Scalar and Momentum transport over Complex Surfaces

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Abstract

Understanding and modeling of scalar and momentum exchanges between rough surfaces and the atmosphere form the overarching goals of this dissertation. Two types of complex surfaces are considered in this study, namely rough surfaces consisting of large bluff-bodies and water surfaces with surface waves. Chapter 1 presents a general review of the theoretical, numerical and experimental studies over the complex surfaces. Chapter 2 outlines the development and improvement of computational method for high-Reynolds number flow over complex-shaped objects. A computationally efficient method has been developed and tested to reduce the Gibbs phenomenon in spectral method used in the context of immersed boundary method. Chapter 3 examines the quality and reliability of wall-modeled large-eddy simulation (LES). The results underline the importance of conducting experimental or numerical studies for convective scalar transfer problems at a Reynolds number commensurate with the flow of interest, and support the use of wall-modeled LES as a technique for that can already capture important aspects of the physics. Chapter 4 studies the similarities and differences of momentum and passive scalar exchanges over large three-dimensional roughness elements of variable geometries in a turbulent channel flow using LES. The turbulent transports of momentum and scalar are similar but strong dissimilarity is noted between the dispersive momentum and scalar fluxes. Increasing frontal density induces a general transition in the flow from a rough boundary layer type to a mixed-layer-like type. This transition results in an increase in the efficiency of turbulent momentum transport, but the reverse occurs for scalars due to reduced contributions of large scale motions in the roughness sublayer. The geometric dependence of momentum and scalar roughness lengths is studied in chapter 5. The scalar roughness length depends on both the geometric parameters and the spatially variable surface scalar transfer coefficients, which cannot be easily determined a priori for a given geometry. Revisiting the surface renewal theory, we derive
a general scaling relation between the logarithmic ratio \( \log(z_{0m}/z_{0s}) \) and \( Re_* \), which explains the results computed from LES. Chapter 6 examines air-wave interactions using the Lake-Atmosphere Turbulent EXchange (LATEX) dataset. The wind waves and swells present in the lake are found to impact the coupling between surface and the air differently. A new relative wind velocity for surface layer similarity formulations is constructed and tested using the data. Finally, conclusions and outlook are presented in the last chapter.
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Chapter 1

Introduction

As the rate of urbanization accelerates, more than half of the global population (54%) now lives in the urban environment and the trend is expected to continue [Nations, 2014]. As succinctly summarized by Oke [2002]: “The process of urbanization produces radical changes in the nature of the surface and atmospheric properties of a region. It involves the transformation of the radiative, thermal, moisture and aerodynamic characteristics and thereby dislocates the natural solar and hydrologic balances.” In addition, the increasingly large number of urban population faces new challenges under the global climate change, such as more frequent heat waves and the need for more efficient energy use [Meehl and Tebaldi, 2004, Lau and Nath, 2012, Fischer et al., 2012, Dai, 2013, Kendon et al., 2014, Güneralp et al., 2015].

To capture the feedback and response of urban environment to the climate [McCarthy et al., 2012, Hamdi et al., 2014], urban areas need to be represented correctly in land-surface models. Over the past decades, numerous urban land-atmosphere models (usually referred to as urban canopy models (UCM) ) that focus on capturing the surface energy balance and lower atmospheric flow dynamics have been developed. These models encompass different levels of complexity and can be integrated into the weather and climate models [Yang et al., 2015a]. For example, the ‘slab’ model

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[Grimmond and Oke, 2002] represents the urban area as a flat surface; whereas many models [Masson, 2000, Ryu et al., 2011, Wang et al., 2013] consider the urban surfaces as arrays of two-dimensional canyons. UCMs rely on parameterization schemes [Jürges, 1924, Mascart and Giordani, 1995] to quantify the turbulent fluxes of momentum and scalars. These parameterization schemes are crucial in determining the surface water and energy balance and in providing accurate representations of the urban environments in weather and climate models. Furthermore, in light of rapid urbanizations, understanding of the turbulent flow and transport processes in urban areas will be essential for building energy studies [Blocken, 2015], designing streets that trap less pollution, parameterizing momentum and scalar fluxes in UCMs and helping to interpret field data measurements in the complex urban environment.

As a first approximation, the flow and transport in the urban atmospheric boundary layer can be formulated as a problem of turbulent shear flows over rough walls. This problem has been an active area of research. Both momentum and scalar exchanges between the wall and the fluid in such flows are of interest in a wide range of disciplines [Belcher et al., 2012]. Previous field experiments over natural vegetation [Poggi et al., 2004a, Katul et al., 1997b], wind tunnel studies over obstacles of regular shapes [Castro et al., 2006], and numerical simulations over three-dimensional roughness elements [Coceal et al., 2007a, Finnigan et al., 2009, Leonardi et al., 2015] have advanced our understanding of this problem significantly. For example, these past studies have underlined the importance of dispersive fluxes inside and close to the roughness canopy [Poggi and Katul, 2008, Poggi et al., 2004a]. Nevertheless, there remains significant gaps in our knowledge, particularly concerning the transport of scalars. Arguably, knowledge of heat and mass (i.e. pollutants and greenhouse gases) transport are essential in quantifying the atmospheric properties of an urbanized region. Much remains to be explored for scalars in comparison to momentum, particularly over urban surfaces, which can be thought of as surfaces consisting of
“large” three-dimensional bluff-body-type roughness elements. Large here implies that the roughness protrudes significantly into the inertial layer and that the details of the flow inside the roughness canopy are important for the applications. This knowledge gap is the primary motivation for this work.

To address the motivations and the knowledge gap, this work adopts a computational fluid dynamics (CFD) approach, using large-eddy simulations (LES) as the primary tool. Comparing to field experiments, which are often limited to point-wise measurements (such as a flux tower) or measurements limited in the canopy or roughness sublayer, numerical simulations can give comprehensive representations of the flow dynamics over complex surfaces. In simulating high Reynolds number flows over geometrically complex surfaces, there are two main challenges that will be briefly outlined here. Subsequent chapters will elaborate on the details of overcoming these challenges.

The first challenge is the Gibbs phenomena that arises from the numerical details of solving the filtered Navier-Stokes equations in LES. To represent the complex geometries of urban surfaces, we use the immersed boundary method (IBM) [Peskin, 2002]. This is an appealing approach because only non body-conformal grids (Cartesian in our case) are required to account for the force exerted by the bluff bodies on the flow, as summarized by Mittal and Iaccarino [2005]. However, discontinuities in quantities of interest (eg. velocity, pressure, or temperature or density) often arise as a result of implementing the IBM. For simulations of incompressible viscous flows that uses spectral discretizations (i.e. Fourier or Chebyshev collocation), discontinuities in the computed variables arising from the IBM lead to a numerical artifact called the Gibbs phenomenon or Gibbs ringing. The resulting unphysical oscillations associated with the function not being smooth and/or periodic can downgrade the numerical accuracy of spectral methods; nevertheless, these methods are very appealing due to their infinite order of accuracy, provided the function is sufficiently smooth [Tadmor,
1986], and to their computational speed (i.e. quadrature in physical space versus Fourier space has $O(N^2)$ and $O(N \log N)$ operations, respectively) [Trefethen, 2000].

As such, it might not be always desirable to forego spectral methods to overcome the errors resulting from Gibbs ringing, particularly in mixed spectral/finite difference codes where Gibbs ringing error is usually restricted to the region of the domain occupied by the solid and does not affect directions where finite difference is used. Therefore, chapter 2 [Li et al., 2016a] is devoted to assess the impact of these errors on the simulated flow and transport, and to develop approaches that can eliminate or at least mitigate them.

The second challenge emerges from the discrepancy in Reynolds number $Re$ between laboratory studies and real atmospheric boundary layer. Wind tunnel studies in the laboratories are very useful because near-surface scalar transfer coefficients can be measured and setups can be varied to study the impacts of topographical complexities [Igarashi, 1985, Aliaga et al., 1994]. However, extending the results of these studies to the real environment has to be handled with caution because of the difference in $Re$. $Re$ based on height of the roughness elements and the bulk velocity can be 3-4 orders of magnitude higher in the typical atmospheric boundary layer than that of common wind tunnels. Unlike momentum exchange, which is fully dominated by form/pressure drag over complex topographies at high $Re$, heat and mass exchanges are always performed by molecular conduction or diffusion in the vicinity of the complex interface and do not lose their dependence on the molecular heat and mass diffusivities at high $Re$. The convective to conductive or diffusive scaling characterized by the Nusselt number ($Nu$) for heat or Sherwood number for mass ($Sh$) in general always has $Re$ dependency [Lienhard, 2013]. This not only imposes difficulty in simply extending results from wind tunnel experiments to the real atmosphere, but also makes verification of LES results extremely challenging.

In particular, to address this challenge, three different experiments were used in this
thesis to verify the LES models for forced convective heat/mass transfer. Chapter 3 [Li et al., 2016b] describes the validation procedures and highlights the importance of $Re$ effect in scalar transport.

After addressing the two main challenges mentioned above, the numerical tool developed is then applied to answer questions about the general differences and similarities between momentum and scalar transport over complex surfaces in chapter 4. The effects of different surface geometries on roughness lengths of momentum and scalars are considered in chapter 5.

Apart from the urban-like surfaces, a completely different type of complex surface considered in this thesis is a lake with surface gravity waves. Based on the available experimental measurements Vercauteren et al. [2008] (LATEX), a hypothesis regarding the surface layer similarity relation is analyzed in detail in chapter 6.
Chapter 2

The impact and treatment of the Gibbs phenomenon in immersed boundary method

2.1 Introduction

Since the immersed boundary method (IBM) was first developed by Peskin [Peskin, 2002], it has been successfully adapted and implemented for flows over various solid objects and complex surfaces [Ye et al., 1999, Fadlun et al., 2000, Tseng et al., 2006, Lundquist et al., 2012]. The details related to implementing the IBM vary with the types of problems being dealt with [Mittal and Iaccarino, 2005], but the main advantage and appeal of this approach continue to be linked to the ability to use Cartesian (non-body conformal) grids and either continuous or discrete forcing to account for the force exerted by the bluff bodies on the flow, as summarized by Mittal and Iaccarino [2005]. Furthermore, the method in general is straightforward to implement in existing codes, and only adds a relatively small computational overhead. However, discontinuities in quantities of interest (eg. velocity, pressure,
or temperature or density) often arise as a result of implementing the IBM. This can give rise to computational challenges, particularly for simulations of incompressible viscous flows that use spectral discretizations (i.e. Fourier or Chebyshev collocation). Discontinuities (as in the case of a wall-modeled large-eddy simulation (LES)) in the computed variables arising from the IBM lead to a numerical artifact called the Gibbs phenomenon or Gibbs ringing [Fornberg, 1998], which refers to the characteristic oscillations in the truncated series expansion of the discontinuous function. The resulting unphysical oscillations associated with the function not being smooth and/or periodic can downgrade the numerical accuracy of spectral methods; nevertheless, these methods are very appealing due to their infinite order of accuracy, provided the function is sufficiently smooth [Tadmor, 1986], and to their computational speed (i.e. quadrature in physical space versus Fourier space has $O(N^2)$ and $O(N \log N)$ operations, respectively) [Trefethen, 2000]. As such, it might not be always desirable to forego spectral methods to overcome the errors resulting from Gibbs ringing, particularly in mixed spectral/finite difference codes where Gibbs ringing error is usually restricted (along the direction using finite difference) to the region of the domain occupied by the solid. Therefore, assessing the impact of these errors on the simulated flow and transport, and developing approaches that can eliminate or at least mitigate them, are important challenges in numerical simulation of fluid flow and transport. Avoiding or reducing Gibbs ringing is of both theoretical and practical interest. It has been extensively studied theoretically for problems that involve non-smooth or non-periodic functions that have analytical expressions [Gottlieb and Shu, 1997, Jung and Shizgal, 2004, Pasquetti, 2004]; however, the approaches proposed for treating the oscillations are not always directly transferable to numerical solutions of discrete functions. For practical computational physics and engineering applications, the challenge imposed by the oscillations associated with the Gibbs ringing spans across different disciplines, such as environmental turbulent
flows [Chester et al., 2007, Tseng et al., 2006], aeroacoustics [Wells and Renaut, 1997, Kaul, 2013] and reactive chemical transport [Adomaitis, 2001], and various strategies have been attempted to mitigate it.

Since Gibbs ringing is essentially related to the slow decay of Fourier coefficients, it is natural to test methods that attenuate the Fourier coefficients at the high frequencies that would be contaminated by the oscillations [Gottlieb and Orszag, 1977]. Applying spectral filters to accomplish that however removes the physical high wavenumber components, and it becomes difficult to assess the accuracy of this type of method in recovering the original function [Mariano et al., 2010]. Goldstein [1993] noted that if the grid resolution is not high enough, more energy will be contained in the higher wavenumbers and thus spectral filtering could reduce the accuracy of the solution. As an alternative remedy, filtering/smoothing in the physical space can also reduce Gibbs ringing by allowing the spectral computations to be applied to a smoothed version/copy of the function. In the IBM implementation of Goldstein [1993], a virtual force inside the bluff body was applied to obtain a smooth velocity field. Lamballais et al. [2008] smeared the immersed boundary force over interfacial computational points by multiplying a Gaussian weight factor according to the distance from the interface. Although it reduces the oscillations, the location of the interface becomes diffuse. It is also worth noting that by using a sixth-order compact scheme of quasi-spectral accuracy, they observed non-negligible Gibbs oscillations that are usually not present with lower-order finite difference scheme. In addition, creating an internal flow field of no physical significance was also applied in direct numerical simulations (DNS) with quasi-spectral method coupled with IBM [Lamballais et al., 2010, Lamballais and Silvestrini, 2002], which offered better regularity across the immersed boundary. Smoothing the velocity field in physical space can also be achieved using a radial basis function interpolation method, as illustrated by Fang et al. [2011], who successfully reduced Gibbs ringing using this
approach. However, the computations needed to find the appropriate radial basis function representations and the iterative procedure in solving the Poisson equation for pressure combine to result in a high computational cost for this method. As a less expensive way to implement the physical space smoothing, Tseng et al. [2006] applied a Laplacian operator iteratively to the velocity field. However, the resulting smoothed field is sensitive to the initial values of the function and the number of iterations.

In general, the concept of smoothing the original function via radial basis functions [Fang et al., 2011], adding a Laplacian operator [Tseng et al., 2006], or through Fourier continuation analysis [Bruno et al., 2007, Bruno and Lyon, 2010] have been demonstrated to be effective in reducing the Gibbs phenomenon whenever the function is non-smooth. However, given some of the challenges of these approaches mentioned above, the purpose of this work is 1) to assess the influence of the Gibbs ringing errors on the simulated velocity and temperature fields in wall-bounded flows over hot bluff bodies to better understand the implications of these errors, and 2) to propose and test a new cost-effective and robust procedure to reduce the resulting oscillations and errors in simulations of high Reynolds number flows with IBM. The findings will be of significant value to the increasing number of scientists who are using the immersed boundary/interface method, combined with high-order numerical schemes, particularly given the relative scarcity of comparable studies that also address the problems of temperature or mass transfer. As we will show in this study, the consequence of Gibbs ringing is even more important for scalar exchanges at the solid-fluid interface.

The outline of the chapter is as follows. In the next section, we describe the new cost-effective smoothing procedure and show some a priori results of its effectiveness in reducing the ringing of the spectrally-computed derivatives of arbitrary discontinuous functions. In section 3, we briefly describe the implementation of the IBM in
an LES code, along with the new smoothing approach. In section 4, we present two a posteriori LES test cases to illustrate the impact of Gibbs ringing on the velocity and temperature fields, and the improvement afforded by the smoothing procedure. Conclusions are drawn in the last section.

2.2 Cubic interpolation smoothing

2.2.1 Gibbs phenomenon and order of accuracy

The Gibbs phenomenon refers to the nonuniform convergence behavior of a Fourier series approximation to the function $f(x)$ being approximated in the neighborhood of a discontinuity $x_0$, in the limit of $K \rightarrow \infty$, where $K$ is the wavenumber in the Fourier series [Gottlieb and Orszag, 1977] (in practice, $K > 2\pi/\Delta$, where $\Delta$ represents the computational mesh resolution). Two characteristics of Gibbs phenomenon are worth noting as summarized by Adomaitis [2001]. The first one is that the Gibbs oscillations do not vanish with increasing number of terms $N$ in the approximation series; instead, the magnitude of the oscillations asymptotically reaches a constant value of approximately 8.9% of the jump magnitude for a discontinuity of the type of a simple Heaviside step function [Mittal and Iaccarino, 2005]. The second one is that the oscillatory behavior extends beyond the discontinuity and influences the function approximation at all points in the physical space. Therefore, using spectral methods to calculate derivatives of quantities that are contaminated by these Gibbs errors will have a global impact on the model performance. To understand the origin of these errors, we point out that the order of accuracy of a spectral approximation of a derivative of order $n$ of a function depends on the smoothness of its higher derivatives of order $> n$ [Gottlieb and Orszag, 1977]. The following theorem puts this in a more formal context:
Let $u \in L^2(\mathbb{R})$ have a $q$th derivative ($q \geq 1$) of bounded variation, and let $w$ be the $q$th spectral derivative of $u$ on the discretized grid with spacing $h$, where $L^2(\mathbb{R})$ is the Hilbert space of complex square-integrable measurable functions, and $h$ is assumed to be the spacing of a uniform mesh, without loss of generality. If $u$ has $p-1$ continuous derivatives in $L^2(\mathbb{R})$ for some $p \geq q+1$ and a $p$th derivative of bounded variation, then the absolute error in the spectral derivatives scales as $|w_j - u^q(x_j)| = O(h^{p-q})$, $h \to 0$, where $u^q(x_j)$ is the exact $q$th derivative of $u$ (for detailed proofs, please refer to [Canuto et al., 1993]). Thus, if a function is not smooth at a point (e.g. the velocity at the solid-fluid interface which has a discontinuous first spatial derivative), its (exact) derivatives will not be continuous and the accuracy of their spectral approximation will therefore be adversely affected. As an example, if one is interested in the first derivative ($q = 1$), then attaining second-order accuracy for a spectral approximation requires that $p - q = 2$, which requires that $p = 3$ and $p - 1 = 2$; i.e. the function must have continuous first and second derivatives.

### 2.2.2 A priori tests of the cubic interpolation method

To obtain second-order accurate first derivatives with Fourier spectral method, the theorem above implies that continuity of the second derivative of a function is required [Trefethen, 2000]. An interpolation method across the discontinuity must therefore not only ensure continuity of the function itself, but also of its higher derivatives. For example, second-order accuracy of the first derivative near the neighborhood of the discontinuity can be accomplished simply by applying a cubic interpolation to the function using two points in the fluid domain from each side of the discontinuity as illustrated in Fig. 2.1. The resulting system is a four-by-four Vandermonde matrix, which is easy to solve. Thus, a uniquely determined cubic polynomial can be found with the four points. This is the interpolation scheme we apply and test a posteriori in this paper in numerical solutions of the Navier-Stokes equations. Note
Figure 2.1: A schematic picture showing the procedure of cubic interpolation smoothing, where two points (in the rectangular box) on each side of the discontinuity are used to construct the cubic polynomial $a_1 x^3 + a_2 x^2 + a_3 x + a_4$ that is then used to construct a smoothed discrete function. The smoothed version of the function is then used in the spectral computations.

that different interpolation methods can be implemented as long as the continuity of the function and an appropriate number of higher derivatives at the interface is ensured. Also note that this method can be adapted to problems where a buffer region is introduced to make the simulation domain physically non-periodic along a direction over which spectral methods are used. As an illustration, we consider the function $f(x) = (\sin(2x) + \sin(4x)) (H(x_1') + H(x_2'))$, where $H$ is the Heaviside step function, $x_1' = x - a$, and $x_2' = x - b$ where $a$ and $b$ are the left and right limits of the introduced discontinuity, respectively (see Fig. 2.2a). Away from the discontinuity, $f(x)$ has finite well-defined analytical derivatives $g(x)$, but Fig.2.2b shows that the derivatives obtained with a spectral method without any treatment are contaminated by Gibbs oscillations, near the discontinuity as well as away from it. These spectral derivatives depart significantly from the analytically computed $g(x)$. If the derivatives inside the discontinuity are not of interest (corresponding for example to velocity derivatives inside a solid region in a flow simulation with IBM), the cubic interpolation approach can be used to obtain second-order accurate derivatives in the region of interest (the fluid region). Fig. 2.2b demonstrates that the cubic in-
Figure 2.2: (a): $f(x) = (\sin(2x) + \sin(4x)) \left( H(x_1') + H(x_2') \right)$, and a smoothed $f(x)$ where the values inside the discontinuity are interpolated using the cubic interpolation. (b): The first derivative of $f(x)$, $g(x)$, computed analytically, using 4th-order finite difference method, using the Fourier spectral method on the original $f(x)$ (No Smooth), and using the Fourier spectral method on the smoothed $f(x)$ (Smooth).

terpolation smoothing procedure very effectively removes the Gibbs oscillations in the derivatives. Computation of the derivatives with a 4th order accurate finite difference scheme on the unsmoothed $f(x)$ are also shown and have larger errors than the spectral method with smoothing; this is consistent with the observation by other investigators (as mentioned in the introduction) that higher-order finite difference schemes are more adversely affected by the discontinuity of the function [Lamballais and Silvestrini, 2002]. However, the errors in the finite difference gradients are related to their stencil, which becomes longer for higher-order schemes, extending into the solid, and are not exactly similar to the Gibbs phenomenon. Fig. 2.3 depicts another test for the function. Similar to Fig. 2.2, the resulting Gibbs oscillation is effectively removed by the cubic interpolation smoothing. Again, the Fourier spectral method outperforms the 4th order finite difference method in achieving a higher accuracy.

Recall from the theorem that the second-order accuracy was the lower limit for the spectral method, but the actual accuracy can be of higher order since the interpolation, while designed to ensure continuity of the second derivative, in practice might
Figure 2.3: (a): \( f(x) = (10x^2)^{-1}(H(x_1') + H(x_2')) \), and a smoothed \( f(x) \) where the values inside the discontinuity are interpolated using the cubic interpolation. (b): The first derivative of \( f(x) \), \( g(x) \), computed analytically, using 4th-order finite difference method, using the Fourier spectral method on the original \( f(x) \) (No Smooth), and using the Fourier spectral method on the smoothed \( f(x) \) (Smooth).

also yield continuity of higher derivatives. The higher order achieved by the smoothed spectral computation is illustrated in Fig. 2.4, which compares the maximum point-wise errors \( \max(|g(x_i) - g_{sp,fd}(x_i)|) \), where \( g(x) \) is the analytically-computed first derivative of \( f(x) \) and \( g_{sp,fd}(x) \) is the derivative calculated using a spectral or finite difference method. In Fig. 2.4a, one can also observe that the error decreases with \( N \) (the number of points used to discretize the function, or numerical resolution) if the cubic interpolation method is applied to the function before calculating the derivatives using Fourier spectral method, second, and fourth order finite differences. The error of the unsmoothed spectral computation on the other hand becomes worse with increasing resolution. Note that unlike the previous figures (Figs. 2.2 and 2.3), the finite-difference gradients in Fig. 2.4a are computed based on the smoothed function. When the unsmoothed function is used (as in Figs. 2.2 and 2.3), the errors of the second and fourth order finite difference methods increase in a similar way to the spectral method without smoothing treatment, as shown in Figure 2.4b. While away from the discontinuity the finite difference methods do not require a smoothing of
the function since their error is local, the maximum error is occurring very near the discontinuity such that the stencil of the finite difference methods extends into the discontinuity and their accuracy is thus reduced. The analysis in Fig. 2.4 is only for $f(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2'))$, but a qualitatively similar trend is obtained for $f(x) = (10x^2)^{-1}(H(x_1') + H(x_2'))$. Our proposed interpolation approach hence also reduces these finite differencing errors near the discontinuity. This a priori test illustrates that estimating the spatial gradient with a spectral method to an adequate degree of accuracy is feasible near a discontinuity through interpolation of the function into the discontinuous region, without any modification to the function outside of that region, in a manner that ensures continuity of the second derivatives. While the derivatives inside the discontinuity are not correct, we reiterate that with the IBM approach this corresponds to regions inside the solid where regardless of the gradients obtained, the velocity is reset to zero by the IBM during time-advancement of the solution. Our method ensures that the computed gradients in the fluid regions are accurate, while maintaining the zero velocity in the solid region (for the pressure solver and wall model) to yield the correct forces on the fluid.

As Lele [1992] pointed out that comparing the Fourier coefficients of the derivative obtained from numerical scheme with the exact coefficients can give some interesting insights. Therefore, we look into the impact of smoothing on the Fourier transform of $g(x)$ for $f(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2'))$ by computing the amplitude and phase of the Fourier coefficients of $g(x)$. We compared the amplitude and the phase of the analytical $g(x)$ with those of $g_{sp}(x)$ (with smoothing) and $g_{sp}^{asm}(x)$ (without smoothing). A fast Fourier transform is applied to the various computed gradients to obtain the amplitude and phase information. Figs.2.5a and b show the excellent agreement in terms of both amplitude and phase when the function is smoothed prior to computing the derivatives. On the other hand, the positive amplitude errors introduced in the high wavenumbers are clearly visible for $g_{sp}^{asm}(x)$ in Fig. 2.5c; the
Figure 2.4: a) The error between approximate values of $g(x)$ and the analytical result as a function of resolution $N$, i.e. the number of collocation points; the finite difference estimates are computed form the smoothed function. b) The errors when no cubic interpolation smoothing is implemented for the finite difference schemes; the errors increases with $N$ for the finite difference methods similarly to the Fourier spectral method without smoothing.

Phase errors also scatter across all wave numbers. Fig. 2.5c gives additional evidence that a cubic interpolation method in physical space will effectively rectify the amplitude error at high wavenumbers and correct for the phase error, which occurs for almost all wavenumbers. The large errors associated with the high wavenumbers (i.e. small spatial scales) when no smoothing is applied will have a profound impact in the subsequent a posteriori tests.

Since eventually the goal is to apply this simple and effective cubic interpolation procedure to turbulent flow simulations, we tested the robustness of this method with the presence of a synthetic turbulent signal added to the original function $f(x)$. The turbulent perturbation signal $f_{turb}(x)$, which is added to the function, follows the 5/3 energy spectrum typical of Kolmogorovs inertial-range turbulence, with a turbulent length scale representative of the one resolved in turbulent simulations such as large eddy simulations. $f(x) + f_{turb}(x)$, with and without smoothing interpolation, are shown in Fig. 2.6. In this case, no analytical derivatives are available, but the figure clearly illustrates that near the discontinuity, the Gibbs oscillations are effectively
Figure 2.5: Comparison of the amplitude (a) and phase (b) of the analytical result $g(x)$ and the one obtained from Fourier spectral method in which the original function $f(x)$ is treated with the proposed method $g_{sp}(x)$; the color bar represents the wavenumber. (c) (d): same as (a) and (b) but without cubic smoothing of the function $f(x)$.

reduced and the FFT with smoothing agrees well with the 4th order finite difference derivatives (based on smoothed function).

