LARGE-EDDY SIMULATION AND MODELLING OF DISSOLVED OXYGEN
TRANSPORT AND DEPLETION IN WATER BODIES

by

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Abstract

In the present doctoral work we have developed and tested a model for dissolved oxygen (DO) transfer from water to underlying flat and cohesive sediment beds populated with DO-absorbing bacteria. The model couples Large-Eddy Simulation (LES) of turbulent transport in the water-column, a biogeochemical model for DO transport and consumption in the sediment, and Darcy’s Law for the pore water-driven solute dispersion and advection. The model’s predictions compare well against experimental data for low friction-Reynolds numbers ($Re_\tau$). The disagreement for higher $Re_\tau$ is investigated by progressively increasing the complexity of the model. A sensitivity analysis shows that the sediment-oxygen uptake (or demand, SOD) is approximately proportional to the bacterial content of the sediment layer, and varies with respect to fluid dynamics conditions, in accordance to classic high-Schmidt-number mass-transfer laws. The non-linear transport dynamics responsible for sustaining a statistically steady SOD are investigated by temporal-and-spatial correlations and with the aid of instantaneous visualizations: the near-wall coherent structures modulate the diffusive sublayer, which exhibits complex spatial and temporal filtering behaviours; its slow and quasi-periodic regeneration cycle determines the streaky structure of the DO field at the sediment-water interface (SWI), retained in the deeper layers of the porous medium. Oxygen depletion dynamics are then simulated by preventing surface re-areation with turbulent mixing driven by an oscillating low-speed current — an idealization of hypolimnnetic DO depletion in the presence of a non-equilibrium periodic forcing. The oxygen distribution exhibits a self-similar pattern of decay with, during the deceleration phase, oscillations modulated by the periodic ejection of peaks of high turbulent mass flux (pumping oxygen towards the SWI), generated at the edge of the diffusive sublayer at the end of the acceleration phase. These fronts of highly turbulent mixing propagate away from the SWI, at approximately constant speed, in layers of below-average oxygen concentration. Finally, the model has been tested in a real geophysical framework, reproducing published in-situ DO measurements of a transitional flow in the bottom boundary layer of lake Alpnach. A simple model for the SOD is then derived for eventual inclusion in RANSE biogeochemical management-type models for similar applications.
Co-Authorship

Significant contributions have been made by my supervisor, Prof. Ugo Piomelli, and my co-supervisor, Prof. Leon Boegman, in helping me develop the computational model, interpreting previous work and new results, critiquing my work and adapting it for journal quality.

Chapter 2 of this thesis will be also referenced in the text as Scalo, et al. (2012b) and has been published as:


Chapter 3 of this thesis will be also referenced in the text as Scalo, et al. (2012a) and has been submitted to ‘Physics of Fluid’ as:

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Chapter 5 of this thesis has been submitted to ‘Limnology and Oceanography’ as:

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<td>$\mu^*_\chi$ (day$^{-1}$)</td>
<td>DO utilization rate</td>
</tr>
<tr>
<td>$K^*_O_2$ (mg l$^{-1}$)</td>
<td>half-saturation coefficient for DO utilization</td>
</tr>
<tr>
<td>$\chi^*$ (mg l$^{-1}$)</td>
<td>concentration of aerobic heterotrophs</td>
</tr>
<tr>
<td>$k^*_d$ (day$^{-1}$)</td>
<td>first order decay coefficient of $\chi^*$</td>
</tr>
<tr>
<td>$D$ (10$^{-9}$ m$^2$s$^{-1}$)</td>
<td>molecular diffusivity of DO</td>
</tr>
<tr>
<td>$\nu$ (10$^{-6}$m$^2$s$^{-1}$)</td>
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</tr>
<tr>
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<td>half-channel height</td>
</tr>
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<td>sediment-layer thickness</td>
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<td>bulk and maximum velocity</td>
</tr>
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<td>$C_b, C_\infty$ (mg l$^{-1}$)</td>
<td>bulk and maximum DO concentration</td>
</tr>
<tr>
<td>$K^*$ (cm$^2$)</td>
<td>intrinsic permeability</td>
</tr>
<tr>
<td>$Re_b, Re_{max}$</td>
<td>$Re_b = U_b \delta / \nu, Re_{max} = U_\infty \delta / \nu$</td>
</tr>
<tr>
<td>$Re_\tau$</td>
<td>$Re_\tau = u_\tau \delta / \nu$</td>
</tr>
<tr>
<td>$Sc$</td>
<td>$Sc = \nu / D$</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>sediment layer porosity</td>
</tr>
<tr>
<td>$\nu_T, \alpha_T$</td>
<td>eddy viscosity and diffusivity</td>
</tr>
<tr>
<td>$\mu_\chi$</td>
<td>$\mu_\chi = \mu^*_\chi \nu / U_b^2$</td>
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<tr>
<td>$K_{O_2}$</td>
<td>$K_{O_2} = K^*_{O_2} / C_b$</td>
</tr>
<tr>
<td>$Y_c$</td>
<td>effective yield for DO utilization</td>
</tr>
<tr>
<td>$\chi$</td>
<td>$\chi = \chi^* / Y_c C_b$</td>
</tr>
<tr>
<td>$k_d$</td>
<td>$k_d = k^*_d \delta / U_b$</td>
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<td>$K$</td>
<td>$K = K^* / \delta^2$</td>
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Chapter 3

\( \mu_\chi^* \) (day\(^{-1}\)) \hspace{1cm} DO utilization rate

\( K_{O_2}^* \) (mg l\(^{-1}\)) \hspace{1cm} half-saturation coefficient for DO utilization

\( \chi^* \) (mg l\(^{-1}\)) \hspace{1cm} concentration of aerobic heterotrophs

\( C_\infty^* \) (mg l\(^{-1}\)) \hspace{1cm} bulk DO concentration

\( \delta \) \hspace{1cm} open channel height

\( \delta_s \) \hspace{1cm} sediment layer thickness

\( U_b \) (m s\(^{-1}\)) \hspace{1cm} bulk velocity

\( \chi \) \hspace{1cm} \( \chi^* = \chi^* \mu^*/Y_c \delta/U_b C_\infty^* \)

\( K_{O_2} \) \hspace{1cm} \( K_{O_2} = K_{O_2}^*/C_\infty^* \)

\( J_{swi} \) \hspace{1cm} dimensionless oxygen flux across the interface

\( c_{swi} \) \hspace{1cm} dimensionless oxygen concentration at the interface

\( \tau_w \) \hspace{1cm} dimensionless wall shear stress

\( \Delta C \) \hspace{1cm} dimensionless oxygen defect at the interface

\( Sh \) \hspace{1cm} Sherwood number

\( K^+ \) \hspace{1cm} mass transfer coefficient

Chapter 4

\( \mu_\chi^* \) (day\(^{-1}\)) \hspace{1cm} DO utilization rate

\( K_{O_2}^* \) (mg l\(^{-1}\)) \hspace{1cm} half-saturation coefficient for DO utilization

\( \chi^* \) (mg l\(^{-1}\)) \hspace{1cm} concentration of aerobic heterotrophs

\( C_\infty^* \) (mg l\(^{-1}\)) \hspace{1cm} bulk DO concentration

\( \delta \) \hspace{1cm} open channel height

\( \delta_s \) \hspace{1cm} sediment layer thickness

\( U_{om}^* \) (m s\(^{-1}\)) \hspace{1cm} amplitude of oscillating free current

\( \chi \) \hspace{1cm} \( \chi = \chi^* \mu^*/Y_c \delta/U_b C_\infty^* \)

\( K_{O_2} \) \hspace{1cm} \( K_{O_2} = K_{O_2}^*/C_\infty^* \)

\( J_{swi} \) \hspace{1cm} dimensionless oxygen flux across the interface

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\( \Delta C \) \hspace{1cm} dimensionless oxygen defect at the interface

\( Sh \) \hspace{1cm} Sherwood number

\( K^+ \) \hspace{1cm} mass transfer coefficient
Chapter 5

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$\mu_0$ (day$^{-1}$)</td>
<td>maximum specific DO utilization</td>
</tr>
<tr>
<td>$\mu$ (mg l$^{-1}$ day$^{-1}$)</td>
<td>maximum oxidation rate, $\mu = \mu_0 \chi / Y_c$</td>
</tr>
<tr>
<td>$\mu_v$ (m$^2$s$^{-1}$)</td>
<td>dynamic viscosity of water</td>
</tr>
<tr>
<td>$C_\infty$ (mg l$^{-1}$)</td>
<td>free stream oxygen concentration</td>
</tr>
<tr>
<td>$K$ (cm$^2$)</td>
<td>intrinsic permeability</td>
</tr>
<tr>
<td>$L_x, L_y, L_z$</td>
<td>box size in W-E, wall-normal, and S-N directions</td>
</tr>
<tr>
<td>$N_x, N_y, N_z$</td>
<td>grid size in respective directions</td>
</tr>
</tbody>
</table>
Chapter 1

General Introduction

1.1 Background and motivation

The presence of dissolved oxygen (DO) in water is critical to the survival of the world’s marine environments. Understanding the mechanisms leading to DO depletion in the water column is of crucial importance to effectively monitor and maintain these delicate ecosystems. Aquatic life can severely suffer from the persistence of low levels of oxygen (or ‘hypoxia’), with harmful consequences for the environment. Areas affected by this phenomenon are known as ‘dead zones’. NOAA estimates the impact on fisheries, tourism and public health to amount to 82 million annually. Also, a recently released report (Committee on Environment and Natural Resources 2010a) has raised awareness of the problem by revealing a tenfold increase over the past 50 years globally and almost thirtyfold in the U.S. alone since 1960; efforts made so far to improve the situation are deemed insufficient. Dead zones are not only present in many coastal environments in North America, including Oregon, Washington, the Gulf of Mexico, the south-mid Atlantic coast and the Great Lakes, but can also be found all over the globe (Figure 1.1) including Southern Japan, England and the Baltic Sea, currently the largest hypoxic area in the world. Further details on the spreading of dead zones in the coastal oceans and their effect on marine ecosystems can be found in Diaz & Rosenberg (2008) and Rabalais, et al. (2010).

The mechanisms leading to oxygen depletion involve a wide range of physical processes. Surface waters are saturated with atmospheric oxygen, which is subsequently transported deeper towards the lake bottom/ocean floor by turbulent motions. Dissolved oxygen acts as a high-Schmidt-number contaminant in water (a passive scalar with very low molecular diffusivity), therefore, away from boundaries, turbulent mixing becomes the dominant transport mechanism. However, a number of physical factors can limit this mixing process, preventing the proper oxygenation of the water column. For instance, stratification can occur, damping turbulence and thereby reducing mixing; this inhibits the vertical DO flux, reducing the oxygen supply to
Figure 1.1: Map of eutrophic and hypoxic coastal systems. Reproduced with permission from Diaz et al. (2010). Data available online at: docs.wri.org

deeper unstratified water layers. Other factors of biogeochemical nature may amplify this problem, such as agricultural, urban and industrial runoff, which release excess nutrients (mainly phosphorous and nitrogen) in nearby rivers, lakes or oceans, overfeeding microscopic aquatic organisms present on the water’s surface (Figure 1.2). This leads to fertilization of algal blooms which can cover an area up to $\sim 100,000$ km$^2$. The result is a severe alteration of the natural ecosystem balance in coastal regions on which a significant portion of the world population relies for their sustenance. The algae eventually die and sink to the (sediment) bed where bacteria feed on them by absorbing dissolved oxygen from the pore water. The bed becomes a sink for the overlying oxygen distribution and when the DO flux across the sediment-water interface (SWI) (and the water-column biological demand) is greater than the flux through the stratified layer (or thermocline) near-bed (or hypolimnetic) oxygen depletion can occur. The amount of DO absorbed by the sediment will, as a result, largely govern the oxygen budget in such bottom water layers (Boudin 1968, Veenstra & Nolen 1991, Patterson, et al. 1985).

Despite the considerable environmental/economical impact of oxygen depletion and the significant effort to characterize the different physical processes involved in DO transport through the water column, across the sediment-water interface and in the sediment layer, a global approach to the problem, which would allow for a better understanding of the interaction among these processes and their relative importance, has not been undertaken. Numerical studies have shown that fully understanding the biological responses to physical variability requires models that couple hydro-dynamics (turbulent mixing), the dynamics of water quality and aquatic organisms, and the complete sediment bio-geochemistry (Koseff, et al. 1993, Boudreau & Jørgensen...
2001, Boegman, et al. 2008a). Turbulence plays a key role in oxygen depletion (Lorke, et al. 2003, Bryant et al. 2010) by driving most (if not all) of the involved governing processes; it therefore requires particular attention.

In the present work we rely on the very accurate characterization of turbulence provided by large-eddy and direct numerical simulations, with the goal of advancing the knowledge in turbulence and in all of the physical processes that interact with it, or are driven by it, in the context of oxygen depletion. These include equilibrium and non-equilibrium turbulent mixing, mass transfer, solute exchange between water and surface layers of sediment beds (hyporheic exchange) and advection and dispersion in porous media. To achieve these objectives, we have designed a computational tool able to resolve the instantaneous distribution of DO by fully coupling the water side and the sediment side governing equations.

From an engineering point of view, this allows for the direct quantification of the DO flux to the sediments (or sediment oxygen demand, SOD) under any prescribed flow conditions and sediment characteristics. The SOD is a critical parameter for the prediction and analysis of oxygen levels in aquatic systems (Wetzel 2001) and currently employed water-quality models for lake or river maintenance would considerably benefit from a parametrization of the SOD based on resolvable turbulent features in the near-wall region, such as wall-shear stress, bulk temperature and oxygen concentration. At present the flux is typically a tune-able parameter, fixed in time (and often in space), and chosen over an order of magnitude scale so that water-quality models can reproduce observations. The variation in observed and model-adopted values motivates the need to develop a time-space variable predictive model for SOD that may be included in a RANSE code. The most advanced aquatic ecosystem model, to our knowledge, is the Computational Aquatic Ecosystem Dynamics
Model (CAEDYM) (Hipsey & Hamilton 2008) which, despite accounting for many components of the DO budget in the water-column (Figure 1.2 (right)), still lacks a parametrization for the SOD based on accurate turbulence modeling.

