.0112</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Error (%)</td>
<td>...</td>
<td>3.4</td>
<td>3.4</td>
<td>5.0</td>
<td>4.3</td>
</tr>
<tr>
<td>2.95</td>
<td>0.0117</td>
<td>0.0114</td>
<td>0.0114</td>
<td>0.0110</td>
<td>0.0112</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Error (%)</td>
<td>...</td>
<td>2.3</td>
<td>2.3</td>
<td>6.0</td>
<td>4.3</td>
</tr>
</tbody>
</table>

As it can be seen from Fig. 2.2, results from all the SGS models are in a reasonable agreement with the DNS data for the mean streamwise velocity profiles. As it is shown on Tab. 2.1, the calculated shear velocities from each scheme has an error of less than 6%. As it can be observed from the streamwise velocity profiles, the SM and SgsKEM started underesolving the mean streamwise velocity profiles in the buffer zone when the grid resolution is decreased from $Y_{min}^+ \approx 0.74$ to $Y_{min}^+ \approx 2.95$. One reason for this could be due to the constant model coefficient which is commonly used by the two models. Moreover, a significant difference has not been identified from the results of the SM and SgsKEM schemes for the entire computational depth.

Fig. 2.3 depicts the x-x component of the resolved Reynolds stress tensor from the two grids. The comparisons between the simulations and the DNS data is quite good for all SGS models for $Y_{min}^+ \approx 0.74$. This shows that all the LES models are efficient enough to capture the streamwise velocity fluctuations for this grid resolution. However as the grid resolution decreases to $Y_{min}^+ \approx 2.95$, the SM and SgsKEM models started underpredicting the $<u'u'>$ profiles in the buffer region. This shows that the SGS contribution is higher for these two schemes compared to the others which use a dynamic model coefficient (DSM, and DMM). Underestimation of the streamwise velocity profiles was also observed from SM and SgsKEM on the buffer region for the coarser grid (Fig. 2.2). The resolved $<u'u'>$ profiles from the DSM have a similar trend to those reported by the previous studies (Gullbrand and Chow, 2003; Ciardi et al., 2005). Gullbrand and Chow (2003) applied a DSM scheme with a finite element method and the $<u'u'>$ profiles from their model also over predicted...
the DNS data. It is clear that the choice of resolution can alter the x-x component of the resolved Reynolds stress tensor.

Figure 2.3: Streamwise velocity fluctuations for $Y_{min}^+ \approx 0.74$ (left) and $Y_{min}^+ \approx 2.95$ (right)

Figure 2.4: Wall normal velocity fluctuations for $Y_{min}^+ \approx 0.74$ (left) and $Y_{min}^+ \approx 2.95$ (right)

The predictions for the wall normal (Fig. 2.4) and spanwise (Fig. 2.5) Reynolds stress components are similar in shape but marginally below the DNS values. Underpredictions of the LES results for these two components could probably be due to the modeled SGS part which was not included during the averaging of the flow variables. Nevertheless, the
DNS gives all scales of turbulence and errors are only due to the numerical scheme, and the imposed initial and boundary conditions. On this study a second order numerical scheme in both time and space was used. Better results can be obtained by using higher orders which can minimize the numerical diffusion. From the four SGS models, DSM and DMM are best in resolving the $< v'v' >$ and $< w'w' >$ components. For both DSM and DMM, the model coefficient, $(C_s \bar{\Delta})^2$, is calculated automatically and both allows SGS energy backscatter to the resolved scales. The DMM differs to DSM due to the application of the scale similarity concept (Bardina et al., 1983). As it can be seen, calculating the model coefficient dynamically is advantageous to get the desired wall normal and spanwise turbulent statistics. Underestimations of $< v'v' >$ and $< w'w' >$ values have also been observed on the previous studies (Holmen et al., 2003; Ciardi et al., 2005), nevertheless the DSM results of Gullbrand and Chow (2003); Winckelmans et al. (2001) overpredicted these two variables compared to the DNS data. Similar to the $< u'u' >$ profiles, the SM and SgsKEM schemes are also more sensitive to the grid resolution for the other turbulence fields.

![Figure 2.5: Spanwise velocity fluctuations for $Y_{min}^+ \approx 0.74$ (left) and $Y_{min}^+ \approx 2.95$ (right)](image-url)
The cross stress components ($<u'v'>$) of the Reynolds stress tensor from each SGS model are shown on Fig. 2.6. For this component, DMM and DSM give results which are in a reasonable agreement with the DNS data. For the finer grid, the location of the peaks are well defined for all of the SGS models. As the grid resolution decreases, again both SgsKEM and SM give poor results.

Figure 2.6: Cross stress profiles for $Y^+_{min} \approx 0.74$ (left) and $Y^+_{min} \approx 2.95$ (right)

It is well known that the scaling of the near-wall turbulent structure is strongly dependent on the nature of flow and the range of Reynolds numbers. To resolve the small scale turbulent eddies around the wall, an adequate grid resolution is required. For most practical flows at high Reynolds numbers, the near wall grid resolution is thus limiting for LES methods. Hence, three approaches are commonly used to bypass this limitation. The first approach consists of keeping a fine grid around the walls but solving the set of equations weakly coupled to the outer flow with a coarse resolution (Piomelli, 1999). The Second is by using a detached eddy simulation (DES) method which switches from LES model in the upper part to RANS in the vicinity of the wall where a finer grid is necessary (Spalart, 2009). The third approach consists of using a relatively coarse grid at the wall and to mimic the dynamical effects of the energy-containing eddies in the wall-layer through
a wall function (Piomelli, 2008; Vuorinen et al., 2015). To assess the performance of each
SGS scheme for a non-wall resolved Large Eddy Simulation, a priori study was performed
with and without a wall function for a near-wall resolution of $Y_{\text{min}}^+ \approx 14$. For the two
cases, the grid spacing, streching, and aspect ratios were kept the same. A wall function
proposed by Spalding (1961) was implemented in OpenFOAM as,

$$Y^+ = U^+ + \frac{1}{E} \left\{ e^{\kappa U^+} - 1 - \kappa U^+ - \frac{1}{2} (\kappa U^+)^2 - \frac{1}{6} (\kappa U^+)^3 \right\}$$

(2.25)

where $\kappa$ is the von Karman constant, $E = 9.8$ is a wall function coefficient, $Y^+ = u_\tau y/\nu$
and $U^+ = u/u_\tau$ are the non-dimensional wall normal coordinate and velocity respectively.

![Figure 2.7: Mean streamwise velocity profiles for LES simulations at $Y_{\text{min}}^+ \approx 14.7$ : left with wall function and right without wall function](image)

Fig. 2.7 depicts the mean streamwise velocity profiles from different SGS schemes for
the computations which were performed with and without a wall function. As it can be
observed from the profiles, the near-wall streamwise velocities are off from the DNS data
for the simulations which were performed without a wall function. Nevertheless the wall
function helps in damping the energy and ultimately with a good estimation of the velocity

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profiles close to the wall. It appears that the SM and SgsKEM models give relatively better values even without a wall function compared to the dynamic models. This could be due to their high dispersion rate around the wall due to the constant model coefficient.

Figure 2.8: Mean streamwise and wall normal turbulent intensity profiles for LES simulations at $Y_{min}^+ \approx 14.7$: left without wall function and right with wall function

Fig. 2.8 and 2.9 show the predictions of the turbulent intensities from simulations with and without a wall function compared to the DNS data. A clear impact of the first grid spacing at the wall for LES is noticeable from these profiles. For the streamwise velocity fluctuations, the wall function mainly helps the DSM scheme to capture the peak values. Moreover, a minor increase in the peaks of $\langle u'u' \rangle$ is achieved by using the wall function for both the SgsKEM and SM schemes. By using the wall function, an improvement in the $\langle v'v' \rangle$ profiles is also shown. For example for the DSM scheme, the wall function
is very efficient to align the axis of $<v'v'>$ profile to the DNS data in the logarithmic region. With the wall function, both the $<w'w'>$ and $<u'v'>$ profiles are resolved well by the DSM. Improvements are also observed for the other models.

Figure 2.9: Spanwise and cross stress turbulent intensity profiles for LES simulations at $Y_{min}^+ \approx 14.7$: left without wall function and right with wall function

2.3.2 Flow over a backward-facing step

The second test case contains a turbulent separating flow over a backward-facing step which was studied experimentally by Jovic and Driver (1994). The height (h) of the step is 0.98 cm. The Reynolds number used in the experiment was $R_{eh} = 5000$ based on the step height and free-stream velocity, $U_o = 7.72$ m/s. The computational domain layout is shown on Fig. 2.10. It consists of a streamwise length $L_x = 30h$, vertical height $L_y = 6h$, and spanwise width $L_z = 4h$. The length of the upstream inlet channel is chosen to be $10h$.
in order to limit the effect of inlet turbulence on the separated region downstream of the sudden expansion.

Large Eddy Simulations were performed using 400 x 140 x 40 grid points along the streamwise, vertical, and spanwise directions, respectively. A pressure outlet (convective condition) was imposed at the downstream location. The flow in the spanwise direction is assumed to be statistically homogeneous (Hungle et al., 1997) and therefore, a periodic boundary condition was used. A no-stress (free slip) wall was applied at the top boundary of the computational domain and a no-slip condition was used for the bottom walls. The inflow velocity field is taken from an instantaneous simulation of a fully developed plane channel flow (Barri et al., 2009) of finite length where periodic boundary conditions were used in the streamwise direction.

![Figure 2.10: The computational domain of the backward-facing step (Hungle et al., 1997)](image)

The simulations were started from a stationary flow field and were allowed to evolve to a statistical steady state for a total computational time of \( \sim 1600h/U_o \). The time step of each simulation was adjusted by keeping the CFL number (Courant et al., 1928) below 0.5. Statistical averaging of the individual flow fields were performed from 1600h/U_o to 4000h/U_o which is approximately 53 ‘flow-through’ times.

Comparisons of the time averaged streamwise velocity profiles at four different locations \( (x/h = -3 \) in the entrance, \( x = 4 \) in the recirculation, \( x/h = 6 \) close to the flow reattachment)
Figure 2.11: Time averaged streamwise velocity profiles

point, and x/h = 10 in the recovery region) between the LES results and the experimental data of Jovic and Driver (1994) are given on Fig. 2.11. Overall, all LES schemes give velocity profiles which are in a good agreement with the experimental data. In the re-attachment region (x/h = 6), it is observed that both the SM, and SgsKEM schemes are not able to capture the mean streamwise velocities close to the bottom wall which is mainly due to the limitations of a constant model coefficient in these two schemes. A transverse flow with negative streamwise velocity is also observed from the profiles of both SM and SgsKEM at x/h = 6 which is an indication of overestimations in the re-attachment lengths.

The mean turbulence fields in terms of the velocity fluctuations for the streamwise \(<u'u'>\) profiles are given on Fig. 2.12. The comparisons were performed at the same four
locations. The numerical $< u'u' >$ predictions from the DSM are in good agreement with the profiles observed with the experimental data both in the re-circulation and recovery regions. Downstream of the sudden expansion, the DMM is found to be dissipative by underpredicting the streamwise velocity fluctuations, however in the entrance region ($x/h = -3$), both the DMM and DSM are shown to be better for the $< u'u' >$ profiles. The peak $< u'u' >$ values predicted by the SM and SgsKEM before the sudden expansion ($x/h = -3$) are lower than the values reported by the experimental data which is also consistent to the values found for these two LES models in the previous section for the wall bounded open channel flow. Downstream of the step, a high rate of velocity damping is
observed for the constant model coefficient LES models (SM and SgsKEM). This high rate of velocity damping gives strong and long re-circulation regions with an overestimation of the streamwise turbulence fields (Fig. 2.12).

Figures 2.13, and 2.14 show the mean representation of the wall normal ($<v'v'>$), and cross-stress ($<u'v'>$) turbulence profiles at the four locations respectively. There are some minor differences in the $<v'v'>$ and $<u'v'>$ profiles from the DSM scheme, but overall it reproduces good turbulent statistics as the experimental data. A slighter underestimation is observed for the two turbulent quantities from the DMM both in the re-circulation and recovery regions. The SM and SgsKEM schemes overpredict the peak values in regions

Figure 2.13: Mean wall normal turbulent profiles
below the sudden expansion. A similar overprediction is also observed for the streamwise turbulent intensities for these two schemes as noted earlier. These comparisons clearly show the advantageous of dynamic model coefficients, and limitations of a constant model coefficient SGS models for resolving complex turbulent flows. It is important to note that using an inlet boundary condition from a periodic boundary simulation of amplitude length is quite adequate to get good predictions of mean flow and turbulent fields both upstream and downstream of the step. According to Aider and Danet (2006), replication of the inlet boundary condition is essential to get good profiles of the hydrodynamic variables below the sudden expansion.

Figure 2.14: Mean cross stress profiles
Table 2.2: Comparisons of reattachment lengths ($X_r/h$)

<table>
<thead>
<tr>
<th>Method</th>
<th>Exp.</th>
<th>SgsKEM</th>
<th>SM</th>
<th>DSM</th>
<th>DMM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_w = 0$</td>
<td>6</td>
<td>7</td>
<td>6.7</td>
<td>6.1</td>
<td>5.6</td>
</tr>
<tr>
<td>Streamline</td>
<td>6</td>
<td>6.8</td>
<td>6.6</td>
<td>5.9</td>
<td>5.4</td>
</tr>
</tbody>
</table>

Figure 2.15: Streamline and instantaneous vorticity contours from SM and SgsKEM

Another important parameter for evaluating the ability of various turbulence models in simulating complex flows with re-circulation and flow separation is the flow reattachment location (Ghosal et al., 1995; Hungle et al., 1997). The reattachment length ($X_r$) is the distance from the step to the point of zero wall shear stress or streamwise velocity. It is known to be one of the key parameters to test the numerical accuracy of SGS models in addition to the mean flow and turbulent fields. We have used two methods to calculate the flow re-attachment location as reported by Hungle et al. (1997); i) the longitudinal distance where the mean streamwise velocity is zero at the first grid point normal to the wall; and ii) the location at which mean streamlines touch the lower wall after the sudden expansion (Fig. 2.15 and 2.16). Tab. 2.2 shows the comparisons of the flow reattachment locations obtained from different LES models. Jovic and Driver (1994) reported a reattachment length of 6 step heights downstream of the step which is close to the values estimated in the current simulation by the DSM scheme. As it can be seen from the table, and the streamline plots,
the SM, and SgsKEM schemes tend to overestimate the flow reattachment location which can also explained by the turbulence fields from the two models as discussed previously. An increase in the reattachment lengths and delay in the transition of the shear layer can possibly be due to the absence of longitudinal turbulent vortices in the recirculation region (Fig. 2.15).

### 2.3.3 Fully developed turbulent flow over a wavy wall

Turbulent flows over wavy surfaces displays characteristics that are not commonly found in flows over flat surfaces (Cherukat et al., 1998). A wavy boundary introduces disturbances into the flow field, which affect different hydrodynamic quantities. Understanding the fundamental flow physics related to the wavy wall helps to elucidate the mechanisms that control separated flows in geophysical and engineering applications.

The computational domain for the current case is similar to the DNS setup of Maαβ and Schumann (1996). The coordinate system and the geometrical parameters are given on Fig. 2.17. The top surface is a flat wall and the bottom boundary has a sinusoidal wavy surface with an amplitude $a$ and wave length $\lambda$. $L(4\lambda)$, $W(2\lambda)$, and $h(\lambda)$ represents the streamwise, spanwise, and wall normal lengths of the flow domain respectively. The lateral domain size was chosen assuming that the length is enough to cover the largest
turbulent structures (Maaβ and Schumann, 1996). The position of the wavy bottom wall $z_w$ is calculated from the streamwise coordinate and wave length by,

$$z_w = \cos \left( \frac{2\pi x}{\lambda} \right)$$  \hspace{1cm} (2.26)

Computations were carried out with different SGS models for an amplitude to wavelength ratio, $a/\lambda = 0.05$, and at a mean flow Reynolds number, $(U.h/\nu) = 6760$ to match the geometrical parameters of Maaβ and Schumann (1996). At this Reynolds number, previous studies (Cherukat et al., 1998; Henn and Sykes, 1999; Yoon et al., 2009) observed an intermittent recirculation due to flow deceleration, separation, reattachment, and acceleration as the particles move from high to low crest locations. A snappyHexMesh utility (OpenCFD, 2013) is used to generate the surface-fitted finite volume grids using STereoLithography (STL) file. The mesh contained about 2.6 million finite volume cells, and the grids were refined close to the wavy surface such that the first point away from the sinsusoidal surface is in the viscous sublayer.

The flow was driven by a pressure gradient in the streamwise direction. At each computational time step, the depth integrated velocity was compared with the value reported in the DNS and the pressure gradient is adjusted by keeping a constant mass flow rate. A no-slip condition is used at the top and bottom walls. The flow is assumed to be statistically
homogeneous in the streamwise and spanwise directions, thus a periodic boundary condition is applied in both directions. The simulations were started from the initial conditions and continued until statistical equilibrium was achieved (approximately 75 ‘flow-through’ times) and averaging of the flow variables was performed for additional 105 ‘flow-through’ times. The LES results are compared to the DNS results of Maaβ and Schumann (1996). All the presented profiles are averaged in the spanwise direction, and over the four surface locations of equal phase angle in the streamwise direction. Since the SgsKEM and SM predict closely similar profiles for the previous two case studies, computations were only performed with the SM scheme in the current case to compare with the dynamic SGS models.

Figure 2.18: Time averaged streamwise velocity profiles
Mean streamwise velocity profiles at four representative locations ($x/\lambda = 0.2$, $x/\lambda = 0.5$, $x/\lambda = 0.7$, and $x/\lambda = 0.9$) within one wave length are compared with the DNS data on Fig. 2.18. As it can be seen, overall the prediction of the streamwise velocity profiles from all SGS models is in fairly good agreement with the DNS data. At $x/\lambda = 0.2$ downstream of the wave crest, a reverse flow with negative streamwise velocity is observed which is an indication of flow separation due to adverse pressure gradient. The DSM and DMM schemes are good schemes in capturing the complex mean flow profiles in the recirculation region compared to the SM which uses a constant model coefficient. At $x/\lambda = 0.5$, the flow is still in the recirculation region subject to a strong reverse flow compared to the values
observed at $x/\lambda = 0.2$. At $x/\lambda = 0.7$ just after the wave trough, all the values of the mean streamwise velocities have only a positive sign showing that this point is outside of the recirculation zone or the flow is already reattached. In the DNS data, the reattachment point was observed close to $x/\lambda = 0.6$. Uphill before the wave crest at $x/\lambda = 0.9$, the fluid moves forward with a positive streamwise velocity and a strong deceleration is clearly observed close to the wavy surface due to the local topography. The streamwise velocity results found in this study are also consistent with the findings of the previous numerical studies (Yoon et al., 2009; Chang et al., 2012; Knotek and Jicha, 2014).