2.3 LES-IBM with cubic interpolation

While in the previous section we illustrated the effectiveness of cubic interpolation in reducing Gibbs ringing errors, the actual application of this method in a turbulent flow simulation code will likely raise additional challenges and it is unclear if the method will work equally well in a posteriori tests. It is also very important to assess the degradation in the quality of the flow simulation due to Gibbs errors, and
Figure 2.6: a) with the superimposed turbulent signal, and its the smoothed version. b) The first derivative $df/dx = g(x)$ using 4th order finite difference method with smoothing, Fourier spectral method without smoothing and with smoothing. For clarity, only the region close to the discontinuity is shown in b. However, the impact of artificial oscillations extends globally.

the benefit of applying the interpolation treatment. To conduct these a posteriori tests, we will consider a pseudospectral large eddy simulation (LES) code with an IBM scheme and apply it to simulate a viscous incompressible flow transporting a passive scalar emitted at the solid surface (e.g. heat from a building wall). We use the wall-modeled LES approach (see [Pope, 2000, Sagaut, 2010]), in which a discrete time momentum forcing is used to simulate the immersed boundary force, such that the velocity field inside the obstacle is zero. We select to test the method in a wall-modeled LES, since tests in DNS or wall-resolved LES are less challenging. The resolved velocity in DNS and wall-resolved LES transitions more gradually to the no-slip condition near the wall, compared with the wall-modeled approach. A sharper transition (in wall-modeled LES) will result in more severe Gibbs ringing and if our proposed method is effective in reducing the Gibbs ringing in wall-modeled LES, we would expect an even better performance in wall-resolved simulations. In addition, based on the a priori tests conducted in previous section as a proof-of-concept of the method proposed, we have assessed the accuracy and consistency of this method in a
simplified setting. Thus, we could further examine the consequence of the proposed method in a challenging scenario, which is the wall-modeled LES. A Lagrangian scale-dependent dynamic subgrid-scale model is used [Bou-Zeid et al., 2005b]. For details of the LES code, please refer to [Albertson and Parlange, 1999]. Here we give a brief description of the LES-IBM code, while detailing the cubic interpolation smoothing treatment. The LES code solves the resolved continuity, Navier-Stokes, and scalar conservation equations (we will omit the usual tilde above the variables that denotes filtering for simplicity, but all the variables we will discuss are the filtered resolved components solved in LES unless otherwise noted):

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

\[
\frac{\partial u_i}{\partial t} + u_j \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = -\frac{\partial p}{\partial x_i} + F_i - \frac{\partial \tau_{ij}}{\partial x_j} \tag{2.2}
\]

\[
\frac{\partial s}{\partial t} + u_i \frac{\partial s}{\partial x_i} = -\frac{\partial q_i^s}{\partial x_i}, \tag{2.3}
\]

where \( t \) denotes time, \( u_i \) is the resolved \( i \)th component of velocity, \( p \) is a modified pressure, \( F_i \) is a body force (that excludes the IBM force but can include gravity and a constant driving pressure gradient for boundary layer flows, for example), \( \tau_{ij} \) is the deviatoric part of the subgrid stress tensor. The density is assumed equal to 1 (all the equations are normalized so the numerical value of the density is irrelevant). In equation 2.3, \( s \) denotes the scalar quantity and \( q_i^s \) is the \( i \)th component of the subgrid scale scalar flux. The Einstein convention is used here, where summation is implied for repeated indices. Since the code uses the second-order Adams-Bashforth time stepping method, the discretized form of equation can be broken into two steps:

\[
u^* = \Delta t \left( \frac{u_i^n}{\Delta t} + \frac{3}{2} RHS^n_i - \frac{1}{2} RHS^{n-1}_i + \frac{1}{2} \frac{\partial p^{n-1}}{\partial x_i} \right), \tag{2.4}
\]
and

\[ u_i^{n+1} = \Delta t \left( \frac{u_i^*}{\Delta t} - \frac{3}{2} \frac{\partial p^n}{\partial x_i} + f_i \right), \tag{2.5} \]

where \( u^* \) is an intermediate velocity, \( n \) refers to the number of the current time step, \( \Delta t \) is the time step; \( RHS_i = -u_j \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) + F_i - \frac{\partial \tau_{ij}}{\partial x_j} \); \( F_i \) is the body force; and \( f_i \) is the immersed boundary force given by:

\[ f_i = \begin{cases} 0 & \text{for points outside the immersed boundary (fluid)}, \\ \frac{3}{2} \frac{\partial p^n}{\partial x_i} - \frac{u^*}{\Delta t} & \text{for points inside the immersed boundary (solid).} \end{cases} \tag{2.6} \]

In our code, the intermediate velocity \( u^\ast \) is set to zero inside the solid area, which simplifies the equation of the body force. Alternative approaches to the implementation of the IBM can be used (e.g. [Fang et al., 2011]), but here we adhere to the implementation detailed by Chester et al. [2007] since our focus is on the Gibbs phenomenon rather than the details of the IBM. Before solving Eq. 2.5 for \( u_i^{n+1} \), we must obtain the pressure field, which is so far unknown for time step \( n \). The divergence of Eq. 2.5 is taken and the resulting Poisson equation is solved for the modified pressure \( p \), while imposing that \( \frac{\partial u_i^{n+1}}{\partial x_i} = \frac{\partial f_i}{\partial x_i} = 0 \) to yield a divergence free velocity field at time \( n + 1 \). The resulting Poisson equation is

\[ \frac{\partial^2 p}{\partial x_i^2} = \begin{cases} \frac{2}{3\Delta t} \frac{\partial u_i^*}{\partial x_i} & \text{for points outside the immersed boundary (fluid)}, \\ 0 & \text{for points inside the immersed boundary (solid).} \end{cases} \tag{2.7} \]

It is also worth noting that if the Gibbs oscillations are present in the velocity gradients, such errors will also propagate spatially by solving the Poisson equation an elliptic PDE resulting in a global influence from these oscillations even along directions that do not use spectral discretization. While vertical derivatives are computed using a second-order centered-difference scheme in the code (and hence no special treatment for the Gibbs phenomenon is required), the Fourier-based pseudospectral
method is used for calculation of the horizontal derivatives. The horizontal partial
derivatives for $u_i$ are computed independently in the $x$ and $y$ directions following:

$$\frac{\partial u_i(x,y,z)}{\partial x} = \sum_{k_x} [\hat{u}_i(k_x,y,z)(i k_x)] e^{i k_x}$$ (2.8)

and

$$\frac{\partial u_i(x,y,z)}{\partial y} = \sum_{k_y} [\hat{u}_i(x,k_y,z)(i k_y)] e^{i k_y}$$ (2.9)

where $\hat{u}_i$ is the wavenumber space representation of $u_i$; $k_x$ and $k_y$ are the wavenumbers in the $x$ and $y$ directions. Note that $x$ and $y$ in equations 2.8 and 2.9 correspond to the quadrature points, where $u_i$ assumes its values. The cubic interpolation method described in the previous session is here applied independently in each of the $x$ and $y$ directions before obtaining the horizontal gradients spectrally using equations 2.8 and 2.9. A level-set method [Chester et al., 2007] that uses a signed distance function is used to define or track the interface where cubic-interpolation smoothing is carried out. Similarly, this same procedure is applied to all other variables for which pseudospectral derivatives are calculated, namely: $\tau_{ij}$ in Eq. 2.2, and $s$ and $q_i^s$ in Eq. 2.3. It is also worth reemphasizing that the interpolated values inside the obstacle will not affect the values outside the obstacle since in the pressure solver and the wall model the zero velocity imposed by the IBM is used, while the smoothed functions are only used when taking the spectral derivatives of the variables indicated above. The desired velocity field will be automatically generated by using the correct immersed boundary force $f_i$. The wall model used in this study is an equilibrium log-law velocity and scalar concentration model to account for the drag and scalar flux that the resolved obstacle surface applies to the surrounding fluid. There is no wall model for a generalized geometry like the ones we use here, but for the very high Reynolds numbers simulations considered here, the first grid point will fall in the inertial layer [Anderson and Meneveau, 2011, Schultz and Flack, 2009], and thus the use of the
equilibrium logarithmic law is justified. Other approaches have been proposed in the literature but since this paper is mainly concerned with the impact and reduction of Gibbs phenomenon, we do not focus on improving or discussing the role of the wall model. The current LES-IBM with the cubic interpolation approach only increases the computational overhead by 3 to 5% in the following numerical tests. In general, it is inexpensive to obtain the desired smoothed fields before the spectral method is used for calculating horizontal derivatives. This is a major advantage of this approach.

2.4 Numerical tests

In this section we consider two test cases, one is the turbulent flow over a staggered array of four cubes (in a periodic domain); the other is the scalar turbulent transfer problem over a single wall-mounted cube. The impact of Gibbs ringing and the improvement in the results associated with the cubic-interpolation IBM-LES are presented.

2.4.1 Flow over staggered cubes

The array of four staggered cubes of height $h$ (used for normalizing the vertical distances from the wall) was selected since it is an extensively studied configuration. Experimental measurements, DNS and LES results under fully rough conditions are all available [Coceal et al., 2007b, Xie and Castro, 2006], serving as a benchmark for detailed assessment of the impact of Gibbs phenomenon. Using the IBM-LES code described in the previous session, we simulated two test cases. The only difference is that smoothing treatment is applied to one of them. A horizontally periodic domain with free-slip impermeable top boundary condition is used for both simulations. The simulations are run for a warm-up period of 50 eddy turnover times defined as $L_z u_*/dt$, where $L_z$ is the depth of the flow (here equal to the height of the domain), $u_*$ the
Figure 2.7: Configuration showing the geometry of four staggered cubes simulated in the two cases. Left: perspective view; right: top-view. Points marked with \( x_1-x_4 \) are locations where the comparisons in subsequent figures were made. The flow enters from the bottom in right panel.

The square root of the total kinematic surface stress generated by the simulation, and \( dt \) the time step. Statistics are computed over the next 50 eddy turnover times to ensure statistical convergence. Fig. 2.7 shows the configuration of the first test case; the points labeled from \( x_1 \) to \( x_4 \) are the locations where profiles of selected parameters were taken for comparison. Fig. 2.8 shows the cross sections in \( x \) and \( y \) directions of the mean streamwise velocity \( u \) from the simulation with smoothing, showing no evidence of Gibbs ringing. The color scale indicates the magnitude of velocity. The mean velocity profiles for both SC and SCS, depicted in Fig. 2.9 show comparable results to [Xie and Castro, 2006]. The means in this paper are taken in time, as surrogates of Reynolds averages, and are denoted either by an overbar \( \bar{\cdot} \) or by angle brackets \( \langle \cdot \rangle \). The discrepancy resulting from the Gibbs ringing in the case without smoothing appears to be minimal. However, these profiles are relatively far from the immersed boundary and as shown in the previous section, the largest error introduced by Gibbs ringing is close to the first point near the discontinuity where the wall modeled stresses and fluxes in LES can be more significantly affected by these inaccuracies. Nevertheless, for this flow, the main surface drag is through the pressure/form drag, which does not seem to be very sensitive to the errors introduced by the Gibbs phenomenon near the wall.
Figure 2.8: The transects of mean streamwise velocity $\langle u \rangle$ along two vertical planes. The measurement points $x_1$-$x_4$ indicated in Fig. 2.7 are labeled. The flow is coming from left to right in the top panel and into the page in the bottom panel. The color scale indicates the magnitude of the velocity.
Figure 2.9: Comparison of the profiles of mean streamwise velocity $u$ to the results of Xie and Castro [35]. These profiles were taken at points $x_1$ (above); $x_2$ (behind); $x_3$ (in front); $x_4$ (in between) labeled in Fig. 2.7. $U_{ref}$ is a reference velocity taken at $z = 2h$. 
To investigate the errors close to the discontinuity, a horizontal transect of both the vertical and horizontal mean velocities, $\langle w \rangle$ and $\langle u \rangle$, are plotted in Fig. 2.10 for the planes immediately below and above the top of the cube along the line that connects the points $x_2$ and $x_3$. These two planes are considered here because they include the most abrupt velocity change associated with the accelerating effect at the cube top, and feature the strongest oscillations. Although the vertical profile of $\langle u \rangle$ shows good agreement with the benchmark results in Fig. 2.9, close to the interface, the presence of oscillations in Fig. 2.10 is clear. This reaffirms that the impact of Gibbs ringing is more pronounced close to the interface. The smoothing is very effective for the plane below the top of the cubes ($z = 0.94h$) and results in velocity trends for both $\langle w \rangle$ and $\langle u \rangle$ that are significantly different (a difference of about 25% for $\langle u \rangle$ above the cube) from the simulation without smoothing. However, notice that for the planes above the top of the cubes $z = 1.06h - 1.12h$, the smoothing method cannot be applied since that plane has no solid region. The sharp change in velocity there is indeed physical (as the flow goes past the top of the cube it changes its speed and direction very fast). Nevertheless, both $\langle w \rangle$ and $\langle u \rangle$ in Fig. 2.10 show less severe effect of ringing when smoothing is applied even above the cubes. Especially for the wake region from $x/h = 3 - 4$, the magenta line showing the smoothing treatment reduces the ringing. For the plane $z = 0.94h$, especially the $\langle w \rangle$ component, shows significant ringing around magnitude close to zero but it is effectively alleviated by the smoothing treatment.

While the impact of Gibbs ringing on the mean parameters was moderate, the associated numerical oscillations would be expected to be more obvious and consequential for the second-order statistics. Gibbs ringing creates oscillations that can cancel out in the mean signal if spatial averaging is performed, thus leading to mean values close to the ones unaffected by the oscillations, but the second-order statistics can be more sensitive to these oscillations since their effect adds up and manifests
itself as higher second-order moments in LES. Figs. 2.11 and 2.12 show the comparisons of the LES-IBM simulated co-variances (stresses) and root-mean-square (rms) velocities to those from LES, DNS and experiments reported by Xie and Castro [2006]. The second-order quantities in these figures represent the statistical characteristics of turbulence. Fig. 2.10 depicts a closer agreement between the total Reynolds stress (i.e. the sum of resolved part and the SGS part) simulated with smoothing and those by Xie and Castro [2006], compared to the simulations without smoothing, showing a more pronounced improvement than the mean profiles in Fig. 2.9. The unsmoothed simulations underestimate the stress near the top of the cubes at locations x1 and x2, and overestimate it at locations x3 and x4. The underestimations can be as large as about 30% of the peak value of the Reynolds stress. The overestimations in x3 and x4 are about 10% of their peak value. Note that we are not only comparing to the experimental results here, which could be contaminated by experimental errors, but also to the DNS and LES of Xie and Castro [2006] that use neither an IBM approach nor spectral numerical methods, and can be as such considered as the reference for these comparisons. At x2 the peak in the total Reynolds stress that occurs just above the top of the cube is better predicted when smoothing is applied. At x3, especially
below the height of the cube, Fig. 2.11 shows that the simulation with smoothing accurately captures the increasing trend of $\langle u'w' \rangle$ below the first minima. Fig. 2.12 shows the root-mean-square (rms) value of both streamwise velocity $\langle u \rangle$ and vertical velocity $\langle w \rangle$ at points x2 and x3. We should acknowledge that this comparison is a bit challenging since for the LES we are only showing the resolved rms velocities (we prefer not to attempt to model the SGS components since we are not certain about the accuracy of the available models in complex terrain), and since these quantities are more sensitive to the Reynolds number differences between experiments, DNS, and LES than the mean velocities or stresses. But the comparison might still be informative. A slightly better agreement with the Xie and Castro [2006] simulations and experimental data is also found here when the smoothing treatment is applied, but the differences are not as significant as with the stresses. As stated previously, the surface drag is dominated by form drag. For a steady constant pressure gradient driven flow, the total wall friction velocity $u_\tau$ is set by the pressure gradient imposed (pressure forcing has to balance surface drag). The friction velocity $u_*$ that the experimental/LES/DNS results of Xie and Castro [2006] is taken as 0.89. The value 0.89 is found for this geometry from theoretical argument given by Coceal et al. [2006], Xie and Castro [2006]. It can be understood as an effective friction velocity of the rough channel flow. This $u_*$ was used to non-dimensionalize the LES/DNS/Experimental results [Xie and Castro, 2006] that we compared with; therefore, we also adopted the same non-dimensionalization for our LES results. Despite the minor influence of the smoothing for these turbulent statistics, the agreement with the experimental/LES/DNS results away from the bottom wall validates the accuracy of our model, while the discrepancy at the bottom wall is related to the fact that the DNS and LES of Xie and Castro [2006] resolve the wall region and are therefore representing the trends in the buffer and viscous sublayer near the wall. On the other hand, our LES
Figure 2.11: Profiles of the Reynolds stress $\left\langle u'w' \right\rangle$ taken at points x1 (above); x2 (behind); x3 (in front); x4 (in between), as labeled in Fig. 2.7.

assumes a much higher Reynolds number, such that the first grid point above the bottom wall is already in the inertial log-region.

The subgrid-scale (SGS) components are also some of the higher order moments that are expected to show sensitivity to Gibbs oscillations in LES. The SGS stress component $\tau_{13}$ is depicted in Fig. 2.13a along a streamwise line behind the cube (point x4) at a height $z = 1.06h$, i.e. immediately above the top plane of the cube. The reduction of the oscillations when smoothing is applied is clear and demonstrates the effectiveness of this smoothing treatment in improving both the resolved and the subgrid scale components. Note the difference of about 100% in the magnitude of the SGS stress near the interfacial computational points. Another key quantity in LES is
Figure 2.12: Profiles of the rms streamwise and vertical velocities $u$ and $w$ taken at points $x2$ (behind); $x3$ (in front); labeled in Fig. 2.7.

the kinetic energy dissipation by the subgrid scales, which is often postulated to be the most important quantity an SGS model should reproduce [Meneveau and Katz, 2000]. Gibbs ringing can lead to excessive spatial gradients and thus to overestimation of the resolved strain rate $S_{ij}$, and this could contribute to an over-estimated SGS dissipation rate of resolved kinetic energy $\epsilon = -\langle \tau_{ij}S_{ij} \rangle$. As can be seen in Fig. 2.13b, the SGS dissipation rate of resolved kinetic energy, depicted along a streamwise line spanning the whole domain just beneath the top of the cube, is strongly overestimated and oscillates significantly when no smoothing is applied. The cubic interpolation smoothing almost eliminates the oscillations and reduces the magnitude of $\epsilon$ significantly. These observations are consistent with the a priori amplitude-phase
analysis, such that the high wavenumber, i.e. small spatial scales, are more prone to the amplitude error. Note that the increase from the first point in front or behind the cube to the next point away from the cube is partially related to the transition from a wall model to an SGS model, and it is difficult to disentangle its effect from that of the Gibbs phenomenon in that region.

To further analyze the details of Gibbs phenomenon on higher order statistics, we consider the radial power spectra of $u$ and $w$ shown in Figs. 2.14 and 2.15, respectively, both with and without smoothing. The radial power spectrum is obtained by time averaging 15 power spectra, each of which is constructed from the instantaneous velocity field in a horizontal plane ($x$-$y$ plane). The radial wavenumber is defined as $k_r = \sqrt{k_x^2 + k_y^2}$. The horizontal axis is the radial wavenumber normalized by $L_x$, which is the streamwise length of the domain. The radial power spectrum will represent the contributions of ringing from both directions across different physical scales. For planes that are below the height of the cubes, the signature of the underlying geometry are shown as the periodic ‘bumps’ in the spectra, where the first bump cor-
responds approximately to the obstacle length scale (indicated by the vertical line) or the harmonics of that scale, and the subsequent bumps are all harmonics of the building length scale. Nevertheless, we can identify two major impacts related to Gibbs phenomenon shown by the velocity spectra in Figs. 2.14 and 2.15. The first impact is the characteristic oscillations near the grid-scale (highest resolved wavenumber) that are clearly seen in the higher peak in the second to last point on the velocity spectra for the unsmoothed case. The $w$ component shows a more pronounced effect, which is eliminated in the simulation with smoothing depicted in 2.15, thus confirming the successful removal of Gibbs oscillations. As shown in Fig. 2.14, the variance of $u$ distributed over the higher wavenumbers (above $k/L_x = 0.1$) is also larger in the case with cubic interpolation. Overall, the presence of Gibbs phenomenon does not change the distribution of energy in larger scales significantly, which explains why the mean and second-order moments were moderately affected by the associated errors. Hence, not much difference in the staggered cube case was found in Figs. 2.9, 2.11 and 2.12 when the mean quantities and second moments were compared with numerical simulations or experiments. On the other hand, the effect is more significant at the smallest scales in the spectra, which explains the strong impact of the smoothing on the SGS quantities that are strongly tied to those smallest resolved scales.

2.4.2 Passive scalar transfer of a single cube

Compared to velocity in incompressible high Reynolds number flows, the transport of scalars (i.e. temperature with small thermal gradients or other passive substances) is more likely to be contaminated by Gibbs ringing. The reasons are two-fold: 1) the strongest influence from the ringing is near the boundary and thus introduce the highest error in the scalar boundary layers around the facets of the cube, where the transfer of scalars is occurring through turbulent diffusion in our wall-modeled LES (and through both viscous and turbulent diffusion in real flows), and 2) unlike
Figure 2.14: Radial power spectra $F_{rad}$ of $u$ without smoothing (left) and with smoothing (right) at four different heights below the obstacle. For clarity, only the higher wavenumber part ($k/L_x > 0.1$) of the spectra is shown.

Figure 2.15: Radial spectra $F_{rad}$ of $w$ without smoothing (left) and with smoothing (right) at four different heights below the obstacle. For clarity, only the higher wavenumber ($k/L_x > 0.1$) part of the spectra is shown.
momentum transfer that occurs through both viscous and pressure drag and that is dominated by pressure drag in high Reynolds number incompressible flows such as the one we simulate here, for scalars, the transfer is mainly through diffusive transport through the boundary layers and large errors associated with Gibbs ringing in those layers can become dominant. The configuration and set up of the numerical test are similar to the one shown for multiple cubes in Fig. 2.7, but here we only have one hot wall-mounted cube. The cube is being heated from interior, where the wall-model of the LES is coupled to a one-dimensional heat conduction equation that assumes a constant core temperature. The fluid temperature initially is 273.15 K, the core temperature is fixed at 348.15 K, and the resulting surface temperature is around 318.15 K. Temperature in this case is modeled as a passive scalar for the purpose of demonstrating the impact of Gibbs phenomenon on scalars in general. The subgrid scale (SGS) model for momentum is the same as the simulation in previous session. An eddy diffusivity model is implemented here as the scalar SGS model, in which the SGS scalar flux is modeled as \( q_s^f = -\nu T/Pr_t \), where \( \nu_t \) is the eddy viscosity obtained from the momentum SGS model and \( Pr_t \), the SGS turbulent Prandtl number set to 0.4. The warm up time is approximately over one eddy turn over time \( (L_x u_s/\Delta t) \) only for this case since reaching a steady state is not essential. One additional eddy turn over time is used to obtain the averaged statistics. Similar to the previous simulations, two cases with and without the smoothing treatment were conducted. Fig. 16 depicts the time-averaged mean passive scalar field across a horizontal \( xy \)-plane. The Gibbs oscillation is almost completely removed in the case with smoothing treatment. More importantly, the development of the thermal boundary layer and thermal wake of the cube are hindered in the simulation with no smoothing due to the oscillations, while their development follows a more physically realistic pattern in the other simulation.

The two simulated cases were only ran for a relatively short period of time, such that the absolute difference in fluid temperature between them remained small.
Therefore, we consider the quantity $\theta''$, defined as $\theta'' = (\theta - \theta_{init})/\langle(\theta)\rangle - \theta_{init}$, where $\theta_{init}$ is the initial air temperature, which is also the air temperature far from the wall, and $\langle(\theta)\rangle$ is the horizontally plane averaged fluid temperature of the case. $\theta''$ represents the relative difference in the rate of heating between the two cases, from the initial conditions which are the same for both cases. Since the set up of this test is such that the temperature increases at closer distances to the cube surface, the decrease in the time-averaged temperature cross-sections in Fig. 2.17a near the cube from the case without smoothing follows a physically incorrect trend. The small oscillations for this case are also clearly visible. These problems are corrected by the smoothing. In general, Gibbs phenomenon results in to 40-50 % less relative temperature increase near the wall. Fig. 2.17b depicts the vertical profile behind of the cube, showing significant differences between the simulations with and without smoothing. The most drastic change is near the top of the cube, where the temperature is expected to increase below the top and then steadily decrease. The results from the case with no smoothing are clearly contaminated by the Gibbs ringing, showing no appreciable increase in temperature. Thus, unlike the velocities shown in previous section, the accuracy of the mean profile of temperature can be more significantly degraded by the Gibbs errors. We have also plotted the radial power spectrum for temperature,
Figure 2.17: a) Normalized temperature $\theta''$ cross-section along the $x$ direction at the spanwise center of the cube and at $z/h = 0.5$. b) The vertical temperature profile at the back of the cube, in the middle of the domain in the cross-stream direction, and at a streamwise distance to the interface of $3\%$ of the size of the cube.

but we do not show it here since it is quite similar to the power spectra for the velocities depicted in Figs. 2.14 and 2.15. The cube-scale still imposes a characteristic signal in the spectra, and the simulation without smoothing yields a spurious increase in variance at small scales due to Gibbs ringing that is removed by the smoothing procedure applied to the other case.