![Figure 1.3](image)

**Figure 1.3**: Effect of Schmidt number on scalar spectrum (Tennekes & Lumley 1972). Reference velocity spectrum or scalar spectrum for $Sc = 1$ (a); Scalar spectrum for $Sc \gg 1$ (b); Scalar spectrum for $Sc \ll 1$ (c); The constants $\alpha$, $\hat{\alpha}$, $\tilde{\alpha}$ are determined with numerical experiments (Borgas et al. 2004)

From a more fundamental fluid mechanics perspective, there is the need for assessing physical assumptions and speculations underlying solute transport models used in environmental flows (high-Schmidt-number mass transfer models) and to understand the predictive capabilities and limitations of commonly adopted numerical strategies. In general, the nature of a high-Schmidt-number contaminant, like dissolved oxygen in water, transported by high-Reynolds-number turbulence, poses fundamental computational and modelling challenges. The very low diffusivity of the scalar field (three orders of magnitude lower than the kinematic viscosity, in the case of dissolved oxygen) causes the presence of a much wider range of scales than in the velocity field. In Figure 1.3 we see the effects of the Schmidt number on the scalar variance spectrum $E(k)$. While the range of scales in the velocity field extends to the Kolmogorov scale $\eta = (\nu/\epsilon)^{1/4}$, for a high-Schmidt-number scalar a new inertial range is present, the viscous-convective subrange, extending to the Batchelor scale $\eta_B = \eta Sc^{-1/2}$ (Batchelor 1959). It is not clear whether sub-Kolmogorov scales are dynamically relevant for the transport and if currently adopted subgrid scale models adequately take into account their effects on the resolved scales. However, in the case of turbulent mass transfer to a solid boundary,
the presence of a very thin diffusive sublayer (i.e. a concentration boundary layer at the wall approximately \(y^+ = 1\) thick) poses considerable computational challenges and the very peculiar physics associated with it imply a redefinition of the understanding of classic turbulent momentum and mass transfer mechanisms (in the case of unitary Prandtl number, for example).

Further modeling and computational challenges, however, arise from the fact that the velocity field alone in lakes or oceans is populated by a multiplicity of scales to be resolved (Figure 1.4). These range from basin-scale waves (order of kilometers) to the velocity viscous sublayer (order of centimeters). For this reason, the large-eddy simulation (LES) technique becomes the ideal candidate to tackle the transport of both the scalar and velocity field and has become a well-established approach in the field, allowing for the estimation of turbulence characteristics in a wide variety of flows. The main idea is to reproduce directly the evolution of those large resolved turbulent scales that are expected to show strong dependence on the initial and boundary conditions driving the flow, while modeling the residual mixing produced by the sub-grid unresolved scales, which might be supposed to exhibit universal characteristics (Kolmogorov 1941a, Kolmogorov 1941b, Kolmogorov 1941c). LES provide three-dimensional, time-dependent solutions of the filtered Navier-Stokes equations with a lower degree of detail with respect to direct numerical simulations (DNS), but, at a significantly lower cost. A DNS of a high-Schmidt-number scalar field would require a grid that is \(Sc^{1/2}\) times finer in each direction than the one used for the velocity field. This can be very demanding from a computational point of view. LES are a feasible alternative since the scalar field and the velocity field share the same integral scale (see Figure 1.3), and the effect of all sub-grid scales (sub-Kolmorogorov and not) are accounted for in the model.

Overall, simulation strategies for hydrodynamic transport processes are relatively well-established and robust. A higher degree of modelling is, however, necessary to describe the transport in the sediment layer, due to the complex physics involved, including biological processes, chemical reactions and flow in porous media. This determines larger uncertainties in the predictions. One of the goals of the present research is to rely on the accurate description of turbulence provided by LES to improve currently adopted models (which are, necessarily, highly parametrized) used to describe momentum and solute transport in the porous sediment layer. The important transport processes are diffusion, mean advection and dispersion. All of these are driven by the instantaneous pressure, velocities and solute concentration distributions at the interface with the fluid. Depending on the sediment grain size, its arrangement, creation and compaction one or more of these processes can be dominant over the others. A detailed description of the mathematical models used to describe these processes can be found in the computational setup section of Chapter 2. While these models could accurately describe the transport away from the interface, the coupling of the fluid and the porous media can much more challenging to model and represents the primary source of errors. For example, the effects of a transition layer between the full Navier-Stokes equations on the water side and the Darcy equations in the porous medium, the Brinkmann layer, should be taken into account to correctly model the
interaction between the two layers. This, in addition to the geometric complexity of the interface, can make the direct modeling of the solute and mass transfer across the interface problematic. However, in this study, simple geometries (flat sediment surface) and first-order boundary condition matching at the interface are used as a first step. From a biochemical perspective, the most advanced DO sediment-absorption model includes a non-linear sink term (oxygen absorption by decomposing organic matter in the sediments is a non-linear function of the oxygen concentration level) whose intensity $\chi$ (the concentration of oxygen-consuming organisms) is not directly measurable (Higashino et al. 2008). While this model, based on Michaelis-Menten kinetics, is fairly robust and is extensively used in field-scale and lab-scale studies, most of the uncertainties in the predictions can be attributed to the aforementioned hyporheic exchange models.
1.2 Thesis Outline

In the present thesis we chose to tackle the problem of oxygen depletion by first developing and validating a computational model based on LES. We then investigate the small-scale transport processes involved in momentum and solute exchange across the sediment-water interface with an idealized computational setup. Finally, we apply the model to geophysically relevant problems where the large-scale variability of the flow, which drives the turbulent mixing, affects the mass transport across the SWI via non-linear mechanisms. Resolving the full range of important transport processes governing oxygen depletion has allowed us to develop a simplified model for the SOD that can be used in field-scale applications.

A more detailed outline of the content of the manuscripts, included in the remainder of this thesis, follows:

- Chapter 2 contains the fundamental work of this project, including the rationale behind the development of the complete model, a detailed description of its mathematical and numerical implementation, its validation and comparison with lab-scale experimental data and a preliminary qualitative analysis of the mass transport physics that this tool has allowed us to reveal. The work is focused on the sediment-layer transport and its interaction with the overlying turbulence;

- Chapter 3 focuses on the water-side-transport dynamics and, in particular, on the relationship between near-wall turbulent structures and high-Schmidt-number mass transfer across the SWI. A comprehensive statistical analysis of the flow structure near the sediment-water interface is carried out to highlight the dynamical relationship between the different small-scale transport processes leading to oxygen depletion in a steady turbulent flow. A conceptual model for the transport is developed, also with the support of instantaneous visualizations. The SOD is directly calculated under different fluid dynamic and sediment-layer conditions and compared with classic heat-and-mass transfer parametrizations;

- Chapter 4 is the first attempt to extend the model to problems of geophysical interest such as oxygen depletion in fully mixed, hypolimnetic layers of water bodies (where the water column is fully mixed and the overlying stratification prevents re-creation). The flow tested is an oscillating boundary layer in the intermittently turbulent regime. In spite of the complex features associated with the highly unsteadiness of the driving current, characterized by non-equilibrium turbulent transport, the resulting oxygen concentration exhibits a well-defined pattern of self-similar decay. The mathematical implications of these findings are explored through an analytical study of the governing equations;

- Chapter 5 contains the results of the direct application of the model to a real transitional oscillatory flow observed in the bottom layer of Lake Alpnach by Bryant et al. (2010). The model is run here in its full complexity. The flow is characterized by transition and laminarization, and its effects on the oxygen transport are explored. A simple parametrization for the SOD, also based on the previous
work carried out in this thesis, is proposed. Please note that for this chapter and this chapter only, all of the primary working quantities are **dimensional** (unless explicitly indicated otherwise), since the corresponding paper is addressed to the community of oceanographers and limnologists rather than turbulence modellers.
Chapter 2

Large-eddy simulation of oxygen transfer to organic sediment beds

2.1 Abstract

We have developed a model for dissolved oxygen (DO) transfer from water to underlying organic sediment beds. The model couples Large-Eddy Simulation (LES) of turbulent transport in the water-column, a biogeochemical model for DO transport and consumption in the sediment, and Darcy’s Law for the porewater-driven transport. The model highlights the spatial and temporal relationship between the turbulent bursting events, the near-wall transport of DO, and the response of the sediment layer. The numerical results — compared to data from laboratory experiments — stress the importance of analyzing instantaneous transport events (not reproducible in a Reynolds-averaged Navier-Stokes model) to better characterize and model the processes that lead to oxygen depletion in the sediment layer. The model’s results are compared against experimental data and the sensitivity to the governing parameters has been tested. As the current velocity increases, the sediment-oxygen demand (SOD) increases more slowly than the friction velocity at the wall, in accordance with classic heat-and-mass-transfer laws. The overall SOD is approximately proportional to the bacterial content of the sediment layer. The predicted mean advective flux in the porous medium and across the sediment-water interface is negligible compared to the total dispersive flux, for permeabilities typical of the sediments used in the experiments ($10^{-7}$ and $10^{-6}$ cm$^2$). Higher permeabilities ($10^{-5}$ cm$^2$) appear to yield results not consistent with experimental data. This computational tool will contribute towards the design of a process-oriented parametrization for the SOD, currently missing in oceanographic applications, that can be easily extended to the transport of other bio-limiting substances.
2.2 Introduction

The presence of dissolved oxygen (DO) in water is critical to the survival of organisms in marine environments. Surface waters are saturated with atmospheric oxygen, which is transported towards the bottom by turbulent motions. A number of physical factors can limit this mixing process. For instance, stratification in the water column damps turbulence, reducing mixing; this inhibits the vertical DO flux, reducing the oxygen supply to deeper unstratified water layers. Other factors of biogeochemical nature may amplify this problem, such as agricultural runoff containing excess nutrients, which fertilize algal blooms. This process can lead to a severe alteration of the natural ecosystem balance in coastal regions (on which a significant portion of the world population relies for their sustenance). The algae eventually die and sink to the bed; in the sediment layer, DO-consuming bacteria feed on them. When the DO flux to the sediments (and biological demand) is greater than the flux through the stratified layer near-bed oxygen depletion can occur. The amount of DO absorbed by the sediment will, as a result, largely govern the oxygen budget in such bottom water layers (Bouldin 1968, Veenstra & Nolen 1991, Patterson et al. 1985); if the lack of oxygen persists, aquatic life may suffer. Areas affected by this phenomenon are known as ‘dead zones’, and can be found in many coastal environments in the ocean (the Gulf of Mexico, Chesapeake Bay, the Baltic sea or the Black Sea) or even in lakes (Lake Erie). Further details on the spreading of dead zones in the coastal oceans and their effect on marine ecosystems can be found in Diaz & Rosenberg (2008) and Rabalais et al. (2010).

Because of the environmental and economical consequences of oxygen depletion, there has been significant effort to understand the processes governing DO transport through the water column and the sediment-water interface and ultimately DO depletion by bacterial absorption in the sediment layer. Being able to model these mechanisms is a necessary step towards the development of prediction tools to improve water-management strategies. Research in this field has been carried out mainly through laboratory and field experiments, and numerical investigations limited to one- or two-dimensional models.

Perhaps the first study of this kind is due to Lorke et al. (2003), who measured and analyzed turbulence induced by oscillatory fluid motions and vertical distribution of DO above and within the sediments in Lake Alpnach (Switzerland). Their analysis focuses on the near-sediment region, and shows how the intensity of the turbulent transport controls the thickness of the diffusive sub-layer, and the diffusive DO flux across the sediment-water interface (SWI). An extension of this work can be found in Bryant et al. (2010) where the transient nature of the sediment oxygen uptake is examined, as well as the importance of characterizing turbulence when correlating it to the oxygen flux to the sediments. This is the first attempt to link sediment oxygen demand (SOD) directly to large-scale dynamics such as oscillatory currents, extending the knowledge of how physical processes can be used to model SOD, taking into account the features of non-equilibrium flows.
The same problem has also been investigated experimentally. Hondzo, et al. (2005) performed DO laboratory measurements in a closed loop recirculating square duct. The oxygen dissolved in the water was absorbed by a synthetically generated sediment layer containing organic compost. They derived a scaling law for the mean DO profiles in water, for Reynolds numbers between 360 and 4000 (based on the half-width of the flume and centreline mean velocity). Using the same experimental setup, O’Connor & Hondzo (2007) analyzed DO depletion mechanisms in the sediment layer. More recently, O’Connor & Hondzo (2008) obtained complete DO measurements (in water and sediments) together with PIV characterization of the turbulent flow in order to correlate the transfer rate of oxygen to the sediments with the Reynolds and Schmidt numbers of the flow. These set of experiments have been chosen as a reference for our numerical study. Their results are compared with semi-empirical solute transport models in turbulent flows (Boudreau & Jørgensen 2001). The experiments show a marked dependence of the DO at the sediment-water interface (SWI) and of the SOD on the turbulent activity in the flow.

The first attempt, to our knowledge, to design a numerical and physical model to reproduce experimental observations such as the ones by Hondzo and co-workers was made by Higashino, et al. (2004), who adopted an unsteady DO diffusion and absorption model coupled with a one-dimensional solution of the Reynolds-Averaged equations for the water-side transport. The biochemical model used for oxygen diffusion and absorption by the sediment layer includes a non-linear sink term and a diffusion term. An extension of this work can be found in Higashino et al. (2008) who performed a simulation of a developing boundary layer, using the algebraic eddy-viscosity model of Dade (1993) to parametrize turbulent transport, coupled with an improved version of the DO sediment absorption model. The new formulation takes into account the biomass concentration of oxygen-consuming bacteria, $\chi^*$, in the sediment layer. Although, in principle, $\chi^* = \chi^*(t)$, this quantity remains nearly constant over typical experimental time scales, and a steady-state value of $\chi^*$ was calibrated to match experimental data. However, their numerical model does not reproduce the observed DO profiles at higher Reynolds numbers; this lack of agreement was attributed to the absence of a model for porewater flow induced transport of DO in the sediment layer.

The influence of porewater flow on solute transport across the SWI was investigated by Higashino, et al. (2009) using an approximate characterization of the turbulent pressure oscillations driving the flow in the sediments according to Darcy’s Law. The interstitial flow was used to predict solute advection across the SWI and effective diffusivity (primarily dispersion) in the sediment layer, $D_e$ (proportional to the intensity of the porewater flow and sediment grain size). Their model resulted in an underestimation of $D_e$ with respect to the empirically-based parametrization of O’Connor & Harvey (2008). Also, the model was not explicitly coupled with a water-side or sediment-side scalar-transport model, so an analysis of the effects of turbulence-driven porewater flow on solute transport was not possible. The highest permeability investigated resulted in a fluctuation intensity of the surface-normal component of the oscillating interstitial velocity of 0.02% of the
friction velocity. More recently Higashino & Stefan (2011) extended the effective diffusivity parametrization of Higashino et al. (2009) and incorporated it into the same RANS model of Higashino et al. (2008) predicting an increase in the sediment oxygen uptake with the sediment permeability. However, the change they obtain in the dissolved oxygen distribution – increased penetration depth and decreased concentration value at the SWI – increases the disagreement between the numerical predictions and the experimental data at higher Reynolds numbers.