Figure 2.20: Mean wall normal turbulent profiles

Streamwise and wall normal turbulent intensity profiles from the three SGS models are compared with the DNS data on Fig. 2.19 and 2.20 respectively. In general most of the
turbulent generation take place in the separate shear layer (between $x/\lambda = 0$ to $x/\lambda = 0.6$), where we can also observe an increase in peak values of the turbulent intensities. From Fig. 2.19, we can see that the DSM scheme is a better scheme in capturing the peak $< u'u' >$ and $< w'w' >$ values throughout the wave crosssection. Results from the Smagorinsky model (SM) show a substantial underestimation of the $< w'w' >$ values in the recirculation region. The dynamic procedure which is used in the DSM and DMM retains the advantages of the spatial scale dependent model variable with improved resolved results in the recirculation and reattachment zones. The SM scheme overestimates the peak $< u'u' >$ values at $x/\lambda = 0.7$ which shows the sensitivity to the model parameter from location to location. In two dimensional-hill LES simulations, Wan et al. (2007) also observed the disadvantages of the Smagorinsky model with a substantial sensitivity to the choice of model parameters in resolving the flow variables.

Fig. 2.21 compares the turbulent cross stress or shear stress profiles ($< u'w' >$) along the four locations. As it can be seen from the figure, the maximum value of $< u'w' >$ occurs away from the wave crest in the recirculation region which is also due to the shear layer as the flow separates. The agreement with the DNS data is overall good for the three SGS models. In all the simulations, good agreements with the DNS were obtained with the Dynamic Smagorinsky Model (DSM). The Dynamic Mixed Smagorinsky Model (DMM) is dissipative compared to DSM. Stoesser et al. (2008) applied different SGS models to study detailed flow and turbulent structures in two dimensional dunes with periodic boundaries and their comparisons show better results with the Dynamic Smagorinsky Model.

The contours of the instantaneous flow structures at certain time from the DSM are given in Fig. 2.22 and 2.23. A diffusive wake layer is observed below the wave crest which is mainly due to the vortices and turbulence generated in the recirculation zone. As it can be seen from the vorticity contours, the turbulence field which is generated in the separated region is advected further downstream and rise to the upper surface due to strong ejection events. The Q-criterion (Hunt et al., 1988) is used to identify the 3D vortex coherent
structures developed over the wavy surface based on the second invariant of the velocity gradient tensor. The coherent structures are visualised as iso-surfaces of $Q = 100$ and they are colored using the vertical coordinate $z$. Strong rollers are formed around the wave crest due to Kelvin-Helmholtz instability. The interaction of these vortex structures with the near wall turbulent structures produces large horseshoe-like structures (marked with circles) in the developing boundary layer.

2.4 Conclusions

Fully developed turbulent flows are investigated using four Large Eddy Simulation models, namely the Smagorinsky Model (SM), the Dynamic Smagorinsky Model (DSM), the Dynamic Mixed Model (DMM), and the SGS Kinetic Energy Model (SgsKEM). Three
numerical cases were chosen based on the previous DNS and experimental studies that include, a fully developed wall bounded channel flow (Moser et al., 1999), flow over a backward-facing step (Jovic and Driver, 1994), and fully developed turbulent flow over a wavy wall (Maaβ and Schumann, 1996). For the first case, three mesh sizes were used to assess the sensitivity of the mean flow and turbulence fields with grid resolution. The DSM and DMM were found to be better closures for simulations that include the laminar sublayer ($Y^{+}_{min} < 5.5$). However, both the SM and SgsKEM schemes are dissipative as the grid resolution decreases. A wall function (Spalding, 1961) was applied for simulations of grid resolutions which are not adequate enough to resolve the laminar sublayer. From the four LES models, the DSM was found to be the best scheme when using a wall function in capturing both the streamwise velocity and peak turbulent intensities.
Figure 2.23: Flow visualisation: instantaneous coherent structures with Q-criterion ($Q = 100$) and typical horseshoe-like structures are marked with circles

The second case (turbulent, separating flow over a backward-facing step) was chosen to evaluate the LES schemes in resolving the mean flow and turbulent fields for applications where there is flow separation and reattachment. Overall, the differences between the numerical and experimental streamwise velocity profiles were small. However, limitations were observed from the constant model coefficient schemes (both SM and SgsKEM) with a reverse flow after the flow reattachment point. For the mean turbulent fields, the DSM was found to be a good scheme both in the recirculation and recovery zones. Compared to the DSM, the DMM underestimates the peak turbulence fields downstream of the sudden expansion. A high velocity damping was observed from both the SM and SgsKEM which leads to strong and long recirculation regions with overestimations of the turbulence fields. The flow reattachment lengths downstream of the backward-facing step from each scheme were also calculated and compared with the experimental data. The flow recovery point from the DSM ($X_r = 6.1$) is close to the value reported by Jovic and Driver (1994), $6$ step heights downstream of the sudden expansion.

The third case (fully developed turbulent flow over a wavy bottom surface) was chosen to explore the feasibility of each LES scheme for geometries which are commonly found in geophysical applications such as, river bedforms and ripples. The predictions of the
streamwise velocity profiles from all SGS models are in fairly good agreement with the DNS data. The DSM was found to be the best model in resolving all the turbulence fields, which is consistent with the results observed during the other case studies presented in this paper. Due to the wavy bottom, most of the turbulence field that is generated in the separated region is either advected further downstream or rises to the upper surface due to ejection events. Strong rollers are formed around the sinusoidal crest due to the Kelvin-Helmholtz instability. The interaction of these vortex structures with the near wall turbulent structures produces large horseshoe-like structures. These 3D turbulent features are going to have significant roles for bedform evolution, sediment suspension, and contaminant mixing.

This is the first study which evaluates these four LES schemes in OpenFOAM using various flow and geometry conditions. The findings of this study should prove useful to the scientific community as a benchmark of LES, mainly for geophysical applications.

2.5 References


Chapter 3
Large eddy simulation of flow and suspended sediment transport in flat-bed turbulent channel flows

3.1 Introduction

A suspended sediment transport process commonly exists in rivers, estuaries, and coastal environments. In the past, different studies have been carried out both theoretical and numerical investigations of flow and sediment transport (Nelson et al., 1995; Zedler and Street, 2006; Werf et al., 2008). In most of these studies, one of the main limitations was the nature of the local coupling between flow, sediment transport, and turbulence. Detailed experimental studies on suspended sediment transport in open channel flows showed the existence of long, persistent sediment streaks close to the bed with a wall coherent structures (Muste et al., 2005; Lyn, 1988). Moreover, the turbulence level in the near-bed region consists of a wide spectrum of scales (Nelson et al., 1993).

To perform numerical simulation of a fluid motion where all turbulent scales are resolved, very fine meshes have to be used (with cell size smaller than the Kolmogorov scale). For this type of solutions, Direct Numerical Simulation (DNS) is required (Moser et al., 1999). In Large Eddy Simulation (LES), only large scales (low frequency modes) are resolved and the small scales are modeled (Fureby et al., 1997a). This approach allows using coarser meshes (compared to DNS) and still gives important information about the majority of turbulence levels. On the other hand, in Reynolds Averaged Navier Stokes (RANS) equations, all turbulence scales are modeled. The RANS methodology can be used when only averaged flow and suspended sediment transport fields are desired.

In most of the previous studies, RANS equations are often employed to study both flow and sediment transport in open channel flows (Johns et al., 1993; Hsu et al., 2003). However, evidences suggest that commonly used RANS models can not represent key tur-
bent quantities in unsteady turbulent boundary layers (Chang and Scotti, 2004). Direct Numerical Simulation (DNS) has also been successfully employed for analysis of sediment transport (Moin and Manesh, 1998; Schmeeckle and Nelson, 2003; Penko et al., 2011). Nevertheless, DNS computations are severely limited to low Reynolds number flows due to small grid size and numerical time step requirements.

To overcome the aforementioned complexities, it is necessary to use an optimal tool for the prediction of sediment transport patterns in flowing waters. Furthermore, the improvement of numerical methods and raise of computing power gives a distinct possibility to develop more advanced models that can give solutions in a relatively short time with reasonable accuracy. The use of Large Eddy Simulation (LES) can resolve a much larger range of smaller scales compared to RANS methods. In recent years, Large Eddy Simulations of flow and sediment transport have successfully been employed in both river and coastal environments. Chou and Fringer (2008) used a Dynamic Mixed Smagorinsky Model (Zang et al., 1993) for suspended sediment transport in channel flows. A detail analysis of both flow and sediment transport was also performed by Zedler and Street (2006) in a turbulent oscillatory flow over ripples.

Due to the spatial and temporal changes in the flow and turbulence fields, the initiation and motion of sediment particles from the bed to the upper parts exhibits a complex dynamics. Understanding these behavior will provide a better insight in the 3D turbulence-sediment interactions leading to attain detailed sediment transport rate parameterizations. Many investigations had given focuses on the relationship between flow and sediment transport based on the local boundary mean shear stress. However, McLean et al. (1994) argued that the nearbed turbulence statistics do not scale with the local mean shear velocity due to the spatial evolution of the turbulence fields. The main goal of the current work is to take the advantage of a Large Eddy Simulation to perform detailed investigations of the instantaneous flow, bed shear stress, and turbulent fields for a fully developed turbulent channel flow. The role of vortex coherent structures for the entrainment of sediment from
the bottom boundary to the upper zones in the water column is demonstrated by superimposing the suspended sediment concentration contours to the instantaneous flow field. Our ultimate long term objective is to implement a three dimensional (3D) coupled flow and sediment transport solver that can be used to understand the interactions of a turbulent flow and sediment transport for complex geometries in geophysical open channel flows such as ripples, and bedforms.

In this study, numerical simulations of flow and suspended sediment transport were performed using a finite volume non-hydrostatic solver OpenFOAM (Open Field Operation and Manipulation) (Weller et al., 1998). The computation was carried out under various flow and median sediment grain sizes. The effect of sediment roughness to the flow field is considered by treating a special boundary condition at the bottom boundary. A generic rough wall formulation which considers three hydraulic roughness regimes (smooth, transitional, and full rough) instead of a full rough regime which was used in many of the previous studies for suspended sediment transport (Chou and Fringer, 2008; Zhu et al., 2013) is applied to account the highly concentrated near-bed sediment particles. The sediment transport module also incorporates mechanisms of gravitational settling, turbulent, and molecular diffusions. To resolve the turbulence levels, both the Dynamic Smagorinsky (DSM) and Subgrid Scale Kinetic Energy (SgsKEM) models are used.

3.2 Numerical model

3.2.1 Governing equations

The governing equations for incompressible unsteady fluid flow are,

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{3.1}
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu_{eff} \frac{\partial u_i}{\partial x_j} \right] + f \tag{3.2}
\]
where \( u \) is velocity vector field, \( p \) is the pressure field, \( f \) is a body force, and \( \nu_{eff} \) is the total viscosity of the fluid which is the sum of molecular and turbulent viscosities.

Suspended sediment transport can be modeled either as a continuum concentration field or as Lagrangian particles (Zedler and Street, 2001). In the continuum approach, the governing formulation is the sediment advection-diffusion equation (Nir and Acrivos, 1990). In this study, a finite volume scalar transport equation of the suspended sediment was implemented in OpenFOAM (Eq. 3.3).

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} (C u_i - C w_s \delta_{j3}) = \frac{\partial}{\partial x_j} \left[ (\nu + \nu_t) \frac{\partial C}{\partial x_j} \right] 
\]  
(3.3)

\[
w_s = \frac{10 \nu}{d_{50}} \left[ \left( 1 + \frac{0.01(S-1)gd_{50}^3}{\nu^2} \right)^{0.5} - 1 \right]
\]  
(3.4)

where \( C \) is local volume of sediment concentration, \( w_s \) is settling velocity of the sediment (van Rijn, 1984), \( S \) is the specific weight of the sediment particle, \( g \) is the gravitational acceleration, \( d_{50} \) is the median grain diameter, \( \nu \) is the fluid kinematic viscosity, \( \delta_{j3} \) is the Kronecker delta with \( j = 3 \), and \( \sigma_c \) is turbulent Schmidt number relating the turbulent diffusivity of the sediment to the eddy viscosity \( \nu_t \).

The advection-diffusion equation assumes that the suspended sediment concentration is low enough to avoid particle-fluid and particle-particle interactions except the gravitational settling (Harris and Grilli, 2014). According to Davies and Li (1997), the continuum formulation of sediment transport can be adopted for low-concentration suspension layers (\( C < 10^{-3} \)) in which the sediment settling velocity is taken as the value for individual grains and Villaret and Davies (1995) pointed out that in practice this formulation is com-
monly used for sediment concentrations (C) up to $10^{-2}$ or larger. The volume of suspended sediment concentrations found in the current study are within the range of $10^{-2}$. For regions directly close to the bottom boundary, where a higher instantaneous dense sediment suspension is expected, a rough wall formulation was implemented to overcome the limitations of the continuum approach by damping the velocity and near-bed turbulence. Many previous studies (Chou and Fringer, 2010, 2008; Harris and Grilli, 2014; Niroshinie et al., 2013; Zedler and Street, 2006; Zhu et al., 2013) have been performed using the current approach and reasonable results in suspended sediment transport were found. In recent studies, two phase flow (Hsu et al., 2003; Jha and Bombardelli, 2010), and discrete element (Schmeeckle, 2014) modeling approaches have been employed to study the sediment transport process at high volume of sediment concentration by incorporating the particle-fluid and particle-particle interactions. Nevertheless, these methods are still under development and their applications are limited to small scale domains due to computational and time step requirements in turbulence resolving simulations.

In LES, large scales are resolved and small ones are modeled. To separate the resolvable scales from the sub-grid scale (SGS), a filtering procedure is needed (Fureby et al., 1997b). The filter cut off should lie in the inertial range of the turbulence spectrum (Eq. 3.5).

$$\bar{f}(x) = \int_D f(x') G(x, x', \bar{\Delta}) \, dx$$

(3.5)

where D is the model domain, $\bar{f}(x)$ is the resolved flow quantity, $x'$ is the location where $\bar{f}(x)$ is considered in the spatial integration, G is a filter function, and $\bar{\Delta}$ is the filter width, i.e., the wavelength of the smallest scale retained by the filtering operation. In this study, a top-hat filter, which is written in one dimension as Eq. 3.6 is used.
\[ G (x - x') = \begin{cases} \frac{1}{\Delta}, & \text{if } |x - x'| \leq \frac{\Delta}{2}, \\ 0, & \text{otherwise} \end{cases} \] (3.6)

The filter function determines the size and structure of the small scales. The most common definition of a filter width is,

\[ \bar{\Delta} = (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}} \] (3.7)

where \( \Delta_x, \Delta_y, \) and \( \Delta_z \) refer to grid spacing in x, y and z directions of 3D space.

To better understand the effect of filter levels within different LES schemes, both the Dynamic Smagorinsky (DSM), and One-equation SGS Kinetic Energy (SgsKEM) Models are used in this study and the simulation results are compared for both the mean flow, suspended sediment, and turbulent quantities. The subgrid scale stress tensor,

\[ (\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{\bar{u}}_i \bar{\bar{u}}_j) \] aids in providing model closure for the LES and is computed through an eddy viscosity approach (Smagorinsky, 1963) and it can be calculated as,

\[ \tau_{ij} = 2\nu_t \bar{S}_{ij} + \frac{1}{3} \delta_{ij} \tau^R_{kk} \] (3.8)

where \( \bar{S}_{ij} \) is defined as,

\[ \bar{S}_{ij} = \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \] (3.9)
The eddy viscosity of the residual turbulent motion, $\nu_t$, is defined as,

$$\nu_t = (C_s \Delta)^2 \sqrt{\langle 2 \bar{S}_{ij} \bar{S}_{ij} \rangle} \quad (3.10)$$

where $C_s$ is the model coefficient. In the original Smagorinsky (1963) formulation, this is the only adjustable parameter and it lies in the approximate ranges of 0.094 to 0.2. However, in the presence of a mean shear rate, Deardorff (1971) found that this value caused excessive damping of large scale motions.

For the DSM, a procedure developed by Germano et al. (1991) and Lilly (1992) was adopted. The constant model coefficient ($C_s$) is no longer taken as constant but allowed to vary in both space and time. The formulation of the dynamic coefficient requires sequential applications of primary and test filters. In the current work, twice the width of the primary filter is used as a test filter. The test filter generates another unknown residual stress tensor and defined as,

$$T_{ij} = \hat{u}_i \hat{u}_j - \hat{\bar{u}}_i \hat{\bar{u}}_j \quad (3.11)$$

The Germano identity between the grid and the test filtered fields, $L_{ij} = T_{ij} - \hat{\tau}_{ij}$ is used to dynamically determine $(C_s \Delta)^2$. The importance of the tensor $L_{ij}$ lies in that it can be expressed in terms of the filtered or resolved velocity $\bar{u}_i$ fields. In terms of the resolved velocity, the Germano identity $L_{ij}$ becomes,

$$L_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \hat{\bar{u}}_j \quad (3.12)$$
The deviatoric portion of $L_{ij}$ can be expressed by test filtering (Eq. 2.6).

$$\hat{\tau}_{ij} = 2(C_s \Delta)^2 |\hat{S}| \hat{S}_{ij}$$  \hspace{1cm} (3.13)

and by modeling the deviatoric part of the test scale stress as,

$$T_{ij} = 2(C_s \Delta)^2 |\hat{S}| \hat{S}_{ij}$$  \hspace{1cm} (3.14)

In Eq. 3.14, the strain rate tensor $\hat{S}_{ij}$, and its norm $|\hat{S}|$ are calculated based on the double filtered velocity $\hat{u}_i$. The model coefficient $(C_s \Delta)^2$ is dynamically computed by minimizing the square of the difference $Q_{ij}Q_{ij}$ (Eq. 3.15) between the modeled and resolved scales (Lilly, 1992), where the difference is given as,

$$Q_{ij} = T_{ij}^R - 2(C_s \Delta)^2 M_{ij}$$  \hspace{1cm} (3.15)

and

$$M_{ij} = |\hat{S}|\hat{S}_{ij} - \beta |\hat{S}| \hat{S}_{ij}$$  \hspace{1cm} (3.16)

where $\beta = \left(\frac{\Delta}{\hat{\Delta}}\right)^2$ is the square of the filter width ratio.
After minimization the dynamic model coefficient becomes,

\[
(C_s \bar{\Delta})^2 = \frac{1}{2} \frac{L_{ij} M_{ij}}{M_{ij} M_{ij}} \tag{3.17}
\]

The model coefficient from Eq. 3.17 can give either positive or negative values in contrary to the constant value used in Smagorinsky (1963) approach.