### 2.5 Conclusions

In this chapter, we propose an approach for reducing the Gibbs phenomenon in simulations of incompressible flows in the context of the immersed boundary method. Compared to the previous solutions to this problem, we have demonstrated that this method is both effective and computationally efficient. The findings are particularly relevant for high Reynolds number incompressible flows in applications in engineering or environmental fluid mechanics and mass transfer problems with the IBM approach.
After a proof-of-concept of the proposed method using a priori tests, the study analyzed and compared the effect of numerical errors caused by the Gibbs phenomenon in both turbulent momentum (where our results were compared to other experimental and numerical results) and scalar transfer problems. The mean velocities and second-order resolved statistics are moderately affected by the Gibbs phenomenon, with the co-variances being more sensitive to the errors than the variances or root-mean-square values. This was illustrated by comparing the various parameters at multiple points to experimental, DNS, and LES results from a code that does not use spectral computations or the IBM approach. The statistics related to the SGS scale were found to be significantly more sensitive to Gibbs errors, this is related to the larger impact of these errors on the smallest resolved scales (highest wavenumbers) as illustrated by both the a priori and the a posteriori tests. Regardless of the magnitude of the impact of the Gibbs phenomenon, our proposed smoothing approach significantly improved the results for all parameters. The second-order resolved statistics showed better agreement with the results from the literature, and the trends were physically more realistic. These conclusions are also supported by the velocity spectra, which illustrated the spurious increase in energy at the smallest resolved scales due to the Gibbs ringing and thus explained why the SGS statistics are the most sensitive to the associated errors. Compared to the impact on momentum, scalar transfer simulations can be much more severely affected by the Gibbs ringing simply because of the nature of transfer mechanism. Our simulations depicted the incorrect physical trend in the temperature profile in the unsmoothed case near the boundary, and how the smoothing approach can correct the problem. Moreover, the noted increase in computational overhead is more than offset by the profoundly improved characterization of scalar fluxes. In general, we can conclude that the Gibbs phenomenon associated with spectral method needs to be assessed and mitigated more carefully when higher-order statistics and scalar transfer are involved.
Chapter 3

Quality and Reliability of LES of Convective Scalar Transfer at High Reynolds Numbers

3.1 Introduction

Convective heat and mass transfer at high Reynolds numbers \((Re \sim 10^6 - 10^8)\) over complex surfaces is of interest for many engineering and environmental applications, such as heat exchanger design, agricultural and urban meteorology, and building energy studies. The latter applications are of growing significance due to rapidly expanding urbanization interacting with global climate change to alter the urban environment and the resource intensity of cities in complex ways. The convective heat transfer coefficient over the exterior surfaces of buildings is a key parameter for modeling the exchange of energy between buildings and their environment. This exchange needs to be quantified to calculate accurate heating and cooling loads [Mirsadeghi et al., 2013, Defraeye et al., 2011b], to assess the energy performance of the building envelope [Palyvos, 2008], and to better simulate the urban environment un-
der a changing climate [Li and Bou-Zeid, 2014]. In addition, with the heat-mass transfer analogy [Chilton and Colburn, 1934], knowledge on the turbulent transfer of temperature (under conditions where it can be considered as a passive scalar) is transferable to studies on the exchange of other scalars, especially carbon dioxide and moisture [Blocken and Carmeliet, 2006], which are important for example for assessing the performance of green roofs [Sun et al., 2014, 2013]. For urban climatological and meteorological studies, it is crucial to simultaneously capture the turbulent heat and water vapor surface fluxes, which are typically parameterized through an urban canopy model (UCM) [Masson, 2000, Wang et al., 2013, Grimmond et al., 2011, 1986] in coarse geophysical simulations. The transfer coefficients for heat and water vapor are important parameters in these UCMs [Hagishima et al., 2005], but their current parameterizations are partially based on experimental results that are over 90 years old [Jürges, 1924]. Improved parameterizations would involve environmental turbulent boundary layer flows over large roughness elements the height of which can be a significant fraction of the total boundary layer depth. Such surfaces are termed very rough in Castro et al. [2006] and the resulting flow differs from the classic rough-wall boundary layers discussed for example in Jiménez [2004] where the height to boundary layer depth ratio is limited to be below 0.025. Advancing our understanding of the fundamental transport processes of heat and moisture over such complex surfaces, and how to model them via transfer coefficients beyond the current state of the science, is hence urgently required in view of the wide range and importance of the related applications. Three different approaches have been traditionally taken to gain a better understanding of the convective transfer coefficients. The first approach is placing scale models in wind tunnels and measuring the convective transfer of either some substance or temperature, while minimizing the effect of buoyancy (which could nonetheless be quite important in real urban terrain). These studies [Aliaga et al., 1994, Igarashi, 1985, Meinders et al., 1998, Meinders and Hanjalić, 1999, Naka-
mura et al., 2001] often considered cases at lower Reynolds numbers (10^3-10^4) (due to length scale limitations), with a developing turbulent boundary layer in a parallel channel flow. Mass transfer experiments, usually with Naphthalene sublimation techniques [Castro et al., 2006, Barlow et al., 2004] or water evaporation [Narita, 2007], were performed to study the mass transfer from surface-mounted cubes in a wind tunnel. These are only some examples of wind tunnel studies from the extensive literature, which was summarized in relatively recent reviews [Defraeye et al., 2011b, Palyvos, 2008]. One advantage of wind tunnel studies is that the spatial variation of heat/mass transfer coefficients along the surfaces of the bluff elements can be accurately measured. The setup of the experiments can also be varied to investigate the effects of different angles of attack [Igarashi, 1985] and geometric configuration of the roughness elements [Aliaga et al., 1994], among other topographically complexities. However, a simple extension of these studies to the environment has to be handled with caution. The Reynolds number of the typical atmospheric boundary layer (ABL) is 3-4 orders of magnitude higher than that of common wind tunnels. Unlike momentum exchange, which is fully dominated by form/pressure drag over complex topographies at high Re, heat and mass exchanges are always performed by molecular conduction or diffusion in the vicinity of the complex interface and do not lose their dependence on the molecular heat and mass diffusivities at high Re. Neither the convective to conductive/diffusive scaling represented by the Nusselt number for heat (Nu) or Sherwood number for mass (Sh), nor the inertial scaling given by the Stanton number (St \sim Nu/Re), become independent of Re in general (See Lienhard [2013]). Re-independence for St might be approached or expected only if the flow over each facet is itself also fully rough [Webb et al., 1971], which is not always the case over urban terrain since the surfaces of building facets might be smooth or transitional. The empirical correlations of Nu, Sh, or St with Re obtained from these scale model experiments are thus not directly applicable to heat or mass transfer from
buildings [Narita, 2007]. In addition, the usually thin inflow turbulent boundary layers [Defraeye et al., 2011b] and the low turbulent intensity levels are further reasons why wind tunnel studies of heat and mass transfer, although providing very valuable insight, have limitations that preclude the direct application of their findings to large scale flows at high $Re$, such as flows in the real natural environment [Test et al., 1981]. Another approach that overcomes the problem of low $Re$ in wind tunnel studies is full-scale experiments conducted outdoors on buildings or structures [Loveday and Taki, 1996, Emmel et al., 2007, Yazdanian and Klems, 1994, Clear et al., 2003, Liu and Harris, 2007]. These field experiments give very valuable information especially on the correlation between the heat transfer coefficient and wind speed, which can be generalized to a power-law relation between $Nu$ and $Re$. One manifestation of the continued dependence of heat and mass exchange on $Re$ is that the exponents in such power laws are themselves $Re$ dependent, and thus these empirical relations apply only in the range of $Re$ in which they were developed. From the perspective of modeling, such full-scale field-derived empirical relations are therefore useful for both building energy simulations and urban climate studies [Mirsadeghi et al., 2013]. However, generalization of the findings can also be challenging due to the influence of the exact shapes of the building facets, the texture/roughness of the building surface materials, and the surrounding structures in the outdoor environment. In addition, the positions at which the temperature and wind velocity are measured vary across different field studies, further complicating inter-comparisons between them to extract more universal empirical relations. Numerical simulations are another useful methodology to study this problem. Reynolds averaged Navier-Stokes (RANS), large-eddy simulations (LES) or direct numerical simulations (DNS) have been carried out in the recent years to study the turbulent transfer of momentum and scalars over rough surfaces with roughness elements that mimic buildings or urban canyons [Park and Baik, 2013, Boppana et al., 2012, Defraeye et al., 2012, Liu et al., 2013]. Since the
computational cost of resolving the viscous layer (i.e. DNS [Leonardi et al., 2003, 2015, Coceal et al., 2007b, 2006] or wall-resolved LES [Pope, 2000]) is too high for applications at Re commensurate with the real-world (limiting these techniques to low Re where the same challenges discussed above for wind tunnels reemerge), wall modeling is often adopted for RANS or wall-modeled LES studies. The ‘law of the wall’ or related equilibrium approaches, which are based on the concept of universal behavior of momentum and scalars in the inertial (logarithmic) layer, are often adopted [Spalding, 1962, Giometto et al., 2016]. These types of wall models have some known caveats in complex flow regions [Launder, 1988]; however, good agreement of models using such equilibrium laws with experiments have been found by both Park and Baik [2013] and Liu and Chung [2012] in their studies of transfer of scalars over geometrically complex surfaces. The application of such equilibrium wall-models in LES pose additional challenges (compared to RANS) that were very comprehensively assessed by Wyngaard et al. [1998]. Various other more sophisticated wall-models that should in principle offer better performance have been proposed such as models that solve the boundary layer equations numerically [Cabot and Moin, 2000] or analytically [Yang et al., 2016, 2015b], or models that use a “customized temperature wall function” (CWF) (though based on low Reynolds number results) [Defraeye et al., 2011a]. Nevertheless, the challenge of wall-modeling in LES remains open [Pope, 2004, PI et al., 2013], even when the very important influence of buoyancy and how to represent it correctly in wall models (particularly for vertical walls) is ignored. This challenge frames the scope and goals of this paper. Given that for studies of turbulent flow and transport over urban-like rough surfaces at high Re wall-modeled LES is a feasible and very appealing tool, there is a growing urgent need to assess its skill in capturing turbulent scalar transport. The near-surface performance is more critical for scalars than for momentum (again due to the dominance of form drag, which is partially resolved in LES, for momentum), and as such the role of the wall-model
is more prominent. But if the shortcomings of current wall models can be investigated, quantified, and potentially overcome, the impact on future studies that focus on scalar transport under high \( Re \) scenarios can be substantial. It is worthwhile to stress again the importance of studying the heat/mass transfer problem at a Reynolds number that is representative of the real problem of interest (which is possible with wall-modeled LES), given that the scalar transfer is inherently \( Re \)-dependent. Therefore, the objective of chapter 3 is to provide a thorough assessment of wall-modeled LES by detailed comparisons to both scale-model and full-scale studies. Knowing the capabilities and limitations of this numerical approach will help to draw more sensible conclusions for future applications in building energy and urban climatology studies. A practical question we seek to answer in this chapter is: are the errors resulting from the parameterization of unresolved scales (wall and subgrid scale models) in LES larger or smaller than the errors involved in extrapolating from low-\( Re \) approaches (DNS or wind tunnels) to high-\( Re \) real world flows, for scalar transfer problems?

### 3.2 Wall-modeled LES and dynamic roughness wall model

The LES code uses the immersed boundary method (IBM) to account for presence of the roughness elements, in which a discrete time momentum forcing is used to simulate the immersed boundary force [Chester et al., 2007, Tseng et al., 2006]. The filtered incompressible continuity, Navier-Stokes and scalar conservation equations (Eq. 3.1 3.3, respectively) are solved assuming hydrostatic equilibrium (we will omit the usual tilde above the variables that denotes filtering for simplicity, but all the variables we will discuss are the filtered/resolved components solved for in LES unless otherwise
\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{3.1}
\]

\[
\frac{\partial u_i}{\partial t} + u_j \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = -\frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + F_i + B_i, \tag{3.2}
\]

\[
\frac{\partial s}{\partial t} + u_i \frac{\partial s}{\partial x_i} = -\frac{\partial q^s_i}{\partial x_i}, \tag{3.3}
\]

where \( t \) denotes time; \( u_i \) is the resolved velocity vector; \( p \) is the modified pressure; \( \tau_{ij} \) is the deviatoric part of the subgrid stress tensor; \( F_i \) is the body force driving the flow (here simply a homogeneous steady horizontal pressure gradient along the \( x \) direction); and \( B_i \) is the immersed boundary force representing the action of the obstacles (buildings) on the fluid. The density is assumed equal to 1 (all the equations are normalized so the numerical value of the density is irrelevant). In Eq. 3.3, \( s \) denotes a passive scalar quantity and \( q^s_i \) is the \( i \)th component of the subgrid scale scalar flux. Although the code can simulate active scalars (see [Kumar et al., 2006, Shah and Bou-Zeid, 2014]), the experimental data we identified for code evaluation were under conditions where buoyancy played an insignificant role. The code uses a pseudo-spectral method for computing the horizontal spatial derivatives on a uniform staggered Cartesian grid. To overcome the Gibbs phenomenon that emerges from the combined application of the IBM method with spectral derivatives, a smoothing approach we developed and detailed in chapter 2 is adopted. Vertical spatial derivatives are obtained from second-order centered finite difference. Second order Adams-Bashforth time integration is used. The subgrid scale (SGS) stress tensor is modeled using the Lagrangian scale-dependent dynamic Smagorinsky model [Bou-Zeid et al., 2005a], while the SGS scalar flux model uses the dynamically computed SGS viscosity with a constant SGS Prandtl number (\( Pr_{SGS} \)) of 0.4 (this is unrelated to the molecular \( Pr \) [Anderson, 2013]). In this study, we adopt a new approach for dynamically evaluating the momentum and scalar roughness lengths in the expression.
of the log-law wall model. The general log-law wall model for momentum and scalars is given by:

\[
\frac{u}{u_*} = \frac{1}{\kappa} \log \left( \frac{z}{z_{0m}} \right) \quad (3.4)
\]

\[
\frac{s_0 - s}{s_*} = \frac{1}{\kappa} \log \left( \frac{z}{z_{0s}} \right) \quad (3.5)
\]

where \( u \) is the local wall-parallel velocity near the wall; \( s_0 \) is the scalar concentration or temperature at the surface; \( u_* \) is the friction velocity calculated as the square root of the kinematic wall shear stress \( \tau_w \); \( s_* \) is the mass flux concentration or heat flux temperature (defined as the kinematic surface flux divided by \( u_* \)); \( z \) is distance away from the wall in the wall-normal direction; \( \kappa = 0.4 \) is the von Karman constant; and \( z_{0m} \) and \( z_{0s} \) are the roughness lengths for momentum and scalars, respectively. These roughness lengths are often chosen according to the roughness types of the surfaces for hydrodynamically rough walls. However, building facets are often hydrodynamically smooth, including the experiments we compare to. Therefore, instead of adopting a fixed roughness, we dynamically model the roughness lengths for momentum and scalars as a function of the viscous length scale \( \nu / u_* \). In fact, it has been shown by Kader and Yaglom [1972] that similar reasoning to the one that yielded the Prandtl-Nikuradse momentum skin friction law for smooth pipe and channel flow can be applied to scalar transfer in a turbulent flow to obtain heat or mass transfer laws for a smooth wall, with some unknown quantities that can be determined from experiments.

Eq. 3.4 can be rewritten following the Prandtl-Nikuradse skin friction law as

\[
\left( \frac{u}{u_*} \right) = A \log \left( \frac{z}{\nu / u_*} \right) + B \quad (3.6)
\]

\[
u_* = \frac{u}{A \log \left( \frac{z e^{B/A}}{\nu / u_*} \right)} = \frac{u}{A \log \left( \frac{z}{z_{0m}} \right)} \quad (3.7)
\]
where $A$ and $B$ are determined from experiments and $z_{0m}$ is given by

$$z_{0m} = \frac{\nu}{u_s} e^{-B/A}. \tag{3.8}$$

The same dimensional analysis can then be similarly developed for scalars:

$$s_0 - s(z) = s_* \psi \left( \frac{u_s z}{\nu}, \frac{\nu}{\chi} \right), \tag{3.9}$$

where $\chi$ is the mass or thermal diffusivity, and $\psi$ is a dimensional analysis function to be determined empirically (with the aid of profile-matching as for velocity). Eq. 3.9 is a general one for turbulent mass or heat transfer in wall-bounded flows. For air, $Pr = 0.7$ and $s_* = q_s / (\rho c_p u_s)$, where $q_s$ is the dynamic heat flux at the wall and $cp$ the heat capacity of the air. The experiments to determine the form of Eq. 3.9, as detailed in [Kader and Yaglom, 1972], then yield the log-law for scalar:

$$\frac{s_0 - s(z)}{s_*} = \alpha \log \left( \frac{z}{\nu/u_s} \right) + \beta \tag{3.10}$$

For air, $\alpha$ and $\beta$ can be found from experiments for heat transfer with weak buoyancy. If $s$ represents air temperature, then the heat flux at the wall is given by

$$\frac{q_s}{\rho c_p} = u_* s_* = u_* \frac{(s_0 - s(z))}{\alpha \log \left( \frac{z e^{\beta/\alpha}}{\nu/u_s} \right) = u_* \frac{(s_0 - s(z))}{\alpha \log \frac{z}{z_{0s}}}, \tag{3.11}$$

where $z_{0s}$ for the scalar can be written as:

$$z_{0s} = \frac{\nu}{u_s} e^{-\beta/\alpha}. \tag{3.12}$$

The roughness length expressions in Eq. 3.8 and Eq. 3.12 should be universal for smooth walls, and thus we can adopt the constants determined by Kader and Yaglom from experiments for fully turbulent flows [61,62] (Table 1 in Kader and Yaglom[61];
A can be viewed as the inverse of the von Krmnn number, but only the ratios $B/A$ and $\beta/\alpha$ influence the results and here we select the same ratio of 3.9/1.8 for both momentum and scalars, which effectively yield

$$z_{0m} = z_{0s} = \frac{\nu}{8.73u_*} \simeq \frac{\nu}{9u_*} \tag{3.13}$$

This result applies for molecular Prandtl of Schmidt numbers $\sim 1$, which is a reasonable approximation for all the tests we conduct in this study. These length scales depend on $u_*$ which varies in space and time over complex geometries. We thus use an explicit approach where $u_*$ form the previous time step is used in Eq. 3.13 to determine $z_{0m}$ at every wall location, and then the updated $z_{0m}$ is used to compute $u_*$ from Eq. 3.7. This dynamic equilibrium wall-model controls the fluxes at the solid-fluid interface, and therefore is important to determine if the LES is able to capture the physics of the flow and reproduce experimental observations. It is important to note here that this model, by construction since it assumes smooth facets, yields a Stanton number that is Re dependent. On the other hand, if the facets were assumed fully rough with constant $z_{0m}$ and $z_{0s}$, the heat transfer regime would become Re independent. We assume the presence of a logarithmic form at the first grid point away from the wall of the solid, which is commonly done in direct forcing immersed boundary method as adopted here.
3.3 Spatial variation of the transfer coefficient compared to a wind tunnel study

3.3.1 Experimental setup of mass transfer over two-dimensional ribs

The dimensional (e.g. in $WK^{-1}m^{-2}$) local heat or mass transfer coefficient is defined as

$$h_c = \frac{q_s}{s_0 - s_{ref}},$$

(3.14)

where $s_{ref}$ is some reference scalar quantity in the fluid. The distributions of the local heat and mass transfer coefficients obtained from detailed scale-model measurements have large spatial variations over the surface of roughness elements due to the highly complex flow patterns involving separations and reattachments in the flow. It is therefore desirable to assess the capability of the wall-modeled LES in predicting these spatial patterns of local heat and mass transfer coefficients. Nevertheless, one here again faces the challenge that the magnitudes of $h_c$ in scaled-model experiments at lower $Re$ and LES at larger $Re$ are not directly comparable due to the dependence of $h_c$ on $Re$. However, since the momentum dynamics are less sensitive to $Re$, the spatial flow patterns should match as long as the scaled-model $Re$ exceeds $\sim 10^5$, and therefore the resulting spatial variation patterns of $h_c$ should be comparable. Therefore, to overcome the magnitude discrepancy and still compare the spatial variabilities, the heat or mass transfer coefficients from different scale-model experiments and numerical simulations are usually normalized for appropriate comparison [Hagishima et al., 2005]. The measurement of mass transfer coefficient from a wind-tunnel study on evaporation of water from two-dimensional roughness (ribs) by Narita [2007] is used here as a benchmark case to assess the LES. The roughness elements, made of acrylic resin of 1mm thickness, were covered with wetted filter
paper. A fine thermistor sensor was inserted just below the paper surface to monitor the surface temperature. The evaporating surface is assumed to be at saturation. A weighing method was used to obtain the evaporation rate and thus the mass transfer coefficient can be estimated by knowing the ambient water vapor concentration. Measurements were conducted at a low relative humidity to keep the experimental error of the transfer coefficient to within 4%. Note that the sharp edges of these 2D ribs fix the separation points to the downstream top corners of each rib, and thus strengthen the insensitivity of the flow patterns to Re and improve the flow simulation results [Temmerman et al., 2003].

### 3.3.2 Numerical model of mass transfer

We considered configurations with three different separation distances between the two-dimensional ribs. Figure 3.1 is a side view of the basic configuration. The rib height $H$ is represented with 16 grid points. We use a horizontally periodic boundary condition for momentum and mass (thus we are simulating infinite repetitions of the patterns shown in Figure 3.1). The longer section behind the ribs is used to ensure that the inflow velocity at the first rib is free of the wake influence from the fifth element. It also mimics the test section surface upstream of the ribs in the open circuit wind tunnel [Narita, 2007]. The experimental Reynolds number is 16000, where velocity is fixed at 4 m/s at the top of the boundary layer and length scale is the rib height. The experiment did not precisely control the humidity in the incoming air in the wind tunnel. Instead, during each run where the evaporation rate was measured, the evaporation rate from a flat plate placed in the free stream was simultaneously recorded for normalizing the measurements. Therefore, we could not replicate the exact details of the mass inflow, but again these only affect the magnitude and not the spatial patterns of the transfer coefficient that we seek to investigate here.
Figure 3.1: Side view of the geometric configuration of the numerical simulations. The cases of $W/H=0.5$, 1 and 2 are shown in the figure from top to bottom. Inflow is from left to right. $N_x$ is the number of grid points in x-direction. $N_z = 80$ total vertical grid points for all three cases.

The top boundary condition in the simulation is slip-free for momentum and zero-flux for the scalar (same top BC for all simulations in this paper). The dimensions of the wind tunnel are 0.9 m in height and 1.8 m in width. The height of the wind tunnel is 15 times the height of the rib $H = 0.06$ m. We have conducted preliminary tests by varying the domain height from 3 times to 10 times $H$ (results not shown here) to test the sensitivity to the domain height. We found that results with domains exceeding 5H in height converge, and therefore we adopt 5H as our domain height in all simulations in this section. The boundary condition on the surfaces of the ribs for water vapor is assumed to be at a constant concentration, which is justified by the saturated state of the wetted surfaces. All cases were run for about 20 eddy turn over times ($L_z/u_*$) and averaged in the y-direction, to reach statistical convergence, which
was further confirmed by ensuring that the velocity profiles reach a steady state, i.e. they become invariable if the averaging time is further increased.

Figure 3.2: Mean (time- and y-averaged) contour plots of \( s/s_0 \) and streamlines. The wind is from left to right. The white spaces represent the transect areas occupied by the solid 2-dimensional ribs. Color scale for the normalized scalar concentration is the same for all three cases.

Figure 3.2 (a)-(c) shows the pseudocolor plots of the scalar concentration normalized by the surface scalar concentration, together with the streamlines. The central vortices in the \( W/H = 0.5 \) and 1 cases are characteristic of the ‘skimming flow’ regime and explain the high concentrations of scalar in the space between the ribs (“the street canyon”), whereas the slightly asymmetric flow field in case \( W/H = 2 \) is evidence of more complex flow interactions in the ‘wake interference regime’ Oke:1978wqba, Perry:1966gqba that allows more exchange between the canyon and the air aloft. The flow patterns are consistent with the regime expected for this geometry. In addition to the more intensive exchanges for the widest canyon, the reduced “emitting surface” to “canyon volume” ratio, \( (W + 2H)/(HW) = H + 2/W \), when \( W \) increases and \( H \) is maintained constant, further explains the reduced con-
centrations in the canyon. Figure 3.3 (a)-(c) shows instantaneous contour of the scalar concentration normalized by the surface scalar concentration, together with the streamlines along one $xz$-slice at a fixed $y$. The instantaneous structures in the scalar concentration field, as well as the streamlines, are generally distinct from their averaged counterparts shown in figure 3.2, particularly for the $W/H = 2$ case. The depicted turbulent structures are important for the vertical exchange; for example, one can observe the strong ejection from the last canyon in figure 3.3(c) for the $W/H = 2$ case. This is consistent with general observations for such kind of type-k roughness where the eddies of scale $H$ are shed out of the cavity, resulting in the more complex flow interactions. The instantaneous vortices inside the canyons for the two other cases, especially $W/H = 1$ in 3.3(b), are somewhat more similar to their time and space averaged counterparts in figure 3.2(b). This dominant mean circulation inside the canyons for these cases might hinder ejections and sweeps near the top of the canyons and reduce the instantaneous exchange between canyons and air above. While we show only one snapshot here; other snapshots we analyzed conveyed the same information. Figure. 3.4 shows the comparisons between the experimental and LES results for the three rib separations, while Table 1 lists the absolute percentage deviation of the LES from the experiments. All quantities are normalized by the average mass transfer coefficient on the floor in between two consecutive ribs. The experimental data are averaged over multiple ribs starting where the transfer coefficient over subsequent ribs converge. To best mimic the experimental data, we average the LES result using relevant quantities from the second to the fifth rib, where the transfer coefficients become independent of location of the ribs. We tested different averaging ranges and the impact on the results is minimal. The resulting general spatial trends for each case, as well as the changes in transfer coefficient patterns as a result of the variation in the separation distance, are adequately captured by the LES. Despite the fact that the leeward transfer coefficient varies quite considerably across
different cases, its variation is captured well: for example, the peak for $W/H=1$ was observed to occur at about $0.4H$ from the bottom and this maximum is also clear in LES. Both the experiment and the LES also show that the decrease along that face at $W/H=0.5$ is more pronounced than $W/H=2$. The variation on the street face (floor between two ribs) is also reasonably captured by the LES. The maximum of the transfer coefficient on the street occurs at about $0.5H$ in the experiments for cases $W/H=1$ and $W/H=2$, which is also the location predicted by the LES. This peak matches the location of the highest wall-parallel velocity produced by the recirculating flow in the canyon. Given the complexity of the wakes and recirculation inside the canyon, the matching of the observed time-averaged transfer coefficients that are modulated by these flow patterns indicate that the wall-modeled LES is capable of reproducing them, as well as the spatial distributions of the local mass transfer they generate inside the canyon. Larger discrepancy between the observations and LES
Figure 3.4: The normalized mass transfer coefficient for different positions across the canyon. \(L\) is the path length along the interface, and a unit \(L/H\) is the length of the dotted line indicated in Fig. 3.1 for case \(W/H=2\) as an example. The white space with no data for the cases in (a) and (b) does not reflect a data gap, but the fact that the street widths are shorter in these cases compared to the case in (c), which we adopt to fix the overall width of the figure.