Although the existence of a direct dependency of the SOD on the turbulence levels has been extensively demonstrated (but not fully understood), in most water-quality models used for lake and ocean management, the SOD is simply a tuneable parameter, fixed in time (and often space), and chosen over an order of magnitude scale so that DO observations can be reproduced. These models typically use the RANS equations, which do not resolve the spatial and temporal characteristics of the boundary layer. In Trolle, et al. (2008) for example, the SOD is fixed to $0.7 \text{g m}^{-2} \text{day}^{-1}$ as a calibration parameter for a one-dimensional water-quality model applied to Lake Ravn (Denmark). In the two-dimensional model applied by Boegman, et al. (2008b) to Lake Erie, SOD=$0.55 \text{g m}^{-2} \text{day}^{-1}$ was used. When SOD is not directly assigned, a simple sediment oxygen flux model is employed that operates by assuming that the flux is only a function of the overlying water temperature and DO concentration (static model) (Hipsey, et al. 2006). Using this model with a three-dimensional hydrodynamic driver Leon, et al. (2011) find good agreement with measured DO profiles in Lake Erie. Such models, however, do not capture any of the boundary layer physics and are still at an early stage of development.

In spite of the availability of field measurements and experimental data, prediction of the various components of the oxygen budget throughout the water column still suffers from many deficiencies, including low-order turbulence modeling of transport dynamics and highly empirical definitions of bio-geochemical parameters characterizing the organic sediment layer. Moreover, no successful attempt has been made to isolate the mechanisms governing DO transfer from water to an organic sediment layer. There is also the need to assess physical assumptions and speculations underlying currently adopted solute-transport models in environmental flows. An investigation method that provides a more detailed description of the turbulent flow (both statistically and instantaneously) than what is available from experimental studies or field measurements, is needed for these purposes. Studies have shown that a full understanding of the biological responses to the varying thermo-fluid dynamic conditions requires physical and numerical models that couple hydro-dynamic transport and the dynamics of water quality and aquatic organisms at all the important scales (Koseff et al. 1993, Boegman et al. 2008a). Being able to resolve the vertical distribution of DO with a fully coupled model would allow for the quantification of the SOD under various fluid flow conditions. The currently employed water-quality models, that tune the SOD such that modeled DO concentration match in-situ observations, would considerably benefit from a process-oriented parametrization of the SOD based on
resolvable flow features in the near-wall region. There is no mechanistic model for SOD based on parameters resolved in currently adopted RANS models.

Within such framework, the present work is aimed at developing a prediction and analysis tool to study oxygen-depletion dynamics with well established eddy-resolving numerical techniques that accurately reproduce the turbulent transport on the water side. Reliable turbulence modeling for the water side transport will help identify and quantify weaknesses in the components of the complete model where the characterization of the governing physical processes is still incomplete. We will focus our analysis on DO transport dynamics of the (non-stratified) near-bed region, and use a simple channel-flow model. Due to the wide range of scales exhibited by the velocity and scalar fields, resolving all the turbulent eddies is infeasible. Large-eddy simulations (LES) will be used to model the transport on the water side, while the diffusion and absorption model proposed by Higashino et al. (2008), together with Darcy’s Law for porewater induced transport, will be used in the governing equations for the sediment side. In the following, we begin by describing the model, which includes the governing equations, the numerical method, and the coupling of the two layers. The comparison between the predictions of our model and the experimental results and a sensitivity test to some of the important model parameters will then be presented. Some remarks and suggestions for further work in this field conclude the article.

2.3 Problem Formulation

In the present work we adopted the large-eddy simulation technique to model the momentum and scalar transport in the fluid, rather than the solution of the RANS equations, to avoid the errors associated with turbulence models and to capture local and instantaneous transport events not present in a RANS solution. Also, in LES only the smaller eddies are modeled, and the motions of the larger eddies (of size comparable to the integral scale) are directly computed extending the range of applicability of the model. In the following, first we discuss the governing equations and the simulation parameters used for the solution of the governing equations in the fluid and in the sediment layer. We then present the computational setup, and the numerical method employed.

2.3.1 Momentum and scalar transport in the fluid

The filtered equations of conservation of mass and momentum can be obtained by applying a filtering operator to the continuity and Navier-Stokes equations (Leonard 1974):
\[
\frac{\partial \bar{u}_i}{\partial x_i} = 0, \quad (2.1)
\]
\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_i} + \frac{1}{Re_b} \nabla^2 \bar{u}_j - f \delta_{ii}, \quad (2.2)
\]

where \(x_1, x_2, \text{ and } x_3\) (or \(x, y\) and \(z\)) are, respectively, the streamwise, wall-normal and spanwise directions, \(\delta_{ij}\) the Kronecker delta and \(\bar{u}_i\) the filtered velocity components in those directions. The filter used is a top-hat filter composed of three one-dimensional 3-point discrete filters. These equations have been made dimensionless by using \(\delta\) (the half-width of the channel) as a reference length scale, and \(U_b\) (the bulk velocity, i.e., the streamwise velocity averaged over the entire domain) as a velocity scale. The Reynolds number is, therefore,

\[
Re_b = \frac{U_b \delta}{\nu}; \quad (2.3)
\]

where \(\nu\) is the kinematic viscosity of water. The forcing term \(f\) in the streamwise momentum equation represents the mean pressure gradient driving the flow. The sub-grid scale (SGS) stresses \(\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j\) are parametrized by an eddy-viscosity model:

\[
\tau_{ij} - \delta_{ij} \tau_{kk}/3 = -2\nu_T \bar{S}_{ij}, \quad \nu_T = C \bar{\Delta}^2 |\bar{S}|, \quad (2.4)
\]

where

\[
\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (2.5)
\]

is the resolved strain-rate tensor and \(|\bar{S}| = (2\bar{S}_{ij} \bar{S}_{ij})^{1/2}\) is its magnitude; \(\bar{\Delta} = (\Delta_x \Delta_y \Delta_z)^{1/3}\) is the filter width. The coefficient \(C\) is evaluated using the dynamic procedure (Germano, et al. 1991, Lilly 1992), and averaged over planes parallel to the wall.

Dissolved oxygen in water behaves like a passive scalar with very low diffusivity, compared with the kinematic viscosity. The filtered transport equation for DO is, therefore,

\[
\frac{\partial \bar{c}}{\partial t} + \frac{\partial \bar{u}_i \bar{c}}{\partial x_i} = \frac{1}{Sc Re_b} \frac{\partial \bar{c}}{\partial x_i} - J_{i}^{sgs}, \quad (2.6)
\]

where \(Sc = \nu/D\) is the Schmidt number and \(\bar{c}\) is the instantaneous filtered scalar concentration field normalized with the bulk DO concentration \(C_b\) defined analogously to \(U_b\). The SGS scalar flux, \(J_{i}^{sgs}\), is also
parametrized by an eddy-diffusivity model:

\[ J_{sgs}^{i} = -\alpha_T \frac{\partial \bar{c}}{\partial x_i}; \quad \alpha_T = C_D \bar{\Sigma}^2 |\bar{S}|. \tag{2.7} \]

The extension of the dynamic model (Germano et al. 1991, Lilly 1992) to the scalar transport at high Schmidt numbers has been shown to be accurate by Zang, et al. (1993), Calmet & Magnaudet (1997) and Na (2004). For this reason we also used the dynamic procedure to determine the model coefficient \( C_D \).

### 2.3.2 Momentum and scalar transport in the sediment

The normalized instantaneous DO concentration level in the sediment layer, \( c_s \), is determined by more complex mechanisms. Dissolved oxygen is transported by diffusion, advection and dispersion, but also depleted by decomposing organic matter. The governing equation for \( c_s \) is

\[ \frac{\partial c_s}{\partial t} + \frac{\partial}{\partial x_i} [u_{si} c_s] = \frac{\partial}{\partial x_i} \left[ \left( \frac{1}{Sc_s Re_b} + D_e \right) \frac{\partial c_s}{\partial x_i} \right] - \dot{c}_s. \tag{2.8} \]

A ‘sediment Schmidt number’ \( Sc_s \) can be defined as (Røy, et al. 2004)

\[ Sc_s = \nu / \phi D_s \tag{2.9} \]

where \( \phi \) is the sediment porosity, \( D_s \) is the effective molecular diffusivity for DO in the porous medium and \( u_{si} \) is the \( i \)-th component of the interstitial velocity field driven by the pressure gradients at the SWI generated by the overlying turbulent flow; the effective diffusivity \( D_e \) — representing dispersion effects — is commonly modeled as the product of a characteristic length scale, \( l_e \), times a velocity scale, \( V_e \) (Freeze & Cherry 1979). In the present work we adopt the parametrization introduced by Higashino & Stefan (2011) for \( D_e \) by extending it to available local and instantaneous quantities obtaining

\[ D_e = \phi^2 d_s (u_{si} u_{si})^{1/2} \tag{2.10} \]

where \( d_s \) is the sediment grain size (proportional to the square root of permeability via the Kozeny-Carmen relationship (Bear 1972)). The DO absorption by organic matter is represented by the sink term, \( \dot{c}_s \), which must be parametrized.

The formulation for the DO advective and diffusive fluxes used here was proposed by Boudreau & Jørgensen (2001). The effective diffusion coefficient inside the sediment, \( D_s \), is lower than in water because molecules must follow a tortuous path around sediment grains. Also, the resulting flux must be reduced by a
factor $\varphi$ to account for the pore-space fraction available to transport in pore water. Several empirical correlations exist between $D_s$, $D$ and $\varphi$ (Boudreau 1996, Iversen & Jørgensen 1993). By using such relationships and the mass conservation constraint at the sediment-water interface (SWI),

$$\frac{1}{Sc \, Re_b} \left( \frac{\partial c_s}{\partial y} \right)_{SWI} = \frac{1}{Sc \, Re_b} \left( \frac{\partial c}{\partial y} \right)_{SWI}$$  \hspace{1cm} (2.11)

it is possible to retrieve the value of the sediment porosity in (2.9) from the measurable slope discontinuity in the mean oxygen profiles at the SWI. The values of porosity used in this paper are calculated based on the correlation between $D_s$, $D$ and $\varphi$ adopted in Higashino et al. (2009) and Higashino & Stefan (2011).

The magnitude of the interstitial flow in the porous medium depends on the permeability. When inertial effects for the fluid occupying the sediment pore-spaces are negligible (for effective grain size, for example, smaller than 1 mm) the flow inside the sediments can be described by Darcy’s Law:

$$u_{si} = -K Re_b \left( \frac{\partial p_s}{\partial x_i} + f \delta_{1i} \right),$$  \hspace{1cm} (2.12)

where

$$K = K^*/\delta^2; \quad p_s = P^*_s/(\rho U_b^2).$$  \hspace{1cm} (2.13)

Here $P^*_s$ is the total pressure, including the gravitational potential, $\rho$ is the density of the water, $K^*$ is the intrinsic permeability of the sediment, and $p_s$ is the normalized pore pressure. The latter can be obtained by combining Darcy’s Law (2.12) with the incompressibility constraint for porewater flow

$$\frac{\partial u_{si}}{\partial x_i} = 0$$  \hspace{1cm} (2.14)

yielding

$$\nabla^2 p_s = 0.$$  \hspace{1cm} (2.15)

Following Higashino et al. (2008), the non-linear sink term $\dot{c}_s$ is parametrized as

$$\dot{c}_s = Re_b \mu_\chi \frac{c_s}{K_{O_2} + c_s} \chi$$  \hspace{1cm} (2.16)

where

$$\mu_\chi = \frac{\mu^*_\chi \nu}{U_b^2}; \quad K_{O_2} = \frac{K_{O_2}^*}{C_b}; \quad \chi = \frac{\chi^*}{Y_c C_b}.$$  \hspace{1cm} (2.17)

The parameters used in (2.17) are $\mu^*_\chi$, maximum specific DO utilization rate (in day$^{-1}$), $K_{O_2}^*$, half-saturation coefficient for DO utilization (in mg l$^{-1}$), $Y_c$ effective yield for the microbial utilization of DO and $\chi^*$, the value of biomass concentration of aerobic heterotrophs (oxygen absorbing organisms). The values of these
### Table 2.1: Dimensional fluid flow and bio-geochemical parameters for oxygen uptake model.

<table>
<thead>
<tr>
<th>Parameter (Unit)</th>
<th>Description</th>
<th>Typical Range</th>
<th>Value adopted</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu^*_\chi$ (day$^{-1}$)</td>
<td>DO utilization rate</td>
<td>0.72 – 13.2</td>
<td>2.4</td>
</tr>
<tr>
<td>$K_{O_2}$ (mg l$^{-1}$)</td>
<td>half-saturation coefficient for DO utilization</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$\chi^*$ (mg l$^{-1}$)</td>
<td>concentration of aerobic heterotrophs</td>
<td>100 – 300</td>
<td>700</td>
</tr>
<tr>
<td>$k^*_d$ (day$^{-1}$)</td>
<td>first order decay coefficient of $\chi^*$</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>$D$ (10$^{-3}$ m$^2$s$^{-1}$)</td>
<td>molecular diffusivity of DO</td>
<td>1.2 – 1.7</td>
<td>2.0 – 3.0</td>
</tr>
<tr>
<td>$\nu$ (10$^{-4}$m$^2$s$^{-1}$)</td>
<td>kinematic viscosity</td>
<td>1.1 – 1.5</td>
<td>0.7 – 0.9</td>
</tr>
<tr>
<td>$\delta$ (cm)</td>
<td>half-channel height</td>
<td>-</td>
<td>7.6</td>
</tr>
<tr>
<td>$\delta_s$ (cm)</td>
<td>sediment-layer thickness</td>
<td>-</td>
<td>2.5</td>
</tr>
<tr>
<td>$U_b, U_\infty$ (cm s$^{-1}$)</td>
<td>bulk and maximum velocity</td>
<td>1-20</td>
<td>5 – 10</td>
</tr>
<tr>
<td>$C_b, C_\infty$ (mg l$^{-1}$)</td>
<td>bulk and maximum DO concentration</td>
<td>6 – 13</td>
<td>2 – 8.2</td>
</tr>
<tr>
<td>$K^*$ (cm$^2$)</td>
<td>intrinsic permeability</td>
<td>10$^{-8}$ – 10$^{-6}$</td>
<td>10$^{-6}$ – 10$^{-5}$</td>
</tr>
</tbody>
</table>

The oxygen absorption rate is taken to be proportional to the level of biomass concentration of oxygen-consuming bacteria, $\chi$, a time dependent quantity whose evolution can be described by a simple logistic model for population growth, giving
\[
\frac{d\chi}{dt} = \left(Re_b \mu_X \frac{c_s}{K_{O_2}} - k_d \right) \left(1 - \frac{\chi}{\chi_{max}} \right) \chi, \tag{2.18}
\]
where $k_d$ is the normalized first-order decay coefficient
\[
k_d = k^*_d \delta / U_b. \tag{2.19}
\]

For the commonly adopted values of the parameters on the right-hand side of (2.18), it can be shown that the timescale over which variations of $\chi$ become significant is of the order of days. Since our simulations span much shorter times, we will assume a constant value of $\chi$ and ignore (2.18), an approach also followed by Higashino et al. (2008).
2.3.3 Computational setup

Numerical Model

The computational setup used is shown in Figure 2.1. The flow is driven by a pressure gradient $f \delta_{1i}$, which is constant in space and adjusted in time to maintain a constant mass flux. The governing equations (2.1), (2.2) and (2.6) are solved on a Cartesian domain. In the streamwise and spanwise directions, $x$ and $z$, periodic boundary conditions are used for all quantities. At the upper and lower walls, the velocity obeys no-slip conditions; for the scalar we use Neumann conditions, with assigned flux. The oxygen dynamically absorbed by the sediment layer across the SWI is reinserted in the flow, at the same rate, from the top boundary by means of an imposed instantaneous flux. Thus, the value of the volume averaged DO concentration is maintained constant and equal to the reference value $C_b$. The oxygen flux assigned at the SWI is calculated based on the coupling between the water and sediment layers, and will be discussed later.