In the SgsKEM, the SGS stress is written in terms of a generalized SGS eddy viscosity representation and its value is computed from the SGS kinetic energy and characteristic grid width (Yoshizawa and Horiuti, 1985). The turbulent SGS viscosity (\(\nu_t\)) is calculated from a transport equation for the SGS kinetic energy, which is assumed to be isotropic (de Villiers, 2006).

\[
\frac{\partial K}{\partial t} + \nabla \cdot (\bar{u}K) - \nabla \cdot (\nu_{eff} \nabla K) = G - \epsilon \tag{3.18}
\]

where K is the subgrid kinetic energy, \(\bar{u}\) is the resolved velocity field, \(\epsilon\) is the turbulent dissipation at the smallest scales, \(\nu_{eff}\) is the effective viscosity of the fluid which is the sum of molecular and turbulent viscosities, and G represents the decay of turbulence from the resolved scales to the subgrid scales through the energy cascade. Furthermore, the dissipation rate and decay of turbulence are calculated as,

\[
\epsilon = C_e K^{3/2} / \bar{\Delta} \tag{3.19}
\]

\[
G = C_k \sqrt{K} \bar{\Delta} |\bar{S}|^2 \tag{3.20}
\]
\[ \nu_t = C_k K^{1/2} \Delta \]  

(3.21)

where \( C_e \) and \( C_k \) are the energy dissipation and turbulence decay coefficients. Different versions of the dynamic SGS models were also proposed (Ghosal et al., 1995; Moin et al., 1991; Vreman et al., 1994).

According to Ghosal et al. (1995), a model based on subgrid kinetic energy reduces the stability issues which are common found in dynamic and dynamic mixed models. However, Fureby et al. (1997a) argued that these types of models are limited due to the discrepancy between the principal axes of the SGS stress and the rate of the strain tensor.

3.2.2 Numerical schemes

OpenFOAM, Open Field Operation and Manipulation (Weller et al., 1998), was used to solve the conservation equations of momentum, continuity, and sediment transport over flatbed open channel flows. It is a freely available tool which has different solvers to simulate specific problems in engineering and fluid mechanics. The equations are well discretized to apply easily for the numerical simulation of partial differential equations. Different libraries within the main system are well linked from which one can easily create solvers and boundary conditions. OpenFOAM can run in both Window and Linux environments. It is parallelized using the Message Passing Interface (MPI). OpenFOAM integrates the equations using Gauss theorem by converting volume integrals to surface integrals. It therefore requires both cell centered and face centered values of different hydrodynamic variables.

The divergence terms of the transport equations are converted to surface integrals using the Gauss divergence theorem (Eq. 3.22 and Eq. 3.23). The surface integrals are then evaluated as fluxes through the surfaces at each face. A second order linear interpolation scheme was used to transfer variables from cell centers to face centers To avoid the spurious oscillations that would occur with the spatial discretization scheme due to shocks, discontinuities or sharp changes in the solution domain, a sweby flux limiter (Sweby, 1984) was
imposed for both momentum and sediment transport equations. For the gradient terms such as $\int_V \frac{\partial p}{\partial x_i} dV$, a second order central difference scheme was applied. The implicit, second order backward scheme was used for the time derivatives. For the laplacian terms such as $\int_V \frac{\partial}{\partial x_j} [\nu_{eff} \frac{\partial u_i}{\partial x_j}] dV$, a second order Gauss scheme with linear interpolation is used. The momentum equation (Eq. 3.2) advances with a velocity pressure coupling via a predictor-corrector procedure based on PISO (Pressure Implicit with Splitting of Operators) of Issa (1986), which re-calculates the velocity field at each time step by correcting the predicted velocity for flux conservation. More details about the available numerical schemes can be found in de Villiers (2006) and Jasak (1996).

$$\int_V \frac{\partial u_i}{\partial x_i} dV = \int_s \bar{u} n dS = 0 \quad (3.22)$$

$$\int_t^{t+\delta t} \left[ \frac{\partial}{\partial t} \int_V \bar{u} dV + \int_V \frac{\partial}{\partial x_j} (u_i u_j) dV \right] dt =$$

$$\int_t^{t+\delta t} \left[ - \int_V \frac{\partial p}{\partial x_i} dV + \int_V \frac{\partial}{\partial x_j} \left( \nu_{eff} \frac{\partial u_i}{\partial x_j} \right) dV \right] dt \quad (3.23)$$

### 3.2.3 Near wall flow and suspended sediment transport

The near-bed region of a turbulent channel with sediment is dominated by a thick layer of sediment. The sediment particles have a significant roughness which damps turbulence in the bottom boundary layer. Therefore, it is required to include this effect to the momentum equation. On this study, the roughness formulation proposed by Cebeci and Bradshaw (1977) is applied. This method considers three distinct roughness zones based of the roughness Reynolds number ($k_s^+ = k_s \frac{u_*}{\nu}$), namely full rough ($k_s^+ > 90$), transitional ($2.25 < k_s^+ \leq 90$), and smooth ($k_s^+ \leq 2.25$). First the three zones are identified based on the computed flow field from the previous time step and then the velocity components at the near wall faces on the bottom first grid point are adjusted based on Eq. 3.24.
\[
\frac{u}{u_\tau} = \begin{cases} 
Y^+, & \text{if } Y^+ \leq Y_i^+ \\
\frac{1}{\kappa} \ln EY^+, & \text{if } Y^+ \geq Y_i^+
\end{cases}
\] (3.24)

where \( u \) is the velocity at the nearest cell center to the bottom boundary with a distance \( y \) from the wall, \( k_s \) is the sediment equivalent roughness, \( Y^+ = \frac{u_{\tau}}{\nu} \) is a non-dimensional distance from the wall, \( u_{\tau} \) is the shear velocity, \( \kappa \) (0.41) is the von Kármán constant, \( Y_i^+ = 11.6 \) and \( E \) (Eq. 3.25) is a roughness parameter which also includes the effect of surface roughness based on Cebeci and Bradshaw (1977).

\[
E = \exp[\kappa (B - \Delta B)]
\] (3.25)

Where \( B = 5.2 \) and \( \Delta B \) is a function which relates the sediment roughness based on the roughness Reynolds number for the three roughness regimes.

\[
\Delta B = \begin{cases} 
0 & k_s^+ \leq 2.25 \\
[B - 8.5 + \frac{1}{\kappa} \ln k_s^+] \sin[0.4258 (\ln k_s^+ 0.811)] & 2.25 < k_s^+ \leq 90 \\
B - 8.5 + \frac{1}{\kappa} \ln k_s^+ & k_s^+ > 90
\end{cases}
\] (3.26)

For a flat bed covered with sand material with median grain size \( d_{50} \), \( k_s \) is assumed to be equal to \( 2.5d_{50} \) (van Rijn, 1984). Therefore, in this work, an equivalent surface roughness of \( 2.5d_{50} \) is considered for each median grain size.
The sediment transport rate in the near-bed grid points of the bottom boundary was calculated using the van Rijn (1984) pick-up formula (Eq. 3.27). This pick-up function has also been employed in previous studies (Chou and Fringer, 2008; Niroshinie et al., 2013; Zhu et al., 2013) for sediment transport rate in the bottom boundary and the results proved that it is applicable for both unsteady and non-uniform flows.

\[
\frac{P_k}{\sqrt{(S - 1)gd_{50}}} = \begin{cases} 
\alpha D^\beta T^\gamma & \theta > \theta_c \\
0 & \theta \leq \theta_c 
\end{cases}
\]  

(3.27)

where \(\alpha, \beta\) and \(\gamma\) are model imperical constants which have values of 0.00033, 0.3, and 1.5 after van Rijn (1984). \(T = (\theta - \theta_c)/\theta_c\) is an excess shear stress parameter. \(D\) is the non-dimensional sediment diameter which is calculated by relating the grain size, molecular viscosity and specific gravity of the sediment.

\[
D = d_{50} \left[ \frac{(S - 1)}{\nu^2} \right]^{1/3}
\]  

(3.28)

\(\theta\) is the instantaneous Shields parameter which is calculated from the wall shear stress, grain size, density of water, and specific gravity of the sediment. \(\theta_c\) (Van Rijn, 1993) is the critical shields parameter for initiation of sediment motion.

\[
\theta = \frac{\tau_b}{(S - 1) \rho g d_{50}}
\]  

(3.29)
3.2.4 Computational domain and parameters

The computation was carried out with four test cases (Tab. 3.1) based on the channel height and median diameter of the suspended sediment particle. Each test case has 1.3 m length and 0.13 m width. For 1565EQ, 1965EQ, and 2565EQ, numerical grids of 260 × 26 × 52 are used in the steamwise, spanwise and wall normal directions respectively. However for 1957EQ, only 48 grids are used in the wall normal direction due to its smaller depth. In the steamwise and spanwise directions, a uniform mesh of size \( \Delta x = \Delta y = 0.005 \) m was used and in the wall normal direction, the grid size was set to \( \Delta z = 0.00125 \) m for all cases. Moreover, the average flowthrough time \( (T_f) \) is calculated by dividing the channel length with the mean velocity of each setup.

Table 3.1: channel test cases (Lyn, 1987, 1988)

<table>
<thead>
<tr>
<th>Experiment</th>
<th>1565EQ</th>
<th>1965EQ</th>
<th>1957EQ</th>
<th>2565EQ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Depth, H (cm)</td>
<td>6.45</td>
<td>6.51</td>
<td>5.72</td>
<td>6.54</td>
</tr>
<tr>
<td>Slope (x 10^{-3})</td>
<td>2.44</td>
<td>2.51</td>
<td>2.95</td>
<td>2.96</td>
</tr>
<tr>
<td>Grain diameter (mm)</td>
<td>0.15</td>
<td>0.19</td>
<td>0.19</td>
<td>0.25</td>
</tr>
<tr>
<td>Bulk discharge (l/s)</td>
<td>10.8</td>
<td>11.05</td>
<td>9.85</td>
<td>12.07</td>
</tr>
<tr>
<td>Mean velocity (m/s)</td>
<td>0.64</td>
<td>0.68</td>
<td>0.66</td>
<td>0.71</td>
</tr>
<tr>
<td>Flowthrough time (s)</td>
<td>2.03</td>
<td>1.91</td>
<td>1.97</td>
<td>1.83</td>
</tr>
</tbody>
</table>

Flow was forced with a constant pressure gradient which gives the mean streamwise velocity at each computational cycle. After the pressure-velocity corrector step, the streamwise velocity is adjusted for a constant mass flow rate by comparing the depth integrated streamwise velocity and the mean velocity from the experiment.

Figure 3.1: Computational domain
A periodic boundary condition is used in the streamwise and spanwise directions. No-slip and free slip conditions are applied for the bottom and top walls respectively. The momentum equation at the first cell is modified based on the rough wall formulation of Cebeci and Bradshaw (1977). We found that the flow gets a false steady solution unless it is provoked with an initial condition that produces some vorticity. According to de Villiers (2006), the near-wall turbulence cycle is naturally initiated through a process of transition that comes as a result of the growth of small initial perturbations or imperfections on the wall boundary. Initial streaks are provided to the initial velocity profile. On Fig.3.2, as can be seen, the solution rapidly became turbulent as the streaks induce vortex formation and further instability. On the figure, t represents the simulation time and $T_f$ is the flowthrough time. An early flow instability was observed in the Dynamic Smagorinsky Model (DSM) compared to the Subgrid Scale Kinetic Energy Model (SgsKEM).

Turbulent eddies are present in turbulent flows which contain turbulent kinetic energy that usually causes turbulent mixing and shear stresses (Rodi et al., 2013). The available kinetic energy is usually transferred from large to small scales of motion (Piomelli, 1999). A turbulence spectrum plot helps to understand the resolved scales of motion based on Kolmogorov hypothesis. Based on this theory, for eddies much smaller than the energy containing eddies and much larger than dissipative scales (of the order of Kolmogorov scales), turbulence is controlled solely by the dissipation rate, and the size of the eddy $(1/k)$, where $k$ is the wave number. In this subrange, the turbulent energy is assumed to follow a $-5/3$ slope (in log-log scale). A reasonable LES scheme is believed to capture part of the flow in the inertial subrange. Fig. 3.3 shows the velocity spectrum plots of the streamwise and vertical velocity profiles. The resolved spectrum using the DSM is found to be higher than the profiles obtained from the SgsKEM. Therefore, the DSM is expected to give higher values of resolved turbulent fields in terms of the velocity fluctuations.

First the hydrodynamic computation was carried out until the flow gets statistically steady state which requires roughly 200 flowthrough ($T_f$) cycles. Once a stable hydrodynam-
namic solution was attained, the wall shear stress ($\tau_b$) and other hydrodynamic quantities which were required for the suspended transport solver are stored. With proper boundary conditions, the suspended sediment transport simulation was started and continued together with the hydrodynamic computation. It was assumed that the channel was initially in clear water condition, therefore suspended sediment concentration ($C$) was set to zero at the beginning of the simulation. At the top boundary of the suspended sediment layer, sediment particles are not allowed to leave from the water surface, a zero sediment flux boundary condition was imposed. At the bottom boundary, the suspended sediment is calculated based on the van Rijn (1984) pick up function (Eq. 3.27).
In order to evaluate the performance of the two LES models for flow and suspended sediment transport, the simulation results are compared with the experimental data of Lyn (1987, 1988) for all cases considered in this study. The experimental data include a mean streamwise velocity, turbulent intensities in the streamwise and spanwise directions, and also mean suspended sediment concentrations.

Figure 3.4 shows comparisons of experimental and modeled values of mean streamwise velocity profiles for each test case. The theoretical log profiles were also calculated from the shear velocities and vertical coordinates for each case. The mean streamwise velocity profiles from both LES schemes are in good agreements with the experimental results. On
the buffer layer, the DSM overpredicts the flow field for all cases. This could be related to limitations of this model to address courser grids during the calculation of the subgrid scale stress. Due to the thick bottom sediment layer and sediment roughness length scale, the cell center of the first bottom grid point is assumed to greater than the grain size of the suspended sediment. It is also observed that the LES models are good in predicting the velocities close to the free surface compared to the theoretical log formulation.

Root mean square (rms) turbulent intensities for the four test cases are shown on Figures 3.5 and 3.6. After temporal and spatial averaging, the actual values are normalized by the wall shear velocity ($u_r$). For resolved turbulent intensities on the streamwise direction
(Figure 2.3), profiles from both the DSM and SgsKEM agree reasonably well with the experimental data. However close to the bottom wall, there is a strong turbulence intensity from the DSM compared to the experimental and SgsKEM values. This overprediction could be related to the modulation of the streamwise velocity field in this region for the DSM as it is shown on Figure 3.4.

Figure 2.5 shows the predicted wall normal turbulence statistics along with the corresponding experimental measurements. It is clearly shown that $<w'>$ profiles from the DSM agrees well with the experimental values in the entire computational domain. In contrast to DSM, the resolved values from the SgsKEM underpredicts the experimental
Figure 3.6: Mean resolved root mean square wall normal turbulent intensities. The experiment didn’t report data for 1565EQ.

Profiles for regions where \( z/h < 0.4 \). Previous studies with a detail comparison of different SGS models (Holmen et al., 2003; Ciardi et al., 2005) also found that LES schemes which use a constant model coefficient tend to give lower values for the spanwise and wall normal components of the Reynolds stress tensor. As it can be noted from both Figures 3.5 and 3.6, the peaks of both turbulence intensities occur in the vicinity of the bottom wall region. This is the area of highest shear where most of the turbulence production occurs and it is important for the enhancement of sediment transport from the bottom boundary to the upper regions of the computational domain.
The sediment concentration profiles for the different cases are shown on Figure 3.7. Profiles which are developed using the theoretical Rouse formulation (Eq. 3.30) are also included for each numerical setup.

\[
C = C_a \left[ \left( \frac{h-z}{z} \right) \left( \frac{a}{h-a} \right) \right]^{-Z} \tag{3.30}
\]

in which,

\[
Z = \frac{w_s}{\beta \kappa u_r} \tag{3.31}
\]
According to Eq. 3.30, the sediment concentration $C$ at a distance $z$ above the bed depends on the total depth $h$ and the reference concentration $C_a$ at the reference height $a$. The exponent $Z$ expresses the ratio of the settling velocity $w_s$ of sediment particles to the product $\beta \kappa u_\tau$ involving the shear velocity $u_\tau$, the von Karman constant $\kappa$, and $\beta$ is the ratio of the sediment diffusivity to the fluid momentum diffusivity.

As can be observed, the concentration profiles from the two LES models are in a good agreement with the experimental data. However, a difference between the Rouse profiles and numerical results are observed. In all the cases except 2565EQ, the Rouse formulation continuously overpredicts the concentration profiles in the mid and upper parts of the computational domain. To mention, the Rouse formulation was developed by considering a uniform steady channel flow. However for turbulent channels at high Reynolds numbers, a perfect steady state and uniform flow solution can not be attained due to the continuous generation of turbulent eddies from the bottom boundary layer. The concentration values from the DSM are also slightly smaller than the values obtained from the SgsKEM for grid points close the bed. This can be correlated to the magnitudes of turbulent intensities in the near-bed region. From the hydrodynamic results, the intensities of both streamwise and spanwise turbulent intensities from the DSM are always greater than the SgsKEM values for $z/h < 0.2$. This could enhance the local ejection and diffusion of suspended sediment and ultimately leading to the underprediction of the local suspended sediment transport.

One of the objectives of this study was also to see the role of sediment grain size on the magnitude of suspended sediment concentration for closely similar hydrodynamic conditions. As it can be noticed from the mean concentration profiles from 1565EQ (0.15 mm median sediment grain size) and 2565EQ (0.25 mm median sediment grain size) on Figure 3.7, a higher suspended sediment concentration is observed for 1565EQ across the channel depth compared to 2565EQ. This is mainly due to the role of gravitational forces on the computation of suspended sediment transport which was included as downward settling flux in the advection-diffusion equation.
Figure 3.8: Temporal evolutions of suspended sediment transport for each median grain size and from the two LES models

Figure 3.8 depicts the temporal evolutions of the suspended sediment which were taken at \( x = 0.65 \) m and averaged laterally for each time step. At the beginning of the simulation, the only source of suspended sediment was the bottom boundary where the suspended sediment transport rate is represented by the pickup function. A sediment particle which is suspended from the bed requires enough amounts of time for full mixing and transport to the other parts of the computational domain. The strength of vortex cores, and both the molecular and turbulent diffusivities have a significant role to distribute the suspended sediment from the sediment source (bottom boundary) to the other parts. On our study,
it was found that the suspended sediment for a typical periodic boundary condition requires at least 50 flowthrough cycles for complete mixing and tp reach a nearly statistically steady state in the vertical direction. Both LES models show different levels of suspended sediment mixing at early periods of the simulations. This could be related to differences in the instantaneous hydrodynamic flow fields which were used as an input variable for the suspended sediment transport solver.