...occurs near the top of the windward facet and on the roof, which can have two possible reasons. One potential reason for this larger discrepancy is the difference in the dominant drag mechanism: while pressure drag dominates at the vertical wall, the viscous drag dominates over the roof [Leonardi and Castro, 2010a]. Another reason is related to our inability to match the experimental inflow conditions in LES exactly, as shown in figure 3.5. The inflow vertical profiles of the normalized mean streamwise velocity and turbulent intensity (\(TI\)) at the upstream of location \(x = 0\) are shown in figure 3.5. The mean velocity in both LES and experiment is normalized by its value at \(z = H\), while the \(TI\) is computed locally. The mass transfer from the roof surface and upper part of the front/windward wall are more dependent on the inflow profile (mean velocity as well as turbulence intensity) than the bottom and the leeward faces.
To test the sensitivity of the mass transfer for the different faces to inflow conditions, another test was conducted also assuming a fully periodic domain but without the long extension. This implies an infinite array of ribs, and is further removed from the actual setup in the wind tunnel. The results from this test (not shown here) indicate that while the absolute value of the error defined as $|(h_{LES} - h_{Exp})/h_{Exp}|$ remained similar for the leeward and bottom faces, the errors on the front and top faces were 3-5 times larger compared to the values presented in table 3.1, which correspond to the basic setup. This further confirms the importance of characterizing the inflow in experiments accurately and reporting it in the associated paper to allow the data to be used for model validation, and supports our explanation that the higher discrepancy in the upper part of the windward facet and on the roof are related to a mismatch in the inflow.
<table>
<thead>
<tr>
<th>W/H=1/2</th>
<th>Leeward</th>
<th>Street</th>
<th>Windward</th>
<th>Roof</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>18.2</td>
<td>15.5</td>
<td>20.3</td>
<td>42.3</td>
<td>25.5</td>
<td></td>
</tr>
<tr>
<td>W/H=1</td>
<td>11.1</td>
<td>12.0</td>
<td>30.2</td>
<td>35.5</td>
<td>22.5</td>
</tr>
<tr>
<td>W/H=2</td>
<td>20.2</td>
<td>22.5</td>
<td>17.4</td>
<td>27.8</td>
<td>22.0</td>
</tr>
</tbody>
</table>

Table 3.1: The absolute percentage deviation (\(\%\)) , \(|(h_{LES}/h_{Exp})| \times 100\), of the averaged transfer coefficient over each facet and all facets combined.

3.4  Facet-averaged heat transfer from a cube compared to a wind tunnel study

3.4.1  Experimental set-up of heat transfer from a single cube

The turbulent forced convective heat transfer over a wall-mounted cube at relatively low Reynolds number has been quite extensively studied as discussed in the introduction. In particular, we will focus on the study by Nakamura et al. [2001] since their experiment was conducted at a relatively high \(Re\) - from 4,200 to 33,000 - despite the fact that it remains orders of magnitude lower than for real buildings. Furthermore, relations between \(Nu\) and \(Re\) for different faces of the cube were proposed in that study, and they will be useful for our comparisons. In this experiment, a copper cube was heated by an embedded heater to maintain the surface temperature approximately constant (within \(\pm 0.5\) °C). The cube, with a dimension of 30 mm, was placed in a low-speed wind tunnel of 4 m height, 3 m width, and 8 m length. A turbulent boundary layer is achieved by placing a horizontal circular cylinder 500 mm upstream from the cube to act as a trip. The diameter of the circular cylinder is 10 mm and the boundary layer depth to cube height ratio varies from 1.5 to 1.83. A temperature difference of approximately 10 °C is maintained between the surface of the cube and the air temperature. \(Re\), defined based on the cube height and the bulk velocity upstream of the cube, was varied to assess how it is related to \(Nu\).
3.4.2 Numerical model of heat transfer from a single cube

For all simulations in this section, a horizontally periodic domain is used. Figure 6 is the schematic drawing of the setup of the numerical simulation. 30 grid points are used along each side of the cube. The domain height is $4H$, where $H$ is dimension of the cube. The upper boundary condition is impermeable with a free-slip for momentum and zero-gradient (no flux) for temperature. Five different simulations were performed at different Reynolds number in our LES by varying the horizontal pressure forcing, which is equivalent to changing the bulk velocity in the inflow. The Reynolds number is defined as $Re = UH/\nu$, where $U$ is the free stream velocity in the wind tunnel. The LES velocity used in $Re$ is taken at the location $(x, z) = (0, 1.5H)$, which provides a reasonable match to the experimental definition. Notice that in the LES setup the wall model defines an inner scale (since we are using a smooth-wall roughness length parameterization that depends on $\nu$), and the nominal $Re$ of the simulations can therefore be determined; viscous stresses are neglected in the numerical integration of the momentum and scalar equations. For all simulated cases, a
constant temperature wall boundary condition is implemented in the wall model. All cases were simulated for a total of 100 eddy turnover times, defined as $L_z/u_*$ (this corresponds to 400 eddy turnover times defined based on the cube scale). After a transient of 50 eddy turnovers, all time-averaged statistics reported were computed using the last 50 eddy turnovers times. Figure 3.7(a) shows a vertical $x - z$ transect along $y = 2H$ (middle of the cube), where both the contour of temperature deviation from the inflow temperature, defined as $(\theta-\theta_i)/\theta_i$, and the velocity streamlines are shown. Similarly, figure 3.7(b) is a horizontal transect at $z = 0.015H$ (near the floor). The temperature deviation contours depict large spatial gradients around the cube. The separation near $z = H/2$, and the reattachment zone near the lower corner of the front face of the cube (figure 3.7(a)) compare well with experimental visualizations [Nakamura et al., 2001, Martinuzzi and Tropea, 1993]. The separation zone and the two counter-rotating vortices shown in figure 3.7(b) near the rear face are also some well-known features of flow around a single cube, as seen for example in flow visualizations in Nakamura et al. [2001] and Martinuzzi and Tropea [1993]. The $Nu-Re$ relation obtained from experimental measurements of Nakamura et al. [2001] follow the classic power law

$$Nu = aRe^m,$$  \hspace{1cm} (3.15)
Table 3.2: The coefficients and exponents in Eq. 3.15 as determined in Nakamura et al. [2001]

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>front</td>
<td>0.71</td>
<td>0.52</td>
</tr>
<tr>
<td>side</td>
<td>0.12</td>
<td>0.70</td>
</tr>
<tr>
<td>rear</td>
<td>0.11</td>
<td>0.67</td>
</tr>
<tr>
<td>top</td>
<td>0.071</td>
<td>0.74</td>
</tr>
<tr>
<td>cube average</td>
<td>0.138</td>
<td>0.68</td>
</tr>
</tbody>
</table>

The coefficients of which are given in table 3.2. Due to the difference in $Re$, these experimental Nu-$Re$ relations of Nakamura et al. are extrapolated to the $Re$ of the LES for comparison. This ignores the well-known dependence of $m$ on $Re$, a caveat we will revisit in the next section. However, this approach was necessary since reducing our $Re$ further to match the experiment would place our first grid point in the viscous or buffer layers and preclude us from testing the wallmodeled LES configurations that we aim to use for full-scale (real-world) applications. Figure 3.8(a) shows the comparisons between the relations proposed by Nakamura et al. [2001], extrapolated to the LES $Re$, for the averaged Nu on different facets and the LES results. Although these experimental relationships were found at $Re$ orders of magnitude smaller, the match between predicted values according to Eq. 3.15 and those obtained from LES is in fact reasonable. The front and leeward faces show higher errors than the other faces, but errors cancel out and cube-averaged fluxes match quite well. This can be interpreted either as giving confidence in the performance of LES, or alternatively in the applicability of extrapolations from low $Re$ studies to the higher $Re$ flows in the real-world. Figure 3.8(b) shows that the ratio of deviation $R_d$ defined as:

$$
R_d = \frac{Nu_{LES}}{Nu_{Exp}}
$$

where the experimental results are the values predicted from Eq. 3.15 and table 3.2, at different $Re$. Except for the front face which is excluded from this comparison,
exchanges from the other faces remain within 50% of the measurements. The most likely reason why the front face deviates the most from the experimental result is that the experimental flow over that face could still be in a regime of laminar or transitional flow. This is strongly suggested by the small experimental exponent, 0.52, which is considerably lower than that expected in turbulent flows, and rather very close to the 0.5 limit expected for laminar flows [Incropera, 2002]. In addition, the turbulent boundary layer depth in the experiment is $1.5\delta/H$, which is different than the fully developed one in LES of $4\delta/H$. It is often of practical interest to

![Figure 3.8](image)

Figure 3.8: (a): $Nu-Re$ relation for different faces using empirical results from Nakamura et al. [2001] i.e. using $m$ and $a$ from table 3.2 and extrapolating to the $Re$ of the LES. (b): Nusselt number of the experiment vs. that from LES. The black lines denote the quantities $Nu_{exp}(1 + Rd)$, where $Rd = \pm 25$ and $\pm 50\%$. The front face is excluded in (b) since its errors are much higher due to the $Re$ discrepancy.

use the cube-averaged or facet-averaged value of the heat transfer coefficient when considering the bulk heat exchange between a building envelope and the surrounding air, despite the high spatial variability. Figure 3.9(a) shows the contours of the heat transfer coefficient normalized by the cube average. Only one side-face is shown because of symmetry. Large deviations from the cube-averaged value occur on the edges as expected. The spatial variation at the intersections between front, top and rear faces is the most prominent. Figure 3.9(b) depicts the heat transfer coefficient normalized by the respective face-averaged values. Despite the large spatial variability at the intersections between different faces, the cyan contour of value 1.1
indicates that the deviation over a large area of each face is only moderate. This implies that for practical applications, point-measured values in the center of a facet or numerically-determined face-averaged values give good estimates of the transfer over larger portions of each facet, despite some loss of information on the higher values near the corners. However, cube-averaged values should not be applied to individual facets. The contour plots in figure 3.9 also compare well qualitatively with results in the experiments of Nakamura et al. [2001]. The wall friction velocity $u_*$ and temperature scale $\theta_*$, where $\theta_* = q_0/(u_* \rho cp)$, are shown in figures 3.10(a) and (b) respectively. The spatial variability patterns of $u_*$ are strongly correlated with those of $h_c$, indicating that the friction velocity has a strong impact on heat transfer as expected. The patterns of $\theta_*$ on the other hand are distinct, with strong heat exchange near the bottom of the all faces due to the horseshoe vortex depicted in figure 3.7. Separate sensitivity tests with varying domain heights of $1.7H$ and $3H$ were also conducted and yielded markedly different results due to the increased flow blockage resulting in higher velocities around the cube. As shown in table 3.3, the shorter domains result in higher $Nu$ as a consequence of these higher velocities. The

Figure 3.9: (a): Local heat transfer coefficient normalized by the cube-averaged value on all four facets. (b): Local heat transfer coefficient normalized by each facet average value.
Figure 3.10: (a): Spatial distribution of the wall friction velocity $u_*$ normalized by the cube average value. (b): Spatial distribution of the wall temperature scale $\theta_*$ normalized by cube average value.

<table>
<thead>
<tr>
<th>$L_z$</th>
<th>Front</th>
<th>Top</th>
<th>Rear</th>
<th>Side</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.7H</td>
<td>+43.8</td>
<td>+54.1</td>
<td>+34.5</td>
<td>+15.0</td>
<td>+32.5</td>
</tr>
<tr>
<td>3.4H</td>
<td>+10.8</td>
<td>+5.60</td>
<td>+6.76</td>
<td>+6.78</td>
<td>+7.34</td>
</tr>
</tbody>
</table>

Table 3.3: Percentage difference between surface averaged Nu compared to case $L_z = 4H$.

much smaller difference between $3H$ and $4H$ compared to $1.7H$ and $4H$ nevertheless indicated that convergence occurs when $L_z \simeq 4H$.

### 3.5 Comparison to full-scale field measurements

Field measurements of heat transfer coefficients provide valuable information to evaluate high-$Re$ numerical models with minimal discrepancy in the Reynolds number. We considered the measurement performed by Hagishima and Tanimoto [2003] in detail for comparison. This outdoor measurement campaign was conducted over two sites: one was on a building roof, and the other on a vertical wall of a cubical extension mounted on a roof. We selected the building roof case for comparison, in which there is a better similarity in the setup between our numerical simulation and the
field experiment. The roof surface energy balance equation, together with the temperature difference between the building surface and air temperature measurement, were used in the experiment to calculate the convective heat transfer coefficient $h_c$. The temperature and wind speed measurements on the roof were positioned at about 10% and 6% of the height of the building respectively. The general $Nu-Re$ relation was deduced from the experimental data and found to follow the power law relation

$$Nu = 0.023Re^{0.891}$$

with $R$-square value of 0.964, irrespective of wind direction variability. The length scale in the Reynolds number is defined as the length from the roof edge considering the wind direction, while the velocity scale is $u_0 = \sqrt{u^2 + v^2 + w^2}$, with the wind components measured by the anemometers. For the comparison between these field measurements and the LES in terms of the fitted relation between the Nusselt and Reynolds numbers, we estimate the Reynolds number based on the same definition of the characteristic length and velocity scales used by Hagishima and Tanimoto [2003]. The same five sets of simulations presented in section 4 are used to estimate the $Nu-Re$ relation. The $h_c$ on the building roof is spatially variable as we showed in previous sections; this affects the field experimental results fitted from measurements at a few points. For accurate comparison, we extract the $h_c$ from the LES roof at the same locations where Hagishima and Tanimoto [2003] acquired measurements on the experimental roof. Figure 3.11 depicts the distribution of the exponent $m$ and coefficient $a$ in $Nu = aRe^m$, found from linear-regression of the LES results at different $Re$ over the roof facet. The red marks denote where the experimental measuring points were positioned, approximately. On average, the spatial variation of the exponent $m$ is about 11%, while a much greater variation is seen in the coefficient $a$, the values of which varied by one order of magnitude. From the roof-averaged LES
results and the ones averaged over the 4 experimental points, we respectively obtain

$$Nu_{\text{roof-average}}^{\text{LES}} = 0.013 Re_{\text{LES}}^{0.88}, \quad Nu_{\text{4 points-average}}^{\text{LES}} = 0.075 Re_{\text{LES}}^{0.88} \quad (3.18)$$

The strong similarity in the exponent values in Eq. 3.17 and Eq. 3.18 indicates that our wall-modeled LES is able to capture the change in heat transfer coefficient well even as the wind speed (i.e. $Re$) varies. The LES values of $a$ (0.013 and 0.075) bracket the experimental value (0.023). We do not anticipate being able to exactly capture the experimental value of $a$, as well as we capture $m$, for several reasons including:

1. Setup conditions in the field experiment and the LES cannot be exactly matched, and $a$ is highly sensitive to these conditions unlike $m$. For example, according to a report by Hagishima and Tanimoto [2003], the 0.25 m protrusion around the building edge induces separation and backflow. The measuring height was 0.60 m above the roof-top but the wake caused by these intrusions can affect the exact magnitude of heat transfer reflected in $a$ (but not its scaling with $Re$ reflected by $m$).

2. The wall-model imposes a thermal roughness length in LES by assuming a smooth wall, but the actual smoothness of the roof used in the Hagishima and Tanimoto [2003] study is not characterized. Some building walls could very well be transitionally or hydrodynamically rough such that the actual roughness length $z_0$ of these surfaces is needed to match $a$, although we point out that this would have also caused discrepancy in $m$.

Therefore, the LES can be expected to quantitatively predict the scaling represented by $m$ in the relation between the wind speed and forced convective heat transfer with high accuracy, but the exact magnitude of $h_c$ for a given wall also requires matching $a$ and is highly dependent on fine details such as wall texture and material, and surrounding obstructions. Table 3.4 gives a summary of results from other field experiments that attempt to relate the heat transfer to change in wind velocity (i.e.
Figure 3.11: Spatial distribution of the best-fit results of $m$ and $a$ on the building roof, where the wind is blowing from bottom to top of the figure. The red dots are the location of the experimental measurements of Hagishima and Tanimoto [2003].

<table>
<thead>
<tr>
<th></th>
<th>Experimental</th>
<th>LES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emmel et al. [2007]</td>
<td>0.85 (Roof)</td>
<td>0.88</td>
</tr>
<tr>
<td>Clear et al. [2003]</td>
<td>0.8 (Roof)</td>
<td>0.88</td>
</tr>
<tr>
<td>Yazdanian and Klems [1994]</td>
<td>0.89 (Windward, low-rise building)</td>
<td>0.89</td>
</tr>
</tbody>
</table>

Table 3.4: The exponent in the $Nu-Re$ relation for different experiments and corresponding values from LES.

Although the experimental conditions and measurement techniques vary across these campaigns, and certainly discrepancies exist among them, there seems to be a consistent power law relation between the forced convective heat transfer and the wind speed with an exponent in the range of 0.67-0.89. The wall-modeled LES considered in this paper is shown to give results that consistently fall within the experimental range. All of the exponents are $< 1$, suggesting that the flow over the surfaces is not in the fully rough regime where the Stanton number would become independent of $Re$.

### 3.6 Discussion and Conclusions

This study assessed the capability of the wall-modeled LES approach to capture the physics of forced convective heat/mass transfer between the surfaces of buildings and the atmosphere. Through detailed comparisons to both wind-tunnel studies and field experiment, we have shown that our LES is able to reasonably predict i) the spatial
variation of the heat/mass transfer coefficient over the different facets of 2D ribs;
ii) the average Nusselt number for a single cube (with larger discrepancy relative
to measurements over the windward face very likely related to the $Re$ discrepancy);
and iii) the power law relation between the Nusselt and Reynolds numbers com-
pared to field measurements. The excellent match of the power law exponent $m$ is
largely attributable to the dynamic wall model we proposed and implemented here.
Returning to the motivating question we asked: “are the errors resulting from the
parameterization of unresolved scales (wall and subgrid scale models) in LES larger
or smaller than the errors involved in extrapolating from low-$Re$ approaches (DNS or
wind tunnels) to high-$Re$ real world flows, for scalar transfer problems?”
, the overall conclusion from out study indicates that the LES, despite its inherent parameteriza-
tions, is more suitable for studying real-world buildings: 1) Wind-tunnel studies result
in $Nu \sim Re^{0.52}$ to $Re^{0.74}$, a significantly lower exponent range than 0.9 observed in
field measurements and LES. This is consistent with the expected trend of a lower $m$
when $Re$ is lower, and suggests that the low-$Re$ effects in the wind tunnel are biasing
the findings and would make them not suitable for extrapolation to the real-world
(yet as mentioned in the introduction some current models rely on such coefficients
empirically determined from water channel studies from 1924 [Jürges, 1924]). As
such, when LES-wind tunnel discrepancies arise, it seem more likely that the errors
are related to the extrapolation of wind tunnel $Nu-Re$ relations outside their range
of validity. 2) There is a strong sensitivity of the heat transfer exchange coefficient to
inflow conditions, and the inflow is wind tunnel studies (or many simulations for that
matter) do not represent realistic upwind conditions in the real world. For building
models and urban microclimate models that often use averaged value for modeling
turbulent heat exchange, based on our simulation results, the use of facet-averaged
values seem to be appropriate, but the relatively large differences among different
facets preclude the use of a single coefficient for the whole building since this would
not capture the large facet-to-facet variations. In addition, we have documented (not surprisingly) that it is important in numerical simulation like LES to match the experimental inflow conditions, especially for the windward faces that are affected the most. For future experimental studies in wind tunnels or field experiments, details such as the inflow profiles in a wind tunnel, measuring positions of wind and temperature, and wind directions should be included so that further validation studies can be conducted with more details of the experimental setup. For the types of numerical experiments considered here, the suitable domain height should be greater than 4 times the height of the obstacle. Another point to note is that the exponent $m$ in $Nu \sim Re^m$ being close to 1.0 (both in building-scale field measurement and LES) is a manifestation of approaching the fully rough limit [Webb et al., 1971], in which the Stanton number is independent of $Re$. However, this limit is not reached suggesting that transitional effects persist. This should not be confused with the building canopy scale flow, which is clearly in the fully rough regime.
Chapter 4

Contrasts between Momentum and Scalar Exchanges over Very Rough Surfaces

The dynamics of turbulent shear flows over rough walls have been an active area of research because of their relevance in the design of engineering systems and in environmental fluid mechanics. Momentum and scalar exchanges between the wall and the fluid in such flows are of interest in a wide range of disciplines [Belcher et al., 2012]. Previous field experiments over natural vegetation [Poggi et al., 2004a, Katul et al., 1997b], wind tunnel studies over obstacles of regular shapes [Castro et al., 2006], and numerical simulations over three-dimensional roughness elements [Coceal et al., 2007a, Finnigan et al., 2009, Leonardi et al., 2015] have advanced our understanding of this problem significantly. For example, these past studies have underlined the importance of dispersive fluxes inside and close to the roughness canopy [Poggi and Katul, 2008, Poggi et al., 2004a]. Nevertheless, there remains significant gaps in our knowledge, particularly concerning the transport of scalars, and how it compares to that of momentum, over surfaces that consist of “large”
three-dimensional bluff-body-type roughness elements. Large here implies that the roughness protrudes significantly into the inertial layer, such that a log-region may not exist, and that the details of the flow inside the roughness canopy are important for the applications. In many natural settings and engineering applications, $H/\delta$ often exceeds 0.1, where $H$ is the roughness height and $\delta$ is depth of the boundary layer. This is a regime sometimes termed the very rough surface [Castro et al., 2006]. Very rough surface is in contrast to previous reviews on rough wall-bounded flows by Jiménez [2004], who limited the discussions of rough-wall boundary layers for $H/\delta < 0.025$, such that the effect of the roughness only extends to less than half of the log-region. Various previous numerical studies [Kanda et al., 2004, Castro et al., 2006, Coceal et al., 2007a, Orlandi and Leonardi, 2008, Giometto et al., 2016] have probed the details of the flow such as the morphology of coherent structures and the effects of the roughness in such regimes. Moreover, recent large eddy simulations (LES) and direct numerical simulations (DNS) [Finnigan et al., 2009, Boppana et al., 2010, 2012, Philips et al., 2013, Park and Baik, 2013, Leonardi et al., 2015] investigated the transport of scalars. However, compared to the extensive number of previous studies focusing on the flow and the momentum transport, research on scalars and their transport in flows over very rough walls remains quite limited. In addition, a comparative analysis of momentum and scalar transport dynamics has not been performed before. These open gaps motivate this chapter: we investigate both momentum and scalars at a very high Reynolds numbers over three-dimensional, large roughness using the LES technique. Particular attentions are paid to regions within the roughness elements and the roughness sublayer, which is below the log-layer and the flow is spatially inhomogeneous. The two research questions we seek answers are:

1. How and why are momentum and scalars transported differently in turbulent shear flows over bluff-body roughness?
2. How does the geometry of this roughness affect the exchanges between the wall and the fluid?

4.1 Numerical setup

The LES code uses the immersed boundary method (IBM) to account for the presence of the roughness elements, in which a discrete-in-time momentum forcing is used to simulate the immersed boundary force [Chester et al., 2007, Tseng et al., 2006]. The non-dimensional filtered incompressible continuity (4.1), Navier-Stokes (4.2), and scalar conservation (4.3) equations are solved assuming hydrostatic equilibrium of the mean flow:

\[
\frac{\partial u_i}{\partial x_i} = 0, \quad (4.1)
\]

\[
\frac{\partial u_i}{\partial t} + u_j \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = - \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + F_i + B_i, \quad (4.2)
\]

\[
\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} = - \frac{\partial q_s^i}{\partial x_i}. \quad (4.3)
\]

All the variables we will discuss are filtered components, so the usual tilde above the symbols are omitted for simplicity. \(x, y\) and \(z\) denote the streamwise, cross-stream and wall-normal directions respectively, and \(u, v\) and \(w\) are the velocity components in these respective directions. \(t\) denotes time; \(u_i\) is the resolved velocity vector; \(x_i\) is the position vector; \(p\) is the modified pressure; \(\tau_{ij}\) is the deviatoric part of the subgrid stress tensor; \(F_i\) is the body force driving the flow (here simply a homogeneous steady horizontal pressure gradient along the \(x\) direction); and \(B_i\) is the immersed boundary force representing the action of the obstacles on the fluid. In (4.3), \(\theta\) denotes a passive scalar concentration, and \(q_s^i\) is the \(i\)th component of the subgrid scale scalar flux. Further numerical details on the code and the subgrid-scale model can be found in Bou-Zeid et al. [2005b], while detailed validations for the flow and
Figure 4.1: Top-view of the ‘repeating unit’ for three cases shown in table 5.1, where shaded areas represent the obstacles: (a) Cube25; (b) Slender32; (c) Wide32. Area highlighted by red-dotted line is the lot area, \( A_t \). Different intermediate cases labeled as Sf in table 4.1 are achieved through varying \( L_{xb} \) and \( L_{yb} \) while keeping \( H \), the obstacle height, constant. Frontal area density, \( \lambda_f \), and plan area density \( \lambda_p \) are defined.

<table>
<thead>
<tr>
<th>Case</th>
<th>( \lambda_p )</th>
<th>( \lambda_f )</th>
<th>( N_x^b, N_y^b, N_z^b )</th>
<th>( N_x, N_y, N_z )</th>
<th>( L_x/\delta )</th>
<th>( L_y/\delta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cube25</td>
<td>0.25</td>
<td>0.25</td>
<td>8, 8, 8</td>
<td>192, 96, 64</td>
<td>3</td>
<td>1.5</td>
</tr>
<tr>
<td>Slender06</td>
<td>0.12</td>
<td>0.06</td>
<td>16, 3, 8</td>
<td>200, 100, 64</td>
<td>3.125</td>
<td>1.5625</td>
</tr>
<tr>
<td>Sf08</td>
<td>0.12</td>
<td>0.08</td>
<td>12, 4, 8</td>
<td>200, 100, 64</td>
<td>3.125</td>
<td>1.5625</td>
</tr>
<tr>
<td>Sf12</td>
<td>0.12</td>
<td>0.12</td>
<td>8, 6, 8</td>
<td>200, 100, 64</td>
<td>3.125</td>
<td>1.5625</td>
</tr>
<tr>
<td>Sf16</td>
<td>0.12</td>
<td>0.16</td>
<td>6, 8, 8</td>
<td>200, 100, 64</td>
<td>3.125</td>
<td>1.5625</td>
</tr>
<tr>
<td>Sf24</td>
<td>0.12</td>
<td>0.24</td>
<td>4, 12, 8</td>
<td>200, 100, 64</td>
<td>3.125</td>
<td>1.5625</td>
</tr>
<tr>
<td>Wide32</td>
<td>0.12</td>
<td>0.32</td>
<td>3, 16, 8</td>
<td>200, 100, 64</td>
<td>3.125</td>
<td>1.5625</td>
</tr>
</tbody>
</table>

Table 4.1: Summary of simulation parameters

Scalar transport can be found in Li et al. [2016a] and Li et al. [2016b], respectively.

The LES uses a wall-model for momentum and scalars that has been developed for a hydrodynamically smooth wall at high Reynolds number (e.g. a realistic building in the atmospheric boundary layer) based on Kader and Yaglom [1972]. Wall modelling for complex walls remains an ongoing area of research [Yang et al., 2015b] and an open challenge; however, the performance of the current approach has been verified and shown to be quite satisfactory in Li et al. [2016b].
To explore the effects of the geometry, we conducted simulations of different cases as summarized in table 4.1. \( \lambda_f \) and \( \lambda_p \) are the frontal area ratio and plan area ratio respectively. \( \lambda_f \) is defined as the total projected frontal area of the roughness elements per unit wall-parallel area (i.e. land area); \( \lambda_p \) is the ratio between the crest plan area (i.e. roof area, shaded in black figure 4.1) and the wall-parallel area. \( N_i^b \) is the number of grid points resolving one obstacle in the \( i \) direction, while \( N_i \) is the total number of computational points in that direction. The two digits at the end of each case name are \( \lambda_f \times 100 \) for that case. The first case is the classic cuboid obstacles, while in the remaining cases we gradually change the horizontal aspect ratio of the obstacles, while maintaining the same height and area (\( \lambda_p \)). Sf stands for ‘Stagger frontal’. Figure 4.1 shows the cubic case and the two extreme aspect ratios of the other cases.