Two main differences exist between the present computational setup and the experimental one used by O’Connor & Hondzo (2008). First, they used a square duct, while we have a plane channel, with no side walls. Second, in the experiment, re-aeration is prevented; thus, the oxygen content slowly decreases when the flume is running; when the flow is quiescent, the DO flux to the sediment layer is negligible. In our calculations, the oxygen content is steady in time, so that a statistical steady state can be achieved. This allows to obtain converged statistical samples more rapidly than if an unsteady calculation were carried out, and ensemble averages were taken.

The experiments were carried out in a recirculating flume configuration. The apparatus was approximately 13 m long and the square duct semi-height was 7.6 cm. A styrofoam layer was used at the top boundary to
prevent re-areation and a finite-length artificially created sediment layer (6.1 m long) was positioned at 4.6 m from the inlet of the flume. The microsensor system used to measure oxygen concentration was positioned at 9.6 m from the inlet. A PIV system was used to measure flow properties.

The numerical model used to compute the flow on the water side is a well-validated finite-difference code (Keating, et al. 2004), based on a staggered grid. Second-order central differences are used for both convective and diffusive terms. The time advancement scheme is a Crank-Nicolson scheme for the wall-normal diffusive term, and a low-storage 3rd-order Runge-Kutta method for the other terms. The solution of the Poisson equation is obtained by Fourier transform of the equation in the spanwise and streamwise direction, followed by a direct solution of the resulting tridiagonal matrix, at each wavenumber. The code is parallelized using the Message Passing Interface (MPI) protocol.

The equations in the sediment layer are solved with the same numerical approach. The scalar and pressure field are located at the cell center and the velocity components at the staggered positions, on the faces of the DO control volumes. The scheme has the same numerical accuracy and stability as the one used on the water side.

Numerical modeling for solute and momentum exchange across the sediment-water interface

An important aspect of the present work is the coupling between the water and sediment layers. We developed a coupling procedure that can enforce the continuity of both the mass flux and the value of oxygen concentration at the SWI. This allows the implicit time-advancement of the solution in both layers (which is required to avoid the viscous time-step limitation caused by the highly stretched meshes near the SWI) while

Figure 2.2: Schematic of the discretization used for the numerical setup of the implicit-two-layer coupling at sediment-water interface.
algebraically independent calculations are performed in the two separate computational domains (water and sediment); thus guaranteeing modularity and simplicity in the implementation of the numerical scheme.

The coupling across the sediment-water interface of the two distinct sets of governing equations for the momentum and solute transport - one for the water-side (2.1),(2.2),(2.6) and the other for the sediment-side transport (2.8),(2.12),(2.15) - can pose some implementation challenges. In order to numerically enforce the continuity of the solute concentration and momentum field (and their respective fluxes) across the SWI a 1D strategy for the coupling (only along \( y \)) has been adopted. This choice is due to the fact that the mass and momentum transport (if present) can occur only across the SWI via the wall-normal component of the respective fluxes. The details of the coupling procedure are described in the following with reference to Figure 2.2.

Let \( \Delta t \) be the time step of the time advancement scheme. The update of the solution in the two layers from time \( n \) to time \( n + 1 \), is carried out via an implicit coupling across the SWI. The instantaneous velocity and oxygen distributions in the two layers are known at time \( n \), i.e. \( c^n, v^n \) on the water side and \( c^n_s, v^n_s \) on the sediment side. The coupling is performed through the following steps:

1. A prediction of the oxygen concentration at the SWI for time \( n + 1 \) is obtained by an explicit update taking into account only the wall-normal components of the total flux; the solution is updated at the closest node to the SWI on the water side (indexes are with references to the figure)

\[
\tau'(+1) = \tau'(1) + \Delta t \frac{1}{S_{Sc} \cdot Re} \left[ \frac{\partial^2 \tau}{\partial y^2} \right]_{+1} - \Delta t \frac{\Delta y}{\Delta y} \left[ \frac{\tau^n(1) \left( c^n(2) + c^n(1) \right)}{2} - \tau^n(0) \left( \frac{\tau^n(1) + \tau^n(0)}{2} \right) \right]
\] (2.20)

and sediment side

\[
c^s(−1) = c^s(−1) + \Delta t \frac{1}{S_{Sc} \cdot Re} \left[ \frac{\partial^2 c^s}{\partial y^2} \right]_{−1} - \Delta t \frac{\Delta y}{\Delta y} \left[ -c^s(−1) \left( \frac{c^s(−2) + c^s(−1)}{2} \right) + c^s(0) \left( \frac{c^s(−1) + c^s(0)}{2} \right) \right]
\] (2.21)

where \( \frac{\partial^2 \tau}{\partial y^2} \bigg|_{+1} \) is a numerical estimate of \( \frac{\partial^2 \tau}{\partial y^2} \) at \( y = +\Delta y_0 / 2 \), linearly dependent on \( \tau^n(0), \tau^n(+1) \) and \( \tau^n(+2) \); likewise, \( \frac{\partial^2 c^s}{\partial y^2} \bigg|_{−1} \) is a numerical estimate of \( \frac{\partial^2 c^s}{\partial y^2} \) at \( y = −\Delta y_0 / 2 \), linearly dependent on \( c^s(0), c^s(−1) \) and \( c^s(−2) \). The final prediction is obtained by averaging the two values
above thus yielding

$$c^*_{swi} = \frac{1}{2} [c^*(1) + c^*(-1)]. \quad (2.22)$$

2. The value of $c^*_{swi}$ is applied as a Dirichlet boundary condition at time $n + 1$ to implicitly update the solution in the sediment layer.

3. An implicit update of the oxygen distribution on the water side is now possible by prescribing the DO flux at time $n + 1$ (extracted from the updated $c_s$ field):

$$\frac{1}{Sc Re_b} \frac{p^{n+1}(1) - p^{n+1}(0)}{\Delta y_0} = \frac{1}{Sc_s Re_b} \frac{c^{n+1}_s(0) - c^{n+1}_s(-1)}{\Delta y_0} \quad (2.23)$$

(the scalar convective flux is treated explicitly everywhere, implicit update is just applied to the diffusive fluxes.)

4. The velocity field is updated; therefore, the pressure distribution $p^{n+1}$ is known in the channel.

5. The governing equations for the interstitial velocity field are directly solved given the fluid-side distribution of pressure fluctuations at the SWI. The boundary conditions for the Laplace equation

$$\hat{\nabla}^2 p^{n+1}_s = 0 \quad (2.24)$$

are

$$\frac{p^{n+1}_s(0) + p^{n+1}_s(-1)}{2} = p^{n+1} + 1; \quad (2.25)$$

$$\hat{\partial} p_s \hat{\partial} y = 0 \quad \text{at} \quad y = -\delta_s/\delta. \quad (2.26)$$

6. The boundary conditions for the velocity field at the next cycle on the water side are

$$v^{n+1}(0) = v^{n+1}_s(-1) = -K Re_b \frac{p^{n+1}_s(0) - p^{n+1}_s(-1)}{\Delta y_0} \quad (2.27)$$

The velocity in the channel is updated implicitly; this strategy introduces a time lag. The only additional numerical accuracy requirement of this scheme is that the grid spacing at the SWI, $\Delta y_0$, must be the same from both sides (see Figure 2.2).

Note that the above procedure results in a time lag (by a fraction of the time step $\Delta t$) between the solution in the water and sediment layer. Since transport dynamics at the SWI exhibit much longer timescales than those in the fluid, the decoupling does not affect the time accuracy of the numerical model: typical values of $\Delta t$, in our simulations, correspond to $1 - 10$ ms of real time.


Table 2.3: Flow characteristics of recirculating flume experiments EXP-2 to EXP-5 in O’Connor & Hondzo (2008). Estimates of $C_b$ have been extracted from Higashino et al. (2008) by matching the steady solution of (2.8) in the sediment layer.

Experimental and field-scale parameters

The numerical study (and, in particular, the range of parameters used) was designed to allow direct comparison to the laboratory data from O’Connor & Hondzo (2008). The flow parameters adopted in these experiments are summarized in Table 2.3. We performed numerical simulations matching the fluid dynamic conditions of the experiments indicated as LES-2, LES-3, LES-4 and LES-5 and the respective parameters are summarized in Table 2.4. Then, only for case LES-3, runs have been repeated at $\chi^* = 500\text{mg/l}$ and $\chi^* = 1000\text{mg/l}$, keeping $\varphi = 0.55$ and $K^* = 0$. Also, for the same case, the sediment properties have been kept constant at $\chi^* = 700\text{mg/l}$, $\varphi = 0.55$ and $K^* = 0$ and $Re_b$ has been changed to $Re_b = 3000$ and then to $Re_b = 9000$, by only changing $U_b$. Finally, for the LES-4 case the effects of permeability have been investigated for $K^* = 10^{-6}\text{cm}^2$ and $K^* = 10^{-5}\text{cm}^2$.

The actual fluid flow characteristics in oceanic environments may differ from the experimental and numerical simulations. Bottom waters can be significantly colder, resulting in a much higher Schmidt number (typically of the order of 1000 for $T = 8^\circ\text{C}$ (Bryant et al. 2010)). The sediment layer surface may not be flat and large scale roughnesses may be present such as mounds, sand ripples and dunes which play an important role in determining advective solute exchange across the SWI (Boudreau & Jørgensen 2001). In small alpine lakes, typically measured free stream and bed shear velocities may be of the order of $0.05\text{ m s}^{-1}$ and $0.001\text{ m s}^{-1}$, respectively (Bryant et al. 2010, Lorke et al. 2003), which are actually lower than what realized experimentally ($0.1\text{ m s}^{-1}$ and $0.005\text{ m s}^{-1}$, respectively). For lakes such as Lake Erie, free-stream velocities in the range of $0.01\text{ m s}^{-1}$ to $10\text{ m s}^{-1}$ can be observed (Bedford & Abdelrhman 1987). In coastal environments current velocities up to $0.12\text{ m s}^{-1}$ have been observed by Chliss & Caldwell (1982) and up to $0.8\text{ m s}^{-1}$ at the edge of tidal bottom boundary layers (Sanford & Lien 1999). Moreover, even if in experimental and numerical studies the velocity scales were to be matched, the length scales of the large eddies governing the transport in the outer region can be of the order of meters in lakes and kilometers in oceans which lead to much higher Reynolds numbers (up to $10^9$ (Hendry & Wunsch 1973)) than what are reproducible in laboratory or numerical experiments. The thickness of the diffusive sub-layer for DO is of the order of millimeters in both field scale and experiments. Bryant et al. (2010) measured thicknesses up to 1 cm due to an abrupt decrease of the turbulent mixing intensity. In spite of these differences, the purpose of this work is to validate the complete model by comparing it to lab experiments, which were performed in
freshwater and at higher temperatures, resulting in lower Schmidt numbers with smooth cohesive sediments and Reynolds numbers in the range $3 - 10 \times 10^3$.

### Simulation parameters

The computations were carried out using domain sizes, on the water side, of dimensions ranging between $16 \times 2 \times 8$ (for the low-$Re_b$ cases) and $6 \times 2 \times 3$ (for the high-$Re_b$ ones); recall that all quantities are normalized by $\delta$, the channel half-width, which in this case is $7.6 \text{ cm}$. The number of grid points used varied between cases, resulting in a streamwise grid spacing, in wall units (indicated by a plus), of $\Delta x^+ \approx 26$ for all cases and in a variable spanwise resolution ranging from $\Delta z^+ \approx 12$ to $\Delta z^+ \approx 6$ where $\Delta x^+ = u_\tau \Delta x/\nu$ and $\Delta z^+ = u_\tau \Delta z/\nu$. This resolution is nearly fine enough to resolve the scales responsible for the dissipation of turbulent kinetic energy; because of the high Sc, however, a range of sub-Kolmogorov scales exists in the DO field that require finer resolution. Previous studies of high-Sc scalar transport in a turbulent channel flow (Calmet & Magnaudet (1997) and Bergant & Tiselj (2007), who both modeled the smallest scalar scales with a sub-grid scale model) show that low-order statistics can be captured very accurately even on coarse grids, and that spectra and scalar variance profiles in the diffusive sublayer and the scalar buffer layer ($y^+ < 5$) are unaffected by the cutoff of sub-Kolmogorov scales. Another issue brought about by the low scalar diffusivity of oxygen is the thinning of the diffusive sublayer; the ratio of diffusive-sublayer thickness to viscous-sublayer thickness scales like $Sc^{-n}$, with $0.5 > n > 0.3$ (Dong, et al. 2003, Schwertfirm & Manhart 2007, Lorke et al. 2003). This results in the need of finer wall-normal resolution near the solid boundaries.

On the sediment side, in all cases, 65 points have been used in the vertical direction, for a sediment layer depth of $\delta_s = 0.33\delta$ and the porosity has been set to $\varphi = 0.55$. Spanwise and streamwise resolution and box size are the same as the water side.

### Table 2.4: Summary of LES parameters matching experimental flow conditions (Table 2.3). See Tables 2.1 and 2.2 for parameter definitions.