Figure 3.9: Instantaneous bed concentration (top) and shear stress (bottom) from SgsKEM for 1565EQ

Figures 3.9 and 3.10 show the instantaneous bed shear stress and concentration fields which were taken from the two LES models roughly at $t/T_f \sim 192$ (after the suspended sediment computation was started) for the 1565EQ. On an average, the sediment is picked fairly uniformly across the channel bed. Furthermore, it is clearly shown that the near-bed suspended sediment is directly correlated to the bed shear stress. A higher spatial variability of suspended sediment concentration is also observed for the DSM compared to the SgsKEM. This is directly related to the differences in the formulations of the SGS stresses for the two LES models. In the DSM, a spatial and time varying model coefficient $(C_s\Delta)^2$ was applied, however the SgsKEM only takes one value of this coefficient for the entire simulation time. At certain location on the bed, it is shown that the suspended
sediment is picked from the bed in local clouds which can possibly be linked to the near-bed turbulence. Furthermore at some grid points, the DSM gives smaller magnitudes of suspended sediment concentration, even close to zero showing that there is no initiation of sediment motion or $\theta \leq \theta_c$.

Figure 3.10: Instantaneous bed concentration (top) and shear stress (bottom) from DSM for 1565EQ

In a fully developed turbulent flow, the spatial and temporal distributions of suspended sediment transport is dependent on the local behavior of the flow field. For example, the geomorphological formation of ripples and dunes is believed to lie in the existence of coherent structures, which are the driving mechanisms for sediment transport and bed deformation (Rodi et al., 2013). Fig. 3.11 shows the interactions of the turbulent flow and sediment transport fields. The instantaneous streamwise velocity, and vorticity at the channel half width are given on the top two contours. The suspended sediment concentration contours at a horizontal and vertical slices are also shown on (c), and (d) respectively. The vectors of the velocity fluctuations are also superimposed to understand the roles of ejection events on the lateral and vertical distribution of the suspended sediment transport. It is clear that the turbulence fields appear to be very important to transport the suspended sediment from the bottom boundary to the upward and lateral directions. Moreover, a higher sediment
concentration is observed in regions where there are strong velocity fluctuation vectors. It can clearly be observed by comparing the instantaneous contour plots of velocity, vorticity and suspended sediment concentration. The existence of strong velocity fluctuation vectors is also an indication of active zones of the flow in terms of lateral and vertical mixings. Some of the vortices in the near wall region are ejected and interact with the flow in the outer region and these vortices are found to be important for the movement and mixing of sediment transport in the high flow speed region. Stoesser et al. (2005) also observed the amalgamation process where the near wall vortices interact with the outer region flow during their growth and movement towards the surface. Therefore, a turbulence resolving scheme is very important to capture the detail physics of a sediment transport process compared to time averaged closure schemes such as RANS.

To understand the role of vortex cores for vertical ejection of suspended sediment transport, it is important to obtain a better insight of the local coherent structures and suspended sediment transport. Vortices are indicative of highly active regions of flow and sediment transport. Zedler and Street (2001) in their studies of sediment transport over
ripples showed that an upward movement of sediment in the flow is directly correlated to vortex-like structures. The Q-criterion (Hunt et al., 1988) is used to visualize the coherent structures of the flow. Figures 3.12 and 3.13 show a zoomed in view of the vortex cores which have been colored by the magnitude of suspended sediment concentration at two different instantaneous periods. For this type of analysis, the results from the SgsKEM and for 1565EQ numerical setup is considered. The velocity vectors are also superimposed to the plane which is perpendicular to the flow direction.

It is clearly shown that the vortex cores which advances diagonally from left to right carry suspended sediment from the near-bed to upper regions. Moreover, the magnitude of suspended sediment concentration is usually greater within the core structures compared to
Figure 3.13: Coherent structures plotted as isosurfaces of $Q = 75 \, \text{s}^{-2}$ and colored by the suspended sediment concentration at $t = 1104.6 \, \text{s}$

the surrounding areas. This is directly related to the ejection of suspended sediment from the highly concentrated near-bed region due to the strong local vorticities. Furthermore a closer comparison of the vortex cores and suspended sediment for the two time steps shows that once bulges of sediment particles are picked up from certain region; they are further transported in the flow direction. As can be seen, the locally ejected suspended sediment is distributed in the nearby fluid zones while the flow progresses to the right. Therefore, turbulence resolving schemes are necessary for an adequate prediction of instantaneous suspended sediment transport process.
3.4 Conclusions

In this paper, Large Eddy Simulation (LES) is applied to study fully developed turbulent channel flow problems together with suspended sediment transport. The simulations were performed using a finite volume non-hydrostatic solver, OpenFOAM under various flow conditions and median sediment grain sizes. The effects of sediment roughness on the flow field are accounted by treating a generic rough wall formulation which considers three classes (smooth, transitional, and fully rough) instead of a full rough regime which was used in most of the previous studies. The suspended sediment transport solver also accounts mechanisms of gravitational settling, turbulent, and molecular diffusions. To resolve the larger turbulence eddies, two LES schemes are applied namely, the Dynamic Smagorinsky (DSM) and Subgrid Scale Kinetic Energy (SgsKEM) models. Before the start of the sediment transport simulation, hydrodynamic computations are carried out for roughly 200 flowthrough cycles to attain a statistically steady state solutions. The channels were initialized with a zero suspended sediment concentration and a pick up function was used at the channel bed to calculate the suspended sediment transport rate. Moreover, at the top boundary of the suspended sediment layer, a zero sediment flux boundary condition was imposed.

The mean velocity and Reynolds stress profiles from both the LES schemes are in a good agreement with the experimental results. Compared to the SgsKEM, the DSM is found to be a better in resolving the turbulence fields for all computational setups. It is also found that the peak turbulence intensities occur in the vicinity of the bottom wall which helps for the enhancement of sediment transport from the bottom boundary to the upper regions. Moreover, the mean suspended sediment concentration profiles from the numerical model agrees well with the experimental profiles. However, the theoretical Rouse profile slightly overpredicts the suspended sediment in the mid and upper channel depths. Due to the differences in the formulations of the SGS stresses, higher spatial variations in suspended sediment transport are observed in the DSM than the SgsKEM. This study also confirmed
that vortex cores have a significant role for the vertical ejection and lateral distribution of suspended sediment transport from the near-bed region.

In conclusion, this study demonstrates that LES is advantageous for solving the complex flow and suspended sediment transport features by resolving the large scale eddies of the turbulent motion. Therefore, the numerical model can be used for further understanding of flow and sediment transport mechanisms in flows where there are higher chances of flow separation and retatchement due to complex geometries.

3.5 References


Chapter 4
Large eddy simulation of turbulent flows over two and three dimensional dunes and implications to sediment transport

4.1 Introduction

Previous studies (Guy et al., 1963; van Rijn, 1984; Nelson et al., 1993; Best, 2005; Chou and Fringer, 2010; Nabi et al., 2013; Khosronejad et al., 2014) showed that if a turbulent flow of sufficient bed shear stress acts on a mobile sediment bed, the excess shear stress initiates the motion of bed materials, causing perturbations which will later evolve either in to two or three dimensional bedforms. The final bedform geometry depends on the level of turbulence, the availability and type of sediment, and the flow depth. For example, the initial response of the bed to low bed shear stresses is to form short, small features called ripples. At higher flow rates, larger features called dunes are formed. Dunes eventually wash out as suspended sediment transport becomes dominant, leading to the near bed flow dominated by a sheet flow sediment transport (Drake and Calantoni, 2001) and the formation of antidunes for flows of high Froude number (Simons and Richardson, 1963). Dunes have an important role on the interaction of near bed flow and sediment transport in fluvial and coastal environments. For example, coastal dunes are one sources of energy dissipation of water waves outside the surf zone in the nearshore. In rivers, the migration of dunes often affects the stability of the bed and banks. Dunes can also change the discharge capacity and water depth of rivers during flooding events (Stoesser et al., 2008).

As the flow passes over the crest of the dune, the velocity of the fluid particle within the boundary layer becomes slower due to the changes in the fluid stresses. This leaves the near-bed fluid with insufficient momentum to overcome the adverse pressure gradient associated with the sharp breakaway of the lee side of the dune (Maddux et al., 2003; Xie et al., 2013).
As a result, the flow detaches from the bed at the dune crest due to the Kelvin-Helmholtz instabilities, creating a separation zone that reattaches four to six dune heights downstream of the dune crest in the trough region (Best, 2005; Stoesser et al., 2008). A shear layer is formed bounding the separation zone, which separates the recirculation flow from the above free stream fluid. The location of the flow reattachment point varies both in the streamwise and spanwise directions based on the dune geometry, and the level of turbulent structures that are generated in the shear layer (Omidyeganeh and Piomelli, 2013b; Xie et al., 2014). Downstream of the flow reattachment region, a new internal boundary layer is formed as the flow accelerates and reestablishes itself to a logarithmic profile before the next dune crest (Nelson et al., 1993; McLean et al., 1994; Maddux et al., 2003; Best, 2005; Venditti, 2007). The sediment transport rate and the morphological evolution of the dune in the lee side is mainly controlled by the streamwise velocity and the magnitude of bed shear stress over the dune crest (McLean et al., 1994; Giri and Shimizu, 2006; Chou and Fringer, 2010; Niroshinie et al., 2013; Omidyeganeh and Piomelli, 2013a; Khosronejad and Sotiropoulos, 2014).

Extensive experimental studies were performed in the past over fixed-bed two dimensional (2D) dunes (Muller and Gyr, 1986; Nelson et al., 1993; McLean et al., 1994; Bennett and Best, 1995; Kadota and Nezu, 1999; Fernandez et al., 2006; Balachandar et al., 2007; Venditti, 2007) and through numerical simulations (Yoon and Patel, 1996; Yue et al., 2005, 2006; Ojha and Mazumder, 2008; Stoesser et al., 2008; Grigoriadis et al., 2009; Omidyeganeh and Piomelli, 2011; Xie et al., 2014). Compared to the two dimensional dunes, few experimental and numerical studies have been conducted over three dimensional (3D) dunes (Maddux et al., 2003; Venditti, 2007; Omidyeganeh and Piomelli, 2013a; Khosronejad and Sotiropoulos, 2014; Xie et al., 2014). Most of these studies were investigated to better understand the relationship between mean flows, turbulent structures, and boundary shear stresses. As stated by Maddux et al. (2003), friction coefficients of three dimensional dunes are higher on average than those of two dimensional dunes when subjected to similar
flows and water depths. However, the turbulence generated over the 3D dune was found to be weaker than the values in 2D dunes. Through numerical simulations over 3D dunes, Omidyeganeh and Piomelli (2013a) observed that the secondary flows across the stream are caused by the three dimensional flow separation together with adverse wall pressure gradient which in turn affects the average reattachment length and the components of channel resistance. Though many insights into these complex flow fields have been gathered from experiments, there are still many unanswered questions about the spatial and temporal sediment transport patterns over complex bedform geometries. The recent developments in advanced computational techniques increases the capability of numerical models for giving detailed flow fields. These computational results can provide useful intuitions of the time dependent three dimensional flow features which are usually difficult to measure in experiments. As it is discussed by Omidyeganeh and Piomelli (2013a), precise measurements of near-wall quantities, including skin friction and form drag were not attained from the experimental and field data which were conducted over three dimensional dunes.

In most of the previous numerical studies for sediment transport (Zedler and Street, 2001, 2006; Chou and Fringer, 2008, 2010; Niroshinie et al., 2013; Zhu et al., 2013; Harris and Grilli, 2014), the advection-diffusion equation is used assuming that the suspended sediment concentration is low enough to avoid particle-fluid and particle-particle interactions except the gravitational settling (Harris and Grilli, 2014). According to Davies and Li (1997), this approach can be used for low-concentration suspension layers (C < 10^{-3}) in which the sediment settling velocity is taken as the value for individual grains. In the bottom boundary layer, the magnitude of sediment concentration is expected to be higher than the upper region of the flow domain. At higher sediment concentration, the fluid-sediment and sediment-sediment interactions changes the physics of the fluid motion field by damping the velocity and near bed turbulence (Ozdemir et al., 2010; Dallali and Armenio, 2014; Yu et al., 2014). A two phase flow (Hsu et al., 2003; Jha and Bombardelli, 2010), and discrete element modeling (Schmeckle, 2014) approaches have also been employed in recent years to
study the sediment transport process at high volume of sediment concentration by incorporating the particle-fluid and particle-particle interactions. Nevertheless, these methods are still under development and their applications are limited to extremely small scale domains due to the computational and time step requirements for turbulence resolving simulations.

In the current study, we implemented a three dimensional robust fluid-sediment mixture method with a well established large eddy simulation (LES) to resolve the large scale turbulence eddies. The coupled flow-sediment transport solver accounts fluid-sediment and sediment-sediment interactions through hindered settling, enhanced viscosity with particle concentration, density stratification through buoyancy effects, and particle pressure similar to the method adopted by Penko et al. (2013) on their numerical simulation of flow and sediment transport over ripple beds.

The motivation of the present study is to apply and demonstrate LES for fully developed turbulent flows over two and three dimensional dunes which can help to further understand the influence of these bedforms on the temporal and spatial variations of the flow and sediment transport field. Due to changes in flow and turbulence fields, the initiation and motion of sediment particles from the bed to the other parts of the flow domain exhibits a complex dynamics. Understanding the behaviors of the turbulence fields above the sediment bed will provide a better insight into 3D turbulence-sediment interactions leading to attain detailed sediment transport rate parameterizations. The near bed flow and shear stress distribution over bedforms is found to be nonuniform due to topographical changes in the bottom boundary layer (Nelson et al., 1993; McLean et al., 1994; Best, 2005; Venditti, 2007). Moreover, the shape of the dune topography controls locations where sediment is eroded and deposited. Most importantly, the distribution of turbulent events and structures are also affected by the shape of the dune bed. In this research, we considered both two and three dimensional dune geometries based on the previous experimental studies of Balachandar et al. (2003) and Maddux et al. (2003), respectively. Large Eddy Simulation (LES) is selected as a turbulent closure scheme due to its ability in resolving a much
larger ranges of useful turbulent scales than the Reynolds Averaged Navier Stokes (RANS) methods. The instantaneous flow fields are investigated together with the occurrence of coherent structures which are identified by a Q-criterion (Hunt et al., 1988). The roles of turbulent coherent structures on the spatial distribution of sediment transport is assessed by superimposing the suspended sediment concentration contours to the instantaneous flow field.

4.2 Mathematical formulation

OpenFOAM, Open Field Operation and Manipulation (Weller et al., 1998), was used to solve the conservation equations of momentum, continuity, and sediment transport over two and three dimensional dunes. The solver is organized with a flexible set of C++ written modules that are used to build solvers to simulate specific problems in engineering and fluid mechanics (Jasak and Weller, 2000). A finite volume numerics is employed to solve the conservation equations in their conservative forms. The fundamental equations are developed within a robust, implicit, pressure-velocity, iterative solution framework, and a domain decomposition method is applied to divide and allocate the flow variables for separate processors during high performance computation.

The fluid-sediment mixture is treated as a continuum which has density and viscosity fields that vary with the instantaneous sediment concentration. Velocity, pressure and other required flow variables are computed from the solutions of the Navier-Stokes equations. The sediment continuity equation (Nir and Acrivos, 1990) is applied to compute the suspended sediment transport, and a new finite volume sediment transport module is implemented in OpenFOAM (Eq. 4.7) that incorporates both hindered settling, and turbulent induced diffusion. The governing equations for the mixture used herein are the full Navier-Stokes equations with the Boussinesq approximation.

\[
\frac{\partial \rho_i}{\partial t} + \frac{\partial \rho \bar{u}_i}{\partial x_i} = 0 \quad (4.1)
\]
where $\overline{u}$ is the filtered velocity vector field, $\rho$ is the mixture density. The time dependent variable mixture density (Penko et al., 2013; Yu et al., 2014) is calculated using the instantaneous sediment volumetric concentration ($C$), sediment particle density ($\rho_s$), and fluid density ($\rho_f$).

$$\rho = C \rho_s + (1 - C) \rho_f$$  \hspace{1cm} (4.2)

The mixture momentum equation is obtained from the sum of sediment particle and fluid phase equations together with the parameterized effects of fluid-sediment, and sediment-sediment interactions.

$$\rho \frac{\partial \overline{u}_i}{\partial t} + \rho \frac{\partial}{\partial x_j} (\overline{u}_i \overline{u}_j) = - \frac{\partial \overline{P}_i}{\partial x_i} + \frac{\partial}{\partial x_j} (2\mu \overline{S}_{ij}) + \frac{\partial \tau_{ij}}{\partial x_i} + F + (\rho_s - \rho_f) C g - S_b \overline{u}_i$$  \hspace{1cm} (4.3)

where $\overline{u}$ is the filtered velocity field, $\overline{P}$ is the pressure field, $g$ is the gravitational acceleration, $F$ is the external driving force, $\mu$ is the molecular viscosity, and $\tau_{ij}$ is the subgrid scale stress which is computed from the resolved velocity field. The fifth term on the right side accounts the sediment induced stratification through buoyancy effects, and the last term considers the particle pressure force which is incorporated to include the roles of sediment-sediment interactions at a higher sediment volume fraction (Penko et al., 2013). $\overline{S}_{ij}$ is the strain rate tensor and it is computed from the resolved velocity fields.

$$\overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)$$  \hspace{1cm} (4.4)
As the volume sediment concentration increases and becomes significant, it is necessary to account for the hydrodynamic interactions of particles, particle rotation, collision between particles, and mechanical interference (Thomas, 1965; Yu et al., 2014), and a rheological model is required to enhance the flow viscosity as a function of the sediment volume concentration (Winterwerp et al., 2012). The rearrangement of particles in suspension increases as the sediment particles shear during the vertical turbulent mixing and lateral movement. Thomas (1965) suggested an exponential function for the enhanced viscosity with polynomial terms which would be proportional to the probability of particles transferring from one shear plane to the other.

\[
\frac{\mu}{\mu_o} = [1 + 2.5C + 10.05C^2 + Aexp(BC)]
\]  

(4.5)

where the coefficients A and B in the formulation take values of 0.00273, and 16.6, respectively, and \(\mu_o\) is the nominal fluid viscosity in clear water conditions.