4.2 Results and discussion

4.2.1 Turbulent transport efficiencies of momentum and scalar

Quadrant analysis is a useful and widely used technique for probing how turbulent motions evolve and transport momentum and scalars in the wall-normal direction [Wallace, 2016]. Thus, we apply this technique here to compare the momentum and scalar turbulent transports. The definition of each quadrant for momentum flux follows previous studies [Katul et al., 1997a,b, Li and Bou-Zeid, 2011]. Q1 events are classified as \( s' > 0 \) and \( w' > 0 \); Q2 as \( s' < 0 \) and \( w' > 0 \); Q3 as \( s' < 0 \) and \( w' < 0 \); Q4 as \( s' < 0 \) and \( w' > 0 \), where \( s \) is \( u \) or \( \theta \). We applied quadrant analysis to time series collected at four representative horizontal locations (\( x_1 \) and \( x_4 \)) indicated in figure 4.1 and at every height, but we will only show results for \( x_2 \) and \( x_3 \) since the
other locations convey the same information. Data were sampled at each time step for a total period of $2T$, where $T$ is one eddy turn over time defined as $\delta/u_\ast$. For the momentum flux, $Q_2$ and $Q_4$ are termed ejections and sweeps respectively; for scalar flux, $Q_1$ (motion that transports higher concentrations of the scalar upward) and $Q_3$ (motion that brings lower concentrations downward) are termed ejections and sweeps, respectively. Compared to other two quadrants, the ejections and sweeps are the dominant events in transporting momentum and scalars.

Figure 4.2 shows the contributions from the various quadrants (momentum in (a) and (c); scalar in (b) and (d)) for case Cube25, where the contribution of quadrant $i$ is defined as $|s'w'|_i/\sum_i|s'w'|$. The contribution of each quadrant to scalar fluxes is broadly similar to that of momentum across all points, though slight differences between momentum and scalars are seen inside the canopy sublayer below $z/H = 1$. The spatial variation across the four different horizontal location in the canopy sublayer is on the other hand significant, underlining the complexity of the flow within these three dimensional roughness arrays. These differences blend away above the canopy. The number of sweeps exceeds that of ejections below $z/H = 1.25$ across all four points (not shown here), indicating that below this height sweeping events are stronger compared to the more frequent and less intense ejections. The crossover point...
at $z/H = 1.25$ is consistent with results for the Reynolds stress from DNS reported by Coceal et al. [2007a] for the same underlying roughness geometry of staggered cubes, although they averaged over all points at a given $z$. It has been previously observed that for momentum transport, the sweeps contribution to total stress dominates over ejections under near-neutral static stability in vegetation canopies [Dupont and Patton, 2012] and in a real city characterized by large roughness elements [Rotach, 1993]. Dominance of sweeps in momentum transport over very rough walls, compared to the dominance of ejections over smooth and less-rough counterparts, is in general agreement with the picture proposed and discussed in detail by Raupach et al. [1996], which adopts a mixing-layer analogy for these very rough walls to account for the differences compared to a typical surface layer. In the outer layer, ejections dominate as typical in smooth-wall boundary layers [Adrian, 2007]. Our results clearly demonstrate that the turbulent transport of passive scalar flux exhibit the same behavior as for momentum. Such similarity between momentum and scalar transport over vegetation canopy has also been observed [Dupont and Patton, 2012], in field measurements in roughness sublayer over an urban area [Wang et al., 2014], and in DNS over two-dimensional bars [Leonardi et al., 2015]. Our present LES results are in agreement with these observed and DNS results.

This general similarity between turbulent transport of momentum and scalar is further confirmed through the analysis of the quadrant-analysis based turbulent transport efficiency for momentum and scalars, defined in [Wyngaard and Moeng, 1992] as $\eta = \frac{F_{\text{total}}}{(F_{\text{ejection}} + F_{\text{sweep}})}$, where $F$ is the (total or from a single quadrant) flux of momentum or scalars. Figures 4.3(a) and (b) show the point-wise efficiencies and an average over the four points $x_1$ to $x_4$, while figure 4.3(c) shows the ratio of the $\eta_m$ to $\eta_s$, averaged over fours points. The spatial variation of efficiencies inside the arrays is again clearly seen: $x_3$ (in front of cube) has the highest efficiency; both $x_4$ (between the cubes) and $x_2$ (downstream of the cube) show a minimum around
4.2.2 The role of dispersive fluxes

An important aspect that sets very rough walls apart is the importance to total transport of the dispersive flux contribution, which arises from the spatial inhomogeneity of the time-average flow field. In the multiply connected space inside the roughness arrays, the spatial averaging and differentiation operations do not commute [Finnigan, 1985, 2003]. Any mean (time-averaged) quantity $\phi$ can be decomposed into $\phi = \langle \phi \rangle + \phi''$, where the brackets represent a spatial average. In this chapter, we consider $\langle \phi \rangle$ representing the planar average over an $x-y$ plane, at a given height. The dispersive fluxes then arise from this spatial averaging of (4.2) and (4.3). Therefore, the spatially-local time averaged (indicated by the overbar) dispersive momentum stress is $\overline{u_i''u_j''}$ and the dispersive scalar flux is $\overline{u_i''\theta''}$, which can then also be spatially averaged over the plane.
Figure 4.4: Ratios of x-y averaged dispersive or turbulent (resolved + subgrid-scale) fluxes for (a) momentum and (b) scalar. ⭐, Slender06; □, Cube25; △, Wide32.

Figure 4.4 shows the ratios $F_{\text{dis}}/F_{\text{total}} = \langle \overline{u'w'} \rangle / (\langle \overline{u'^2} \rangle + \langle \overline{u'w'} \rangle)$ and $F_{\text{turb}}/F_{\text{total}} = \langle \overline{w' \theta'} \rangle / (\langle \overline{w'^2} \rangle + \langle \overline{w' \theta'} \rangle)$ in (a) and their counterparts $\langle \overline{w' \theta'} \rangle / (\langle \overline{w'^2} \rangle + \langle \overline{w' \theta'} \rangle)$ and $\langle \overline{w' \theta'} \rangle / (\langle \overline{w'^2} \rangle + \langle \overline{w' \theta'} \rangle)$ in (b) for three cases (Slender06, Cube25 and Wide32). A none-exhaustive list of previous studies on the momentum dispersive fluxes [Poggi et al., 2004a, Christen and Vogt, 2004, Coceal et al., 2007b, Martilli and Santiago, 2007, Poggi and Katul, 2008, Leonardi et al., 2015, Giometto et al., 2016] and a few on dispersive scalar fluxes [Christen and Vogt, 2004, Leonardi et al., 2015] have demonstrated their importance within the canopy sublayer, as well as in the roughness sublayer. Similar to previous findings, our simulations also indicate that the dispersive fluxes are significant within the roughness arrays. The dispersive flux can contribute up to 50% to the total momentum or scalar flux below the roughness elements height for some cases. Note that Leonardi et al. [2015] and Coceal et al. [2007b] commented that the dispersive fluxes are only important on the intermediate time scales. We performed our analysis for the time averaged quantities over time spans of approximately $H/U_b = 2000$ ($U_b$ is the bulk velocity) and longer than the $H/U_b = 600$ suggested in Leonardi et al. [2015]. Still, temporal averaging for large $H/U_b$ gives converging results of the dispersive fluxes that continue to show that
Figure 4.5: Normalized dispersive stress and flux for three cases: color scale indicates \((s'' w'')_N = s'' w'' / (\langle s'' w'' \rangle_{z=H} + \langle s'' w' \rangle_{z=H})\) for \(s = u\) or \(\theta\). Lines with arrows are the \(\bar{u}\) and \(\bar{w}\) streamlines.

The differences between dispersive momentum stress and scalar flux are studied in detail in figure 4.5, showing the normalized dispersive stress and scalar flux over an \(x-z\) cross section indicated by the blue line in figure 5.1. We remind the reader here that the total flux, the denominator in the normalization, is negative (downward) for momentum and positive for the passive scalar (upward, emission by the wall). The pseudocolor plots and streamlines are spatially averaged across all repeating units in the domain for better convergence. The strongest dispersive stress fractions are concentrated behind and in front of the obstacles in figure 4.5 (a, c and e). The Slender06 case, even though with the same \(\lambda_p\) as Wide32, has larger dispersive stress fractions that also impact a large area within the gap, which explain why this case has the highest fraction in figure 4.4a. The most important conclusion however that one can draw from figure 4.5 is that, unlike turbulent fluxes, dispersive fluxes of momentum and scalars are quite distinct. The difference between \(\langle w' u' \rangle\) and \(\langle w' \theta' \rangle\) across three cases is the most pronounced in front of the obstacle, where the mean recirculation pattern results in counter gradient dispersive momentum transport.
(fluid slowed by the pressure field being advected upward) but down gradient scalar transport (low concentration fluid transported downwards). This difference emerges from the non-local action of pressure on momentum (the fluid streamwise velocity has to decrease as it approaches the windward face even before it contacts that face), but its absence from the dynamics of scalars (the fluid has to “touch” the surface to uptake scalars). The sign of the dispersive fluxes is thus always the same as the total fluxes, while there is partial cancelation of dispersive fluxes for momentum. A consequence of this is that, as $\lambda_f$ increases, the mean circulation in the canopy sublayer leads to an increase of the scalar dispersive flux contribution, while for the dispersive momentum flux the dispersive contribution decreases (in agreement with Poggi et al. [2004b]) due to this cancelation effect.

### 4.2.3 The effect of roughness types

Now we turn our attention to the second question raised in the introduction: how do changes in roughness geometry affect the exchanges between the wall and the fluid?. The parameter space that characterizes the surface geometry is large. Previous studies have investigated height variations [Yang et al., 2016], as well shapes [Leonardi et al., 2015, Yang et al., 2016] of regular [Kanda et al., 2004, Placidi and Ganapathisubramani, 2015] or irregular [Chester et al., 2007] surface roughness elements. We do not aim to comprehensively examine the parameter space in this paper, but we are rather interested in the general transition of the flow as the roughness, conserving the same area density $\lambda_p$, changes from slender elements with low $\lambda_f$, to wide ones with high $\lambda_f$. The previous figures and discussion already provided some insights; for example, figure 4.4a showed that Slender06 has the highest dispersive momentum flux contributions compared to the other two cases for $z/H < 1.5$, but at higher wall-normal distance, Wide32 is the largest. Whereas for scalar dispersive fluxes in figure 4.4b, Wide32 has the highest dispersive contribution
Figure 4.6: Shear length scale, $L_s$ and the correlation coefficient $r_{uw}$ for cases listed in table 4.1 inside the roughness elements and Slender06 has the highest near $z/H = 1$.

Figure 4.6 shows the shear scale $L_s$, a basic length scale in canopy flows analogous to the vorticity thickness defined in a plane mixing layer, as a function of the frontal blockage ratio $\lambda_f$. It is defined as $L_s = \frac{\bar{u}}{du/dz}$, here computed at $z = H$. $L_s$ decreases with increasing $\lambda_f$, which signifies a larger shear strength and hence more deviation from the classical surface layer profile as the blockage increases. While $L_s$ for Slender06 and Wide32 differ significantly, additional intermediate cases show a monotonic decrease with $\lambda_f$. The correlation coefficient $r_{uw}$ between vertical and horizontal turbulent fluctuations is also computed just above $H$, and depicted in figure 4.6. It can be interpreted as a vertical momentum transport efficiency. As $\lambda_f$ increases, $-r_{uw}$ increases to approximately 0.46, a value consistent with what is typically found in canopy flow and mixing layer flow ($-r_{uw} = 0.5$) [Finnigan, 2003]. The dynamics of this kind of ‘obstructed shear flow’ as termed by Ghisalberti [2009], can be characterized by a few velocity and length scales; a key one among which is the penetration depth ($\delta_e$) of the vortices into the obstruction. $L_s$ defined here is analogous to $\delta_e$. It is worth noting that obstacles in all the cases presented in figure 4.6 have the same plan area density (i.e. $\lambda_p = 0.12$); but by changing $\lambda_f$, we
are observing a transition from a boundary-layer canonical flow, to a mixing-layer one.

Another parameter that can help shed light on the effect of the blockage ratio of the roughness on the flow is the skewness shown in figure 4.7. Slender06 has close to zero skewness of $u'$ and $w'$ (figures 4.7a and b) in the roughness sublayer but higher values are observed as $\lambda_f$ increases in cases Cube25 and Wide32, more typical of canopy flows [Raupach, 1981, Rotach, 1993, Finnigan, 2003]. This is consistent with the previous quadrant analysis for Cube25, showing the dominance of sweeps in the canopy and approximately equal contributions of ejections and sweeps in Slender06 (results not shown). The variation in skewness presents further evidence of the role of frontal area, and hence pressure drag, in dictating the characteristics of the roughness sublayer dynamics. There is also a good correspondence between $w'$ and $\theta'$. The negative skewness for $\theta'$ in figure 4.7c signifies dominance of downward events that tend to bring down cooler fluid regardless of the underlying surface geometry. This is similar to findings for temperature, as a passive scalar, over rough surfaces in the DNS by [Orlandi and Leonardi, 2008].

Finally, the effects of geometry on scalar and momentum fluxes can be examined using the correlation spectrum defined as $R_{XY} = C_{oXY} / (\Gamma_X \Gamma_Y)$, where $C_{oXY}$ is the
Figure 4.8: Correlation spectra $R_{uw}$ in (a)-(c) for different cases; $R_{\theta w}$ in (d)-(f) for different cases. The dotted vertical black lines correspond to $\Delta z/\delta$, $H/\delta$, $3H/\delta$ and $L_x/\delta$ as labeled in (a); solid horizontal black line denotes the height of the obstacles.

cospectrum of time series $X$ and $Y$, $\Gamma_X$ and $\Gamma_Y$ are the power spectra of $X$ and $Y$, respectively. Physically, it can be interpreted as the spectral representation of the correlation between $X$ and $Y$. For $Y$ being vertical velocity fluctuation $w'$ and $X$ being $u'$ or $\theta'$, $R_{XY}$ is interpreted as a transport efficiency in the spectral space.

Point-wise (at $x_1$-$x_4$, and all heights) time series of relevant quantities are recorded at a frequency of 25 Hz. The total length of the time series defined in time unit $L_z/U_0$ is about 60, where $U_0$ is the free stream velocity. Using Taylor’s hypothesis to convert time to length scale with $U_0$ and performing ensemble average using 20 shorter time series at each representative point $x_i$, the correlation spectra are shown in figure 4.8, where only results at $x_3$ (in front of the obstacle) are presented; similar conclusions can be obtained from other points. Eddies of large scales (close to $\delta = L_z$) contribute to the efficient transport of both momentum, and scalars, but a wider range of scales contribute to $R_{\theta w}$. Higher correlation spectra values can be noted for scalars.
for all three cases between $H/\delta$ and $3H/\delta$. In general, from figure 4.8a to c, larger scale motions ($O(\lambda_x/\delta) = 1$) are efficient in transporting momentum even below the canopy, particularly for the Wide32 case. The situation for $R_{\theta w}$ is opposite to $R_{uw}$, and large scale motions are found to contribute most efficiently for the Slender06 in figure 4.8d.

In summary, figure 4.8 shows the change in length scales that contribute to the efficiencies across different geometries. From such change in length scales, we clearly see how distinct surface geometries affect momentum and scalar transports.

### 4.3 Conclusion

We use LES to compare and contrast the transport of momentum and passive scalars over very rough surfaces consisting of three-dimensional cuboid roughness elements. The paper focuses on answering two main questions about the contrasts between momentum and scalar exchanges over rough surfaces in the canopy and roughness sublayers; and the effect of surface geometry on transport. Turbulent transport of momentum and passive scalar are found to be similar as evidenced by quadrant analysis, but the dispersive fluxes (which are non-negligible) differ considerably. The scalar dispersive fluxes on denser canopy are found to be more important than that for sparse one, which is opposite to the behavior of dispersive momentum flux. In addition, we observe a general transitioning behavior from a canonical surface layer dynamics to a typical mixing layer flow or ‘obstructed shear flow’ when the frontal area ratio $\lambda_f$, that is the blockage by the roughness, increases while the planar density of the roughness, $\lambda_p$, is maintained constant. This highlights the dominant role of pressure drag in the divergent dynamics of momentum and scalar transport. Furthermore, contrary to the behavior of momentum, transport efficiencies for scalars measured by the correlation coefficient decrease in response to higher $\lambda_f$. This is
mainly a result of the reduced contribution from large scale motions in the roughness sublayer.

Although we only simulated flows with fixed boundary concentrations, the results about similarity in turbulent and dissimilarity in dispersive transport should hold regardless of the scalar boundary condition. On the other hand, if the scalar concentration influences buoyancy (e.g. temperature), the active role of the scalars will then have a strong impact on the dynamics and the present results might not hold [Li and Bou-Zeid, 2011]. The findings from this paper, especially the scalar dispersive flux contribution over dense canopy, can inform the interpretation of experimental measurements, which are often point-wise data where dispersive fluxes cannot be estimated: such measurement in the canopy and roughness sublayers are missing nearly half of the total fluxes. Our finding can also guide model development since current parameterizations do not distinguish between turbulent and dispersive fluxes, but as our analyses show their physics are quite different and this difference is not the same for momentum and scalars.
Chapter 5

On the Momentum and Scalar Roughness Lengths of Urban Surfaces

5.1 Introduction

The roughness lengths in the Monin-Obukhov similarity theory play a central role in modeling surface-atmosphere interactions. As such, intensive research efforts have been undertaken for measuring and parameterizing these roughness lengths, or the corresponding bulk transfer coefficients over urban surfaces [Kastner-Klein and Rotach, 2004, De Ridder, 2006, Kanda et al., 2007b, Demuzere et al., 2008]. The geometric parameters of the underlying surfaces are often used in such parameterizations. Especially for momentum roughness length $z_{0m}$, a significant progress has been achieved, such as studies by Macdonald et al. [1998], Kanda et al. [2013], Yang et al. [2016] and more examples are given in reviews [Grimmond and Oke, 1999a, Barlow and Coceal, 2009].

On the other hand, there have been significantly fewer studies on the scalar rough-
ness lengths over rough surfaces such as built terrain, despite their importance in modeling turbulent fluxes in urban land-atmosphere models [Demuzere et al., 2008, Ryu et al., 2011, Wang et al., 2013]. These scalar roughness lengths, $z_{0s}$, are usually related to their momentum counterparts, $z_{0m}$, via $\kappa B^{-1} = \log(z_{om}/z_{os})$, where $\kappa$ is the von Karman constant. From field measurement results, we know that many factors can affect the values of $\kappa B^{-1}$. For example, Moriwaki and Kanda [2006] reported field measurements at a suburban site in Tokyo, Japan and concluded that the values of $\kappa B^{-1}$ for heat and water vapor varied with heat sources distribution and surface water availability. Voogt and Grimmond [2000] observed that the method of surface temperature determination also affects the value of $\kappa B^{-1}$ for heat. In terms of the geometric effects on scalar transport, using an outdoor urban scaled-model, [Kanda et al., 2007a] showed that the the logarithmic ratio $\kappa B^{-1}$ follows a universal parameterization even for surfaces of different geometries. In addition to field experiments, wind tunnel experiments on bluff-bodies that are heated or coated with some passive scalars have also advanced our knowledge of the underlying physics. For example, bluff-bodies coated with naphthalene [Barlow et al., 2004] or wetted with water [Ikegaya et al., 2012, Chung et al., 2015] were used to investigate the dependence of scalar transfer coefficients on roughness packing density, height variations, orientations and distributions of scalar sources. Numerical approaches, namely large eddy simulations, were also used by Anderson [2013] to simulate flow and scalar transport over different fractal surfaces; they found that the usually-assumed constant value for $\kappa B^{-1}$ may not hold. Demuzere et al. [2008] conducted sensitivity study in mesoscale model and showed that the model for $\kappa B^{-1}$ by Zilitinkevich et al. [2001] gives the best performance.

However, these phenomenological formulations for the dependence (of lack thereof) of $z_{0s}$, or the ratio between $z_{0m}$ and $z_{0s}$, on the surface geometry still lack an overarching theoretical framework. To develop such theory, more studies are needed.
that systematically vary the geometric properties and document the ensuing changes in the roughness lengths, especially $z_{0s}$, for very rough surfaces like built terrain and at a comparable Reynolds number ($Re$) to that of real urban environments. This study aims to bridge these two research gaps by conducting large-eddy simulations of flow and passive scalar transport over cuboidal roughness elements representing an idealization of individual buildings at high $Re$. Furthermore, we investigate and attempt to explain the different sensitivities of $z_{0m}$ and $z_{0s}$ to changes in surface geometry. The two driving research questions are: (1) Why and how do the geometric parameters of rough surfaces impact momentum and scalar roughness lengths? (2) How do the logarithmic ratio between momentum and scalar roughness lengths over very rough surfaces?

5.2 Numerical Setup

Large-eddy simulation (LES) remains the most appropriate tool to simulate the complex turbulent flows and transports over urban terrain since direct numerical simulations cannot attain the realistic $Re$ values needed to faithfully capture the flow physics [PI et al., 2013, Li et al., 2016b]. Thus, it has been widely used to study this problem [Kanda et al., 2004, Bou-Zeid et al., 2009, Giometto et al., 2016]. The LES model used here implements the immersed boundary method (IBM) to resolve the bluff-body obstacles explicitly. The non-dimensional filtered incompressible continuity (5.1), Navier-Stokes (5.2) and scalar conservation (5.3) equations are solved assuming hydrostatic equilibrium of the mean flow:

$$\frac{\partial u_i}{\partial x_i} = 0,$$

(5.1)
\[
\frac{\partial u_i}{\partial t} + u_j \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = -\frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + F_i + B_i, \tag{5.2}
\]

\[
\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} = -\frac{\partial q^i_s}{\partial x_i}, \tag{5.3}
\]

where \(x, y, z\) denote the streamwise, cross-stream and wall-normal directions respectively, and \(u, v, w\) are the velocity components in these respective directions. \(t\) denotes time; \(u_i\) is the resolved velocity vector; \(p\) is the modified pressure; \(\tau_{ij}\) is the deviatoric part of the subgrid stress tensor; \(F_i\) is the body force driving the flow (here simply a homogeneous steady horizontal pressure gradient along the \(x\) direction); and \(B_i\) is the immersed boundary force representing the action of the obstacles on the fluid. In (5.3), \(\theta\) denotes the concentration of a passive scalar quantity and \(q^i_s\) is the \(i\)th component of the subgrid scale scalar flux. All the variables we will use and discuss are the filtered components, although the usual tilde on top will be omitted for notational simplicity. Equations 5.1-5.3 are pre-normalized by the friction velocity that accounts for the total (viscous and form) surface drag \(u_*\), the boundary-layer depth \(\delta\), air density \(\rho\) and a reference scalar quantity \(\theta_0\).

In this study, the passive scalar \(\theta\) will be considered as temperature assuming very weak heating that does not induce significant buoyant force; the results would be applicable to all other passive scalars such as water vapor. However, future extension to include buoyant forces under strong heating is naturally very important. An isothermal boundary condition of 330K is imposed on all surfaces. Horizontal periodic boundary conditions are applied to all quantities. The top boundary conditions are zero stress and no-penetration (zero normal velocity). Details of the numerical procedures Chester et al. [2007], Li et al. [2016a] and subgrid scale model Bou-Zeid et al. [2005b] will not be presented here and can be found in the cited papers. The code has been verified [Li et al., 2016a,b] for its good performance in simulating both momentum and scalar transports.

Three categories of surfaces with different plan area density, \(\lambda_p\) and frontal area den-
sity, $\lambda_f$, are considered. In the first category (see figure 5.1a), $\lambda_p$ and $\lambda_f$ are varied simultaneously and $\lambda_p \equiv \lambda_f$ and this category is called “Variable P lan and F rontal area density” (VPF). In the second category (see figure 5.1b), $\lambda_f$ is kept constant at 0.25 but $\lambda_p$ is varied, and it is called “Variable P lan area density” (VP). In the third category (see figure 5.1c), $\lambda_p$ is kept constant at 0.12 but $\lambda_f$ is varied, and it is called “Variable F rontal area density” (VF). A few different cases within each category are considered. The simulation parameters are summarized in table 5.1. Table 5.1 lists the simulation parameters.

**Figure 5.1:** Schematic picture showing a “repeating unit” of different geometric setups, where shaded areas represent the obstacle. $H$ is height of the obstacle. The black, orange and green lines illustrate three different variations of geometry within each category. (a) VPF; (b) VP; (c) VF.

### 5.3 Roughness lengths determined from LES

#### 5.3.1 Momentum roughness length and parameterization

Under the framework of Monin-Obukhov similarity theory, the $x$-$y$ plane-averaged mean profiles of stream-wise velocity $\bar{u}$ and scalar $\bar{\theta}$ under neutral stability simplify to the classic log-laws given by (here $\langle \rangle$ represents averaging in the $x$-$y$ plane):

$$\frac{\langle \bar{u} \rangle}{u_*} = \frac{1}{\kappa} \log \left( \frac{z - d}{z_{0m}} \right)$$  \hspace{1cm} (5.4)
Table 5.1: Summary of simulation parameters: $N_i^b$ is the number of points of one obstacle in $i$ direction; $N_i$ is the number of points for the domain. The numbers at the end of the case names represent the first two decimal values of $\lambda_p$ or $\lambda_f$.

\[
\left\langle \bar{\theta} - \bar{\theta}_s \right\rangle T^* = \frac{1}{\kappa} \log \left( \frac{z - d}{z_0} \right), \quad (5.5)
\]

where $d$ is the displacement height; $\bar{\theta}_s$ is the surface scalar value (in this case temperature); $T^* = \frac{F_s}{u_*}$ where $F_s$ being the kinematic surface scalar flux; $\kappa$ is the von Karman constant. Adopting different procedures in calculating $z_{0m}$ can lead to different results [Leonardi and Castro, 2010b]. To understand the implications, we first used a procedure that is similar to previous studies [Kanda et al., 2004, Bou-Zeid et al., 2009, Placidi and Ganapathisubramani, 2015, Yang et al., 2016] by least-square fitting of the log-law from $z = 1.5H$ to $2.0H$ with a constant $\kappa = 0.4$ and the pre-normalized velocity $\left\langle \bar{u} \right\rangle / u_*$ directly from the output of LES. This procedure yields $d$ and $z_{0m}$. We then applied a second method called “drag moment” to calculate the displacement height according to Jackson [1981], before determining $z_{0m}$ alone using least-square fitting from $z = 1.5H$ to $2.0H$. $d'$ denotes the displacement.
height obtained from this method. $d'$ is equivalent to the mean level of momentum absorption by the surface [Leonardi and Castro, 2010b], which can be calculated as $d' = \int_0^H zD(z)dz/\int_0^H D(z)dz$, where $D(z)$ is the total drag acting at height $z$. In this study, we use the resolved plus the subgrid-scale momentum fluxes to compute $D(z)$. $d$ and $d'$ together with $z_{0m}$ determined from these two methods are shown in Fig. 5.2. As a comparison, the models for $d$ and $z_{0m}$ by Macdonald et al. [1998] are also plotted in Fig. 5.2. The values of $d$ from direct fitting are mostly larger than both $d'$ [Jackson, 1981] and the model of Macdonald et al. [1998], in agreement with the findings from Kanda et al. [2004] (Figs. 5.2d, 5.2e and 5.2f). The largest discrepancies between $d$ and $d'$ are observed for low values of $\lambda_p$, and especially for the cases RSF in which $\lambda_p = 0.12$.