<table>
<thead>
<tr>
<th>LES run</th>
<th>$Re_b$</th>
<th>$Re_{\tau}$</th>
<th>$Re_{max}$</th>
<th>$Sc$</th>
<th>$\chi^*$ (mg l$^{-1}$)</th>
<th>$K^*$ (cm$^2$)</th>
<th>Domain size</th>
<th>Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES-2</td>
<td>3900</td>
<td>241</td>
<td>4534</td>
<td>358</td>
<td>700</td>
<td>0</td>
<td>$12\times2\times6$</td>
<td>$128\times128\times128$</td>
</tr>
<tr>
<td>LES-3</td>
<td>6137</td>
<td>360</td>
<td>7124</td>
<td>291</td>
<td>700</td>
<td>0</td>
<td>$8\times2\times4$</td>
<td>$128\times128\times128$</td>
</tr>
<tr>
<td>LES-3 (low-$Re$)</td>
<td>3000</td>
<td>188</td>
<td>3500</td>
<td>291</td>
<td>700</td>
<td>0</td>
<td>$16\times2\times8$</td>
<td>$128\times128\times128$</td>
</tr>
<tr>
<td>LES-3 (high-$Re$)</td>
<td>9000</td>
<td>510</td>
<td>10500</td>
<td>291</td>
<td>700</td>
<td>0</td>
<td>$6\times2\times3$</td>
<td>$128\times128\times128$</td>
</tr>
<tr>
<td>LES-3 (low-$\chi$)</td>
<td>6137</td>
<td>360</td>
<td>7124</td>
<td>291</td>
<td>500</td>
<td>0</td>
<td>$8\times2\times4$</td>
<td>$128\times128\times128$</td>
</tr>
<tr>
<td>LES-3 (high-$\chi$)</td>
<td>6137</td>
<td>360</td>
<td>7124</td>
<td>291</td>
<td>1000</td>
<td>0</td>
<td>$8\times2\times4$</td>
<td>$128\times128\times128$</td>
</tr>
<tr>
<td>LES-3</td>
<td>9019</td>
<td>515</td>
<td>10314</td>
<td>218</td>
<td>700</td>
<td>$10^{-6}$</td>
<td>$6\times2\times3$</td>
<td>$128\times192\times256$</td>
</tr>
<tr>
<td>LES-4 (K-6)</td>
<td>9019</td>
<td>515</td>
<td>10314</td>
<td>218</td>
<td>700</td>
<td>$10^{-6}$</td>
<td>$6\times2\times3$</td>
<td>$128\times192\times256$</td>
</tr>
<tr>
<td>LES-4 (K-5)</td>
<td>9019</td>
<td>515</td>
<td>10314</td>
<td>218</td>
<td>700</td>
<td>$10^{-6}$</td>
<td>$6\times2\times3$</td>
<td>$128\times192\times256$</td>
</tr>
<tr>
<td>LES-5</td>
<td>11285</td>
<td>630</td>
<td>12861</td>
<td>188</td>
<td>700</td>
<td>0</td>
<td>$6\times2\times3$</td>
<td>$128\times192\times256$</td>
</tr>
</tbody>
</table>
2.4 Results and discussion

2.4.1 Validation and grid convergence test

To validate the velocity statistics we compare in Figure 2.3 the mean velocity and trace of the Reynolds-stress tensor $q^2 = \langle u'_i u'_i \rangle$ with direct simulation data at comparable Reynolds numbers (Moser et al. 1999a). All quantities are normalized by $u_\tau$ and $\nu$, and are averaged spatially over planes parallel to the wall and in time over 240 samples for a total averaging of 1200 $\delta/U_b$ time units for the low $Re_b$ case, and 400 time units for the high $Re_b$. To test for grid convergence of the scalar statistics we compare in Figure 2.4 LES of passive-scalar transport at $Re_\tau = 400$ with progressively refined grids to assess the effects of the unresolved scales on the resolved quantities for the scalar. Neumann boundary conditions were applied at the solid wall for this test. The results confirm that first-order moments are insensitive to the grid resolution, provided that the diffusive sub-layer, whose thickness is known a priori in channel flow, is resolved. A slight grid dependency can still be observed in the scalar variance profiles which collapse, for every grid, over more than 99 % of the channel height, varying only in part of the diffusive sub-layer (by 5 % in the last refinement step) where scalar fluctuations are inactive and not statistically relevant for transport dynamics. The presence of the sediment layer, which damps oscillations via the sink term (2.16), is expected to improve the near-wall convergence.
2.4.2 Instantaneous flow characteristics

We want to highlight the three-dimensional and instantaneous nature of the data generated by the LES by looking at visualizations extracted from case LES-4 (K-6), which includes all the transport processes that have been implemented in our model. Data from a RANS simulation of the same problem would be steady and one-dimensional (all quantities vary only along $y$) and would not allow for the analysis of the flow features, which exhibits a multiplicity of scales both in space and time.

The spatial distribution of the diffusive flux at the SWI (Figure 2.5(a)) reveals very fine organized structures, similar to the ones observable in the DO concentration contours (Figure 2.5(b)) and in the vertical velocity fluctuations (Figure 2.5(c)) at $y = 0.01$; this is the edge of the diffusive sub-layer, which can be identified as the location where the turbulent flux reaches its freestream value (shown later). Vertical velocity fluctuations here play an important role in the transport governed by turbulent motions convecting, on average, patches of high DO concentration towards the SWI and low DO concentration towards the bulk flow.

Contours of instantaneous velocity and scalar fluctuations have also been extracted in the plane $y = -0.0025$ in the sediment layer (Figure 2.6). The scalar field exhibits the same elongated structure in the
streamwise direction both above (Figure 2.5 (b)) and below (Figure 2.6 (b)) the SWI. The porewater-flow-enhanced effective diffusion in the porous medium (relative here to a permeability of \( K^* = 10^{-6} \text{cm}^2 \) or \( K = 1.7 \times 10^{-8} \)) smooths out spatial gradients in the scalar field whereas higher levels of fluctuation intensity on the water side, especially due to spanwise variations in DO concentration, are evident from the visualizations; in spite of the overall higher variance, relatively extended regions of (approximately) constant DO concentration are visible on the water side. This is the signature of internal intermittency effects, which are emphasized in the high-Sc limit (Antonia & Orlandi 2003); intermittency cannot occur in the sediment layer, where no scalar-variance-production mechanisms are present. The velocity fluctuation field does not preserve its structure in the sediment layer, where it becomes more disorganized. This is due to the elliptic nature of the equations governing the advective transport here (2.15); the higher wave-numbers are damped faster with depth, and, in this case, the signature of the pressure gradients, driving the flow at the SWI, disappears rapidly as the fluid penetrates into the permeable layer. The velocity and scalar field in the sediment appear rather uncorrelated as confirmed later.

2.4.3 Comparison with experimental data

We now compare predictions of the present model with the experimental results reported by O’Connor & Hondzo (2008). We attempt to reproduce the flow characteristics of experiments EXP-2, EXP-3, EXP-4 and EXP-5 (Table 2.3), which were carried out over several months and the water temperature varied from \( T = 25^\circ \text{C} \) to \( T = 37^\circ \text{C} \), with our model runs LES-2, LES-3, LES-4 and LES-5, respectively (Table 2.4). Kinematic viscosity and oxygen molecular diffusivity were both affected by the changes in temperature, resulting in Schmidt numbers decreasing, in time, from 358 to 188. The water, with an initial homogeneous oxygen concentration, was forced to recirculate in a square duct over an artificially created organic sediment layer. The bulk decay of oxygen in the recirculating water during each experiment is ignored as it occurs over timescales much longer than the measurements and our numerical simulations; therefore, we maintain \( C_b \) constant for each experiment. DO-concentration profiles were experimentally measured in both water and sediment. The position of the sediment-water interface was determined from the gradient discontinuity in the mean oxygen profile, after an initial optical inspection. Experiment EXP-1 was not considered in our study, since (due to the low Reynolds number) the flow was probably transitional in the experiment (see the discussion in Higashino et al. (2008)). The fluid dynamic conditions in our model were set to match the centreline velocity, the viscosity and oxygen diffusivity, the duct height and the sediment depth of the reference experiments (a discussion on the effects of the duct geometry is included below). Values of intrinsic permeability in the experiment are not given and are difficult to estimate, even when the sediment composition is given. Therefore, in our model, we first neglected the effects of porewater flow (2.12) or, equivalently, we set \( K^* = 0 \). Values of porosity and bacterial population were calibrated by matching the
numerical results against data for EXP-2; the resulting values ($\chi^* = 700 \text{ mg/l}$ and $\varphi = 0.55$) were used for all the calculations. Note that the value of $\chi^*$ is somewhat larger than those typically found in the literature (Table 2.1) but smaller than the value $\chi^* = 1000 \text{ mg/l}$ used in the RANS calculations of Higashino et al. (2008). Also, the uncertainty on the value of $\mu_\chi^*$ (see Table 2.1) is rather high and affects the product $\chi \mu_\chi$ (or $\chi^* \mu_\chi^*$) in (2.16), which is the only parameter that ultimately matters for the sediment oxygen uptake.

In Figure 2.7(a) we compare the mean concentration profile computed from the LES-2 run with the experimental data for case EXP-2 ($Re_{max} = 4500$ and $Sc = 360$). Since this case is used to determine the values of $\chi^*$ and $\varphi$, the calculations give good agreement (by design) with the experiments. In Figure 2.7(b) we present the same comparison between simulations and experiments for EXP-3 ($Re_{max} = 7100$ and $Sc = 290$). The agreement is still very good; in particular, the model predicts the correct DO penetration depth into the sediments and thickness of the oxygen diffusive sub-layer. The value of the error bar at the SWI was taken from Figure 9 of Higashino et al. (2008), and reduced with the distance from the SWI, consistent with Figure 1 in Røy et al. (2004).

When the Reynolds number is further increased, however, the quality of the agreement begins to deteriorate (see the comparison between LES-4 and LES-5 with EXP-4 and EXP-5 in Figures 2.7(c) and (d)). In the experimental results, as the Reynolds number increases, the position of the SWI becomes less defined and the increasing experimental uncertainty does not allow an accurate estimate of the material properties needed to run the numerical model, specifically the porosity, calculated from the experimental mean gradient discontinuity at the SWI. To establish if experimental uncertainty in the determination of the position of the SWI could have contributed to the observed disagreement, the experimental profiles from EXP-4 and EXP-5 were shifted vertically until the best match was found with the model predictions LES-4 and LES-5. This is obtained with a vertical shift of $+0.003 \delta$ (0.23 mm) and $+0.0015 \delta$ (0.11 mm), respectively, for EXP-4 and EXP-5 (shifted data are shown with open circles and no error-bars). These values are well within measurement error. Acceptable agreement is recovered between LES-4 and EXP-4 after the shifting, but the gradient discontinuity at the SWI (which is always present in our model and is governed by the porosity) is barely distinguishable, especially for EXP-5, in the experimental data. The fact that the discontinuity becomes gradually less defined in the measured data as $Re$ is increased cannot be attributed to pre-resuspension phenomena such as bed-load transport, since estimates for the values of the mobility Shields parameter for the EXP-4 and EXP-5 experiments are below the critical level (see Quaresma, et al. (2007) and Boegman & Ivey (2009)).

While we believe the present model for the transport on the fluid side to be accurate, an improved biogeochemical model for the DO transport and absorption may be required. The sediment layer may have porosity, permeability and bacterial population variable, for example, with depth which can affect the predicted oxygen profile dramatically. These variations could be easily implemented in the model but, at this
stage, any functional form adopted for these material properties would be completely arbitrary and specific measurements are required. The disagreement between numerical and laboratory data can, therefore, be solved in the framework of a collaborative approach between numerical modellers and experimentalist. The following sections explore the model’s sensitivity to the governing fluid dynamic and geochemical parameters in an attempt to explain the observed discrepancies and investigate the simulated physics of transport.

2.4.4 Effects of microbial biomass concentration

The effect of the bacterial population $\chi^*$ on the oxygen concentration is examined in Figure 2.8. Variations up to 100 % of the bacterial population (from case LES-3 (low-$\chi$) to case LES-3 (high-$\chi$)) only result in a limited variation of the value of dissolved oxygen at the sediment-water interface (less than 10 %). On the other hand, the SOD, coinciding with the freestream value of the turbulent flux in Figure 2.8 (c), exhibits an almost linear dependency from $\chi^*$. Increasing the value of the bacterial population by 40 %, from case LES-3 (low-$\chi$) to case LES-3, and by 43 %, from LES-3 to LES-3 (high-$\chi$), determines an enhancement of the SOD by approximately 17 % and 14 %, respectively. Sources of non-linearity are, however, present in the functional form used for the absorption term (2.16), often simplified to a constant term in field-scale applications (Lorke et al. 2003, Bryant et al. 2010), and intrinsically present in the turbulent transport dynamics on the water side. Values of resolved scalar rms increase with $\chi^*$, consistent with what is observed in field data (Lorrai, et al. 2010).

2.4.5 Effects of Reynolds number

In Figure 2.9 we show the effects of increasing flow velocity (and Reynolds number) on DO concentration for bulk Reynolds numbers of 3000, 6100 and 9000. This corresponds to an overall increase in the friction velocity (or $Re_\tau$; Table 2.2) by a factor of 2.7 (Table 2.4). The DO at the SWI is higher as $Re_b$ is increased and the turbulent transport on the water side becomes more intense, in agreement with the observations of Bryant et al. (2010). As $Re_b$ increases the DO flux to the sediment, across the SWI, increases due to the thinning of the diffusive sub-layer and the resulting higher oxygen uptake by the sediment layer can only be sustained by higher DO concentration at the SWI and higher penetration depth. However, the mean DO response to $Re_b$ increases becomes less pronounced at higher $Re_b$. This is consistent with classical results in heat and mass transfer (Pinczewski & Sideman 1974, Schwertfirm & Manhart 2007) where the gain in mass transfer rate across the interface, as mixing on the fluid side is enhanced, is reduced at higher Reynolds numbers. The limiting factor for the sediment uptake lies in the nature of the fluid side transport, regardless of the presence of an underlying absorbing medium.

We conclude that, overall, the model reacts as expected to changes in turbulent activity. The resolved
scalar rms peak approaches the SWI as the Reynolds number is increased (thinning of the diffusive sub-layer is predicted by the model); the total value of the scalar turbulent flux (non-dimensionalized by $C_b U_b$) is reduced by the increased Reynolds number (reduced mean scalar gradient at the wall). This is understood by analyzing the dimensionless governing equations: as the reference current velocity $U_b$ is increased the non-dimensional value of the DO utilization rate $\mu_\chi = \mu_\chi^* \nu / U_b^2$ is reduced. The SOD dimensional counterpart (that can be obtained by multiplying the free-stream value of the total turbulent flux in Figure 2.9 (c) by $C_b U_b$) does, however, increase as observed experimentally.

### 2.4.6 Effects of pore-water-flow-induced transport

To this point the effects of porewater induced solute transport in the sediment layer — advection and dispersion — have not been considered (i.e., the results shown have been for $K^* = 0$). Higashino et al. (2008), who modeled the turbulent transport with an algebraic RANS model in a developing flat plate boundary layer, also observed disagreement between their model and the experimental data for the higher Reynolds number cases. They argued that the reason for such discrepancies is that the permeability of the sediment layer was not fully taken into account. Velocity fluctuations are expected to penetrate in the sediments extending the turbulence-driven transport to this layer. Moreover, the newly introduced advective flux should increase the value of the oxygen concentration at the SWI. Subsequent investigations by the same author showed no improvement for small $K^*$, worsening of the agreement for higher $K^*$ as anticipated in the Introduction.