In addition to the enhanced viscosity, it is necessary to account the particle-particle interaction through particle pressure term when the sediment concentration is high. An exponential function was used in the previous studies for the parameterization of particle pressure (Buyevich, 1999; Penko et al., 2013). A formulation similar to Penko et al. (2013) is used here to include the damping effect of the sediment particles on the flowing fluid.

\[
S_b = \gamma(C)^8
\]  

(4.6)

where \(\gamma\) is an empirical parameter with a value of 0.3 that reduces the resolved velocity in
high sediment concentrated flow zones.

Suspended sediment transport can be modeled either as a continuum concentration field or as Lagrangian particles (Zedler and Street, 2001). In the continuum approach, the governing formulation is the sediment advection-diffusion equation (Nir and Acrivos, 1990). In this study, a finite volume scalar transport equation of the suspended sediment is implemented in OpenFOAM (Eq. 4.7).

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} ( C u_i - C w_s \delta_{j3} ) = \frac{\partial}{\partial x_j} \left[ (\nu + \frac{\nu_t}{\sigma_c}) \frac{\partial C}{\partial x_j} \right]
\]  (4.7)

where \( C \) is local volume of sediment concentration, \( w_s \) is the concentration dependent settling velocity (Richardson and Zaki, 1954), \( \nu \) is the fluid kinematic viscosity, \( \delta_{j3} \) is Lronecker delta with \( j = 3 \), and \( \sigma_c \) is the turbulent Schmidt number relating the turbulent diffusivity of the sediment to the eddy viscosity \( \nu_t \).

For single particles, the settling velocity \( (w_{s0}) \) can be calculated by equating the balance of gravity and drag forces using a drag coefficient for spherical particles (van Rijn, 1984; Nielsen et al., 2002). When suspended sediment concentrations become significant, the settling velocity of sediment particles is hindered by the intra-particle interaction (Richardson and Zaki, 1954), can even become negligible close to a highly concentrated near-bed region (Li and Davies, 2001).

\[
w_s = w_{s0}(1 - C)^q
\]  (4.8)

\[
w_{s0} = \frac{10\nu}{d_{50}} \left[ \left( 1 + \frac{0.01(S - 1)gd_{50}^3}{\nu^2} \right)^{0.5} - 1 \right]
\]  (4.9)
where $S$ is the specific weight of the sediment particle, $g$ is the gravitational acceleration, $d_{50}$ is the median grain diameter, and $q$ is the empirical constant which is calculated based on the particle Reynolds number ($\text{Re}_p = \frac{d_{50}|\text{W}|}{\nu}$).

$$q = \begin{cases} 
4.35R_e_p^{-0.03} & 0.2 < \text{Re}_p \leq 1 \\
4.45R_e_p^{-0.1} & 1 < \text{Re}_p \leq 500 \\
2.39 & \text{Re}_p \geq 500 
\end{cases} \quad (4.10)$$

LES allows the prediction of turbulent flows for a wide variety of flows by using grids that are fine enough to resolve the large scales of turbulence while modeling the dissipation and mixing in the subgrid scales (Scalo et al., 2013). The conservation equations of continuity and momentum are obtained by filtering the Navier Stokes equations (Fureby et al., 1997). In this study, the Dynamic Smagorinsky Model (DSM) which was initially proposed by (Germano et al., 1991) and later improved by Lilly (1992) is used. Agegnehu and Willson (2015) have performed detailed evaluations of LES schemes for fully developed turbulent flows over a wall bounded channel, a backward facing step, and a wavy wall and it was found that the DSM is the best scheme in resolving the mean flow and turbulence fields. This scheme employs a dynamic model coefficient, which varies both in space and time based on the resolved velocity fields, and the geometry of the flow domain at two filter levels (Zang et al., 1993). It assumes that the behavior of the resolved scales is similar to the subgrid scales (Gullbrand and Chow, 2003). In this study, twice the width of the primary filter ($\bar{\Delta}$) is used as a test filter ($\hat{\Delta}$).

The subgrid scale stress tensor, $(\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j)$ aids in providing a model closure for the LES and it is computed through an eddy viscosity concept (Smagorinsky, 1963) by,
\[ \tau_{ij} = 2 \nu_t \bar{S}_{ij} + \frac{1}{3} \delta_{ij} R_{kk} \]  

(4.11)

where \( \bar{S}_{ij} \) is defined as,

\[ \bar{S}_{ij} = \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \]  

(4.12)

The eddy viscosity of the residual turbulent motion, \( \nu_t \), is defined as,

\[ \nu_t = \left( C_s \Delta \right)^2 \sqrt{2 \bar{S}_{ij} \bar{S}_{ij}} \]  

(4.13)

where \( C_s \) is the model coefficient. In the original Smagorinsky (1963) formulation, this is the only adjustable parameter and it lies in the approximate ranges of 0.094 to 0.2. However, in the presence of a mean shear rate, Agegnehu and Willson (2015) and Deardorff (1971) found that this value can cause excessive damping of the large scale motions.

Due to the sequential applications of primary and test filters, an additional unknown residual stress can be modeled at the higher filter (test filter) level, and defined as,

\[ T_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \]  

(4.14)

The germano identity between the grid (primary) and the test filtered fields, \( L_{ij} = T_{ij} - \hat{\tau}_{ij} \) is used to dynamically determine \( \left( C_s \Delta \right)^2 \). The importance of the tensor \( L_{ij} \) lies in that it
can be expressed in terms of the resolved velocity $\pi$ fields, which becomes,

\[ L_{ij} = \widehat{u_i} \widehat{u_j} - \widehat{u_i} \widehat{u_j} \]  

(4.15)

The deviatoric portion of $L_{ij}$ can be expressed by test filtering (Eq. 2.6).

\[ \hat{\tau}_{ij} = 2(C_s \hat{\Delta})^2 |\bar{S}| \bar{S}_{ij} \]  

(4.16)

and by modeling the deviatoric part of the test scale stress as,

\[ T_{ij} = 2(C_s \hat{\Delta})^2 |\bar{S}| \tilde{S}_{ij} \]  

(4.17)

In Eq. 4.17, the strain rate tensor $\tilde{S}_{ij}$, and its norm $|\bar{S}|$ are calculated based on the double filtered velocity $\widehat{u}_i$. The model coefficient $(C_s \Delta)^2$ is dynamically computed by minimizing the square of the difference $Q_{ij}Q_{ij}$ (Eq. 4.18) between the modeled and resolved scales (Lilly, 1992), where the difference is given as,

\[ Q_{ij} = T_{ij}^R - 2(C_s \hat{\Delta})^2 M_{ij} \]  

(4.18)

and
where $\beta = \left( \frac{\tilde{\Delta}}{\Delta} \right)^2$ is the square of the filter width ratio. After minimization, the dynamic model coefficient becomes,

$$
(C_s \tilde{\Delta})^2 = \frac{1}{2} \frac{L_{ij} M_{ij}}{M_{ij} M_{ij}}
$$

(4.20)

The model coefficient from Eq. 4.20 can give either positive or negative values in contrast to the constant value used in Smagorinsky (1963) approach.

**Near bed suspended sediment transport**

The sediment transport rate from the bottom boundary was calculated using the van Rijn (1984) pick-up function (Eq. 4.21). This pick-up function ($P_k$) has also been employed in the previous studies (Zedler and Street, 2006; Chou and Fringer, 2008; Zhu et al., 2013; Niroshinie et al., 2013) for sediment transport rate in both unidirectional and oscillatory flows and the results demonstrated that it is applicable for both unsteady and non-uniform conditions.

$$
\frac{P_k}{\sqrt{(S-1)g d_{50}}} = \begin{cases} 
\alpha D^\beta T^\gamma & \theta > \theta_c \\
0 & \theta \leq \theta_c 
\end{cases}
$$

(4.21)

where $\alpha, \beta$ and $\gamma$ are model empirical constants which have values of 0.00033, 0.3, and 1.5 after van Rijn (1984), $\theta$ is the instantaneous Shields parameter which is calculated from
the wall shear stress, grain size, density of water, and specific gravity of the sediment (Eq. 4.22), $T = (\theta - \theta_c)/\theta_c$ is an excess shear stress parameter, $\theta_c$ (Van Rijn, 1993) being the critical shields parameter for initiation of sediment motion, and $D$ is the non-dimensional sediment diameter which is calculated by relating the grain size, molecular viscosity and specific gravity of the sediment (Eq. 4.23). In this study, a 0.1 mm grain size sediment with specific gravity of 2.65 is considered for both two and three dimensional dunes.

$$\theta = \frac{\tau_b}{(S - 1) \rho g d_{50}}$$

(4.22)

$$D = d_{50} [(S - 1)/\nu^2]^{1/3}$$

(4.23)

To solve the conservation equations, the values of the flow variables are required at the face centers. A second order linear central differencing scheme was applied in this study. To avoid the spurious oscillations that would occur with the spatial discretization scheme due to shocks, discontinuities or sharp changes in the solution domain, a sweby flux limiter (Sweby, 1984) was imposed for both momentum and sediment transport equations. A standard second order finite volume discretization of Gaussian integration scheme (Gauss linear) was used for the gradient terms such as $\nabla \cdot \bar{P}$. For finite volume discretization, surface normal gradients are evaluated at the cell faces (de Villiers, 2006). The surface normal gradient is then the gradient component which is normal to the cell faces. For this study, an explicit non-orthogonal correction scheme is used (Jasak, 1996). The implicit, second order backward scheme is applied for the temporal derivatives. The Gauss scheme is the only available scheme for the laplacian terms such as $\int_V \frac{\partial}{\partial x_j} (2\mu \bar{S}_{ij}) \, dV$. The pressure
implicit with splitting of operator algorithm (PISO) algorithm of Issa (1986) was employed for the pressure-velocity coupling. More details about the available numerical schemes can be found in (de Villiers, 2006; Jasak, 1996).

Two numerical cases are considered in the current study, a two dimensional dune (Balachandar et al., 2003) and a three dimensional dune (Maddux et al., 2003), to understand the effects of bedform geometry on the temporal and spatial variations of the flow and sediment transport fields. In the next sections, detailed descriptions of computational setups, boundary conditions, and numerical results will be discussed for both cases.

4.3 Results and discussion

4.3.1 Fully developed turbulent flow over two-dimensional dunes

The dune geometry and flow conditions for simulations over two-dimensional dunes are the same as the experiments performed by Balachandar et al. (2003). Experimental measurements were carried out on the 17th dune of a 22 train of identical non-mobile dunes mounted in a hydraulic flume. Streamwise and vertical velocity profiles were collected at six selected centerline locations. The dune height, k, is 20 mm and its wave length, \( \lambda \), is 20k (400 mm). The Reynolds number is close to 58,000 based on the water depth and free surface velocity \( U_0 \). The dune geometry is defined in (Fig. 4.1), where x, y, and z are aligned with the streamline, spanwise, and wall normal directions. The computational domain consists of two dune wave lengths in the streamwise, 8k in the spanwise, and 6.6k in the vertical directions, respectively. The lateral domain size was chosen assuming that the length is enough to cover the largest turbulent structures. Numerical simulations were also performed in this dune geometry without sediment transport by previous researchers (Yue et al., 2005, 2006).

A no-slip boundary condition was applied to the bottom wall, and periodic boundary conditions were used for both the stream & spanwise directions. The free surface was assumed as a flat plane of symmetry with a zero stress condition. The dynamic effects of the free surface variation in the rigid lid condition are accounted through pressure variations
Figure 4.1: Schematic geometry of the two-dimensional dune (not to scale)

(Stoesser et al., 2008). The vertical velocity as well as the wall normal derivatives of the streamwise and spanwise velocities are set to zero at the top wall. The dynamic free surface variation for the current case study is reported to be negligible (less than 2% of the flow depth) and the effect of the rigid lid boundary is assumed to be small on the continuity and turbulent structures (Zedler and Street, 2006; Bhaganagar and Hsu, 2009; Grigoriadis et al., 2009; Omidyeganeh and Piomelli, 2011). The flow is driven by a pressure gradient that maintains a constant flow rate in time. At each computational time step, the depth integrated streamwise velocity was calculated and compared with the experimental value.

A snappyHexMesh utility (OpenCFD, 2013) was used to generate the surface-fitted finite volume grids using STereoLithography (STL) file. The mesh contained about 4.5 million finite volume cells, and the grids were refined close to the dune surface such that the first point away from the bottom wall is in the viscous sublayer. At the beginning of each numerical computation, the grid quality was tested in terms of the non-orthogonality and skewness limits and LES computations were performed using the Dynamic Smagorinsky Model (DSM). For the given computational domain, each simulation requires nearly 100 flowthrough times ($\lambda/U_0$) or nearly 100 seconds before it reaches statistically-steady state.
Flow fields were collected for about 150 flowthrough times to remove any transient effects. As stated before, an instantaneous shear stress dependent sediment pick up function was applied at each computational time step based on the van Rijn (1984) formulation. The clear water numerical results are also validated with the experimental data of Balachandar et al. (2003) for both the mean velocity and turbulence fields.

The numerical model described in the previous section is used to investigate the modulations of turbulence due to the existence of sediment particles by modifying the conservation laws through sediment induced density stratification (Thomas, 1965; Chou et al., 2014; Yu et al., 2014), enhanced viscosity (Penko et al., 2013; Yu et al., 2014), and particle pressure at relatively high sediment concentration (Penko et al., 2013). The effect of sediment particles on different hydrodynamic variables was studied by comparing with the sediment free (clear water) and sediment induced stratification simulation results.

The velocity at the free surface, $U_0$ was used to get the dimensionless velocity, and turbulence components. The horizontal, and vertical distances are normalized by the dune height, $k$. The comparison of the LES results with the experimental data at the six LDV measurement locations for the streamwise velocity component are presented on Fig. 4.2. As it can be seen, results from the numerical computation are in excellent agreements with the experimental measurements showing that the numerical schemes and grid resolutions are adequate enough to capture the mean flow fields. A slight underprediction is observed from the numerical results at $x/h = 12$ which might be due to a leak or any continuity defect during the experiment. A similar profile was also observed in previous studies (Yue et al., 2006; Stoesser et al., 2008) at this location. Stoesser et al. (2008) discussed the limitations of the experiment at certain locations where mass conservation was not satisfied due to measurement inconsistencies. The negative reverse flow, downstream of the dune crest at $x/h = 2$, and 4 shows that these two stations are located within the recirculation region.

The numerical results obtained from the simulations of sediment free, and sediment induced stratification with enhanced viscosity show that the overall effect of the sediment
particles on the mean streamwise velocity fields is insignificant (Fig. 4.2). However, the sediment particles can potentially reduce the strength of flow recirculation (looking at the computed velocity profiles at x/h = 2) and can also reduce the speed of the flow in the upper flow zone.

The mean turbulence fields in terms of the velocity fluctuations for the normalized streamwise profiles ($u'/U_0$) are given on Fig. 4.3. The comparisons were performed at the same six locations. The numerical $u'$ predictions are in good agreement with the experimental profiles both in the re-circulation and recovery regions, showing that the dynamics of the shear layer is well captured. Overall, most of the turbulent generation takes place in
the separating shear layer (between $x/k = 0$ to $x/k = 6$), where an increase in peak values of the streamwise turbulent intensities are observed. A pronounced difference is observed between results of sediment free and sediment induced stratification with enhanced viscosity simulations. As can be seen, the sediment particles attenuate and damps the peak streamwise velocity fluctuation in the turbulence production region. Ozdemir et al. (2010) and Yu et al. (2014) also observed that the attenuation of turbulence caused by sediment induced stratification occurs mostly in the upper zone, while the enhanced viscosity attenuates the turbulence mainly occurs in the near bed region due to the high sediment concentration.
Figure 4.4: Comparisons of wall normal component of turbulent intensities: LES with clear water (symbols), LES with sediment transport (solid lines), experimental data (circles)

Predictions of the time averaged wall normal ($w'/U_0$) and the turbulent shear stress ($u'w'/{U_0}^2$) components are given on Fig. 4.4 & 4.5, respectively. Similar to the streamwise velocity fluctuations, the comparisons of these two statistical flow variables are also in excellent agreements with the clear water experimental data at all the six vertical locations. A slighter overestimation is observed for the ($u'w'/U_0^2$) component in the recirculation and recovery regions, which could be due to the less dissipative nature of the LES scheme in the flow separation zone. Moreover, the maximum values of $u'w'/U_0^2$ occurs downstream of the dune crest due to the generation of turbulence in the shear layer as the flow separates. As a result of the enhanced viscosity, sediment induced stratification and particle pressure
effects, a significant reduction of the peak turbulence levels is observed on both the wall normal and Reynolds shear stress profiles. This can potentially reduce the vertical mixing and turbulent suspension of sediment particles in the flow field.

![Figure 4.5: Comparisons of Reynolds shear stress profiles: LES with clear water (symbols), LES with sediment transport (solid lines), experimental data (circles)](image)

Fig. 4.6 gives the instantaneous contours of streamwise velocity, spanwise vorticity, suspended sediment concentration, and subgrid scale kinetic energy at a specific simulation time along the dune centerline. As can be observed, the flow travels downstream, forming a strong shear layer on the lee side of dunes. Moreover, at this instant of time, there is strong spatial variability of the simulated fields and the complexity level increases in the recirculation region downstream of the dune crest. Similar to the previous studies
strong span-wise vortices are generated in the shear layer separating from the dune crest due to the Kelvin-Helmholtz instability. The vortices are transported downstream with the flow and become responsible for a high rate of subgrid scale kinetic energy, and suspended sediment transport. Overall, the regions behind the dune crest and the flow reattachment regions are the main sources of suspended sediment transport. In the flow recovery zone and dune crest, a higher rate of suspended sediment diffusion is observed which could be mainly due to the formation of horseshoe like vortex structures with ejection events \( u' < 0, w' > 0 \). It is also clear that the turbulence fields are very important to transport the suspended sediment transport from the bottom boundary layer to upward and laterally.