Figure 5.2: $z_{0m}$ and $d$ determined with direct fitting from $z = 1.5H$ to $2H$ (filled circle) and drag moment using method by Jackson [1981]. Red-dotted line shows results using models for $d$ and $z_{0m}$ by Macdonald et al. [1998], with $Cd = 1.2$, $\kappa = 0.4$, $\beta = 1$ and $A = 4.43$. (a) and (d) for category VPF; (a) and (d) for category VPF; (b) and (e) for category VP; (c) and (f) for category VF.

Cases in category VPF ($\lambda_p = \lambda_f$) show a peak in $z_{0m}$ between $\lambda_p = \lambda_f = 0.25$ and 0.31 (see Fig. 5.2a). This peak in $z_{0m}$ has been observed in many previous studies.
(Kanda et al. [2004], Hagishima et al. [2009], Leonardi and Castro [2010b]) for arrays of cubical roughness, in which $\lambda_p$ and $\lambda_f$ are always equal. It is not surprising that the peak value reported here is different than the cubical arrays considered by previous studies since the obstacles considered in VPF are not cubes. The effects of separately changing $\lambda_f$ and $\lambda_p$ have also been studied by Placidi and Ganapathisubramani [2015] in wind-tunnel measurements of obstacles made of LEGO bricks. The results shown in figure 5.2b is consistent with their findings of monotonically decreasing trend of $z_{0m}$ with increasing $\lambda_p$. In the category VF (varying $\lambda_f$) the direct fitting method gives a monotonically increasing $z_{0m}$ for increasing $\lambda_f$ but the drag moment method shows a slight peak at around $\lambda_f=0.24$. Both methods however suggest a plateauing of $z_{0m}$ when $\lambda_f$ exceeds 0.25. Qualitatively, Figs. 5.2b and 5.2c demonstrate the opposing effects of $\lambda_p$ and $\lambda_f$ on $z_{0m}$.

For large roughness elements in a high $Re$ flow, the frictional (viscous) drag is much smaller than the pressure drag ($< 7\%$), as demonstrated by Leonardi and Castro [2010b]. Thus, it is here appropriate to model the total surface stress using the inertial quadratic drag law (force on a single element is $0.5A_f\rho C_d\bar{u}^2$), where $A_f$ is the frontal area of one element and $C_d$ is a constant drag coefficient, which is a common approach in rough-wall modelling [Macdonald et al., 1998, Coceal and Belcher, 2004, Di Sabatino et al., 2008]. Substituting $u_*$ from Eq. 5.4 and invoking the force balance between $\rho u_*^2$ on the lot area $A_t$ and the pressure drag yields

$$z_{0m} = (z - d) \exp \left(-\kappa (0.5\lambda_f C_d)^{-1/2}\right).$$  \hspace{1cm} (5.6)

Thus, according to Eq. 5.6, $d$ and $\lambda_f$ directly affect $z_{0m}$. Furthermore, $z_{0m}$ depends explicitly on $\lambda_f$ but not $\lambda_p$. This is consistent with the consensus that $\lambda_f$ is the most important surface morphometric parameter to characterize the momentum transfer.
[Grimmond and Oke, 1999b]. \( d \) in general depends on the surface morphology. As shown in Yang et al. [2016], changes in mutual sheltering among roughness elements is the primary effect that explains the variations in \( d \). Stronger sheltering effect shifts \( d \) (the center of drag force acting inside the canopy layer) upward. In the VP suite of simulations (varying \( \lambda_p \) by changing the separation between roughness elements in streamwise direction), mutual sheltering increases with higher \( \lambda_p \). In this scenario, \( \lambda_f \) is kept constant; variations of \( z_{0m} \) are mainly related to changes in \( d \). Therefore, for constant \( \lambda_f \), increase in \( d \) with \( \lambda_p \) results in decreasing trend in \( z_{0m} \) (Fig. 5.2b).

In category VF, although the mutual sheltering among roughness elements varies for each case (see Fig. 5.1) as \( \lambda_f \) is independently varied, the exponential dependence of \( \lambda_f \) dictates the change in \( z_{0m} \) (Fig. 5.2c). In category VPF, the competing effect of \( \lambda_f \) and \( \lambda_p \) on \( z_{0m} \) gives rise to the characteristic non-monotonic trend (Fig. 5.2a). The model by Macdonald et al. [1998], which only use two parameters (\( \lambda_p \) and \( \lambda_f \)) qualitatively captures the responses of \( z_{0m} \) to variable geometries. For applications in highly heterogeneous urban morphology, more involved modelling may be required; for example, models that explicitly account for the mutual interactions between roughness [Yang et al., 2016] or the statistical properties of the rough surface [Kanda et al., 2013]. Nevertheless, a geometrically-based model is a viable approach to model \( z_{0m} \).

### 5.3.2 Scalar roughness lengths and parameterization

Next, we consider the scalar roughness length \( z_{0s} \) determined from LES in Figs. 5.3a-c. Least-square regression is carried out using the normalized scalar profile (i.e. \( \frac{\langle \theta_s - \theta \rangle}{\theta_s} \) in Eq. 5.5); here also \( d \) could be determined either through the fitting or using the drag moment approach. Physically, \( z_{0s} \) is the height at which the extrapolated normalized scalar profile becomes zero. Thus, at \( z = d + z_{0s} \), \( \theta(z) = \theta_s \) (= 330 K
in our simulations). To gain some physical insights into the variations in $z_{0s}$ with changing geometry, we consider the scalar flux balance within a control volume (CV) that extends from $z = 0$ to some height $z_{ref}$ in the inertial sublayer. The scalar flux at the top of this CV (upward in this case due to higher prescribed surface temperature) is balanced by the total surface fluxes inside it under steady state, $F_s$. Using the commonly adopted bulk transfer relation for the surface scalar flux, this leads to

$$A_t F_s = \int_A C_f(x,y,z) \Delta \theta(x,y,z) \langle \bar{u}(z) \rangle \, dA,$$

where $A_t$ is the lot area, $C_f$ is a bulk scalar transfer coefficient that is in general a function of position; $z$ is some elevation above the canopy sublayer (e.g. the top of the CV $z_{ref}$); and $\Delta \theta(x,y,z)$ is $\langle \bar{\theta}_s(x,y,z) - \bar{\theta}(z) \rangle$. For the cuboidal underlying surface roughness elements, $A_t F_s$ can also be computed as summation of contributions from each facet; thus Eq. 5.7 can be rewritten as

$$A_t F_s = \sum_i A_i C_{fi} \langle \bar{u}(z) \rangle \Delta \theta_i(z),$$

where $A_i$ is surface area of the $i$th facet; $C_{fi}$ can be considered as the average bulk scalar transfer coefficient for the $i$th facet; and $\Delta \theta_i(z)$ is the difference between the average $i$th facet temperature and $\langle \bar{\theta}(z) \rangle$. Manipulating Eqs. 5.5, 5.6 and 5.8, leads to

$$z_{0s} = (z - d) \exp \left( -\kappa \left( \sum_i \lambda_i C_{fi} \frac{\Delta \theta_i(z)}{\Delta \theta(x,y,z)} \right)^{-1} (0.5 \lambda_f C_d)^{1/2} \right),$$

where $\lambda_i = A_i/A_t$. $\sum_i \lambda_i$ is ratio of the total surface area to the lot area $A_t$. The dependence on $\frac{\Delta \theta_i(z)}{\Delta \theta(x,y,z)}$ drops out from Eq. 5.9 because of the isothermal boundary condition imposed in this case (see Eq. 5.10), but in general $z_{0s}$ depends on the
surface temperature distribution.

\[ z_{0s} = (z - d) \exp \left( -\kappa \left( \sum_i \lambda_i C_{fi} \right)^{-1} (0.5\lambda_f C_d)^{1/2} \right) \]  

(5.10)

Figure 5.3: (a)(b)(c): \( z_{0s} \) determined using least-square regression using \( d \) directly fitted (filled circle) and \( d' \) (filled triangle). (d)(e)(f): the logarithmic ratio \( z_{0m} \) to \( z_{0s} \).

From Eq. 5.10, we can make a few useful observations. The first is that, compared to Eq. 5.6 for \( z_{0m} \), \( z_{0s} \) depends on the ratio between \( (\lambda_f^N)^{1/2} \) to \( \lambda_i^N \), where \( N \) denotes “normalization” by \( C_d \) and \( C_{fi} \), respectively. Therefore, in category VP, for constant \( \lambda_f \), \( z_{0s} \) increases with \( \lambda_p \) (see Fig. 5.3) as a direct result of the increasing total surface area. The exponential dependence of \( \lambda_i \) outweighs the decreasing factor \( z - d \).

Variations of \( z_{0s} \) in category VF can also be explained similarly by considering the ratio \( (\lambda_f)^{1/2} \) to \( \sum_i \lambda_i \) as a first order approximation. The monotonically decreasing \( z_{0s} \) with \( \lambda_f \) is consistent with decreasing values of \( (\lambda_f)^{1/2}/\sum_i \lambda_i \) (i.e. \( (\lambda_f)^{1/2}/\sum_i \lambda_i \) decreases from 0.30 to 0.14 for cases VF08 to VF32). In category VPF where
\( \lambda_f = \lambda_p \), there is no general explanation since more factors are involved as both geometric parameters change. Overall, this simple analysis shows that \( z_{0s} \) has a different geometric dependence compared to \( z_{0m} \). In addition, the surface scalar transfer coefficients \( C_f(x, y, z) \) normalized by the average value of the five facets can be spatially highly variable as shown in Fig.5.4. The scalar fluxes on each facet as well as for the bottom surfaces are normalized by the average from the five facets of the cuboid. Two examples from all the simulations (VP31 and VF12) are shown. The surface scalar transfer coefficients for each facet differ drastically.

Thus, it is rather challenging to parameterize the scalar surface fluxes using a succinct model based entirely on morphometric parameters. This is in contrast to momentum flux, in which the pressure drag can be related to the frontal area

![Figure 5.4: Surface scalar transfer coefficients normalized by the cuboid-averaged value on all five facets and the bottom surface. (a): VP31; (b): VF12.](image-url)


directly; therefore allowing more straight-forward parameterization of $z_{om}$ based on geometric parameters. However, modelling of the logarithmic ratio between $z_{om}$ and $z_{0s}$ has been a common approach in the literature. The models for $\log(z_{om}/z_{0s})$, which is often referred to as $\kappa B^{-1}$, based on experimental results and theoretical considerations [Brutsaert, 1965, Zilitinkevich et al., 2001] continue to be an active subject of research. The next section presents a model for $\kappa B^{-1}$ by applying the surface renewal theory over three-dimensional large roughness elements.

5.4 Surface renewal theory on very roughness surface

Surface renewal theory models the process of scalar transport across an interface. It is based on the surface scouring by eddies, assumed to occur randomly. The eddies come in contact with the surface for some time interval before they are swept away and replaced by new ones. During that interval, the flow near the surface is laminar and the upward diffusion of the scalar is imply by molecular diffusion. Since Danckwerts [1951] first introduced a statistical model that accounts for the time duration over which eddies are in contact with the surface (i.e. internal between renewals), extending the theory into turbulent transport of scalars has been successfully carried out in atmospheric boundary layer [Brutsaert, 1975b, Clayson et al., 1996, Katul et al., 1996, Snyder et al., 1996, Denby and Snellen, 2002, Castellvi et al., 2008]. Most applications of the surface renewal theory are limited to the “natural rough” surfaces such at over ocean surface [Clayson et al., 1996], glacier surface [Denby and Snellen, 2002] and forests [Katul et al., 1996]. In the context of the urban surface, large bluff-body objects can be taller than 2.5% of the typically rough wall boundary layer thickness and their effect can extend to about three times their height, and
hence more than half of the thickness of the logarithmic layer can be affected by these roughness elements [Harman et al., 2004].

In the framework of the surface renewal theory, an eddy places a mass of air in contact with the surface for an interval $dt$, before it is replenished by the scouring from a new one; and the process repeats. The scouring-replenishing process can be considered as a surface renewal event and the rate of occurrence of the surface renewal event is assumed to follow an exponential distribution [Danckwerts, 1951]. Thus, $\phi(t) = s \exp(-st)$ is the probability density function for the rate of occurrence of the surface renewal event, where $s$ is the rate parameter. Physically, $1/s$ is the characteristic time that an eddy remains in contact with the surface before it is swept away.

The rate parameter $s$ has to be chosen appropriately, with the understanding that the organized eddy motions (namely sweeps and ejections) account for the scouring motions that transport scalar across the interface. Previous studies over large bluff-body obstacles [Leonardi et al., 2015, Li and Bou-Zeid, in preparation] demonstrated that sweeps and ejections indeed dominate in the roughness sublayer for turbulent scalar transport. Therefore, the time scale $1/s$ should be chosen to represent the duration of the ejection-sweep cycles, which are driven by the mean shear stress at the canopy-air interface [Paw et al., 1995, Katul et al., 1996]. Here, we choose $1/s \propto u_\tau/z_{0m}$, where $u_\tau = \sqrt{-\tau(z = H)/\rho}$ and $\tau(z = H)$ is the mean Reynolds stress at the top of the canopy layer. A crucial difference between the current analysis and the related derivation proposed in Brutsaert [1975b] is the choice of time scale $1/s$. In the paper by Brutsaert [1975b], the time scale $1/s$ follows from the inner layer time scale $1/s \propto (\nu/\epsilon)^{1/2}$, where $\epsilon$ is the rate of energy dissipation and $\nu$ is kinematic viscosity.

Very close to the interface of large bluff bodies with air, similar to natural surfaces considered in Brutsaert [1975b], the small eddies (corresponding to the viscous and buffer layers) are responsible for eddy scouring and they scale with the viscous fluid properties (depicted as the smaller gray arrows in Fig. 5.5); however, the additional
large organized eddy motions in the roughness sublayers (colored arrows in Fig. 5.5) are the main structures accounting for the turbulent renewal over very rough. We hypothesize here that it is this large-scale renewal that is the most restricting of the two for very rough surfaces, and that its rate should be used in formulating an exchange law for such surfaces.

Figure 5.5: Schematic picture showing the canopy, roughness sublayer and inertial sublayer.

Close to the surface, diffusion/conduction is the only process whereby scalars are transported. The rate of molecular diffusion/conduction in the $z$ direction is given by $-\rho \alpha (\partial c/\partial z)$. Thus, the total scalar flux from the surface averaged over the surface renewal events is $-\int_0^\infty \rho \alpha \phi(t) (\partial c/\partial z) dt$ at $z = 0$. Given that $\phi(t) = s \exp(-st)$, the total scalar flux is:

$$ F_c = -\rho \alpha s \int_0^\infty \exp(-st) (\partial c/\partial z)|_{z=0} dt. \quad (5.11) $$

Assuming the flow is one dimensional and solving

$$ \frac{\partial c}{\partial t} = \alpha \frac{\partial^2 c}{\partial z^2} \quad (5.12) $$
for boundary conditions

\[ c = c_a, \, z > 0, \, t = 0 \]
\[ c = c_a, \, z \gg 0, \, t > 0 \]
\[ c = c_s, \, z = 0, \, t > 0, \]

where \( c_a \) is the mean scalar concentration in the inertial later (above the canopy sublayer) where the fresh air brought by new eddies originates, \( c_s \) is the scalar concentration of the surface, and \( \alpha \) is the molecular diffusivity, gives

\[
\left. \frac{\partial c}{\partial z} \right|_{z=0} = \frac{(c_a - c_s)}{(\alpha \pi t)^{1/2}},
\]

which can be substituted into (5.11) to obtain:

\[
F_c = \rho(\alpha s)^{1/2}(c_s - c_a).
\] (5.13)

Using the time scale \( t_0 = A/s = Au_r/z_{0m} \) (where \( A \) is a proportionality constant) and defining the interfacial Sherwood number (e.g. if \( c \) is some passive scalar) as \( Sh = \frac{F_c}{\rho u_r(c_s - c_a)} \), Eq. (5.13) can then be reformulated as:

\[
Sh = A \rho \left( \frac{z_{0m} u_r}{\nu} \right)^{-1/2} \left( \frac{\alpha}{\nu} \right)^{-1/2}.
\] (5.14)

In addition, \( z_{0m} \) and \( z_{0s} \) can be related to the interfacial \( Sh \) and \( C_d \) [Anderson, 2013] as

\[
z_{0s} = z_{0m} \exp \left[ -\kappa \left( Sh^{-1} - C_d^{-1/2} \right) \right],
\] (5.15)
in which $Sh^{-1} - C_d^{-1/2}$ is usually referred to as $B^{-1}$, i.e. $z_{0s} = z_{0m} \exp[-\kappa B^{-1}]$. From the last two equations we can now obtain:

$$B^{-1} = Sh^{-1} - C_d^{-1/2} = C_1 Re_*^{1/2} + C_2,$$

(5.16)

In the fully rough limit, $C_d$ is constant with respect to $Re$ (i.e. only depends on the geometry of the surface) and thus $C_2 = -C_d^{-1/2}$ is a constant. This explains why $B^{-1}$ is usually modelled as a function of the roughness Reynolds number $Re_* = \frac{z_{0m} u_*}{\nu}$ in practical applications, where $C_1 = (A\rho)^{-1} \left( \frac{\nu}{\epsilon} \right)^{1/2}$ and $C_2$ are constants depending on the details of the surface roughness and the fluid properties.

Fig. 5.6 shows the calculated $B^{-1}$ from LES results for all the three-dimensional rough surfaces in Table.5.1, in addition to results from simulations of flow over two-dimensional bars of variable height to gap-width ratios. Models from Brutsaert [1965, 1975b] and Owen and Thomson [1963] as well as the $Re_*^{1/2}$ line are also shown in Fig.5.6. The model by Brutsaert [1965, 1975b], which adopts the time scale $(\nu/\epsilon)^{1/2}$ in the surface renewal model, results in $B^{-1} = C_1 Re_*^{-1/4} + C_2$ instead of $Re_*^{-1/2}$ in Eq.5.16. Model by Owen and Thomson [1963] postulated $B^{-1} = c_1 Re_*^m (Pr)^n$ by considering the Reynolds analogy for a rough surface, where the constants $m = 0.45$, $n = 0.8$ and $c_1 = 0.45 - 0.7$ are found from experimental data. Fig.5.6 shows that surfaces of three-dimensional roughness elements closely follow the relation $B^{-1} \propto Re_*^{1/2}$ or $Re_*^{0.45}$ (slopes are too close to distinguish the match quality). Considering a least-square fitting of the models $B^{-1} \propto Re_*^{1/2}$ versus $B^{-1} \propto Re_*^{1/4}$ for all cases of the three-dimensional roughness, the R-squares are 0.70 and 0.46 respectively.

### 5.5 Conclusion

We conducted large-eddy simulations for urban-like surfaces consisting of arrays of very large cuboids that intruded well into the inertial layer. Both the momentum
and scalar roughness lengths are computed for the various geometries to inform surface-layer similarity relations. In particular, we independently vary the frontal area density $\lambda_f$ and the plan area density $\lambda_p$. The variations in $z_{0m}$ can be understood as resulting from the combined effects of increasing $\lambda_f$ and decreasing $\lambda_p$. Models based on morphometric parameters can qualitatively capture the trend in $z_{0m}$. In contrast, the scalar roughness length $z_{0s}$, not only depends on the geometric parameters, but it also varies with the surface exchanges coefficients, which show significant spatial heterogeneities for individual facet of the obstacle. Thus, it is in general much more challenging to derive a purely morphometrically-based model for the scalar roughness length.

In addition, we demonstrate that using the surface renewal theory and choosing the velocity scale $u_\tau$ and length scale $z_{0m}$ as the characteristic scales for the roughness sublayer, the logarithmic ratio $\log(z_{0m}/z_{0s})$ follows $Re_s^{1/2}$. Eq.5.16 is similar to the model proposed by Zilitinkevich et al. [2001], which did not adopt the surface renewal approach was rather based on dimensional arguments. However, both
approaches arrive at a similar conclusion. For applications in realistic urban settings, morphometrically-derived models for $z_{0m}$ can be useful. They can be then combined with the present results for $\log(z_{0m}/z_{0s})$ to model $z_{0s}$. 
Chapter 6

Signatures of Air-Wave Interactions over a Lake

6.1 Introduction

The exchanges of momentum, heat and passive scalars between the atmosphere and the underlying earth surfaces play a central role in a wide range of geophysical and environmental systems. Their accurate measurement and modeling have thus been the subject of many studies in numerous fields such as oceanic and atmospheric sciences, hydrology, ecology, and limnology. Water surfaces, unlike land surfaces, are continuously changing in response to the momentum and energy exchanges at the air-water interface [Belcher and Hunt, 1998, Hara and Belcher, 2002, Kudryavtsev and Makin, 2004]. The main framework to relate these air-water exchanges to the properties and conditions of the lower atmosphere and the surface, including water surfaces, remains the Monin-Obukhov similarity theory (MOST) via the following equations:

\[ \bar{u} = \frac{u_*}{\kappa} \left[ \log \left( \frac{z}{z_0m} \right) - \Psi_m \left( \frac{z}{L} \right) \right], \]  \hspace{1cm} (6.1)
\[ \bar{\theta} - \theta_s = \frac{-H}{\kappa u_* \rho C_p} \left[ \log \left( \frac{z}{z_0 h} \right) - \Psi_h \left( \frac{z}{L} \right) \right], \quad (6.2) \]

\[ \bar{q} - q_s = \frac{-E}{\kappa u_* \rho} \left[ \log \left( \frac{z}{z_0 v} \right) - \Psi_v \left( \frac{z}{L} \right) \right]. \quad (6.3) \]

In the above, the overbars denote mean air properties; \( u_* \) is the friction velocity; \( \kappa \) is the von Karman constant; \( \theta \) is the potential temperature and \( q \) the relative humidity of the air at a height \( z \), while the same symbols with a subscript \( s \) denote surface level values; \( u \) is streamwise wind speed at a height \( z \); \( H \) and \( E \) are the sensible heat and water vapor fluxes; \( \rho \) and \( C_p \) are the density and specific heat at constant pressure of air; and \( z_{0m}, z_{0h} \) and \( z_{0v} \) are, respectively, the roughness lengths for momentum, heat and water vapor. \( \Psi_m, \Psi_h, \) and \( \Psi_v \) are the stability correction functions of MOST that vary with the stability parameter \( z/L \), where \( L = -\theta_r u_*^3 / (\kappa g w' \theta_v') \) is the Obukhov length, \( w' \theta_v' \) is kinematic (surface) buoyancy flux where the primes denote the turbulent perturbation components, \( \theta_v \) the virtual potential temperature, \( \theta_r \) the reference temperature, and \( g \) the gravitational acceleration. Knowing the profiles (left hand side of Eqs. 6.1-6.3) allows one to compute the fluxes that appear on the right hand side if the roughness lengths are known, hence the keen interest in understanding and parameterizing these lengths that characterize the earth surface.

The parameterization of the momentum roughness length \( z_{0m} \), or equivalently the drag coefficient, over water surface remains an active research topic. Apart from the Charnock’s relation [Charnock, 1955] for \( z_{0m} \), other models have been proposed that include wave surface state parameters such as wave period, wave age and wave steepness ([Brutsaert and Toba, 1986, Nordeng, 1991, Ataktürk and Katsaros, 1999, Pan et al., 2005, Zhao et al., 2015]. However, no universally accepted relation between \( z_{0m} \) and surface wave state has yet been formulated. Recent numerical and experimental studies have advanced our fundamental understanding of air-water interactions,
especially the impact of the direction of wave propagation on momentum transport, raising the potential for improved models for the roughness length. Experimental measurements over open sea or large lakes have shown that the direction of wave propagation can impact the angle between the surface stress vector and the mean wind direction [Geernaert et al., 1993, Rieder and Smith, 1998, Drennan et al., 1999, Grachev and Fairall, 2001]. The observation that the directionality of wave propagation significantly alters the momentum transport was also demonstrated in the LES study by Sullivan et al. [2008]. The wind-following and wind-opposing waves were found to modulate the near-surface pressure field differently; this field generates the so-called pressure or form drag. Sullivan and McWilliams [2010] summarized numerical and experimental results that demonstrate that the momentum transport efficiency decreases with the ratio of the wave phase speed to the wind speed projected onto the direction of wave propagation (from field measurements that contain directional wave spectra). However, more analyses remain needed to fully elucidate the physical attributes of momentum transport under different surface wave conditions, and subsequently improve the parameterizations of surface drag. This open challenge is the first motivation of the present study, which is discussed in detail in chapter 6.

On the other hand, scalar transport and the associated scalar roughness lengths over water have not been investigated nearly as often as momentum. Theoretical analyses of the relative magnitudes of \(z_{om}, z_{oh}\) and \(z_{ov}\) [Garratt and Hicks, 1973, Brutsaert, 1975a] have attempted to propose different functional relations between these roughness lengths that depend on the roughness Reynolds number, \(Re_* = u_* z_{om}/\nu\), which is a good estimate of the ratio of form drag to viscous drag (\(\nu\) is the kinematic viscosity of air). Previous studies proposed models of \(\log(z_{om}/z_{oh})\) as power law functions of \(Re_*\) [Owen and Thomson, 1963, Sheriff and Gumley, 1966, Brutsaert, 1975b, Zilitinkevich, Grachev, and Fairall, 2001]. However, different approaches and
assumptions lead to different exponents in these power laws, and testing against experimental results to differentiate the skills of these various approaches remain lacking. This gap is the second motivation for our work in chapter 6.

In chapter 6, we use the field data from the Lake-Atmosphere Turbulent EXchange (LATEX) field measurement campaign [Vercauteren et al., 2008] over lake Geneva that has the desirable feature of a relatively simple wave field (we will come back to this point in later section in chapter 6). The problem of momentum exchange between atmosphere and underlying water surfaces is revisited in this chapter by thoroughly examining the signatures of air-wave interactions. We then implement an approach for computing the surface temperature and humidity based on heat and water vapor flux measurements that reduces the error in the computation of the temperature and humidity gradients, allowing more robust estimates of the scalar roughness lengths. These experimentally determined roughness lengths are then used to test the various models proposed for the ratio of momentum to scalar roughness lengths.