To shed some light on these issues we have investigated the effects of advection and dispersion — both processes governed by the permeability — in the sediment for case LES-4. Figure 2.10 shows the effects of non-zero permeability on the DO distribution. Values of intrinsic permeability up to $K^* = 10^{-6}$ cm² ($K^* = 0$ corresponding to no porewater flow in the sediment layer) do not affect the mean DO distribution significantly. If the permeability is furthermore increased to $K^* = 10^{-5}$ cm² the effective diffusivity in the sediment layer increases dramatically, increasing the SOD and, consequently, the flux on the water-side. This leads to rather low values of oxygen concentration at the interface that are not consistent with the experimental observations at higher Reynolds numbers and is similar to what was observed by Higashino & Stefan (2011). Moreover, typical values of permeability for sediments of the type used in the experiments are between one and two orders of magnitude lower than this value (Boudreau & Jørgensen 2001, Huettel & Gust 1992, Wiebke Ziebis & Förster 1996).

In Figure 2.11 we show the rms velocity fluctuations and the DO fluxes on the sediment side for runs LES-4 ($K^* - 6$) and LES-4 ($K^* - 5$). All of these quantities are maximum at the SWI where the direct forcing by the turbulent pressure waves from the water side takes place. The values of velocity rms are negligible with respect to the corresponding water side quantities. The correlation between fluctuations of the vertical
component of the interstitial velocity and scalar fluctuations (not available in a RANS code) in the sediment layer creates an advective flux (mean advection is zero in the porous medium), shown in Figure 2.11 (b) (amplified by a factor of 100). Its value is negligible with respect to the diffusive and dispersive fluxes (between 2 or 3 orders of magnitude lower). Since the magnitude of the effective diffusivity directly depends on the intensity of the porewater flow based on (2.10) the model yields a strong discontinuity in the DO total diffusivity across the SWI, from purely molecular to fully dispersive, that is evident in Figure 2.10 (a).

The pressure is continuous across the SWI, as shown in Figure 2.12(a). The interstitial flow in the sediment layer is driven from high pressure to low pressure regions; however, its intensity is too low (of the order of $10^{-5}U_b$ for the run LES-4 ($K$-6)) to significantly affect the net mass-transfer rate across the interface. The corresponding DO concentration contours in Figure 2.12(b) are consistent with the near-wall high-Schmidt-number transport dynamics described by Pinczewski & Sideman (1974): regions of above-average pressure at the wall, like the ones at $x = 1.1$ (bursting events), are caused by eddies, rich in oxygen, that are strong enough to reach the SWI, and that, only after some time, cause the thinning of the diffusive sublayer (enhancing the instantaneous mass-transfer rate across the SWI). The existence of such time lag (due to diffusive transport times) explains why in Figure 2.12 a patch of high pressure, traveling in the direction of the mean current at approximately the friction velocity, is leading an elongated streak (from $x = 0$ to $x = 1.1$) of higher-than-average mass flux at the SWI, also visible in Figure 2.5(a); since both pressure and DO concentration fields are advected downstream, the time lag between the occurrences of these two events determines the observed shift in space, which is a function of the Schmidt and Reynolds numbers.

The DO penetration depth in the sediment layer and DO concentration at the SWI, are not immediately affected by instantaneous variations in water-side transport dynamics. This is due to the long diffusive time scales, associated with the transport in the porous medium and across the diffusive sub-layer, compared to the ones characterizing the turbulent transport above it. This determines a time lag between the sequence of small-scale transport processes (water-side turbulent transport, transfer across the SWI and transport in the porous medium) that ultimately leads to DO consumption in the sediment layer. The sediment layer retains the signature of the overlying turbulent transport events.

2.4.7 Effect of duct geometry

Another potential reason for the disagreement between the model and the experiments is the effect of the duct geometry. The experiments were carried out in a square duct, our calculations in a plane channel. We have also performed simulations of the flow field only in a square duct, for $Re_{max} = 3000$ and 4600 and compared them with the channel flow calculations (at the same Reynolds numbers). We notice that in every case (and, more remarkably, in the higher Reynolds number case) the channel flow exhibits a more extended turbulent mixed region, than the one present in the symmetry plane of a square duct, indicative of more efficient local
transport of momentum from the centerline towards the wall for the channel flow. LES of cases EXP-4 and EXP-5, performed in a square duct configuration, would therefore cause the numerical predictions to either remain unchanged, or further deviate from the observations (which exhibit a more extended region of turbulent mixed DO concentration than the simulations). We therefore conclude that the cause for observed disagreement for the higher Reynolds number cases should not be sought in the geometry of the flow duct.

2.5 Conclusions

We developed a model for dissolved oxygen (DO) transfer, from water to underlying organic sediment beds that, for the first time, couples Large-Eddy Simulation (LES) of turbulent transport on the water side with existing biogeochemical models for the transport and the DO bacterial absorption in the sediment bed. As opposed to a RANS model, LES provides unsteady and time-resolved data allowing us to visualize and analyze instantaneous events in the flow, such as bursts. This allows us to determine the role of turbulent coherent structures in controlling the diffusive sublayer thickness and, thus, sustaining the mass-transfer rate across the SWI, or, equivalently, the sediment oxygen demand (SOD). Differences between the characteristic time scales of the transport in the sediment layer, with respect to the overlying turbulent flow, are also quantified. Instantaneous visualizations of the velocity and concentration fluctuations reveal a flow pattern organization (determined by near-wall coherent motions) that is still retained at the SWI and leaves its signature within the sediment layer. Relying on an accurate description of the flow, on the water-side, has also the advantage of better describing turbulence-driven transport processes in the sediment layer, improving, therefore, the prediction of the SOD. These include porewater-flow driven advection and dispersion, which directly depend on the instantaneous pressure distribution at the sediment-water interface (SWI), not available in a RANS code.

The computational tool presented here can be applied to investigate the modeling issues of near-wall oxygen depletion and transfer dynamics in water-bodies. Very good agreement is found with experiments at low and intermediate Reynolds numbers (cases EXP-2 and EXP-3). For higher \( Re_b \) the agreement between experiments and simulations is recovered by applying a vertical shift to the data of 0.23 and 0.11 mm for cases EXP-4 and EXP-5, respectively. A sensitivity analysis, to all of the important material properties (including bacterial population, current intensity, permeability), has been carried out to try to explain such discrepancies and, at the same time, to estimate the relative importance of the different physical processes involved in the problem. The SOD response to changes in bacterial population is almost linear, whereas increases in the current intensity reveal slow gains in the overall DO depletion rate, despite the presence of an absorbing sediment layer. Transport dynamics on the water side are consistent with classic heat-and-mass transfer laws. Investigating the effects of a variable intrinsic permeability \( K^* \) has revealed that mean
pore-water flow advection in the sediment layer, for the smooth organic sediments investigated here (clayey sand), is not an important process; dispersion, on the other hand, becomes important for permeabilities of $K^* \geq 10^{-5} \text{cm}^2$ which leads to oxygen distributions that appear unrealistic for our case.

Future research, at lab scale, should focus on higher Reynolds numbers ($Re_{max} > 7000$) where numerical predictions are not consistent with experimental observations. Application of a fully coupled numerical and mathematical model to represent experiments like the ones presented here, requires, among other things, accurate measurements of porosity (or, mean profiles slope discontinuity at the SWI) and permeability, the most critical sediment layer material properties determining the mean oxygen distribution. Values of $\chi^*$ are currently an output of calibration procedures performed with models like ours and are not easily determined a priori. Higher-order statistics (scalar variance and turbulent flux profiles) have to be measured and compared to companion numerical predictions; particular attention must be taken in order to avoid sediment resuspension or pre-resuspension phenomena that would lead to bi-phasic flow that is too difficult to account for in the model; at least at this stage of development. Additional experiments with permeable sands and carefully measured pore-water-flow intensities would help understand the limits of applicability of the currently adopted numerical approach. Also, a special effort should be made by experimentalists who wish to collaborate with computational modelers in trying to adopt geometries amenable to LES and DNS studies, such as high-aspect-ratio ducts (well-approximated by a doubly-periodic channel flow). All of the aforementioned suggestions can facilitate a synergistic interaction between experimental and numerical investigations. The goal is to avoid potential sources of disagreement between the two approaches, contaminating the analysis of the problem, which is already sufficiently complicated by a broad spectrum of physical processes. This joint effort is required to develop accurate numerical models for oxygen transport that can be adopted to calibrate RANS models for field scale applications such as water-quality management. An eddy-resolving model like LES is the ideal candidate for this task, as it can provide sufficient detail to carry out in-depth analysis of the governing mechanisms for oxygen transport and depletion at reasonable computational costs.

The thus-obtained numerical model for oxygen transport could be easily extended to multiple species and contaminants transported in the fluid and in the porous medium, by taking into account, for example, the complete sediment bio-geochemistry. This extension, although rather straightforward, would significantly broaden the scope of the developed model to problems where more accurate biochemical descriptions are required. The development and validation of the current numerical setup is a crucial step towards the design of accurately time-resolving transport models for solute exchange across the interface between fluid and porous media.
Figure 2.5: Contour plots of diffusive flux at SWI (a), scalar concentration fluctuations (b) and vertical velocity fluctuations (c) at edge of the diffusive sublayer \((y = 0.01\) plane), for case LES-4 \((K-6)\). The location of the \(z = 0.57\) plane is indicated with a dashed black line. Note that the DO flux is scaled with \(C_b U_b = 0.37 \text{ mg l}^{-1} \text{ m s}^{-1}\), the oxygen concentration field with \(C_b = 4.5 \text{ mg l}^{-1}\), the velocity fluctuating field with \(U_b = 8.3 \text{ cm s}^{-1}\) and the coordinates \(x, z\) with \(\delta = 7.6 \text{ cm}\).

Figure 2.6: Contours of vertical interstitial velocity (a) and scalar concentration (b) at \(y = -0.0025\) for case LES-4 \((K-6)\). The location of the \(z = 0.57\) plane is indicated with a dashed black line. Note that the velocity fluctuating field is scaled with \(U_b = 8.3 \text{ cm s}^{-1}\), the oxygen concentration field with \(C_b = 4.5 \text{ mg l}^{-1}\) and the coordinates \(x, z\) with \(\delta = 7.6 \text{ cm}\).
Figure 2.7: Comparison between the channel flow model (—) and experiments (■) for cases (a) LES-2 and EXP-2, (b) LES-3 and EXP-3, (c) LES-4 and EXP-4, (d) LES-5 and EXP-5. ○ Experimental results shifted upwards by $0.003\delta$ (0.23 mm) in (c), and $0.0015\delta$ (0.11 mm) in (d).

Figure 2.8: Effect of $\chi$; (a) Mean scalar profile; (b) rms intensity; (c) total turbulent flux. —— LES-3 (low-$\chi$); —— LES-3; —— LES-3 (high-$\chi$).
Figure 2.9: Effect of Reynolds number; (a) Mean scalar profile; (b) rms intensity; (c) total turbulent flux. - - - LES-3 (high-\(Re\)), --- LES-3, -- -- LES-3 (low-\(Re\)).

Figure 2.10: Effect of intrinsic permeability; (a) Mean scalar profile; (b) rms intensity; (c) total turbulent flux. LES-4 --- LES-4 \((K^* = 0)\), \(\cdots \cdots \cdot \) LES-4 \((K^* = 10^{-6} \text{cm}^2)\), \(\cdots \cdots \cdot \) LES-4 \((K^* = 10^{-5} \text{cm}^2)\).
Figure 2.11: Fluid statistics in the sediment layer for calculations including the porewater flow for LES-4 ($K_{-6}$) and LES-4 ($K_{-5}$) runs shown without and with circle markers respectively. (a) rms velocity fluctuations; $v_{rms}$, $u_{rms}$, $w_{rms}$; (b) comparison between total diffusive and dispersive flux and $- - -$ advective flux (amplified by $\times 100$) in the sediment layer.
Figure 2.12: Contours of instantaneous pressure (a) and DO concentration with (estimated) thickness of the diffusive sub-layer (white dashed line) (b) in the \( z = 0.57 \) plane with velocity vector plot (velocity vectors in sediments are amplified by \( \times 1000 \) for clarity) for case LES-4 \((K-6)\) at \( K^* = 10^{-6}\)cm\(^2\) \((K = 1.7 \times 10^{-8})\). Note that the pressure field is scaled with \( \rho U_b^2 = 6.9 \) Pa, the oxygen concentration field with \( C_b = 4.5 \) mg l\(^{-1}\) and the coordinates \( x, y \) with \( \delta = 7.6 \) cm.
Chapter 3

High-Schmidt-number mass transport mechanisms from a turbulent flow to absorbing sediments

3.1 Abstract

We have investigated the mechanisms involved in dissolved oxygen (DO) transfer from a turbulent flow to an underlying organic sediment bed populated with DO-absorbing bacteria. Our numerical study relies on a previously developed and tested computational tool that couples a bio-geochemical model for the sediment layer and large-eddy simulation for transport on the water side. Simulations have been carried out in an open channel configuration for different Reynolds numbers ($Re_{\tau} = 180 - 1000$), Schmidt numbers ($Sc = 400 - 1000$) and bacterial populations ($\chi^* = 100 - 700$ mg$l^{-1}$). We show that the average oxygen flux across the sediment-water interface (SWI) changes with $Re_{\tau}$ and $Sc$, in good agreement with classic heat-and-mass-transfer parametrizations. Time correlations at the SWI show that intermittent peaks in the wall-shear stress initiate the mass transfer and modulate its distribution in space and time. The diffusive sublayer acts as a de-noising filter with respect to the overlying turbulence; the instantaneous mass flux is not affected by low-amplitude background fluctuations in the wall-shear stress but, on the other hand, it is receptive to energetic and coherent near-wall transport events, in agreement with the surface renewal theory. The three transport processes involved in DO depletion (turbulent transport, molecular transport across the diffusive sublayer, and absorption in the organic sediment layer) exhibit distinct temporal and spatial scales. The rapidly evolving near-wall high-speed (low-speed) streaks transport patches of fluid to (away from) the edge of the diffusive sublayer, leaving slowly-regenerating elongated patches of positive (negative) DO concentration fluctuations.
and mass flux at the SWI. The sediment surface retains the signature of the overlying turbulent transport over long time scales, allowed by the slow bacterial absorption.

3.2 Introduction

The prediction of dissolved oxygen (DO) levels is critical for preserving and monitoring marine ecosystems. Oxygen evolves in water bodies as a high-Schmidt-number passive scalar with saturation levels highly dependent on temperature. It is entrained at the surface and transported across the water column by the turbulent motions. Many natural factors can interfere with this mixing process such as stratification, which damps the turbulent motion, reducing the supply of oxygen to the near-bed region where decomposition of organic matter in the sediment layer by oxygen-consuming bacteria can cause DO concentration to drop to unsustainable levels for aquatic life; anoxic ‘dead zones’ are then formed, with considerable economical and environmental impacts. The characterization of the physical processes involved in this problem is twofold: i) the governing mechanisms in high-Schmidt-number mass transfer from a turbulent flow to a solid boundary need to be identified and the adequacy of currently adopted models assessed; ii) the transport in the sediment layer (bio-geochemical characterization) and its interaction with the overlying turbulent field need to be modeled.