![Contour plots of streamwise velocity, spanwise vorticity, suspended sediment concentration, and subgrid scale kinetic energy](image)

Figure 4.6: Contours of instantaneous: a) streamwise velocity, b) spanwise vorticity, c) suspended sediment concentration, and d) subgrid scale kinetic energy

To get a better insight into the role of vortex coherent structures on the vertical ejection and lateral distribution of suspended sediment transport, a Q-criterion (Hunt et al., 1988) is applied, based on the second invariant of the velocity gradient tensor, to visualize the coherent structures of the turbulent flow field. The vectors of the velocity fluctuations are also superimposed to understand the roles of ejection and sweep events for spatial
distribution of suspended sediment transport. As can be seen on Fig. 4.7, the turbulence field, which is generated in the separated region, is advected further downstream and rises to the upper region of the flow zone in the form of large horseshoe-like structures. Frias and Abad (2013) also observed the amalgamation process where the near wall eddies interact with the outer region flow during their growth and movement towards the surface. Vortices are indicative of highly dynamic zones of flow and sediment transport. For example, Zedler and Street (2001) observe in their studies of sediment transport over ripples with LES that an upward movement of sediment is directly correlated to vortex-like structures. As it can be seen on Fig. 4.7, the vortex cores advance diagonally by carrying suspended sediment from the near bed region to upper zones. Moreover, the suspended sediment concentration is usually greater within the core structures compared to the surrounding areas which is mainly due to the ejection of suspended sediment transport from the near bed region. Stronger velocity perturbation vectors are also observed around the large horseshoe-like structures.

The local flow and sediment transport dynamics over river and coastal dunes exhibit a highly complex process that varies with the near bed turbulence, topography, and grain size distribution (Nelson et al., 1993; McLean et al., 1994; Nelson et al., 1995; Nielsen et al., 2002). Better insights on the spatial and temporal variability of the flow turbulence, bed shear stress, and other related hydrodynamic variables above the dune surface can provide important details, which can help to better understand the roles of near bed turbulence on sediment transport and the vice versa (Singh et al., 2012; Keylock et al., 2013). Fig. 4.8 gives the instantaneous contours of near bed spanwise vorticity, shear stress, sediment transport, and concentration dependent viscosity. As can be seen, the numerical model results show strong spatial variabilities across the dune bed. Lower values of near bed vorticity, and shear stress are observed between the dune crest and the flow reattachment point where a strong shear layer was generated. The near bed sediment concentration is also minimum on these areas. Both the shear stress and vorticity fields increase between the
Figure 4.7: a) vortex coherent structures colored by suspended sediment concentration, b) suspended sediment concentration at a lateral slice (x = 0.6m) with the perturbation velocity vectors, and coherent structures \((Q = 300s^{-2})\)

flow recovery region and dune crest, giving a higher magnitude of sediment concentration. From previous numerical and experimental studies (Zedler and Street, 2001; Best, 2005; Frias and Abad, 2013), it is known that the low and high shear stress regions correspond to deposition, and erosion processes, respectively. An increase in flow viscosity is also observed in regions with higher sediment concentration, indicating that sediment transport can attenuate turbulence and finally laminarize the flow at a higher volume of sediment concentration. Ozdemir et al. (2010); Yu et al. (2014) also observed flow laminarization
when the sediment concentration becomes more significant, $O(100)$ g/l due to the fluid-particle interaction.

![Figure 4.8](image)

Figure 4.8: a) vorticity b) shear stress c) suspended sediment concentration d) concentration dependent viscosity

### 4.3.2 LES of a turbulent flow over three-dimensional dunes

Three dimensional LES simulation was performed to understand the interaction between turbulent flow and the dune three dimensionality based on experiments described in Maddux et al. (2003), where detailed measurements were collected over 3D dunes placed in a laboratory flume. The computational domain layout is given on Fig. 4.9. Each dune has a lee side slope angle of $30^0$, a mean wavelength of $\lambda_m = 0.8\text{m}$, mean dune crest height of $H_m = 0.04\text{m}$, and a dune width of $w = 0.9\text{m}$. The stoss side was a half-cosine wave running from the trough to the crest. Dune three dimensionality was applied as a full cosine wave in the spanwise direction, superimposed into the two dimensional dune. These stationary dunes were created to resemble the real sinuous-crested three dimensional dunes as observed both in the field and flumes with mobile sediments (Blom et al., 2003; Giri and Shimizu, 2006; Venditti, 2007; Coleman and Nikora, 2011). The height of the crests of the dunes above the troughs, $H$, varied in the cross-stream direction from 0.02 to 0.06m, and
successive crest lines were 180\(^\circ\) out of phase to immediately follow a dune of high middle and low sides with low middle and high sides. The crest-to-crest wavelength, \(\lambda\), varied from 0.73 to 0.87 m in the cross-stream direction. The mean water depth, \(d\) during the experiment was 0.173 m, with the ratio of the mean water depth to the mean dune height, i.e. \(d/H_m\), being 4.3. The steepness of the dunes varied in the spanwise direction with \(H/\lambda\) values ranging from 0.02 to 0.08, which is also in the range of dune steepness values reported for actual open channel flow dune shapes (Julien and Klaassen, 1995; Karim, 1999; Best, 2005; Tuijnder et al., 2009). The Reynolds number (Re) and Froude number (Fr), based on the mean bulk flow velocity \(U_0 = 0.357 \text{ m/s}\) and the mean water depth \(d\), are 62,000 and 0.275, respectively.

![Figure 4.9: Schematic geometry of a three dimensional dune](image)

Large Eddy Simulations were performed using closely four million finite volume cells for flow and suspended sediment transport computations. The flow in the streamwise direction is assumed to be statistically homogeneous (Yue et al., 2006; Stoesser et al., 2008; Omidyeganeh and Piomelli, 2013a,b; Xie et al., 2013, 2014) and therefore a periodic bound-
ary condition was used. A no-stress (free slip) wall was applied in the spanwise direction which is consistent to the condition imposed during the experimental data collection at the side walls of the flume. A no-slip condition was used at the dune surface for the flow, and the van Rijn (1984) pick-up function (Eq. 4.21) was applied to calculate the sediment transport rate. The variation of the free surface compared to the local water depth is small for the considered domain (Maddux et al., 2003), and a rigid lid was imposed for the flow at the top boundary. The rigid lid accounts any free surface effects through the pressure (Stoesser et al., 2008) and any error introduced to the continuity error was assumed negligible. A rigid lid condition has been successfully used in previous LES studies for open channel flows in three and two dimensional dunes (Yue et al., 2006; Zedler and Street, 2006; Stoesser et al., 2008; Omidyeganeh and Piomelli, 2013a,b; Xie et al., 2013, 2014). For the suspended sediment transport, a zero sediment flux condition was considered at the top boundary (Wu et al., 2000; Zedler and Street, 2006; Zhu et al., 2013).

![Streamwise velocity profiles at the centerline node, Y = 0](image1)

![Streamwise velocity profiles at Y = 0.225m](image2)

Figure 4.10: Comparisons of mean streamwise velocity profiles between the experimental measurements and numerical results

The time averaged streamwise velocity profiles from the numerical model and the experimental data are presented on Fig. 4.10 at various points across the dune cross-section.
In order to show the flow response to the effects of three dimensionality of the dune geometry, the mean velocities at two spanwise locations (i.e. the centreline $y = 0$m and the crest line $y = 0.225$m) are also included for comparison. The numerical model captured the streamwise velocity profiles at both locations with a reasonable agreement. In general, the streamwise velocity is higher in the stoss side of the highest dune crest due to its lower depth for the same volume flow rate. On the lee side, the speed of the fluid becomes slower due to the development of a shear layer and local adverse pressure gradient. A flow reversal is also observed on these regions indicating flow separation and recirculation. Downstream of the dune crest, after 4 to 6 dune heights, the flow again reattaches which is consistent to what was observed in the previous studies (Nelson et al., 1993; McLean et al., 1994; Venditti, 2007; Stoesser et al., 2008; Omidyeganeh and Piomelli, 2013a; Xie et al., 2013, 2014). As can be seen from the velocity profiles at the two locations ($y = 0$m and $y = 0.225$m), the fluid becomes slower behind the lowest dune crest compared to the node of the highest crestline, showing the effects of dune three dimensionality in the cross-stream (span wise) direction.

Fig. 4.11 shows the comparisons between the predicted Reynolds shear stresses ($u'w'$) and the corresponding experimental measurements. Overall, good agreement is achieved between the modeled and observed profiles, although there are minor over-predictions in the shear layer downstream of the dune crests. Xie et al. (2014) also performed LES on the same dune geometry and their numerical results also showed similar discrepancies on this region compared to the experimental measurements. The experimental data were collected over two individual dunes and over one-quarter width of the flume from $y = -0.225$m to $y = 0$m (Maddux et al., 2003) and the velocity results from the measurement regions have been transposed to the entire flume width assuming that the flow is symmetric about the flume centerline and that no walls are present. This might be partly responsible for the differences between the numerical and experimental results. A shear layer was formed downstream of the dune crest which is due to vortices and generated turbulent structures.
Figure 4.11: Comparisons of mean Reynolds shear stress profiles between the experimental measurements and numerical results at $y = 0$ m (centerline) and $y = 0.225$ m in the separation zone. Maximum shear ($u'w'$) and normal ($u'u'$) stresses are observed to occur downstream of the highest dune crest (Fig. 4.12) which is mainly due to the high level of energy dissipation and turbulent generation in the separating shear layer. According to Omidyeganeh and Piomelli (2013a), secondary flows are greater and more structured over saddle or lobe shaped crestlines and these currents control the downstream sediment transport and morphological features.

Figure 4.12: Contours of mean streamwise velocity fluctuation (left) and Reynolds stress (right) in a longitudinal plane

Fig. 4.13 shows sample visualizations of the instantaneous streamwise velocity, span-
wise vorticity, isosurface of coherent flow structures, and suspended sediment transport. As can be seen in the streamwise velocity field, a negative transverse flow is observed on the lee side with a longest recirculation after the highest crestlines. This energy dissipation controls both lateral and vertical mixing processes that are elucidated by the generation of local vortices, turbulent sweeps, and ejections. Compared to the stoss side, strong vortices are generated downstream of the dune crest due to the Kelvin-Helmholtz instability and these vortical structures are transported towards the reattachment region as the flow progresses further downstream. Due to the instability of the separated shear layer, roller type coherent flow structures are formed after the dune crest and these vortical structures interact with the near wall turbulence producing horse-shoe like turbulent flow structures in the developing boundary layer on the stoss side of the dune. Similar findings were also observed in the previous numerical studies of both two and three dimensional dunes (Frias and Abad, 2013; Omidyeganeh and Piomelli, 2013a; Anderson and Chamecki, 2014). In LES studies of two dimensional dunes, Frias and Abad (2013) observed that the horse-shoe like structures interact with the free surface creating a boils which are believed to be responsible for the formation of the water surface gradients in open channel flows. As can be seen from the sediment concentration contours, the mixing and transport of the instantaneous sediment transport process is directly related to the formation of vortical and coherent structures. Experimental studies on migrating bedforms (Papanicolaou et al., 2001; Venditti et al., 2005; van der Werf et al., 2008; Nelson et al., 2009; Singh et al., 2009, 2012; Celik et al., 2013) also showed that the changes in dune shape and size mainly depend on the level of flow turbulence, availability of sediment, and grain size distribution. These instantaneous profiles offer an insight into the complexity and spatial variability of the flow, turbulence, and sediment transport fields, which are extremely useful for bedform migration and sediment transport processes for typical geophysical flows.

Fig. 4.14 shows contours of the instantaneous sediment concentration together with the perturbation velocity vectors at four different slices in the cross-stream direction. Stong
spatial variations of the sediment transport process is clearly shown both in the spanwise and vertical directions at all slices. The bursting process associated with the flow field at this instant can also be observed from the velocity fluctuation vectors. Turbulent ejection events \((u' < 0, w' > 0)\) play a significant role for the vertical suspension and mixing of sediment from the near bed region (Zedler and Street, 2006). For example at \(x = 2.6\)m, close to the flow reattachment region, the roller type coherent flow structures which were generated downstream of the dune crest (Fig. 4.13, c) start interacting with the near wall turbulence in the reattachment and developing regions, forming horse-shoe like vortical structures which play a major role in the suspension of sediment through ejection events. As was observed in previous studies (Drake et al., 1988; Zedler and Street, 2001; Bauer et al., 2013), sweeps \((u' > 0, w' < 0)\) transport the fluid and sediment particles towards the bottom boundary and they are commonly responsible for bed load transport in saltation dominated flows. Overall, the local rate of sediment transport patterns are strongly dependent on the shape of the bedform geometry and the level and nature of turbulent structures associated with the flow field.
In geophysical flows, the near bed hydrodynamic fields play a significant role on bedform evolution, as well as the initiation and transport of sediment from the lower regions to the other parts of the flow domain (Singh et al., 2012). The temporal and spatial variations of the boundary shear stress also depends on the intensity and distribution of the turbulent eddies which, in turn, controls the total amount of sediment transport and formation of bedforms (a larger rate of sediment transport is expected at a higher boundary shear stress). Fig. 4.15 shows the boundary shear stress at the dune surface together with the suspended sediment concentration, vorticity magnitude, and concentration dependent viscosity (Thomas, 1965). Higher shear stress and vorticity fields are observed in the developing boundary layer after the flow reattachment point. However, the shear stress decreases in the recirculation region due to energy dissipation, adverse pressure gradient, and Kelvin-Helmholtz instability. Similar to the findings of the previous studies (Venditti et al., 2005; Zedler and Street, 2006; Frias and Abad, 2013), a higher boundary shear stress region is responsible for sediment suspension and erosion processes, whereas deposition
and downward particle motion dominate in areas with low shear stress and sweep events. The flow viscosity also increases with sediment concentration, showing that the suspended sediment can attenuate turbulence and laminarize the flow for concentrated sediment beds.

Figure 4.15: Contours of instantaneous simulated near-bed hydrodynamic fields: a) Bed shear stress b) sediment concentration c) vorticity magnitude d) concentration dependent viscosity

4.4 Conclusions

Developments in advanced computational techniques have increased the capability of numerical models for providing detailed flow fields and the coupling of flow and transport processes. Computational results can provide useful insights of the time dependent three dimensional flow features which are usually difficult to measure in experiments. In this study, LES together with mixture theory is applied for fully developed turbulent flows over two and three dimensional dunes to understand the temporal and spatial interactions of flow and sediment transport fields. LES is selected as a turbulent closure scheme due to its ability in resolving a much larger range of useful turbulent scales which are vital to understand fluid and sediment motions in complex geometries. A three dimensional fluid-sediment mixture method is implemented in a non-hydrostatic, finite volume software,
OpenFOAM. The coupled solver accounts for fluid-sediment and sediment-sediment interactions through enhanced viscosity with particle concentration, density stratification, and particle pressure similar to the method adopted by Penko et al. (2013). Hindered settling was also applied based on the Richardson and Zaki (1954) formulation to account the intra-particle interaction when the suspended sediment concentration becomes significant. An instantaneous shear stress dependent sediment pick up function (van Rijn, 1984) was used to calculate suspended sediment transport from the bottom boundary layer. To elucidate the effect of sediment particles on different hydrodynamic variables, separate simulations were performed with sediment free (clear water) and sediment induced stratification over two and three dimensional dunes.

The clear water numerical results are compared with the experimental data of Balachandar et al. (2003) and Maddux et al. (2003) for two and three dimensional dunes, respectively. Good agreements were achieved for the mean velocity, and Reynolds stress profiles for the two cases showing that the numerical schemes and grid resolutions are adequate enough to capture the mean flow fields. On the lee side of the dunes, the speed of the fluid become slower with a flow reversal due to the development of a shear layer and local adverse pressure gradient. Strong cross-stream variations of flow and turbulence fields are observed over the 3D dunes. For instance, the fluid becomes slower behind the lowest dune crest compared to the node of the highest crestline. Maximum shear and normal stresses are developed downstream of the highest dune crest due to high energy dissipation. These type of hydrodynamic features were not observed in the two dimensional dune simulations.

As a result of the enhanced viscosity, sediment induced stratification, and particle pressure effects, a reduction on the peak turbulence levels is shown for both the wall normal and Reynolds shear stress components. These phenomena can potentially decrease the vertical mixing and turbulent suspension of sediment particles in the flow field. However, the effect of sediment concentration for the time averaged streamwise velocity fields is insignificant, most likely due to the small magnitude of solid volume fraction used here. In
previous studies (Ozdemir et al., 2010; Yu et al., 2014), flow laminarization and velocity damping were observed when the sediment concentration becomes more significant, O (100) g/l.

The instantaneous flow and sediment transport fields are investigated together with the existence of coherent structures which are identified by a Q criterion. The impacts of vortex structures on the spatial and temporal variations of sediment transport are assessed by superimposing the suspended sediment concentration contours to the instantaneous flow field. Strong spanwise vortices are generated in the shear layer separating from the dune crest due to the Kelvin-Helmholtz instability. These vortices are transported further downstream and become responsible for a higher suspended sediment transport rate. The upslopes behind the dune crest and the flow reattachment regions are found to be the main sources of suspended sediment transport due to the higher magnitude of bed shear stress. Horseshoe like vortex structures together with ejection events \((u' < 0, w' > 0)\), are responsible for the vertical and lateral transport of suspended sediment from the near bed region. Stronger velocity perturbation vectors are also observed around the horseshoe-like structures, demonstrating that these areas are highly dynamic zones of flow and sediment transport. Compared to 2D dunes, strong spatial variations of the sediment transport process is clearly shown in both the spanwise and vertical directions over 3D dunes.

In conclusion, this study demonstrates that LES is advantageous for solving the complex flow and sediment transport dynamics by resolving the large scale eddies of the turbulent motion and that, when coupled with a sediment transport model, can provide valuable insights into three dimensional turbulence-sediment interactions. Therefore, the current approach should prove useful to extend the study of morphodynamics and bedform evolution, where the bed features change both in space and time due the resolved scales of the turbulent flow, availability of sediment, and grain size distribution.

4.5 References


Yue, W., Lin, C.-L., Patel, V. C., 2005. Large eddy simulation of turbulent open-channel flow with free surface simulated by level set method. Physics of Fluids 17 (2), –.


Chapter 5
Three dimensional hydrodynamic simulations to gain insights on the effects of vertical distortion in hydraulic physical models

5.1 Introduction

Physical models are valuable experimental tools for finding technically and economically optimal solutions of engineering hydraulic problems in a reasonably short period of time. Physical models are commonly used to i) duplicate a flow phenomenon observed in a prototype through small scale laboratory experiments, ii) examine the performance of different hydraulic structures or to find alternate countermeasures for a final design to be implemented, and iii) elucidate model and prototype performances under various hydrodynamic and sediment conditions. Geometrically distorted models have a large horizontal to vertical scale ratio (greater than unity) in order to model bigger prototypes, while maintaining adequate model flow depth for fully turbulent conditions (Peakall et al., 1996; Julien, 2002). Scale effects arise due to differences in force ratios between the model and its real-world prototype. The hydraulic similarity in the vertical direction is usually affected in distorted physical models (Peakall et al., 1996; Fang et al., 2008; Lu et al., 2013; Zhao et al., 2013). Deviations in the vertical velocity profile brings differences not only in the turbulence structures but also in the scaled sediment transport rates between the physical model results and prototype measurements.