In this chapter, we examine the momentum and scalar exchanges between water surface and the air in detail. Specifically, the impact of surface wave states on the momentum exchange is analyzed in detail. The Monin-Obukhov similarity relations in the atmospheric surface layer for momentum, heat and water vapor are repeated here:

\[
\bar{u} = \frac{u_*}{\kappa} \left[ \log \left( \frac{z}{z_{0m}} \right) - \Psi_m \left( \frac{z}{L} \right) \right],
\]

\[
\bar{\theta} - \theta_s = \frac{-H}{\kappa u_* \rho c_p} \left[ \log \left( \frac{z}{z_{0h}} \right) - \Psi_h \left( \frac{z}{L} \right) \right],
\]

\[
\bar{q} - q_s = \frac{-E}{\kappa u_* \rho} \left[ \log \left( \frac{z}{z_{0v}} \right) - \Psi_v \left( \frac{z}{L} \right) \right].
\]
The chapter is organized as follows: section two describes the experimental details and basic analyses of the measurements; section three discusses the impact of surface wave states on momentum exchange and proposes a modified surface layer similarity relation; section four focuses on details of the computation and analysis of scalar exchange and the corresponding roughness lengths.

6.2 Experimental setup

The Lake-Atmosphere Turbulent EXchange (LATEX) field measurement campaign took place over Lake Geneva, Switzerland, between August and October of 2006 (DOY 226 to DOY 298). Four pairs of Campbell Scientific CSAT3 sonic anemometers and Licor LI7500 open path CO2/H2O analysers were deployed on a tower fixed to the bottom of the lake at $z = 1.66, 2.31, 2.96, 3.61$ m above mean water surface. The tower is at about 100 m from the northern shore of the lake, which at that location is over 10 km wide. All CSAT3/LI7500 pairs were oriented in the same direction, away from the shore, and we filter out data when the wind is coming from the back of the tower such that the open water fetch of our measurements is over 10 km. This large fetch implies that all measurements are well within the internal equilibrium layer of the lake [Brutsaert, 1998, Bou-Zeid et al., 2004]. The instantaneous water surface elevation directly under the atmospheric turbulence measurements was measured using a high-frequency submersible level transducer (Pressure Systems Inc., model 735; 0.05% accuracy) mounted 1.15 m below the surface. Other deployed instruments relevant to this study were used to measure air temperature and relative humidity (Rotronic hygroclip S3 at 3.05 m), the surface water temperature (Apogee Instruments IRTS-P infrared thermocouple), and the lake current (Nortek Lake current profiler). For a detailed experimental setup of
The setup thus allows the measurement of the fluxes of momentum \( (\overline{u'w'^2} + \overline{v'w'^2})^{1/2} = u^* \), sensible heat \( H \), and water vapor \( E \) using the eddy covariance technique and the data from the CSAT3/LI7500 pairs. Double angle rotation, linear detrending, and the Webb correction [Webb et al., 1980] for the scalar fluxes were applied to the data. Tests confirm that the fluxes computed at the four levels are in excellent agreement (as they should be in the constant flux layer); therefore, the averages of the four measurements of the different fluxes are used, though using the individual measurements from each height gives essentially very similar results. The fluxes, along with the mean potential temperature averaged over the 4 levels and used as reference temperature, are then used to determine the value of the Obukhov length \( L \) used in Eq. 6.4 to Eq. 6.6.

To distinguish the influence of waves from other influences, in various parts of this chapter we also compare the LATEX results to those obtained over a vineyard (see full site and description in Li and Bou-Zeid [2011]; the sensors used and data analysis procedures are exactly the same as for the lake data. This allows us to confirm whether a given observation results from the interaction with waves (present only over the lake) or from other factors such static stability (present in both datasets). We selected the vineyard data measured at a height of 2.4 m (comparable to the measurement height over the lake) using a set-up near the edge of the site, such that the measurements are not directly influenced by the movements of the vegetation since the footprint mainly features much shorter grass vegetation.
6.3 Basic analyses

As mentioned in the introduction, the wave field over smaller water bodies is less complicated than the open sea, where most field measurements have been conducted previously. Field measurements over open sea are subjected to many complicating factors such as wave breaking, sea sprays and wave nonlinear interactions [Janssen, 2004]. Furthermore, over open seas, wind waves [Drennan et al., 2003] and swells [Drennan et al., 1999, Smedman et al., 1999] coexist. Wind waves are generated by spatially and temporally local wind, whereas swells have been generated at a distant location and/or during previous times and have propagated to the studied locations. When they coexist, it is difficult to disentangle the influence of different types of waves on momentum transport. However, for smaller water bodies such as lake Geneva, the generated waves tend to travel to the shore in relatively short time period, quickly dissipating a large fraction of their energy. Thus, the wave field would be dominated by wind waves during high wind periods and by swell for a short period after the wind dies down. A small-scale water body (but not too small so as to allow wave formation and propagation) thus presents an auspicious scenario to study momentum transfer from air to water without the distractions and added complexity of a wave field with multiple interacting wave types. However, relatively few studies have been conducted over lakes to take advantage of this feature [Ataktürk and Katsaros, 1999], hence the appeal of using the LATEX dataset.

Since the surface of the lake mostly consisted of one of those two types of waves (wind waves or swells), it could be conceptualized as consisting of a statistically homogeneous two-dimensional wave field represented by a characteristic significant wave height, wave period, wave length and phase speed associated with these significant waves. Therefore, one can infer the conditions of the underling wave field based on the level transducer measurement (except direction of propagation), thereby distinguishing between wind waves and swell. The level measurements allow us to compute
the significant wave height, $H_s$ (as the average of the highest one-third of wave height [Holthuijsen, 2010]), and the period $T$ (as the average of the period of the highest one-third of waves.) and associated frequency $\omega_s = 2\pi/T$. The wave steepness, $S$, is then given by the ratio of the significant wave height $H_s$ and the significant wave length $\lambda$, where $\lambda$ is obtained from the full dispersion relation [Lighthill, 2001]:

$$\omega_s^2 = \frac{2\pi g}{\lambda} \tanh \left( \frac{2\pi}{\lambda} d \right), \quad (6.7)$$

where $d$ is the average water depth at the measurement site, which was approximately 3.5 m. We evaluated the effect of the accuracy of water depth determination on the wavelength obtained and found the results were insensitive to small water depth variations. We also attempted an alternative method where $\omega_s$ is computed as the peak frequency from the wave energy spectra. This approach gives overall similar results. However, since the first method accounts for a range of important frequencies, it is a better statistical representation of the entire wave field compared to the single value corresponding to the peak frequency. The short wind waves and the longer, less steep swell can be clearly distinguished by the two branches in Fig. 6.1. The short winds waves eventually reach equilibrium with air and according to Pierson and Moskowitz [1964], the waves are fully developed when the wave age $c_p/U_a$ is approximately 1.2, where $c_p$ is the wave phase speed and $U_a$ is the mean wind speed at some reference height. Usually $U_a$ is taken as the wind speed at 10 m under neutral conditions [Rutgersson and Smedman, 2001], $U_{N10}$. Typically, the fully developed waves (i.e. swell) propagate at speeds larger than 1.2 $U_{N10}$, and their direction of propagation is independent of the local wind direction. To account for the directional information of wave propagation, we adopt the criterion for categorizing a wave as swell to be $|c_p/U_{N10} \cos \theta| > 1.2$, where $\theta$ is the angle between wave propagation and mean wind, similar to [Sullivan et al., 2008, Sullivan and McWilliams, 2010] (we will elaborate
Figure 6.1: Significant wave height versus significant wavelength. The higher branch corresponds to wind waves that directly respond to local atmospheric forcing and that have high wave steepness. The lower branch waves are referred to as swell; they are due to waves generated non-locally (swell persisting from previous higher wind periods or potentially boat wakes). The color scale indicates wave steepness $S$.

on how $\theta$ is determined in section 6.4.2.)

Fig. 6.2 depicts how the wave properties are linked to the turbulent structures in the atmospheric boundary layer (ABL), specifically the streamwise size of the structures

Figure 6.2: Autocorrelation of the mean wind for different surface wave characteristics. a) With changing wave steepness. b) Averaged autocorrelation over wind waves (young) and swell (old).
as educed from the autocorrelation function. Taylor’s frozen turbulence hypothesis was used to convert time series to spatial series [Stull, 2012]. Fig. 6.2(a) shows that, as the waves steepen, the spatial autocorrelation of the streamwise wind speed $u$, $\rho_{uu}(L)$ where $L$ is separation distance, decreases. Comparison between the lake and vineyard data (not shown here) reveal that $\rho_{uu}$ is significantly more sensitive to wind speed over the lake than over the vineyard, suggesting that the modulation of the lake surface by wind results in a feedback that influences turbulent structures in the ABL. Averaging separately over all periods of wind waves (i.e. young wave) and swell (old wave), defined according to the aforementioned criterion, gives distinctive integral spatial scales as depicted in Fig. 6.2(b); the young waves are associated with active strong winds with an integral spatial scale of 189 m, while over the old waves the integral scale increases to 532 m. The integral time scales also follow a similar trend, suggesting the existence of larger and more persistent turbulence structures over swell.

6.4 Coupling between surface waves and momentum transport

In the previous section, we demonstrated that wave properties are associated with distinctive turbulent structures: active waves with shorter structure and swell with longer structures. The state of the surface and the atmosphere interact and evolve together, rather than one dictating the properties of the other. In this section, we aim to investigate the influence of surface wave properties on momentum transport to further understand this interaction.
6.4.1 The angle between the mean wind and stress vectors

It has been widely reported in the literature [Weber, 1999], that there often is a large misalignment between the mean horizontal wind vector $\vec{u}$ and the surface stress vector $-\vec{\tau}$ (in this paper $\vec{\tau}$ is defined as the stress from air on water, and thus $-\vec{\tau}$ is from water on air, $\vec{\tau} = \vec{\tau}_x + \vec{\tau}_y = -\rho \langle u'w' \rangle \hat{x} - \rho \langle v'w' \rangle \hat{y}$, where $\hat{x}$ and $\hat{y}$ are the unit vectors). The angle of misalignment $\alpha$ between $\vec{u}$ and $\vec{\tau}$ is defined as:

$$\alpha = \begin{cases} 
\arctan \left( \frac{v'w'}{u'w'} \right) - \arctan \left( \bar{v}/\bar{u} \right), & \text{for } v'w' < 0 \text{ and } u'w' < 0 \\
\pi + \arctan \left( \frac{v'w'}{u'w'} \right) - \arctan \left( \bar{v}/\bar{u} \right), & \text{for } v'w' < 0 \text{ and } u'w' > 0 \\
\arctan \left( \frac{v'w'}{u'w'} \right) - \arctan \left( \bar{v}/\bar{u} \right), & \text{for } v'w' > 0 \text{ and } u'w' < 0 \\
-\pi + \arctan \left( \frac{v'w'}{u'w'} \right) - \arctan \left( \bar{v}/\bar{u} \right), & \text{for } v'w' > 0 \text{ and } u'w' > 0 
\end{cases}$$ (6.8)

This definition of $\alpha$ is more clearly illustrated in Fig. 6.3, with subplots (a) to (d) respectively depicting the four lines in Eq. 6.8. Various reasons for this angle misalignment have been discussed previously in the literature. As mentioned in the introduction Geernaert et al. [1993] and Rieder et al. [1994] attributed high values of $\alpha$ in measurements over sea surface to the swell not traveling in the same direction as the mean wind. Mahrt et al. [2001], however, found that the Ekman turning effect on momentum transport by large convective eddies to be the reason for the misalignment. Recently, Bernardes and Dias [2010] reported that the misalignment increases with atmospheric instability and the observed ‘misalignment’ is due to statistical error. To tackle this question, we examine the relation between the surface wave age $c/u_*$ and $\alpha$ in Fig. 6.4. In this section, and to ensure the fluxes are well-resolved by the instruments and minimize the impact of statistical errors, we filtered out the momentum fluxes to exclude periods of exceptionally small components of stress, which corresponds to both $\langle u'w' \rangle$ and $\langle v'w' \rangle$ being smaller than $10^{-4} \, m^2s^{-2}$. This prevents potential contamination from measurement errors associated with small
Figure 6.3: Schematic diagram showing four quadrants (a)-(d), which are defined in Eq. 6.8. \( \hat{x} \) and \( \hat{y} \) are the unit vectors in the streamwise direction of \( \bar{u} \) and cross-stream direction of \( \bar{v} \). \( \vec{\tau} \) is defined as the stress from air on water; \( \tau_x \) and \( \tau_y \) are the stress magnitudes along \( \hat{x} \) and \( \hat{y} \) directions.

surface shear stress. The results confirm that \( \alpha \) varies with wave age. This angle has a much larger variability for swell (which can be identified by their lower steepness as depicted by their green-blue marker color) compared to wind waves (high steepness). This finding is consistent with previous studies conducted over ocean [Donelan and Drennan, 1997, Kudryavtsev and Makin, 2004], where the presence of counter-, cross- and following-swells was identified from directional wave spectra. Fig. 6.4 also indicates that for wind waves, which correspond to larger wave steepness \( S \) (i.e. the higher branch in Fig. 6.1) the variability of \( \alpha \) is smaller (less than 30°). The fact that \( \alpha \) is not exactly zero for these wind wave cases may be due to 1) the fluctuation of the mean wind direction within the time period of averaging or its spatial variability over the upwind fetch, 2) measurement errors, 3) the Ekman turning effect described above, 4) the simplicity of the assumption of a monochromatic uniform wave field. The ensure that this variability of alignment is truly caused by wave properties and

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not by stability that happens to be correlated with wind speed and thus wave properties, we contrast the variation of $\alpha$ with stability for both the lake and the vineyard in Fig. 6.5. Overall, at a given range of stability (especially $z/L < 0.1$), $\alpha$ spans a much wider range for the lake than for the vineyard. The difference is not clear under stable conditions due to stronger winds over the lake, which results in waves aligned with the wind, but very obvious during unstable conditions. This proves that the wave field plays a key role in the wind-stress misalignment, independently of stability, errors, or Ekman turning. To explore the impact of this misalignment further, we computed the momentum transport efficiency $\eta_c$, where the vertical transport of streamwise momentum $\langle u'w' \rangle$ is considered. The efficiency is defined as the ratio of the total flux over the down-gradient flux (from ejections and sweeps only):

$$\eta_c = \frac{F_{\text{total}}}{F_{\text{downgradient}}} = \frac{\langle u'c' \rangle}{\langle u'c' \rangle_{\text{ejections}} + \langle u'c' \rangle_{\text{sweeps}}}$$  \hspace{1cm} (6.9)
It has been previously shown in Li and Bou-Zeid [2011], using the same two data sets used here, that momentum transfer efficiency decreases with instability. This trend is not surprisingly reproduced here in Fig. 6.6 (for now only consider the data points with $45^\circ < \alpha < 45^\circ$, where the misalignment of wind and stress is not significant). However, another factor that clearly plays an important role is the stress vector orientation relative to the mean wind. This is amply demonstrated in Fig. 6.6 in the stability range $10 < z/L < 0.5$. At a fixed stability, large $\alpha$ corresponds to small $\eta_m$, and vice versa. Negative efficiencies are observed for a few cases when $\alpha$ is greater than $90^\circ$, which implies upward momentum transport (the blue points) where inward and outward interaction dominate. This is not surprising as it is a direct consequence of the method used to compute $\alpha$ in Eq. 6.8; however, the variations in the magnitude of the efficiency are independent of this method. Fig. 6.6 also shows that under stable condition, there is a slight decrease in $\eta_m$ with increasing stability and angle, but the strong winds during night-time result in wind-stress alignment and thus the effect is clearer under unstable conditions. It is worth noting that the Furnas lake studied in Bernardes and Dias [2010] is smaller than the lake Geneva. Their measurement also has a smaller fetch (3km vs. 10km). Therefore, swell conditions, which are the main contributing factors to the significant misalignment observed in
LATEX, might occur very rarely or not at all in their data and thus the role of waves in inducing wind-street misalignment might not be clear. This can be the reason why the results of stress vector misalignment in LATEX are more similar to those in open sea [Geernaert et al., 1993, Grachev and Fairall, 2001], where both stress angle misalignment and upward momentum transport have been reported. A similar plot as in Fig. 6.6 for the vineyard data (not shown here) confirms that, on average, $\eta_m$ is larger than that for the lake since the stress angle misalignment over the vineyard is much smaller and does not result in reduced transport efficiency. Fig. 6.2 is re-

![Figure 6.6: $\alpha$ under different stability conditions. Color scale indicates the momentum transfer efficiency defined in Eq. 6.9.](image)

plotted in Fig. 6.7 but each point is colored with $\eta_m$. One interesting feature that can be identified in Fig. 6.7 is that the higher branch (wind-wave) always has a high momentum transport efficiency $\eta_m$ (greater than 0.5), where as the lower branch (swell) has a much larger variability in $\eta_m$. The previous results thus clearly show that swells result in very atypical air-water momentum transfer that might not conform to the similarity theories developed over land and wind waves. In the next section, we attempt to explore how the most widely used of these theories, MOST, fails under swell conditions, and how it might be reformulated.
6.4.2 Decomposition of stress and modified MOST

To explain this widely observed phenomenon of stress-wind misalignment and the marked decrease in momentum transport efficiency with increasing $\alpha$, we examine the physical origins of the surface stress vector $\vec{\tau}$. For a turbulent flow over any surface, the total surface stress (exactly at the surface) is a vector sum of the viscous drag $\vec{\tau}_v$ and the pressure (or form) drag $\vec{\tau}_p$. Over a fixed surface, this stress is then transmitted upwards in the lower atmosphere by pressure modulations, viscous fluxes, and turbulent fluxes, the later dominating as one moves away from the surface. For an undulating water surface, the pressure modulations (resulting from pressure gradients) in the air generate a wave-induced stress component; thus, over a water surface, the total stress can be expressed as a vector sum of shear stress (which includes viscous and turbulent flux contributions) and wave stress [Phillips, 1977], i.e. $\vec{\tau} = \vec{\tau}_{\text{shear}} + \vec{\tau}_{\text{wave}}$. Irrespective of near surface processes that generate and transmit the stress, “sufficiently” away from the surface in the ABL, this stress is transmitted primarily via turbulent fluxes since the viscous fluxes become negligible.
at high Reynolds numbers and the wave induced pressure perturbations generating the wave stress dissipate (except maybe in a very stable boundary layer). However, in the constant stress layer, this stress away from the surface remains equal (as a vector and under steady-state conditions) to the stress generated at the surface by viscous and pressure drag.

Over a very rough surface, the surface pressure drag is expected to dominate over viscous drag. This pressure stress at the surface is simply given by the surface integral \( \tau_p = \frac{1}{A} \int_S -p \bar{n} dA \), where \( \bar{n} \) is the normal unit vector of the surface, and \( p \) is the stagnation pressure due to the background pressure and the dynamic pressure that is generated (via the Euler equation in streamline coordinates) from the change in the air velocity at the surface to match the surface velocity (no slip condition relative to the velocity of the water surface, which is different from but related to wave phase speed), as well as from the asymmetrical curvature of the streamlines around the wave (which is also dictated by wave shape and phase speed). Given the above, one can conclude that the horizontal form drag over waves must (1) be perpendicular to wave crests (i.e. aligned with the wave propagation direction since \( \bar{n} \) has no component along the wave crests), (see Fig. 6.8), (2) depend only on the wind speed component that is aligned with the wave propagation direction since it is the one that generates the dynamic pressure and (3) depend on the relative difference between that aligned wind speed and wave phase speed since the dynamic pressure is induced when the velocity and direction of streamlines are modified by the traveling wave. Therefore, one can anticipate that the dynamic pressure \( p_d \) will be proportional to \( (|\bar{u}| \cos \theta - |c|)^2 \), where \( |\bar{u}| \) and \( |c| \) are the magnitudes of the two velocity vectors and \( \theta \) the angle between them (the information on the direction \( u \) relative to \( c \), e.g. opposing or following swell, is here included through \( \cos(\theta) \) since the absolute values of the velocities are used).

In LATEX, we found almost no correlation between \( w' \) and \( h \) (the surface elevation),
even when the two time series were lagged relative to each other in both directions by a variable time. Therefore, we can infer that the measured $\vec{\tau}$ was above the inner region, where the wave-induced component of stress is significant [Belcher and Hunt, 1993, Kudryavtsev and Makin, 2004]. In addition, the measurements were very far above the viscous sublayer, which only spans a few millimeters in the ABL, so no viscous contribution to the measured stress is expected. Therefore, the measurements are “sufficiently” far away from the surface such that the turbulent stress should be the main stress component and can be viewed as a very good surrogate for the total surface stress.

In addition, we make the following assumptions in order to pursue this analysis further: 1. There is no overlap between periods of wind-wave and swell. This implies that $\vec{\tau}$ is either due to wind wave or swell. For small water bodies such as a lake, the wave field is less complex than that in open oceans since generated waves tend to travel to the shore in relatively short times, quickly dissipating most of their energy making very long-lived swell unsustainable. Furthermore, analyses of the wave spectra and of the probability distribution functions of wave periods (not shown here) demonstrate that in the vast majority of the cases, a dominant type/length of waves exists in our measurements. 2. $\vec{\tau}$ is aligned with the wave propagation direction since it primarily results from the form drag at the surface. For periods where the wave height is small, viscous drag contribution could be significant; under such conditions, the velocity gradient vector producing the viscous stresses in the viscous sublayer will be modulated by the flow structures in the wave sublayer. This will result in viscous stress alignment somewhere between the wave propagation direction and the mean wind direction. This might induce some misalignment between the stress and wave propagation directions but for the purpose of this analysis, this misalignment cannot be accounted for and is expected to be relatively small. However, this assumption can be easily relaxed if the present analysis is applied to experimental data with
wave direction measurement, which were not available from LATEX (but again the “simplicity” of wave fields in LATEX is a feature we aim to exploit in this study). In addition, wave-resolving simulations can shed further light on the magnitude as well as the direction of the viscous stress component.

Similar to the method used by Grachev et al. [2003], we decompose the stress $\vec{\tau}$ along the wind-wave direction ($\vec{\tau}_{ww}$); and along the swell propagation direction ($\vec{\tau}_{sw}$). There can be three different cases, namely wind waves (WW), counter swells (CS) and following swells (FS), as shown in Fig. 6.8. The following subsections explain the three cases sequentially.

![Diagram](image)

Figure 6.8: Orientations of wind, stress, and waves. The dotted lines in (a1)-(c1) represent wave crests of an idealized monochromatic wave. (a1) wind wave (WW), (b1) counter swell (CS), and (c1) following swell (FS). (a2) shows the relative velocity scale for cases corresponding to (a1) and (c1), respectively. $\vec{\tau}_{ww}$ and $\vec{\tau}_{sw}$ are the stress components under wind-wave and swell conditions; only one of them can be non-zero since we assume that the two conditions do not overlap. Also recall that $\alpha$ is the angle between wind $\vec{u}$ and stress $\vec{\tau}$, while $\theta$ is the angle between wind $\vec{u}$ and wave propagation direction; $U_r$ is the velocity of air projected onto the direction of $c$.  

$\tau = \tau_{ww}; \tau_{sw} \approx 0$

$\tau = \tau_{sw}; \tau_{ww} \approx 0$

$\tau = \tau_{ww}; \tau_{sw} \approx 0$
**Wind wave case (WW)**

The wind wave (WW) case is depicted in Fig. 6.8(a1). Under WW conditions, $\vec{\tau}_{ww} = \vec{\tau}$ and $\vec{\tau}_{sw} \approx 0$ as illustrated in Fig. 6.8(a1). As explained in previous section, wind waves are locally generated. In general, $\alpha$ is small; the stress vector aligns with the mean wind. As shown in Fig. 6.8(a2), for wind waves, the stress-wind angle $\alpha$ is equal to the wave-wind angle $\theta$. The wind speed also generally exceeds the phase speed under such conditions. This case corresponds to the upper branch shown in Fig. 6.7.

**Counter swell case (CS)**

This case is shown in Fig. 6.8(b1). Under counter swell (CS) conditions, the component of $c$ projected along the $x$ direction is opposite to the direction of $\bar{u}$. The swell travels faster than the surface mean wind and it propagates at an obtuse angle ($> 90^\circ$) with respect to the direction of $\bar{u}$. Therefore, the relative velocity $U_r$ is given by as illustrated in the vector diagram in Fig. 6.8(b2). $U_r$ is the velocity of air in the reference frame of the propagating wave. For CS case, $|\alpha| < 90^\circ$ and the maximum magnitude of $U_r$ is achieved when $\alpha = 0$ and thus $\theta = 180^\circ$, which physically corresponds to swell propagating exactly opposite to the mean wind speed. The resulting magnitude of $U_r$ for this particular alignment is given by $c - \bar{u}\cos(180^\circ) = c + \bar{u}$.

Such variation of $U_r$ impacts the surface pressure drag (see also Phillips [1977, page 131, Eq.4.4.31], where it is concluded that the mean surface pressure scale follows $\langle P \rangle \sim \rho U_r^2$). Since here $U_r > \bar{u}$, one expects strong momentum transfer and higher momentum transfer efficiencies compared to the scenario without influence of the swell. As $\alpha$ decreases, momentum transfer is enhanced, vice versa. Therefore, in the lower branch of Fig. 6.7, periods of CS conditions give rise to a large range of variability in $\eta_m$.

Other observational evidence and numerical simulations support this conclusion. For
example, Donelan and Drennan [1997] reported a significant increase in the bulk momentum transfer coefficient ($C_m$) under swell that can be categorized as counter swell (CS) on open ocean. Similar conclusion is reached for idealized waves propagating in opposite direction to the wind [Sullivan et al., 2008].

**Following swell case (FS)**

Fig. 6.8(c1) depicts another category of swell conditions, called following swell (FS), where the component of $c$ decomposed along $x$ direction is in the same direction as $\bar{u}$. The swell travels faster than the surface mean wind and it propagates at an *acute* angle ($< 90^\circ$) with respect to direction of $\bar{u}$, which results in the swell providing momentum to the air. $U_r$ (i.e. velocity of air in the reference frame of propagating wave) is here too given by $U_r = \bar{u} \cos(\pi - \alpha) - c = \bar{u} \cos(\theta) - c$ as illustrated in the vector diagram in Fig. 6.8(c2). However, in the FS case, $|\alpha| > 180^\circ$, thus the maximum value of $|U_r|$ is $c$, occurring where for $\alpha = 180^\circ$ and $\theta = 0^\circ$, in which the wave propagation direction is perfectly aligned with $\bar{u}$.

Referring back to the lower branch in Fig. 6.7, there are several cases with negative $\eta_m$, signifying upward momentum transport. Upward momentum transport has been observed under following swell conditions in previous experiments [Drennan et al., 1999, Grachev and Fairall, 2001, Rutgersson and Smedman, 2001] as well as in numerical studies [Sullivan et al., 2008].