The mechanisms of high-Schmidt-number mass transfer from a turbulent flow to a solid boundary involve many fundamental aspects of near-wall turbulence, such as the interaction between the viscous sublayer and buffer-layer events (Fage & Townend 1932, Lin, et al. 1953). Einstein & Li (1956) were perhaps the first to propose a one-dimensional model describing the cyclic growth (slow development and abrupt breakdown) of the viscous sublayer. The effects of the unsteadiness of the viscous sublayer on high-Schmidt-number mass-transfer mechanisms was subsequently investigated by Hanratty (1956) who proposed a similar one-dimensional model for the unsteady growth of the diffusive sublayer: the near-wall region is pictured as a series of periodically renewing patches of fluid transporting the free-stream concentration value, stagnating at the wall (where molecular mass transfer occurs) and then being ejected to the outer region. This was the seminal idea of what is more recently referred to as the “surface renewal theory” (Boudreau & Jørgensen 2001). Reiss & Hanratty (1962) extended this work by directly measuring the instantaneous mass-transfer rate to a solid boundary and relating it to the overlying fluctuating velocity field. Their results highlight the role of velocity fluctuations remaining active in the lowest layers of the viscous sublayer. Sirkar & Hanratty (1970) carried out experiments at $Sc = 2300$, which supported the correlation between the instantaneous mass flux and the low frequency spanwise velocity fluctuations persisting in the viscous sublayer. Also, streamwise velocity fluctuations were claimed not to be effective in controlling the mass transfer and are neglected in their transport model. Pinczewski & Sideman (1974) extended the model of Hanratty (1956) to
a concentration boundary layer developing both in space and time, being renewed by quasi-periodic bursting events. A parametrization in closed form is obtained relating the average mass transfer to the mean wall-shear stress and \( Sc \). The emphasis, in their work, is on the Schmidt number effects: as \( Sc \) increases, the diffusive sublayer layer acts as a progressively stronger limiting layer for the mass transfer; only a fraction of the eddies (the most energetic ones) successfully modulate the diffusive sublayer thickness, and, therefore, the mass flux. Shaw & Hanratty (1977a) pointed out the strong similarity between the spatial distribution of the overlying streamwise-oriented vortices and the mass flux at the wall, which evolves over longer time-scales. Time spectra of mass-transfer fluctuations are shown to scale with \( Sc \). Previous studies from the same group (Shaw & Hanratty 1964, Sirkar & Hanratty 1970) confirm the reduced transverse spatial extent of the mass flux distribution at the wall with respect to the overlying turbulent structures. Investigations of high-Schmidt-number mass transfer to a pipe wall were carried out by Campbell & Hanratty (1983b) stressing the strong relation between the low-pass filtered transverse velocity gradient fluctuations at the wall and the corresponding concentration fluctuations, in line with Sirkar & Hanratty (1970). In conclusion it is established that mass transfer is controlled by the low frequency component of the velocity fluctuations in quasi-streamwise vortices and that the diffusive sublayer acts as a low-pass filter. The same authors, in a separate work (Campbell & Hanratty 1983a), confirm this picture with a non-linear numerical model for the diffusive sublayer forced by experimentally extracted velocity data. All indications support the idea that mass transfer at the wall is not controlled by the most energetic velocity fluctuations (Campbell 1981), but it is instead dominated by the low-frequency component of the velocity field and that, as \( Sc \) increases, progressively fewer turbulent transport events reach the thinner diffusive sublayer and, therefore, govern the mass transfer.

The aforementioned experimental investigations come with numerous challenges. Measurement of the very small length scales and time scales of the scalar field represents, perhaps, the most severe one. Moreover, in the case of oxygen concentration measurements, involving both the fluid side and the sediment layer, the presence of an interface between two media can cause measurement difficulties (Røy et al. 2004, O’Connor & Hondzo 2008). Numerical investigations have analogous difficulties. Accuracy can be an issue, as high-Schmidt-number passive scalar exhibits a range of sub-Kolmogorov scales extending as far as the Batchelor scale \( \eta_B = \eta/\sqrt{Sc} \) where \( \eta \) is the Kolmogorov length scale; resolving the complete range of scales can become an unfeasible option. When modelling unresolved scales, establishing the adequacy of grid resolution can, therefore, be problematic. These issues have been addressed by several researchers in the past. The suitability of large-eddy simulation (LES) for investigating high-Schmidt-number mass transfer was first tested by Calmet & Magnaudet (1997) and later by Dong et al. (2003). Their results confirmed the suitability of LES in predicting, with very good accuracy, the essential characteristics of a high-Schmidt-number scalar field such as the mass flux at the solid wall. A hybrid approach has been adopted by Bergant & Tiselj (2007)
who performed DNS of the velocity field with an LES-like formulation for the scalar field up to $Re_\tau = 400$ and $Sc = 200$. They showed that low order statistics are captured very accurately and that spectra and scalar variance profiles in the diffusive sublayer are unaffected by the grid cutoff of sub-Kolmogorov scales. Schwertfirm & Manhart (2007) performed a fully resolved DNS at $Re_\tau = 180$ up to $Sc = 49$ by adopting a hierarchical grid approach. A scaling law for the mass-transfer coefficient with $Sc$ is derived and compared with classic experimental correlations. More recently, Hasegawa & Kasagi (2009) adopted a similar numerical approach to perform simulations up to $Sc = 400$. With the aid of the generated data, a one-dimensional linear model has been derived reproducing the frequency response of the fluctuating mass-transfer rate at the wall to the overlying turbulent velocity fluctuations.

All of the previously mentioned work focused on aspects of high-Schmidt-number mass-transfer exclusively connected to turbulence. However, the presence of a porous and mass-absorbing sediment layer, in the case of oxygen transport, raises questions as to how turbulence interacts with it. In the sediment, solutes dissolved in the pore water, in general, diffuse through the porous medium (at a slower rate than in pure water), disperse and are advected by interstitial flow (typically modeled by Darcy’s Law for low permeabilities). In the case of dissolved oxygen in marine environments absorption by bacterial decomposition may also occur (Higashino et al. 2008). However, for flat and cohesive beds the dominant processes are diffusion and absorption (Scalo et al. 2012b). Advection becomes particularly important in presence of large-scale bed roughness. This causes persistent pressure differences at the sediment-water interface (SWI) driving a mean interstitial current that transports solutes in the underlying bed (Boudreau & Jørgensen 2001). Dispersion effects are important for highly permeable sediment beds and, like advection, are driven by pore water flow (O’Connor & Hondzo 2007, Higashino et al. 2008, Higashino et al. 2009, Higashino & Stefan 2011).

In the present work we adopt the model developed by Scalo et al. (2012b) to study the turbulence-driven small-scale transport processes involved in oxygen transfer to smooth and cohesive organic sediment layers and their sensitivity to the governing parameters such as $Re_\tau$, $Sc$ and $\chi^*$ (oxygen absorbing bacterial population density). The present work is the natural extension of previous experimental (O’Connor & Hondzo 2008), numerical (Higashino et al. 2008) and field-scale (Lorke et al. 2003) studies to a numerical investigation based on an eddy resolving method.

In the following we begin by describing the complete transport model and the problem setup. Results are then presented for all cases investigated showing first order statistics and temporal and spatial correlations at the SWI. A conceptual model for the transport is deduced from the presented data and confirmed by the instantaneous visualizations.
3.3 Problem Formulation

The filtered conservation equations of mass and momentum can be obtained by applying a filtering operator \( \overline{\nabla} \) to the governing equations (Leonard 1974), resulting in:

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

\[
\frac{\partial \pi_j}{\partial t} + \frac{\partial \pi_i \pi_j}{\partial x_i} = -\frac{\partial \pi}{\partial x_j} - \frac{\partial r_{ij}}{\partial x_i} + \frac{1}{Re_b} \nabla^2 \pi_j - f \delta_{ij} \tag{3.2}
\]

where \( x_1, x_2 \) and \( x_3 \) (or \( x, y \) and \( z \)) are, respectively, the streamwise, wall-normal and spanwise directions, and \( \pi_i \) the filtered velocity components in those directions. These equations have been made dimensionless by using \( \delta \) (height of the open channel) as reference length scale, and \( U_b \) (the volume average streamwise velocity component) as velocity scale. The bulk Reynolds number is \( Re_b = U_b \delta / \nu \); where \( \nu \) is the kinematic viscosity of water. The forcing term \( f \) in the streamwise momentum equation represents the normalized mean pressure gradient driving the flow. The sub-grid scale (SGS) stresses are modeled using the dynamic procedure (Germano et al. 1991, Lilly 1992).

Oxygen dissolved in water behaves like a passive scalar with very low molecular diffusivity, \( D \), compared to the kinematic viscosity. The filtered transport equation for DO is, therefore,

\[
\frac{\partial c}{\partial t} + \frac{\partial \pi_i c}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \frac{1}{Sc Re_b} \frac{\partial \pi}{\partial x_i} - J_{gs}^{s} \right] \tag{3.3}
\]

where \( Sc = \nu / D \) is the Schmidt number and \( \pi \) is the instantaneous filtered scalar concentration field normalized with the freestream DO concentration \( C^\infty_\infty \). The SGS scalar flux, \( J_{gs}^{s} \), is also modeled with the same approach used for the velocity field.

The normalized instantaneous DO concentration in the sediment layer, \( c_s \), is determined by more complex mechanisms. Dissolved oxygen is diffused but it is also depleted by decomposing organic matter. Advection and dispersion effects can be neglected for smooth and cohesive beds and will not be included in the present simulations. The momentum and mass (DO) exchange across the SWI will, therefore, be exclusively molecular. The governing equation for \( c_s \) is

\[
\frac{\partial c_s}{\partial t} = \frac{\partial}{\partial x_1} \left[ F(\phi) \frac{\partial c_s}{\partial x_1} \right] - \dot{c}_s \tag{3.4}
\]

where \( F(\phi) \) is a function of the sediment porosity \( \phi \) which accounts for the reduction of the molecular diffusivity due to porosity and tortuosity. A commonly used approximation in the field for this function is \( F(\phi) = \phi^2 \) (valid for \( \phi < 0.7 \)) (Higashino & Stefan 2011). It is possible to retrieve the value of the sediment porosity from the measurable slope discontinuity in the mean oxygen profiles at the SWI by imposing the
continuity of the mass flux from both sides of the SWI (Røy et al. 2004). The DO absorption by organic matter is represented by the sink term, $\dot{c}_s$, which must be modeled. The parametrization for the non-linear sink term, $\dot{c}_s$, due to Higashino et al. (Higashino et al. 2008), is

$$\dot{c}_s = \chi \frac{c_s}{K_{O_2} + c_s} \quad (3.5)$$

where

$$\chi = \frac{\chi^* \mu^* \delta}{Y_c U_b C_\infty} \quad (3.6)$$

and

$$K_{O_2} = \frac{K^*_{O_2}}{C_\infty}. \quad (3.7)$$

The parameters used in (3.6) and (3.7) are $\mu^*$, maximum specific DO utilization rate (in day$^{-1}$), $K^*_{O_2}$, half-saturation coefficient for DO utilization (in mg$l^{-1}$), $Y_c$, effective yield for the microbial utilization of DO and $\chi^*$, biomass concentration of oxygen absorbing organisms (currently not directly measurable). The values for these constants suggested by Higashino et al. (2008) are shown in Table 3.1. We assume a constant and uniform value of $\chi^*$ within the sediment layer.

### 3.4 Computational Setup

The computational setup used is shown in Figure 3.1. The flow is driven by a uniform pressure gradient $f$ dynamically adjusted in order to achieve the desired flow rate. The governing equations (3.1), (3.2) and (3.3) are solved in a Cartesian domain. In the streamwise and spanwise directions, $x$ and $z$, periodic boundary conditions are used for all quantities. The velocity obeys no-slip conditions at the lower wall, and, at the top boundary, free-slip conditions; for the scalar field we use Neumann conditions at the SWI with a flux that varies in space and time obtained by solving the sediment layer transport equation (3.4). Further details regarding the numerical strategy adopted for the coupling between the sediment layer and the water side and comparison with experiments can be found in Scalo et al. (2012b). The oxygen dynamically absorbed by the sediment layer across the SWI is reinserted in the flow, at the same rate, from the top boundary by means of an imposed instantaneous flux. The value of the volume averaged DO concentration is maintained constant and equal to the initial value.
The numerical model used to compute the flow on the water side is a well-validated finite-difference code (Keating et al. 2004), based on a staggered grid. Second-order central differences are used for both convective and diffusive terms. A Crank-Nicolson scheme is used for the wall-normal diffusive term, and a low-storage third-order Runge-Kutta method for the other terms. The solution of the Poisson equation is obtained by Fourier transform of the equation in the spanwise and streamwise directions, followed by a direct solution of the resulting tridiagonal matrix, at each wavenumber. The code is parallelized using the MPI protocol. The equations in the sediment layer are solved with the same numerical approach as adopted for the water side and have the same accuracy and stability properties.

We performed numerical simulations of an open channel flow by adjusting the forcing term in (3.2) in order to obtain four different friction Reynolds numbers $Re_\tau = 180, 400, 620$ and $1000$. This resulted in four velocity fields each simultaneously transporting 6 scalar fields, one for every combination of three Schmidt numbers, $Sc = 400, 690, 1020$ (corresponding to water temperatures of $25^\circ C, 15^\circ C$ and $8^\circ C$ and to dissolved oxygen saturation levels of $C_\infty^* \simeq 8.3, 10.1, and 12 \text{mg l}^{-1}$), and two bacterial populations, $\chi^* = 100$ and $700 \text{mg l}^{-1}$ (Table 3.2). A porosity of $\varphi = 0.55$ has been used for all cases. The domain size has been chosen in order to accommodate the large structures; the near-wall streaks and the elongated concentration patches at the SWI (shown later). The grid size has been chosen accordingly to keep the resolution at a DNS level ($\Delta x^+ \simeq 5$ and $\Delta z^+ \simeq 3$) for the velocity field for cases $Re_\tau = 180$ and 400 and (very fine) LES resolution ($\Delta x^+ \simeq 23$ and $\Delta z^+ \simeq 10$) for cases $Re_\tau = 620$ and 1000. The sub-grid scale closure is therefore used, for the velocity field, only for the higher Reynolds number cases. The coarsest resolution adopted here accurately describes the concentration field as shown by Scalo et al. (Scalo, et al. 2011) and by Calmet and Magnaudet (Calmet & Magnaudet 1997). The hybrid approach used for the finer simulations is similar to one proposed by Bergant et. al (Bergant & Tiselj 2007). The resolution in the wall-normal direction has been chosen, for every Reynolds number, based on the expected diffusive sublayer thickness at $Sc = 1020$. In all cases the sediment layer depth is fixed to $\delta_{sed} = 0.3 \delta$ (see Figure 3.1) and discretized with 65 grid points. The sediment layer shares the same spanwise and streamwise resolution of the water side as well as the wall-normal resolution at the SWI.
3.5 Results

The discussion of data extracted from the simulations is organized as follows. First, mean profiles of the scalar concentration are shown and the correspondent sediment oxygen uptake is plotted as a function of $Re_\tau$ and $Sc$ and compared to heat-and-mass-transfer laws available in literature (Section 3.5.1); then, a statistical analysis of the temporal and spatial structure of the near-wall transport is carried out focusing on auto- and cross-correlation functions between the streamwise component of the wall-shear stress, $\tau_w(x, z; t) = Re_b^{-1} \frac{\partial u}{\partial y}$, the DO concentration field at the SWI, $c_{swi}(x, z; t)$, and the instantaneous mass flux across the SWI, $J_{swi}(x, z; t) = (Re_b Sc)^{-1} \frac{\partial c}{\partial y}$ (Section 3.5.2 and 3.5.3); finally, a conceptual model for oxygen depletion is illustrated and instantaneous visualizations are shown to support the global picture arising from the results (Section 3.6).