Fang et al. (2008) applied a three dimensional numerical simulation using a Reynolds Averaged Navier Stokes (RANS) approach to model flow and sediment transport processes in a flatbed channel under different distorted scales and found that the discrepancies between the distorted and the undistorted models for the streamwise velocity profiles are negligible, while differences were observed for the velocities in the vertical direction. Fur-
thermore, it was shown that the spatial distributions of sediment erosion and deposition rates are affected with different levels of distortion. The sediment suspension decreases with distortion while the deposition rate increases. According to Lu et al. (2013), the effect of distortion on bed load is observed in sediment movement and transport rates due to increases of vertical and horizontal slopes at the riverbed. Furthermore, it was noted that the secondary flow pattern in the meandering reach could be affected by distortion, and part of the fully developed secondary flow moved downstream as the distortion ratio increases. Zhao et al. (2013) developed a mathematical function for Chezy coefficient using distortion ratio, water depth in the prototype, and the roughness height and showed that the Chezy coefficient is greater than unity for distorted models and it should be adjusted based on the distortion ratio and bed roughness. The scaling and self-similarity study by Ercan et al. (2014) on unsteady open channel flows through one-parameter Lie group scaling transformations recommended the use of equal scaling ratios of channel depth and width to get better flow characteristics in the cross-stream direction than the traditional approach for distorted hydraulic models. Moreover, Carr et al. (2015) extended the findings of Ercan et al. (2014) for one dimensional non-equilibrium suspended sediment transport by applying Lie group scaling on the governing equations and boundary conditions. The new concept is believed to give better results for sediment grain size scaling compared to the limitations of previous methods that use light weight and larger diameter based on the Shields parameter $\theta$ (Shields, 1936), particle Reynolds number $R_{e*}$, and relative particle fall velocity $w_s/U_*$ (Abderrezzak et al., 2014).

A new Expanded Small Scale Physical Model (ESSPM) of the Lower Mississippi River has been designed to improve our ability to physically model the flow and sediment (sand) transport in the Lower Mississippi River. This model extends from Donaldsonville, LA to the Gulf of Mexico (Fig. 1). The mean flow in the ESSPM is designed to maintain Froude number (F) similarity between the prototype and the model, their ratio being equal to unity. Similar to previous studies (Wallerstein et al., 2001; Abderrezzak et al.,
2014; Gorrick and Rodríguez, 2014), the flow Reynolds number is relaxed, ensuring fully turbulent flow conditions in both the prototype and the model. The model is designed with different geometric scales in the horizontal (1:6000) and vertical (1:400) directions. These scales are chosen to achieve rough turbulent flow conditions and sediment movement in the ESSPM for the prototype to be studied. The geometric distortion, which is the ratio of vertical to horizontal scales, corresponding to the ESSPM is fifteen. The scaling differences and distortion may limit the model's ability to replicate some of the complex hydrodynamic and sediment transport processes. This study first focuses on a description of the similarity laws that were used in the ESSPM design and what limitations are expected due to the use of a distorted scale. A three-dimensional computational fluid dynamics (CFD) software is used to quantitatively study the impacts of scaling and distortion on the hydrodynamics by comparing velocities, turbulent structures, boundary shear stress, and sediment transport distributions.

A large eddy simulation (LES) scheme is used as a turbulence closure in this study. The use of LES resolves a much larger range of turbulence scales than Reynolds Averaged equations (RANS) in which all turbulence scales are modeled. Unsteady simulations using LES give vital turbulent quantities which help to understand particle and fluid motions over complex geometries. In many of the previous numerical studies for sediment transport, RANS equations are often employed (Johns et al., 1993; Hsu et al., 2003). However, evidences suggest that commonly used RANS models can not represent key turbulent quantities in unsteady boundary layers (Chang and Scotti, 2004).

5.1.1 Physical model dimensionless parameters

For open channel flows with a movable-bed, a number of variables control both the hydraulics and transport of sediment including: fluid viscosity ($\mu$), fluid density ($\rho$), hydraulic radius (R), surface roughness (Ks), channel bed slope (So), mean velocity (U), gravitational acceleration (g), sediment density ($\rho_s$), and sediment grain size (D). These variables can be combined to drive dimensionless relationships that characterise an inde-
Figure 5.1: ESSPM domain (not to scale, source??)

ependent phenomenon, \( A \), to be studied (Peakall et al., 1996; Ettema et al., 2000).

\[
A = f(\mu, \rho, R, K_s, S_o, U, g, \rho_s, D) \tag{5.1}
\]

Nine independent variables (Eq. 5.1) and three fundamental dimensions (Length, Mass, and Time) can be rearranged through the Buckingham-Pi (\( \pi \)) theorem into a set of new six dimensionless parameters,

\[
\Pi_A = f \left( \frac{\rho U}{\mu}, \frac{U}{\sqrt{gR}}, \frac{K_s}{R}, \frac{\rho \left( \sqrt{gRS_0} \right) D}{\mu}, \frac{D}{R}, \frac{\rho (gRS_0)}{(\rho_s - \rho) gD} \right) \tag{5.2}
\]

In Equation 5.2, \( \sqrt{gRS_0} \) represents the shear velocity (\( U_* \)) of the flowing fluid and therefore, the dimensionless parameters can be further simplified into,
\[ \Pi_A = f \left[ \frac{\rho RU}{\mu}, \frac{U}{\sqrt{gR}}, \frac{K_s}{R}, \frac{U_s}{D}, \frac{D}{R}, \frac{\rho U_s^2}{(\rho_u - \rho) gD} \right] \] (5.3)

or

\[ \Pi_A = f \left[ \text{Re}, F, \frac{K_s}{R}, \text{Re}_s, \frac{R}{D}, \theta \right] \] (5.4)

The six independent dimensionless parameters in Eq. 5.4 represent the flow Reynolds number (Re), the Froude number (F), the relative roughness of the channel bed (Ks/R), the grain Reynolds number (Re_s), the relative roughness of the grain sediment (D/R), and the Shields parameter (\theta).

Most physical models are designed to ensure Froude number similarity between prototypes and models. Distorted models which are constructed through this dimensionless parameter are assumed to simulate bulk one dimensional hydrodynamic properties (Peakall et al., 1996; Ettema et al., 2000; Julien, 2002; García et al., 2008). Scaling of two and three dimensional flow variables may not be accounted in these models and therefore, special considerations should be taken to model diffusion, turbulent mixing, vorticity, and others.

5.1.2 Model scaling and similitude

In order to achieve a complete similarity between model and prototype behavior, hydraulic physical models should display geometric, kinematic, and dynamic similitude (Peakall et al., 1996; Wallerstein et al., 2001; Chanson and Gualtieri, 2008; Heller, 2011; Gallisdorfer et al., 2014). For geometric similitude, homologous spatial dimensions between the prototype and the model must have equal scale factors and shape. The kinematic similitude governs motions of physical phenomena, for example, velocity fields of a fluid between
the prototype and its scaled model, with a similar scale factor. Correspondence between the prototype (subscript \( p \)) and the model (subscript \( m \)) is determined by a scale function, \( E(S) \) which is defined as,

\[
E(s) = \frac{S_m}{S_p} \quad (5.5)
\]

where \( S \) is an independent variable that represents a specific property in open channel flows to attain similitude between the prototype and model.

The sediment material is designed to preserve incipient motion and sediment re-suspension between the prototype and the model. The Shields parameter (Eq. 6) and grain Reynolds number (Eq. 7) should be preserved to ensure the same bed state in the model as in the prototype (Gill and Pugh, 2009; Abderrezzak et al., 2014), i.e.,

\[
E(\theta) = E \left( \frac{\rho U^2}{(\rho_s - \rho)gD} \right) = 1 \quad (5.6)
\]

and

\[
E(Re_s) = E \left( \frac{\rho U_s D}{\mu} \right) = 1 \quad (5.7)
\]

Equation (5.8), which is a mathematical correlation between the sediment density and grain size can be obtained from Eqs. 5.6 and 5.7 and allows one to choose from available sediment grain sizes and densities.
The model sediment density is taken as $1.05\rho$ and the ESSPM is designed to predict sediment transport processes for sand with a median grain size ($D_{50}$) in the order of 0.0004 m to 0.00045 m. Table (5.1) summarizes the important scaling functions and values used in the ESSPM for both the flow and sediment transport processes.

Table 5.1: Fundamental scaling functions and their values in the ESSPM

<table>
<thead>
<tr>
<th>Flow/Sediment parameter</th>
<th>scaling function, $E(S)$</th>
<th>scaling value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal length</td>
<td>$E(L)$</td>
<td>1:6000</td>
</tr>
<tr>
<td>Vertical length</td>
<td>$E(H)$</td>
<td>1:400</td>
</tr>
<tr>
<td>Velocity</td>
<td>$E(U) = E(H)^{1/2}$</td>
<td>1:20</td>
</tr>
<tr>
<td>Hydraulic time</td>
<td>$E(T) = E(L)*E(H)^{-1/2}$</td>
<td>1:300</td>
</tr>
<tr>
<td>Flow rate</td>
<td>$E(Q) = E(L)^{3/2}E(H)^{3/2}$</td>
<td>1:48 x 10^6</td>
</tr>
<tr>
<td>Sediment grain size</td>
<td>$E(D) = E(\rho_s - \rho)^{-1/3}$</td>
<td>3.2:1</td>
</tr>
<tr>
<td>Sediment density</td>
<td>$E(\rho_s)$</td>
<td>1:2.52</td>
</tr>
</tbody>
</table>

Due to the advances in computational power in recent years, numerical models have been largely used to aid our understanding of flow, turbulence and sediment transport processes in river environments (Miyawaki et al., 2010; Van Balen et al., 2010; Constantinescu et al., 2011; Simeonov et al., 2013). The motivation of this study is to elucidate the effect of distortion scales on the velocity, suspended sediment transport, and turbulence fields through detailed numerical simulations. Three dimensional hydrodynamic simulations were performed using the geometry and flow conditions of a $\sim$10 meters of ESSPM of the Lower Mississippi River to understand the effect of distortion scales on different
hydrodynamic variables. A detailed analysis was carried out by running simulations at two distortion scales (i.e., 15, the design distortion and 7.5). These two numerical cases are chosen considering the available computational resources and grid requirements to achieve adequate results using large eddy simulation (LES). OpenFOAM (Weller et al., 1998), a three dimensional, finite volume, and non-hydrostatic model is used and Large Eddy Simulation (LES) is chosen to resolve the turbulence eddies. Comparisons are made of (i) the velocity components at typical cross-sections, (ii) the turbulent fields in terms of velocity fluctuations, and (iii) the boundary shear stress. Conclusions are drawn regarding differences in the vertical velocity fields and the possible effects on the sediment transport processes. Moreover, locations in the study reach where additional turbulence is generated due to local topographical effects will be identified and discussed.

5.2 Mathematical formulation and Computational setup

A three dimensional software, OpenFOAM, Open Field Operation and Manipulation (Weller et al., 1998) is used. A finite volume numeric is employed to solve the conservation equations in their conservative forms. The fundamental equations are developed within a robust, implicit, pressure-velocity, iterative solution framework, and a domain decomposition method is applied to divide and allocate the flow variables for separate processors during high performance computation. Unsteady open channel flows can be described by the Navier Stokes equations, which are conservations of mass and momentum for an incompressible fluid flow. A large eddy simulation approach is applied in this study and the conservation equations are based on the filtered Navier Stokes equations, given as:

\[
\frac{\partial \bar{u}_i}{\partial x_i} = 0
\]  (5.9)
\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\overline{u}_i \overline{u}_j) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(2\nu \overline{S}_{ij}) + \frac{\partial \tau_{ij}}{\partial x_i} + F \tag{5.10}
\]

where \(\overline{u}\) is the filtered velocity field, \(\overline{p}\) is the pressure field, \(g\) is the gravitational acceleration, \(F\) is the external driving force, \(\mu\) is the molecular viscosity, \(\tau_{ij}\) is the subgrid scale stress which is computed from the resolved velocity field, \(\overline{S}_{ij}\) and is the resolved strain rate tensor which is computed from the resolved velocity field as:

\[
\overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \tag{5.11}
\]

As has been described previously, the flow in the ESSPM is designed to be fully turbulent at typical flows when the sediment is mobile. A large eddy simulation scheme that was developed by Germano et al. (1991) and modified by Lilly (1992), which is often called Dynamic Smagorinsky Model (DSM), is used as a turbulence closure in this study. Agegnehu and Willson (2015) have performed detailed evaluations of LES schemes for fully developed turbulent flows over a wall bounded channel, a backward facing step, and a wavy wall and through comparisons with experimental and direct numerical simulation (DNS) data, it was found that the DSM is the best scheme in resolving the mean flow and turbulence fields. LES allows the prediction of turbulence for a wide variety of flows by resolving the large scales while modelling the dissipation and mixing ranges through a subgrid scale stress model (Scalo et al., 2013). The conservation equations of continuity and momentum are obtained by filtering the Navier Stokes equations (Fureby et al., 1997). DSM requires sequential applications of two filter levels on the Navier Stokes equations, primary and test filters. In the current study, twice the width of the primary filter is applied for the test
filter. During the numerical solution, the momentum equation advances with a velocity pressure coupling via a predictor-corrector procedure based on PISO (Pressure Implicit with Splitting of Operators) of Issa (1986).

The conservation of the suspended sediment transport is computed with the advection-diffusion equation. A finite volume scalar transport equation of suspended sediment is implemented in OpenFOAM (Eq. 5.12).

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} \left( C u_i - C w_s \delta_{j3} \right) = \frac{\partial}{\partial x_j} \left[ \left( \nu + \nu_t \sigma_c \right) \frac{\partial C}{\partial x_j} \right]
\]  

(5.12)

where \(C\) is local volume of sediment concentration, \(w_s\) is the settling velocity (van Rijn, 1984), \(\nu\) is the fluid kinematic viscosity, \(\delta_{j3}\) is Lronecker delta with \(j = 3\), and \(\sigma_c\) is the turbulent Schmidt number relating the turbulent diffusivity of the sediment to the eddy viscosity \(\nu_t\).

OpenFOAM supports both structured and unstructured meshes. About six million finite volume numerical cells were used for the 3D computation. The grid was generated using the river bathymetry data which was obtained from C & C Technologies, Inc. The survey data includes the part of the Lower Mississippi River from Grayville to Harvey, LA, which is about 10 meters reach length in the ESSPM. The overall study area is divided into seven panels, where each of them comprises nearly four million nodes of STereoLithography (STL) files. The mesh is refined around the solid walls (Fig. 5.2) to capture the small scales of turbulence around the boundary layers. The banks and the channel bed were treated as a no slip condition. The free surface is assumed to be an impermeable rigid lid where a free-slip condition is used. In this study, the free surface variation is relatively small compared to the flow depth and therefore, the effect of the rigid lid boundary on the continuity and generation of turbulent structures is assumed negligible. Previous studies (Constantinescu
et al., 2011; Meselhe et al., 2012) applied a similar approach for river flows and adequate numerical results were obtained at a reasonable computational cost compared to the Volume of Fluid (VOF) or any other free surface capturing methods. For the inflow (upstream), a flow rate type boundary is imposed. To account the inlet turbulence, synthetic randomly distributed eddies (Lund et al., 1998) are applied on the mean inlet velocity field. The perturbations are generated by considering the collective effect of all eddies on the velocity profiles in the inlet plane, controlled by the target turbulent statistics (2-5% for this case). At the downstream (outflow), the zero gradient (convective) boundary condition is used. This boundary condition assumes all the hydrodynamic variables reaching the boundary leave the computational domain freely. A wall function (Spalding, 1961) that links the laminar sub-layer with the log layer is applied to reduce the computational and time step requirements around the solid walls. This formulation accounts the velocity at the first grid point away from the wall by logarithmic and exponential functions using the shear velocity.

For the suspended sediment transport, a zero sediment flux condition is considered at the top boundary. At the upstream inlet boundary, a suspended sediment concentration input of 0.06621kgm$^{-3}$ is used (Thomas, 2014). For the solid and downstream outlet boundaries, a Neumann condition is imposed.

5.3 Results and discussion

Using the three dimensional model, numerical computations were carried out at distortion scales of 15, the design distortion and 7.5 (Tab. 5.2). A flow rate of about 23,124 m$^2$s$^{-1}$ in the prototype is scaled for each case and used as an inflow boundary condition. Moreover, the Reynolds number was kept constant by using an equal scale in the vertical direction for both cases. Before direct comparisons of the results from the two distortion scales, an illustration on the structure of the instantaneous flow and turbulence at a typical channel section from the distortion of 15 is described by presenting the visualizations of instantaneous velocity magnitude, vorticity magnitude, and three dimensional vortex struc-
tures. To get better insights into the generation of vortex coherent structures and their role on the vertical and lateral mixing processes, a Q-criterion (Hunt et al., 1988) is applied, based on the second invariant of the velocity gradient tensor. Throughout the paper, the velocity, boundary shear stress, and velocity fluctuation fields are non-dimensionalized with the bulk velocity at the inflow upstream boundary ($U_i$).

Table 5.2: Model parameters used for each distortion scale

<table>
<thead>
<tr>
<th>Distortion</th>
<th>Horizontal scale</th>
<th>Vertical scale</th>
<th>Flow rate (ft³s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>6000</td>
<td>400</td>
<td>0.017</td>
</tr>
<tr>
<td>7.5</td>
<td>3000</td>
<td>400</td>
<td>0.034</td>
</tr>
</tbody>
</table>

Figures 5.3 and 5.4 show the representation of the resolved instantaneous flow physics for the distortion scale of 15. Upstream of the channel bend, the streamwise velocity in the inner (left) bank is found to be higher than that on the outer bank. As the flow approaches the bend, the deceleration rate increases rapidly due to local changes in water depth and topographical channel curvature. As the flow passes over the channel bend, the velocity of the fluid particle within the boundary layer becomes slower due to the changes in the fluid stresses. This leaves the fluid insufficient momentum to overcome the adverse
pressure gradient, creating a strong separation zone. As can be seen from the individual cross-sections (Fig. 5.4), the energy dissipation controls both lateral and vertical mixing processes that are elucidated by the generation of local vortices, turbulent sweeps, ejections, and three dimensional vortex coherent structures. Due to the instability of the separated shear layer, roller type coherent vortex structures are formed after the channel bend and these vortical structures interact with the boundary layer turbulence forming horse-shoe like turbulent flow structures (Fig. 5.4c) in the downstream developing boundary layer. Frias and Abad (2013) observed that the horse-shoe like structures interact with the free surface creating boils which are believed to be responsible for the formation of the water surface gradients in open channel flows.