**Brief summary of three cases (WW, CW and FW)**

Overall, we can summarize the analyses above using the schematic diagram in Fig. 6.9. From information on stress-wind angle, one can infer the change in both momentum transport efficiency and direction. For $|\alpha| < 90^\circ$, the momentum transport is from air to surface and the efficiency increases as $|\alpha|$ tends to zero. On the other hand, for $|\alpha| > 90^\circ$, the momentum transport is from surface to air and the efficiency
increases as $|\alpha|$ tends to 180°. For $|\alpha| = 90°$, there is no distinction between the counter and the following swell cases. However, as $|\alpha|$ tends to 90°, the transport efficiency is expected to decrease due to the drop in form drag as the wind becomes aligned along the wave crests. Fig. 6.6 clearly demonstrates the transition between a dominance of ejections and sweeps over inward and outward interactions to a balance as $|\alpha|$ goes from 0 to 90°, to a dominance of inward and outward interactions that results in a net upward momentum transfer as increases towards 180°.

Despite the assumptions and simplifications, the aforementioned conceptual framework can provide a consistent explanation of the LATEX results. We consider the bulk momentum transfer coefficient $C_m$, where $C_m$ is defined as:

$$C_m = \frac{\text{sign}(\langle v'w' \rangle + \langle u'w' \rangle) \times \left( \langle v'w' \rangle^2 + \langle u'w' \rangle^2 \right)}{\bar{u}(z)^2}. \quad (6.10)$$

The statistics of the mean $C_m$ for different scenarios are shown in Fig. 6.10. The counter swell (CS) shown in Fig. 6.10(b) has a higher mean $C_m$ than wind wave (WW) cases in Fig. 6.10(a). As increases, $C_m$ shifts towards lower values (Fig. 6.10(c)). Finally, as $\alpha$ exceeds 90°, $C_m$ becomes negative for the following swell (FS) cases (Fig. 6.10(d)).
6.4.3 A modified formulation for MOST

Given the analyses in the previous sections, water surfaces would seem to require a modified relative velocity $U_r$ in the formulation of surface-air exchange models. Under conditions where MOST remains valid, the relevant velocity that results in momentum exchanges as pointed out above is not $U$, but rather the velocity in a frame of reference at rest with respect to the crests and troughs of the surface waves, which is $U_r$. Since $\alpha$ is directly measurable by the sonic anemometers, we can now propose that the formulation of MOST for momentum over moving waves should be modified to:

$$|\bar{u}\cos \theta - c| = \frac{u_s}{\kappa} \left( \log \left( \frac{z}{z_{0mr}} \right) + \Psi \left( \frac{z}{L} \right) \right).$$  \quad (6.11)
Hence, \( z_{omr} \) is the height at which \( \bar{u} \cos \theta = \bar{c} \), which is also called ‘critical height’ [Phillips, 1977, Belcher and Hunt, 1998] and is physically different from the roughness length \( z_m \) typically used in MOST. The absolute value accounts for the fact that \( u_* \) by convention is calculated as the square-root of the magnitude of \( \tau \). There are studies on MOST being inapplicable during strong swell conditions [Drennan et al., 1999, Smedman et al., 2009], but it is beyond the scope of this paper to delve into this issue and the conclusions in those studies might have been due to the use of the classical MOST formulation. One should also note here that, in addition to the phase speed, the waves could also have a mean current component that should be added to \( c \) to represent the velocity of the surface waves. However, measurements of the mean current with the profiler during LATEX show that its speed is at least two orders smaller than \( \bar{u} \) or \( c \). We also estimated the Lagrangian velocity of water particles at the surface, which was, as expected, also much smaller than \( \bar{u} \) or \( c \).

Sonic measurements at four different levels allow us to evaluate the modified momentum equation for MOST (Eq. 6.11) that uses \( U_r \), and compare it with the classical form that uses \( \bar{u} \). At any one instant, there are four measurements at different levels, under the same atmospheric conditions. The stability-modified log-law (here written with any characteristic flow speed \( U_c \), that can be either \( U_r \) or \( \bar{u} \)) is given by:

\[
\frac{U_c(z)}{u_*} = \kappa^{-1} \left( \log \left( \frac{z}{z_{0m}} \right) - \Psi \left( \frac{z}{L} \right) \right) = \kappa^{-1} \left( \log(z) - \log(z_{0m}) - \Psi \left( \frac{z}{L} \right) \right). \tag{6.12}
\]

Since \( \Psi(z = 0) = 0 \), the intercept of this log-law is only affected by the state of the surface given by \( z_{0m} \). Given the uncertainty in the estimate of \( z_{0m} \), it is better to use the equivalent formulation of this law between two heights above the surface (yielding 6 different measurements from the 4 levels of LATEX):

\[
\frac{U_c(z_1) - U_c(z_2)}{u_*} = \kappa^{-1} \left( \log(z_1) - \log(z_2) + \Psi \left( \frac{z_1}{L} \right) - \Psi \left( \frac{z_2}{L} \right) \right).
\tag{6.13}
\]
Note that the wave speed $c$ cancels out since it is also related to the ‘surface state’, which is identical for the four different heights.

We do the same procedure for all the time periods (15-min average periods) for the entire LATEX measurements. To test if the modified MOST for water surfaces is better, we can write Eqs. 6.12 or 6.13 with $U_c = \bar{u}$ or $U_c = U_r$, and then check which form better yields (i) the correct slope which should be given by $\kappa^{-1}$ (ii) a better fit to the data with lower fitting residuals. To that end, a least-square error minimization can be applied to Eq. (10) for each time period $(t)$, which we can write in a general form

$$U_D^j(t) = B_1(t)Z_D^j(t),$$

(6.14)

where the left-hand side is either $U_D^j = \frac{\langle u(z_k^1) - u(z_k^2) \rangle}{u_*}$ or $U_D^j = \frac{|\cos(\alpha)\langle u(z_k^1) \rangle| - |\cos(\alpha)\langle u(z_k^2) \rangle|}{u_*}$; $j$ is 1-6 depending on which two levels are chosen to take the differences; $t$ is time; and $B_1$ is the slope to be deduced from the least-square fitting (a value is obtained for every time period) and it is expected to yield a value of $\kappa^{-1}$. Thus, what we are minimizing is the sum of the square errors over the 6 two-level differences, for each time period independently. $\alpha$ is computed from the height-averaged stress components to reduce the bias that occurs in the lateral direction when double-rotation in $y$ and $z$ is applied [Grachev et al., 2003]. To ensure the robustness of this statistical test and the validity of the constant stress layer assumption, we impose an additional criterion commonly used for the evaluation of the von Karman constant from atmospheric surface layer data [Andreas et al., 2006]. Specifically, we limit the data used to cases in which the median of the measured $u_*(z)$ only deviates by 10% from the least-square fitted $u_{s0}$, where $u_*(z) = az + u_{s0}$ and $a$ is a constant obtained from the least-square fitting. This limits the number of periods to 163. A least-square error minimization with respect to $B_1$ in Eq. 6.14 over these 15-minute periods is carried out using both velocity scales. A better model will give a smaller mean square-error (MSE) for the residuals, as well as a von Karman constant closer to the widely-observed value in
wall-bounded flows, i.e. between 0.38 and 0.42. For each period, MSE is calculated and the probability distributions of MSE for both models are shown in Fig. 6.11. Overall, the modified MOST leads to lower MSE, in which the average MSE is 0.135 compared to 0.153 for the conventional MOST. Estimate of the von Karman constant is calculated by inverse of the average of the slope $B_1$. Modified MOST yields $\kappa = 0.387$ and $\kappa = 0.366$ for the conventional MOST. The results demonstrate that the modified MOST matches the experimental observations better than the classical form.

This analysis suggests that for water surfaces, in which wave propagation can sometimes misalign with the mean wind direction, the appropriate velocity scale that accounts for the pressure drag that dominates in this case should be formulated as $|\bar{u} \cos \theta - c|$. The Monin-Obukhov similarity theory, when applied over water surfaces, thus needs to be modified accordingly. In reality, especially over open sea, when the wind wave and swells coexist, the appropriate angle $\theta$ should be derived from the proper wave directional information, such as from wave directional spectra or from wave models in numerical simulations.

$z_{om}$ and $z_{omr}$ calculated from Eqs. 6.4 and 6.11 respectively are compared in Fig. 6.11.

![Figure 6.11: Histogram of mean square error for the modified MOST and the conventional MOST.](image)

Figure 6.11: Histogram of mean square error for the modified MOST and the conventional MOST.
6.12 as a function of $z/L$. Note that using the different velocity scales in the two forms of MOST results in different physical interpretations of the momentum roughness lengths; $z_{0mr}$ as mentioned before is the critical height and contains additional information on the moving waves. The range of $z_{0mr}$ is greater than that of $z_0m$, since they have different physical meanings. However, Fig. 6.12 suggests that $z_{0mr}$ (Fig. 6.12(b)) may result in better collapse of the data with changing stability than $z_0m$ (Fig. 6.12(a)). Parameterizations for $z_{0mr}$ might thus be more universal than those for $z_0m$, but require more results from observational data and numerical simulations and are hence beyond the scope of the current work.

6.5 Scalar transport over lake surface

Now we turn our attention to the scalar roughness lengths using LATEX measurements. In Eq. 6.5 and Eq. 6.6 the friction velocity $u_*$, kinematic sensible heat flux $H/\rho C_p$ and kinematic water vapour flux $E/\rho$ can all be taken as averages over the four measurement heights. To compute the scalar roughness lengths, the temperature and humidity at both the surface and some height $z$ are required to relate the
Figure 6.12: (a) \( \log(z_{0m}) \) and (b) \( \log(z_{0mr}) \) as functions of stability. The circles are bin-averages results according to different stability ranges, and the error bars show the standard deviation.

gradients to fluxes. Therefore, accurate and precise measurements of scalar gradients are crucial to determine \( z_{0h} \) and \( z_{0v} \). LATEX setup included many instruments that measured this surface temperatures as well as air temperature and specific humidity at different positions (see [Vercauteren et al., 2009]); therefore, we were able to explore the optimal combinations of temperature sensors that yields the most accurate temperature gradients using the criterion that when plotting the sensible heat flux versus this temperature gradient, the intercept should be as close to zero as possible. Theoretically, the intercept should be zero if there is no bias in temperature and flux measurements; however, as illustrated by Vercauteren et al. [2009], given the small magnitude of air-water temperature differences and the large uncertainties in temperature measurements relative to these air-water differences, the uncertainty in the gradients will be quite significant. A method to compute a surface temperature that would be consistent with the computed fluxes and that can reduce the uncertainties in the gradients is to obtain the surface temperature from a Bowen’s ratio expression (Eq. 6.15 below) where it is assumed that the turbulent transfer coefficients are the
same for both heat and water vapor (for LATEX, this was shown to be a very good assumption for most conditions by Li and Bou-Zeid [2011]). Given that the viscous sublayer can be assumed to be saturated with water vapor, the Bowen’s ratio for LATEX can be directly computed from the fluxes determined by the eddy-covariance method:

\[
Bo = \frac{H}{LE} = \gamma \frac{T_s - \bar{T}}{e^*_{s} - \bar{e}} = \gamma \frac{T_s - \bar{T}}{f(T_s) - \bar{e}},
\]

(6.15)

where \(e^*_s = f(T_s)\) is the saturated surface water vapor pressure in hPa at \(T_s\), \(\bar{e}\) and \(\bar{T}\) are the water vapor pressure and temperature of the air at measurement level, and \(\gamma\) is the psychometric constant, given by \(\gamma = C_p \rho / 0.622 L_e\). \(\rho\) is pressure (hPa) and \(L_e = 2.453 \times 10^6\) J/kg is the latent heat of evaporation of water at 20°C. In Eq. 6.15, \(e^*_s\) is a function of \(T_s\). The only unknown in the above equation is hence \(T_s\), which can be determined by solving the equation using the polynomial form of the Clausius-Claperyon equation suggested by Brutsaert [2005]. Furthermore, the Rotronic Hygroclip air temperature and water vapor pressure are used for \(\bar{T}\) and \(\bar{e}\) since the instrument should yield more accurate means than the CSAT3 or LI7500. This sensor is located at a distance \(z = 3.05\) m above the mean water surface. Using the same criterion that the linear relation between \(H\) and temperature difference should give an intercept close to zero, we observed that air-water temperature difference using the \(T_s\) calculated based on Bowen ratio and the air temperature given by Rotronic sensor indeed yields the smallest intercept (1.5 W m\(^2\)) compared to other combinations we tested; therefore, we conclude that this combination is the most suitable to compute the temperature and humidity differences needed in to calculate the scalar roughness lengths \(z_0h\) and \(z_0v\). Furthermore, this approach has already been used by Bintanja and Van Den Broeke [1995] to compute the scalar roughness lengths. Notice that to account for the effect of different stability conditions needed in the various equations, we adopted the forms of the functions \(\Psi_m\), \(\Psi_h\) and \(\Psi_v\) given by Brutsaert [1992].

First, we analyze the scalar transfer efficiency defined similarly to Eq. 6.9. Fig. 2.13
shows that water vapor transport efficiency decreases as the atmosphere transitions from unstable to neutral to stable. The trend is consistent with the findings of Li and Bou-Zeid [2011], where it was attributed to the coherent structures changing from hair-pin vortices to plumes and thermals. Compared to the momentum transport efficiency in to Fig. 6.6, the variations of scalar efficiency are not sensitive to $\alpha$. The interfacial scalar transport is not through pressure drag as for momentum, but rather through viscous transport near the interface and as such it does not depend on the relative angle between wind and waves. Similar results were obtained for temperature transport efficiency, but are not shown here.

Figure 6.13: Transport efficiency for water vapor under different stability conditions and wind-stress angles.

Next, we consider the existing parameterizations of momentum to scalar roughness length ratios. Since all the models for the relation between momentum and scalar roughness lengths are based on the classical form of MOST, we use $z_{0m}$ calculated from Eq. 6.4 for the following analyses. It is widely usually postulated that $\log(z_{0m}/z_{0h})$ and $\log(z_{0m}/z_{0v})$ depend on a roughness Reynolds number such as $Re_* = u_* z_{0m}/\nu$. In the case of temperature, $\log(z_{0m}/z_{0h})$ indicates the roughness-layer temperature increment [Zilitinkevich et al., 2001] defined as: $\delta \theta = \theta_s - \theta_0 = \frac{H}{u_* k} \log \frac{z_{0m}}{z_{0h}}$, where $\theta_s$ is the surface temperature and $\theta_0$ is the so-called aerodynamic surface temperature,
which is the potential temperature extrapolated logarithmically downward to the level \( z = z_{0m} \) (a similar interpretation can be done for humidity). We compared different models proposed in the literature to our data in Fig. 6.14. Fig. 6.14(a) shows the comparisons between LATEX results and various models summarized in Table 6.1, with the model coefficients taken exactly as reported in the original papers for these models. However, due to different data sets used in developing these models and fitting their parameters, it is difficult to assess the performance of the various formulations from LATEX. To have a fairer comparison, the coefficients in different models were re-determined using a least-square fitting to LATEX data (resulting model expressions are shown in the third column in Table 6.1). Fig. 6.14(b) shows the comparison of these refitted models with LATEX coefficients. The Brutsaert and Sherrif&Gumley models outperform the other two, with R-square values of 0.36 and 0.39 respectively. The major discrepancy between these two models, compared to the other two (Zilitinkevich et al. and Thomson&Owen) is in the exponents relating the roughness ratio to \( Re^* \). These exponents are obtained based on various theoretical arguments and were not changed in the recalibration of the models with LATEX data. This discrepancy seems to be most significant in the transitional and smooth regimes (Fig 6.14(b)), defined as the regimes where the wave heights are very small, on the order of the depth of the viscous sublayer. This remain a poorly understood problem that warrants further investigations to pin down its physics.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Original Relation</th>
<th>LATEX Fitted Relation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brutsaert [1975a,b]</td>
<td>( 7.3 Re^{1/4} Pr^{1/2} - 5 )</td>
<td>( 10.7 Re^{1/4} Pr^{1/2} - 11.2 )</td>
</tr>
<tr>
<td></td>
<td>( 2.4 Re^{0.45} Pr^{4/5} )</td>
<td>( 3.39 Re^{0.45} Pr^{4/5} )</td>
</tr>
<tr>
<td>Sheriff and Gumley [1966]</td>
<td>( 7.78 Re^{0.199} - 4.65 )</td>
<td>( 12.5 Re^{0.199} - 14.6 )</td>
</tr>
<tr>
<td>Zilitinkevich et al. [2001]</td>
<td>( \kappa(4.0 Re^{0.5} - 3.2) ) (heat)</td>
<td>( \kappa(4.87 Re^{0.5} - 5.05) ) (heat)</td>
</tr>
<tr>
<td></td>
<td>( \kappa(4.0 Re^{0.5} - 4.2) ) (water vapor)</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.1: Models for \( \log(z_{0m}/z_0) \) and \( \log(z_{0m}/z_0v) \) proposed in the literature, and model with coefficients refitted using LATEX data.
Figure 6.14: Comparisons between models and LATEX measurements, where the \( Re_* \)-bin-averaged results are the solid dots. \( z_{0s} \) is either \( z_{0h} \) or \( z_{0v} \). The error bars of the bin-averaged points show the standard deviation of data in that bin. The dotted line marks the smooth (\( Re_* < 0.135 \)), transitional (0.135 < \( Re_* < 2.2 \)) and the rough (\( Re_* > 2.2 \)) regions. (a): Lines represent models as reported in the literature. (b): Lines represent corresponding model in (a) with coefficients determined by fitting to LATEX data.

### 6.6 Summary and conclusions

The aim of this study is to understand the influence of surface wave states on air-water exchanges of momentum, heat and humidity. The relatively simple wave field over a lake, where wind wave and swell rarely coexist, motivated the use of the Lake-Atmosphere Turbulent EXchanges (LATEX) Experiment data for the analyses. Swell was found to correspond to larger and more persistent coherent structures in the overlying ABL, as deduced from analyses of the wind velocity autocorrelation. The magnitude and variability of the surface stress-wind angle are much larger over swell than over wind waves, which is consistent with previous studies over open oceans and large lake. The dependence of momentum transport efficiency on this angle was thoroughly examined and contrasted with results from data collected over a vineyard. LATEX results indicate that the wind-stress misalignment over swell causes a
drastic reduction in the efficiency of momentum transport, independently from other factors such as static stability. To explain these observations, we sought to develop a conceptual framework for the basic physical attributes of air-wave interaction during the experiment. This framework distinguishes between following and counter swell, and postulates that the surface drag is dominated by pressure/form drag (and therefore the surface stress is aligned with the wave propagation direction), that the measured eddy-covariance fluxes capture the totality of the momentum and scalar transports, and that one type of waves - either swell or wind waves - dominate during any given 15-minute period. The framework explains the observed large variability of stress-wind angle, the drop in momentum transport efficiency under counter-swell conditions when the wind and waves are highly misaligned, and the occurrence of upward momentum transfer under following-swell conditions. More importantly, it leads to a modified form of Monin-Obukhov similarity theory, where the flow velocity scale is taken to be $U_r = |\bar{u} \cos(\theta) - c|$. Statistical analyses show that using this velocity scale results in better fit to the field experimental data and yields von Karman constant values that are closer to those reported in the literature for various wall-bounded flows.

The momentum and scalar roughness lengths were also determined from the LATEX measurements. We tested various existing models for $z_{0m}/z_{0h}$ or $z_{0m}/z_{0v}$. The models by Brutsaert [1975a,b] and Sheriff and Gumley [1966] were found to outperform the other two by Sheriff and Gumley [1966] and Zilitinkevich et al. [2001], especially in the smooth and transitional regimes.

The findings of this study are limited by the lack of observations of the direction of wave propagation. More experimental measurements and numerical simulations that include the directional information of the surface wave will be useful to evaluate the modified relative velocity scale proposed here. The result shown using experimental data in this chapter can also be useful to develop wall-model in large-eddy simula-
tion over waves. For example, as shown by Yang et al. [2013], wall-models based on wave-wind relative motion (but with no information on directionality) [Kitaigorodskii and Volkov, 1965], achieves the best performance in a wind-wave coupled large-eddy simulation.
Chapter 7

Conclusion

Motivated by the knowledge gap in exchanges of scalars between geometrically complex surfaces and the lower atmosphere, this work started by addressing the two challenges outlined in the introduction. One challenge is related to the numerical approach (the Gibbs phenomenon) and the other is the discrepancy in Reynolds number, which inherently exists in the physics of the problem. To overcome the first numerical challenge, we proposed and tested a computationally efficient and practical approach to alleviate the Gibbs phenomenon in simulations of incompressible flows in the context of the immersed boundary method. The findings are applicable for high Reynolds number incompressible flows in engineering or environmental fluid mechanics and mass transfer problems with the immersed boundary method (IBM) approach. The Gibbs phenomenon is demonstrated to introduce significant errors in the statistics related to the subgrid scales. In particular, scalar transfer simulations are more prone to Gibbs errors but the proposed method gives the correct physical trend. While we tested our method in a wall-modeled LES code, application to RANS, wall-resolved LES or DNS should be very comparable and the benefits should be similar. Overall, the results from this chapter indicate that momentum is less prone to be affected severely by errors associated with Gibbs phenomenon. compared
to scalars. This means that scalar dispersion problems using IBM combined with spectral discretization method have to be cautiously handled. This is especially relevant to studies of any scalar dispersion problems using similar numerical approaches. The second challenge with regard to scalar exchanges is explored in great detail in chapter 3. We verified the LES model with improved computational method to study high Reynolds number forced convective heat/mass transfer in rough-wall boundary layers. Three different experimental measurements from the literature are used to assess the capability of wall-modeled LES approach. We have shown that our LES predicts the spatial variation of the heat/mass transfer comparing to a wind-tunnel measurements; the average Nusselt number on different facets of a single cube (larger discrepancy over the windward face likely to be related to the mismatch between Reynolds number in the laboratory experiments and our LES); and excellent match of the the power law relation between the Nusselt and the Reynolds number compared to field experiments. The overall conclusion from our study indicates that the LES, despite its inherent parameterizations, is suitable for studying real-world buildings. Going forward, the results gives us confidence in the capability of LES and the potential for using the technique to develop a better understanding of coupled scalar and momentum transfer at high-$Re$ over complex topographies, and to formulate improved spatially-averaged surface exchange models to be used in coarse atmospheric models (weather or climate) where the buildings cannot be resolved. Wall-modeled LES can be a viable approach to provide reliable schemes for turbulent fluxes parameterization, especially in the context of improving the urban land-atmosphere models such as the urban canopy model. Moreover, this study highlights the importance of $Re$ in applying results of scalar transfer from wind-tunnel studies. If one is to develop scalar fluxes parameterizations for urban environments based on wind-tunnel or direct numerical simulations (that often have much lower $Re$ based on
building height and bulk wind speed), the effects of $Re$ have to be properly factored in.

Despite the complex geometries in realistic urban environments, results from chapters 4 and 5 over idealized geometries shed some light into the impact of roughness geometry on scalars and momentum exchanges. Firstly, as a consequence of pressure/form drag dominating the transfer of momentum at high Reynolds number, we demonstrated the important dynamical consequence of the frontal area density $\lambda_f$. $\lambda_f$ dictates the magnitude of the form drag and it is also the key parameter influencing the transitioning behavior from a canonical rough-wall surface layer to a mixing layer. In terms of parameterizing the momentum roughness length $z_{0m}$ in the Monin-Obukhov framework, knowledge of $\lambda_f$ is useful to parameterize $z_{0m}$ based on morphometric models. Secondly, there is no pressure/form drag equivalence for scalar transfer, therefore the frontal area density $\lambda_f$ does not affect the scalars in the same way as momentum. The different implications of $\lambda_f$ for momentum and scalars are not adequately emphasized by previous studies. As a result, parameterizing the scalar roughness lengths based on purely geometric parameters is extremely difficult because scalar transfer depends on the local scalar transfer coefficients over all surfaces of the roughness elements and they are spatially heterogeneous. Thirdly, even though it is hard to directly connect the geometric parameters to scalar transfer, this work has demonstrated the potential to invoke the surface renewal theory, which has not been applied previously to very rough surfaces like the urban case. Predictions from the surface renewal theory for the scalar roughness length compare well with results directly calculated from LES. These three main points summarized above suggest that it is important to relate the geometric forms to the fundamental transfer mechanisms of momentum and scalars. Although the parameter space for surface geometry is enormous, starting from idealized setups, a lot can be learned in terms of the dynamical consequences of some important parameters. In this study, the effect
of varying the distribution of geometric parameters are not considered. However, it will be one step closer to the realistic complex urban surfaces if this effect is taken into account. This is an area of on-going research and there are still many open questions. The dissimilarity between momentum and scalars are explored in chapter 4, where we delve into studying the general distinctions between their exchanges particularly in the canopy and roughness sublayers. As one of the very few studies that study both the scalars and momentum numerically over very rough surfaces, we demonstrated the similarity in turbulent exchanges between momentum and scalars but the dispersive fluxes, which can be half of the total fluxes, differ between momentum and scalars. The findings can inform interpretations of field measurements in real urban canopy layers and development of models for the dispersive fluxes. Throughout this work, only passive scalars are considered; however, the effects of stability in the atmospheric boundary layer will be the next step in future studies. As shown by Li and Bou-Zeid [2011], the dissimilarities between momentum and scalars become notable under unstable conditions over a lake and vineyard. Nevertheless, few studies have examined the role of buoyancy in the context of surfaces that consist of large bluff-bodies. In order to understand more about the interactions between different types of complex surfaces and turbulent flows, this study also examines the air-water exchanges of momentum and scalars (temperature and water vapour) in chapter 6, using the Lake-Atmosphere Turbulent EXchange (LATEX) dataset. Different types of waves (wind waves vs. swells) present on the lake surface are found to impact the momentum transport differently. The stress aligns with wind in the presence of wind waves, but a wide range of stress-wind angle misalignment is observed during swell. Momentum transport efficiency decreases with significant stress-wind misalignment, suggesting strong coupling between surface waves and momentum exchange. A new relative wind velocity for surface layer similarity formulations is formulated and tested using the data. Momentum exchanges at the water surfaces present an extremely challeng-
ing scenario because of the undulating surface. In our study, we are limited by the lack of wave direction measurement as well as near surface velocity measurements. Nevertheless, this study is a starting point to examine if there are some new velocity scales present for the undulating water surface, which could impact how similarity theory is formulated. In the future, experimental data and numerical simulations that include the directional information of the surface wave and the wind will be useful to evaluate the modified relative velocity scale proposed.

As a final remark, the results from this work identified some major challenges in studying scalar transport over complex surfaces compared to momentum, such as effects of the Reynolds number and the spatially variable surface transfer properties. Despite the difficulties, LES developed and verified here can be a promising tool for future studies especially those that aim at improving the parameterization schemes in land-atmosphere models.
Bibliography


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