The hydrodynamic sensitivities to distortion levels were assessed by comparing the mean velocity profiles, turbulent intensities, bed shear stresses, and suspended sediment concentrations. Figure 5.5 shows comparisons of mean horizontal velocity profiles, which were taken from the three sample cross-sections on the computational domain (Fig. 5.2).
Figure 5.4: Velocity magnitude (top left), vorticity magnitude (top right), and isosurface of vortex coherent structures at Q = 4 s^{-2} (bottom)

Overall, the difference in horizontal velocity profiles from the two distortion levels is small. Fang et al. (2008) also performed numerical simulations over a flatbed channel at different distortion scales and their findings also showed that the effect of distortion on the streamwise (horizontal) velocity fields is negligible. However, deviations are observed around the
banks on the development and shape of the boundary layer. The difference elucidates the limitations of Froude number scaling on the balances of near wall energy dissipation and turbulence generation which mainly control bank erosion and deposition processes in natural river systems.

Figure 5.5: Comparisons of horizontal velocity profiles: (a) Section 1 at distortion 15, (b) Section 1 at distortion 7.5, (c) Section 2 at distortion 15, (d) Section 2 at distortion 7.5, (e) Section 3 at distortion 15, and f) Section 3 at distortion 7.5

Comparisons of mean vertical velocity profiles from the two distortion scales are presented on Fig. 5.6. It is clearly shown that the magnitude of the vertical velocity profile (both negative and positive) changes with the distortion levels. For example, at distortion scale of 15 on the third cross-section (Fig. 5.6e), positive and negative vertical velocities are attained around the banks and centreline, respectively. However, at distortion scale of 7.5, negative vertical velocities are observed over the right bank and strong positive vertical velocities extend from the bottom bed to the left bank (Fig. 5.6f). Significant differences on the vertical velocity profile are also observed at the other two cross-sections. The deviations in the vertical velocity profiles have implications on the cross-sectional distribution of
Figure 5.6: Comparisons of vertical velocity profiles: (a) section 1 at distortion 15, (b) section 1 at distortion 7.5, (c) section 2 at distortion 15, (d) section 2 at distortion 7.5, (e) section 3 at distortion 15, and f) section 3 at distortion 7.5

suspended sediment transport, bed evolution, and sandbar formation. Moreover, the rate of mass and momentum exchange over the vertical direction can be affected due to vertical distortion. For example, Fang et al. (2008) observed an increase in bed thickness with distortion together with suspended sediment transport variations in the vertical direction. Lu et al. (2013), through experimental investigations, have also showed the effects of physical model distortion for the kinematics of suspended sediment transport.

The cross-sectional variation of turbulence levels in terms of velocity fluctuations from the two distortion scales are given on Fig. 5.7 in terms of time averaged horizontal ($\langle u'u' \rangle$) and vertical ($\langle w'w' \rangle$) velocity fluctuations. For the horizontal velocity fluctuations, deviations are observed mainly around the boundary layers (banks and bed) which could be related to the differences on the formation of shear layer as shown previously in the mean horizontal velocity profiles. For instance, at the distortion scale of 15 over Section 1, higher values of $\langle u'u' \rangle$ are observed close to the free surface and
Figure 5.7: Comparisons of horizontal (top) and vertical (bottom) velocity fluctuations: (a) Section 1 at distortion 15, (b) section 1 at distortion 7.5, (c) section 2 at distortion 15, (d) section 2 at distortion 7.5, (e) section 3 at distortion 15, and (f) section 3 at distortion 7.5
left bank, however, lower magnitudes of $< uu >$ are established at identical locations for a distortion scale of 7.5. Similar to the vertical velocity profiles, overestimations of the $< w'w' >$ profiles are also observed with vertical distortion at two typical cross-sections. At a distortion scale of 7.5, the peak $< w'w' >$ values decrease almost by half compared to the values observed at a distortion scale of 15 for both Sections 1 and 3. At Section 2, the maximum $< w'w' >$ values are formed away from the boundary layer towards the channel centre when the vertical distortion is 15. However, the spatial distribution of peak $< w'w' >$ values extends from right to left banks for a distortion scale of 7.5. As observed from $< u'u' >$ and $< w'w' >$ profiles, distortion can limit the proper representation of flow, sediment transport, and solute mixing processes in the vertical and lateral directions.

The calculated boundary shear stresses for the two distortion cases will be compared in order to elucidate the impact of distortion on the underlying morphodynamics phenomena and other related mechanisms. Bed shear stress is an important parameter in river flows to understand streambed erosion and deposition processes. Figure 5.8 shows the bed shear stress contours on a typical part of the computational domain for the two distortion scales. In river flows, the inner and outer banks are usually represented by slow and fast moving flows, respectively and the magnitude of boundary shear stress is related to the development of the shear layers and production of turbulent kinetic energy. Downstream of the bends, the distribution of the bed shear stress is highly heterogeneous due to the acceleration of the flow field introduced by the spatially variable roughness elements. Very low shear stress areas around channel bends are introduced due to the flow separation that creates a free shear layer along the recirculation region. These areas play a key role on the formation of sandbars in fluvial environments. As can be seen from Figure 8a and 8b, differences are observed on both the magnitude and spatial distribution of the bed/bank shear stress. For example, the cross-stream variation of bed shear stress is greater at the distortion scale of 7.5 compared to similar points at a distortion scale of 15. This is probably due to differences in channel widths, strength of spanwise vortices, and the induced local pressure gradient.
Figure 5.8: Bed shear stress on a typical part of the computational domain: (a) for distortion of 15 and (b) for distortion of 7.5 (note: for visualization purposes, different horizontal scalings were used on the two figures)

for the two cases. The width to depth ratio at the distortion scale of 7.5 is twice greater than the corresponding cross-sections at a distortion scale of 15.

Figures 5.9 and 5.10 show the time averaged suspended sediment concentration contours at a vertical slice near channel mid depth and at two typical cross-sections (sections 1 and 2) for distortion scales of 15 and 7.5, respectively. The suspended sediment concentra-
tion magnitude is higher around the inner banks due to slowly flowing fluid that introduces low boundary shear stresses and flow separation. In many natural rivers, sandbars are commonly observed in the inner side of meandering streams (Abad et al., 2013; Gutierrez et al., 2014). As has been discussed earlier, outer banks are expected to have lower suspended sediment concentration due to strong erosion. The outer bends are always critical for bank stability and scour protection. The outer bends are always critical for bank stability and scour protection. Suspended sediment transport is stronger around the inner banks for the distortion scale of 7.5 than the distortion scale of 15, indicating that distortion can alter the scaling of the channel deposition and erosion processes. Moreover, suspended sediment transport deviations are also observed in the cross-stream and vertical directions. Overall, the simulated results show a strong vertical mixing for the distortion scale of 15 than the distortion scale of 7.5.

5.4 Conclusions

Due to developments in High Performance Computing and advanced numerical techniques, versatile three dimensional simulations allow investigations of turbulent flows in
complex geometric domains. The numerical models can give detailed flow fields to shed light into the spatial and temporal flow and sediment transport features which are commonly difficult to measure with experiments. Three dimensional hydrodynamic simulations were performed using the geometry and flow conditions of a 10 meter section of the Expanded Small Scale Physical Model (ESSPM) of the Lower Mississippi River to understand the effect of vertical distortion on various hydrodynamic variables. Analysis and comparisons are carried out at two distortion scales (i.e., 15, the design distortion and 7.5) using turbulence resolving simulations. A non-hydrostatic and finite volume software, OpenFOAM together with Large Eddy Simulation are applied in this study. A total of 5,389,563 finite volume cells were generated for the 3D computation using the river bathymetry data. The mesh was refined around solid walls to capture the small scale turbulence levels.

From the instantaneous flow and turbulence fields at typical channel sections, the streamwise velocity in the inner bank is found to be higher than that on the outer bank upstream of a bend and as the flow further approaches the bend, the deceleration rate increases and finally forms a strong recirculation zone. Due to the instability of the separated
shear layer, roller type coherent vortex structures are also formed after the channel bend. The instantaneous results elucidate the complexity of the three dimensional flow within the channel, and provide better insights on the underlying physical mechanisms on river flow hydrodynamics and sandbar formation.

The sensitivity of different flow variables to distortion levels were assessed by comparing the mean velocity profiles, turbulent intensities, boundary shear stresses, and suspended sediment concentrations. Overall, the difference in horizontal velocity profiles from the two distortion levels is small and for the mean horizontal velocity fluctuations ($u'u'$), deviations are mainly around the boundary layers (banks and bed) which could be related to the differences on the formation of the shear layers. At cross-sections, however, significant deviations are observed for the vertical velocity profile both in terms of magnitude and spatial distribution. Overestimations are also shown for the $w'w'$ profiles with the vertical distortion. Moreover, the cross-stream variation of boundary shear stress is higher for the distortion scale of 7.5 compared to similar locations at a distortion scale of 15. Due to the deviations in vertical velocity, turbulence structure, and boundary shear stress fields, implications are also shown for the suspended sediment transport fields, both in regions of sediment erosion and deposition.

**Notation**

- $C =$ volume of sediment concentration (-)
- $D =$ sediment grain size (m)
- $F =$ Froude number (-)
- $g =$ gravity acceleration (ms$^{-2}$)
- $Ks =$ surface roughness (m)
- $p =$ filtered pressure field (m$^2$s$^{-2}$)
- $R =$ hydraulic radius (m)
- $Re =$ flow Reynolds number (-)
- $Re_*$ = grain Reynolds number (-)
So = channel bed slope (-)
\( \overline{S}_{ij} \) = resolved strain rate tensor (m-1s-1)
t = time (s)
\( \overline{u}_i \) = filtered velocity components (ms\(^{-1}\))
u = horizontal velocity component (ms\(^{-1}\))
v = spanwise velocity component (ms\(^{-1}\))
w = vertical velocity component (ms\(^{-1}\))
U = bulk velocity (ms\(^{-1}\))
\( U_i \) = inflow bulk velocity (ms\(^{-1}\))
\( U_{mag} \) = velocity magnitude (ms\(^{-1}\))
\( U_\ast \) = shear velocity (ms\(^{-1}\))
\( \nu_t \) = turbulent eddy viscosity (m\(^2\)s\(^{-1}\))
\( \rho \) = fluid density (kgm\(^{-3}\))
\( \rho_s \) = sediment density (kgm\(^{-3}\))
\( \sigma_c \) = turbulent Schmidt number (-)
\( \tau \) = bed shear stress (Pa)
\( \tau_{ij} \) = subgrid scale stress (m\(^2\)s\(^{-2}\))
\( \theta \) = shields parameter (-)
\( \mu \) = fluid viscosity (kgm\(^{-1}\)s\(^{-1}\))
\(<\>\) = time averaging

5.5 References


Thomas, W. A., 2014. Hec-6T sediment study: Sand inflow to expanded small scale physical model. Mobile Boundary Hydraulics, PPLC, Clinton MS 39060.


Chapter 6
Conclusions and recommendations

Flow and sediment transport processes in open channel flows are among the most complex and least understood processes in nature. It is very difficult to find analytical solutions for most problems in hydraulics and it is also not easy to obtain three dimensional numerical solutions without high performance computing. With the recent advancements in computational power, numerical models have been greatly improved and widely used to solve problems in open channel flows that have great practical importance. To develop better and feasible solutions, a good understanding of the flow physics is required. Computational results can provide useful insights of the time dependent three dimensional flow features which are usually difficult to measure in experiments. The main objective of this dissertation is to better understand the interaction of flow and sediment transport processes using detailed three dimensional numerical computation together with Large Eddy Simulation (LES). As a contribution, a new three dimensional fluid-sediment mixture method is implemented in a non-hydrostatic, finite volume software, OpenFOAM. The coupled solver accounts for fluid-sediment and sediment-sediment interactions through enhanced viscosity with particle concentration, density stratification, and particle pressure. This approach handles complex geometries at a resolution sufficient enough to resolve turbulent flows at high Reynolds numbers. The concluding remarks for the dissertation are the following:

The predictive capabilities of various Large Eddy Simulations (LES) schemes for fully developed turbulent flows are evaluated aiming to choose a scheme that can be used to investigate flow and sediment transport processes in geophysical applications at relatively high Reynolds numbers with an optimum grid resolution. Four Subgrid Scale stress (SGS) models are utilized for simulations of fully developed turbulent flows over a wall bounded channel, a backward-facing step, and a wavy wall. A detailed analysis and evaluation of the mean velocity and turbulence fields from the Smagorinsky Model (SM), the Dynamic
Smagorinsky Model (DSM), the Dynamic Mixed Model (DMM), and the SGS Kinetic Energy Model (SgsKEM) were performed using available experimental and DNS data. Both the DSM and DMM give better results for simulations that include the laminar sublayer ($Y^+ < 5.5$). However, the SM and SgsKEM schemes are found to be dissipative as the grid resolution decreases. A wall function is also a useful alternative to capture the peak turbulent fields, and mean velocity profiles when the grid resolution is not adequate enough to resolve the laminar sublayer. For separating flows, the DSM is a best scheme for both the mean velocity and turbulence fields in the recirculation and recovery zones. For example in the backward-facing step flow, the DSM predicts a flow reattachment point ($X_r$) of 6.1 which is close to the value reported in the experimental data ($X_r = 6$).

The advantages of a Large Eddy Simulation is taken to perform detailed investigations of the instantaneous flow, bed shear stress, and turbulent fields for fully developed turbulent flat-bed channel flows and to elucidate the role of vortex coherent structures for the entrainment of suspended sediment transport from the bottom boundary layer. The advection-diffusion equation is solved for suspended sediment transport and a sediment pick up function is applied to calculate the sediment transport rate from the bottom boundary layer. The effect of sediment roughness on the flow is accounted using a rough wall formulation which considers three distinct roughness zones. Both suspended sediment and flow quantities are validated by comparing the model results with experimental data. The simulated results are in good agreements with the observed experimental values. It is also shown that the vortex cores have a significant role for the upward movement and lateral distribution of sediment transport. Moreover, the spatial and temporal evolutions of suspended sediment transport from the bed is directly related to the magnitude of excess bed shear stress.

In open channel flows, the near bed hydrodynamic fields play a significant role on bedform evolution, as well as the initiation and transport of sediment from the lower regions to the other parts of the flow domain. The temporal and spatial variations of the
boundary shear stress also depends on the intensity and distribution of the turbulent eddies which, in turn, controls the total amount of sediment transport and formation of bedforms. Applications of LES has been further extended for fully developed turbulent flows over two and three dimensional dunes to understand the time dependent three dimensional flow and sediment transport features. Stronger cross-stream variations of flow and turbulence fields are observed over the 3D dunes than over the 2D dune shapes, which are mainly due to the effects of bedform three dimensionality. As a result of the flow-sediment mixture, the peak values of the normal and Reynolds shear stress components are reduced, which can potentially lead to flow laminarization and velocity damping at higher volume of solid fraction. Strong spanwise vortices are generated in the shear layer separating from the dune crest due to the Kelvin-Helmholtz instability. These vortices are transported further downstream and become responsible for a higher suspended sediment transport rate.

Three dimensional hydrodynamic simulations are also conducted using the geometry and flow conditions of a ~10 meter section of the Expanded Small Scale Physical Model (ESSPM) of the Lower Mississippi River to gain insights on the effects of model distortion on various hydrodynamic variables. Analysis and comparisons are carried out at two distortion scales (i.e., 15, the design distortion and 7.5) using turbulence resolving simulations. Overall, the difference in horizontal mean velocity profiles and velocity fluctuations ($\langle u' u' \rangle$) from the two distortion levels is small, supporting the ability of a distorted models to replicate bulk $1 - D$ sediment transport. Minor deviations are shown mainly around the boundary layers (banks and bed) which could be related to the differences on the formation of shear layers. At cross-sections, however, significant deviations are observed for the vertical velocity profile both in terms of magnitude and spatial distribution. Overestimations are also shown for the vertical velocity fluctuations ($\langle w' w' \rangle$) profiles with the vertical distortion. Moreover, the cross-stream variation of boundary shear stress is higher for the distortion scale of 7.5 compared to similar locations at a distortion scale of 15.
The work presented in this dissertation provides a foundation for applications of Large Eddy Simulation to understand and answer a range of flow and sediment transport processes in typical open channel flows for geophysical applications. Detailed investigations are performed on the unsteady features and, in particular, turbulent structures of the flow to demonstrate the great potential of eddy resolving methods for situations where these features play an important role. In conclusion, this study demonstrates that LES is advantageous for solving the complex flow and sediment transport dynamics by resolving the large scale eddies.

Future work

The results in this study show the complexities introduced to the flow field due to topography changes and dune three-dimensionality for fixed beds. However, bed deformation, fluid flow, and sediment transport processes occur at the same time. As the flow develops and interact with the bed, sediment is transported due to the excess bed shear stress, causing boundary deformation and at the same time affecting the flow field. Therefore, an extension of the current approach will provide invaluable insights to study morphodynamics and bedform evolution, where the bed features change both in space and time due the resolved scales of the turbulent flow, availability of sediment, and grain size distribution.

Simulation of moving or deformable boundaries is computationally difficult and expensive due to mesh reconstruction at each time step. Body-fitted grids generate structured or unstructured meshes that conform to the shape of the object. These grids have limitations due to non-orthogonally and skewness effects which are also critical for Large Eddy Simulation formulations. As an alternative, the use of an immersed boundary method, which enables to represent a body of any shape within the context of Cartesian grids significantly simplifies and decreases the solution procedure for moving boundaries.

In most of the sediment transport studies, the total sediment transport is divided into bedload and suspended load components. Invoking the dilute suspension, the suspended sediment transport is usually solved through the advection-diffusion equation. Empirical
parameterizations of bedload transport rate and pickup functions are commonly used under uniform-steady flow and single grain size assumptions. At higher sediment concentration, however, the fluid-sediment and sediment-sediment interactions changes the physics of the fluid motion field by damping the velocity and turbulence. Discrete element modeling is usually applied in a particle tracking framework, which is very effective for limited number of particles for extremely small domains or high density ratios such as gas-solid flows. In many geophysical applications, both the suspended and bedload sediment transport rates are significant, moreover the scale of the problem under consideration is very large. Therefore, the current method can be extended to an Eulerian method with a two phase flow approach to model complicated sediment transport processes. A two-phase model can resolve the sediment concentrated region by including closures of particle stresses and fluid interactions in the governing equations without the need to divide the sediment transport into bedload and suspended load components.
Vita

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