3.5.1 Mean profiles and average mass flux across the sediment-water interface

The mean velocity and concentration profiles in Figure 3.2 reveal the reduced thickness of the diffusive sublayer with respect to the velocity boundary layer. The oxygen concentration at the SWI increases with $Re_\tau$ and the diffusive sublayer becomes progressively thinner. The most dramatic change in the oxygen distribution occurs from $Re_\tau = 180$ to $Re_\tau = 400$; further increases in the wall-shear stress ($Re_\tau > 400$) result in less evident changes in the DO field, as Reynolds number effects become less significant. This also increases the magnitude of the diffusive flux of oxygen across the SWI and, therefore, the sediment oxygen uptake. The DO penetration depth exhibits a reduced sensitivity to the increasing wall-shear stress; changes in Schmidt number, on the other hand, equally affect both sides of the SWI. Lower $Sc$ result in more intense molecular transport causing, for a given $Re_\tau$, thickening of the diffusive sublayer on the water side and larger penetration depths into the sediment layer. Also, the mean value of oxygen at the SWI decreases for lower $Sc$,.
Figure 3.2: Mean velocity profiles (—) and mean profiles of oxygen concentration for $\chi^* = 700 \text{mg l}^{-1}$ (---) and $\chi^* = 100 \text{mg l}^{-1}$ (----) for $Re_\tau = 180, 400, 620$ and $1000$ (shown by arrow); $Sc = 400$ (a) and $Sc = 1020$ (b).

as the concentration boundary layer from the water side becomes thicker. Overall, Schmidt number effects are stronger at lower Reynolds numbers.

It is of particular interest in geophysical applications to parametrize the average mass flux $\langle J_{swi} \rangle$ as a function of $Sc$ and $Re_\tau$. A commonly used dimensionless quantity in the field is the Sherwood number (O’Connor & Hondzo 2008) defined, in our normalization, as

$$Sh = \frac{Re_b Sc}{\Delta C} \langle J_{swi} \rangle \quad (3.8)$$

with $\Delta C = 1 - \langle c_{swi} \rangle$. As shown in Figure 3.3 the variation of the Sherwood number with $Re_\tau$, predicted by our LES is not significantly affected by the Schmidt number (the effects of varying the bacterial population, $\chi^*$, are absorbed when normalizing by $\Delta C$); results are in fair agreement with other parametrizations found in heat-and-mass-transfer literature — despite the presence of an organic mass-absorbing sediment layer — such as the one by Shaw & Hanratty (1977b)

$$K^+ = 0.0889 Sc^{-0.704} \quad (3.9)$$

where, in our normalization

$$K^+ = \langle J_{swi} \rangle / u_\tau \Delta C. \quad (3.10)$$

Good agreement is also found with the semi-analytical model suggested by Pinczewski & Sideman (1974)

$$Sh = 0.0102 Re_b^{9/10} Sc^{1/3}. \quad (3.11)$$
Figure 3.3: Sherwood number, $Sh$, as a function of $Re_τ$ and $Sc$; oxygen flux at the sediment-water interface for all cases in Table 3.2 (●), correlation (3.9) by Shaw & Hanratty (1977b) (---) and correlation (3.11) by Pinczewski & Sideman (1974) (----) for $Sc = 400$ and $Sc = 1020$. The trend with $Sc$ is shown for all data by the arrow, the effects of the bacterial population, $χ^*$, are absorbed by the normalization (3.8).

Figure 3.4: $K^+$ as a function of $Sc$ and $Re_τ$; oxygen flux at the sediment-water interface for all cases in Table 3.2 (●), correlation (3.9) by Shaw & Hanratty (1977b) (---), correlation proposed by Schwertfirm & Manhart (2007) (——) fitted from their DNS data at $Re_τ = 180$ and $Sc = 1, 3, 10, 25, 49$ (⋄), companion LES at $Sc = 3, 49, 1000$ (■), correlation (3.11) by Pinczewski & Sideman (1974)(-----).
The sediment oxygen uptake, measured by the Sherwood number, increases super-linearly with respect to $Re_\tau$. The agreement is not as satisfactory when results are compared to similar semi-empirical models such as the one suggested by O’Connor & Hondzo (2008).

The same data in Figure 3.3 is recast in terms of $K^+$ and plotted in Figure 3.4 together with a correlation proposed by Schwertfirm & Manhart (2007), derived by fitting their (full) DNS data for $Sc = 1, 3, 10, 25, 49$ at $Re_\tau = 180$, and companion LES simulations at $\Delta x^+ = 12$, $\Delta z^+ = 6$. The agreement between DNS results and LES for $Sc = 3$ and 49 is remarkable. Very good agreement is also found between the mass flux predicted by the LES at $Sc = 1000$ and the aforementioned correlation. The DO flux to the sediment shows a clear trend with $Re_\tau$, on the $K^+$ vs $Sc$ plane, as highlighted by the inset image and is in good agreement with the correlations (3.9) and (3.11).

Further discussions on this topic are out of the scope of the present work which is primarily focused on the study of the near-wall transport dynamics involved in oxygen depletion (carried out in the remainder of the paper). Future investigations will, however, include the effects of dispersion in the sediment layer (which introduces the bed’s intrinsic permeability, $K^*$, as a new parameter (Boudreau & Jørgensen 2001)).

3.5.2 The temporal structure of the near-wall transport

The time series in Figure 3.5 shows the essential mechanisms driving the mass transfer in this problem. Energetic sweeps resulting in peaks in the wall-shear-stress distribution initiate the transport of DO which occurs across the diffusive sublayer and the SWI, from the turbulent core of the channel to the sediment layer. Every strong peak is followed by correspondent increments in the mass flux $J_{swi}$ (integral response) which are delayed in time. The latter causes even smoother increases in the DO level at the SWI, $c_{swi}$, further delayed in time. The mass flux (or, equivalently, the diffusive sublayer thickness) appears to be almost exclusively modulated by the most intense sweeps, penetrating violently across the viscous sublayer, in agreement with Hanratty (1956) and Pinczewski & Sideman (1974). The delay between peaks in $J_{swi}$ and peaks in $c_{swi}$ is due to the fact that increments in mass flux at the SWI instantaneously increase the supply of oxygen to the sediment layer, but not its oxygen level. The latter takes some time to increase as mass is transferred across the diffusive sublayer and the interface by molecular transport. Time cross-correlations (Figure 3.6 (a))

$$C_1(\tau) = \frac{\langle \tau_w(x, z; t + \tau) J_{swi}(x, z; t) \rangle}{\langle \tau_w J_{swi} \rangle}$$

$$C_2(\tau) = \frac{\langle J_{swi}(x, z; t + \tau) c_{swi}(x, z; t) \rangle}{\langle J_{swi} c_{swi} \rangle}$$

allow the quantification of the time shift between the three signals, supporting the cause-and-effect relationship deduced from the time series in Figure (3.5).

The three signals shown in Figure 3.5 exhibit three visibly distinct characteristic time scales. This is
Figure 3.5: Time series of instantaneous wall-shear stress, $\tau_w$ (---), mass flux, $J_{swi}$ (---), and oxygen concentration, $c_{swi}$ (---) at one point on the sediment-water interface, normalized by mean and standard deviation for $Re_{\tau} = 400$, $\chi^* = 100 \text{ mg l}^{-1}$, $Sc = 400$.

Figure 3.6: Time cross-correlations $C_1(\tau)$ and $C_2(\tau)$ (shifted by 2 for clarity) (a) and auto-correlation functions (b) $R_0(\tau)$, $R_1(\tau)$ and $R_2(\tau)$ for $Re_{\tau} = 400$ and $\chi^* = 100 \text{ mg l}^{-1}$; $Sc = 400$ (---), $Sc = 690$ (---), $Sc = 1020$ (---) (trend shown by arrow).

confirmed by the time autocorrelations (Figure 3.6 (b))

$$R_0(\tau) = \frac{\langle \tau_w(x, z; t + \tau) \rangle}{\langle \tau_w \rangle}$$

(3.14)

$$R_1(\tau) = \frac{\langle J_{swi}(x, z; t + \tau) J_{swi}(x, z; t) \rangle}{\langle J_{swi} J_{swi} \rangle}$$

(3.15)

$$R_2(\tau) = \frac{\langle c_{swi}(x, z; t + \tau) c_{swi}(x, z; t) \rangle}{\langle c_{swi} c_{swi} \rangle}$$

(3.16)

where the integral time scales of $J_{swi}$ and $c_{swi}$ are more than an order of magnitude longer than the ones associated with $\tau_w$. Increasing $Sc$ results in a slower response of the diffusive sublayer and oxygen concentration in the sediment layer to the overlying turbulent forcing. The effects of $Sc$ are not visible to the same extent in spatial correlations of the same instantaneous quantities (not shown).
Figure 3.7: Streamwise autocorrelation functions $R_0(\Delta x)$ (----), $R_1(\Delta x)$ (---) and $R_2(\Delta x)$ (-----); for $Sc = 400$ and $\chi^* = 100 \text{mg l}^{-1}$; $Re_\tau = 180$ (a), $Re_\tau = 400$ (b), $Re_\tau = 620$ (c) and $Re_\tau = 1000$ (d).

### 3.5.3 The spatial structure of the near-wall transport

The streamwise autocorrelation functions (Figure 3.7)

\[
R_0(\Delta x) = \frac{\langle \tau_w(x + \Delta x, z; t)\tau_w(x, z; t) \rangle}{\langle \tau_w^2 \rangle}
\]

\[
R_1(\Delta x) = \frac{\langle J_{swi}(x + \Delta x, z; t)J_{swi}(x, z; t) \rangle}{\langle J_{swi}^2 \rangle}
\]

\[
R_2(\Delta x) = \frac{\langle c_{swi}(x + \Delta x, z; t)c_{swi}(x, z; t) \rangle}{\langle c_{swi}^2 \rangle}
\]

are consistent with the considerations made in Section 3.5.2. The concentration fluctuations at the SWI exhibit an extended streamwise coherence that required a longer computational domain (Table 3.2) in that direction. The instantaneous mass flux exhibits shorter length scales in the streamwise direction with respect to the scalar concentration; however, as $Re_\tau$ increases, the characteristic streamwise extension of patches of $J_{swi}$ is systematically reduced, falling below the wall-shear-stress integral length scale. This behaviour is the sign of the diffusive sublayer becoming gradually thinner with respect to the viscous sublayer as $Re_\tau$ increases: eddies penetrate, on average, less frequently into the thinner diffusive sublayer, therefore, not sustaining the streamwise extension of patches of positive mass flux fluctuation (see discussion in Section 3.6).

Dependence on the Schmidt number of the spatial correlations is very minimal, probably due to the cut-off of the sub-Kolmogorov scales. The effect is only visible for the $Re_\tau = 180$ case and for the autocorrelation of $c_{swi}$ (not shown). Overall, the effect of an increasing $Sc$ is to prolong the characteristic spatial scales in the direction of the mean flow.
3.6 A conceptual model for the transport

Figures 3.8 (a) to (h) illustrate a conceptual model for the transport that can be extracted from the results shown so far. We have shown that the mass transfer is initiated by the stronger sweeps, those that penetrate deeper into the viscous sublayer and control the instantaneous diffusive sublayer thickness, and, therefore, the flux to the sediment layer. In this section we want to idealize the different stages of the mass transfer across the SWI following a significant bursting event.

During a sweep (Figure 3.8 (a)) a patch of positive wall-shear-stress fluctuation (statistically correlated with a negative fluctuation in the wall-normal velocity above) is created at the wall. If the inertia of the high-momentum fluid particles is sufficiently high, these will carry high concentration values through the viscous sublayer, and down towards the edge of the diffusive sublayer (Figure 3.8 (b)), where a diffusive front (headed towards the wall) is created.

The local peak in the wall-shear stress thus created is, therefore, followed by an increase of the mass flux, after, on average, a delay of $\sim 0.1 \delta/u_\tau$ or large-eddy turnover times (LETOTs) (Figure 3.6 (a), Figure 3.8 (c)). As a result, patches of high wall-shear stress precede, in the direction of the mean flow, those of positive mass flux which persist at the SWI given their longer characteristics time scales (Figure 3.6 (b)). For higher Reynolds numbers we expect the delay to be reduced and the extension of these patches to approach those of the wall-shear stress, as suggested by the streamwise auto-correlation functions (Figure 3.7).

At this stage the diffusive flux at the control point has been enhanced (Figure 3.8 (d)), patches of positive wall-shear stress have rapidly disappeared due to instabilities (Figure 3.8 (e)) and transfer across the SWI will occur (Figure 3.8 (f)). However, given the extremely low diffusivity there will be a time lag between positive fluctuations in the flux and the corresponding increase in the concentration (Figure 3.6 (a)). The result is a prolonged streamwise extensions of these patches (with respect to the overlying turbulent structures) whose persistence at the SWI is allowed by the long time scales of bacterial absorption. This leads to the final state shown in Figure 3.8 (g) where patches of high wall-flux, preceding patches of above-average oxygen concentration at the SWI, persist at the interface in locations where rapidly evolving high speed streaks have, previously, reached the maximum intensity.

Instantaneous visualizations (Figure 3.9) confirm the dynamics of transport explained above. The mass transfer is initiated by strong bursting events, such as the positive fluctuation patch of $\tau_w$ initially located at $x = 2.3$, $z = 0.7$ at time $t = 0$ (transport event shown by a black arrow). There are no simultaneous traces of this event in the mass flux distribution or the concentration contours. After some time, at $t = 0.056 \delta/u_\tau$, the quickly evolving patch has reached the location $x = 3.2$ leaving behind a first trace of above-average mass flux starting to appear at $x = 2.9$. After $\Delta t = 0.0388 \delta/u_\tau$, at time $t = 0.095 \delta/u_\tau$, the high-speed streak starts to break up due to instabilities; on the other hand, the above-average mass flux patch is still
Figure 3.8: Illustration of a conceptual model for the dissolved oxygen (DO) transfer from a turbulent flow to underlying absorbing sediment layers; generation of a high-speed streak (close to the wall) associated with a positive fluctuation of DO at the edge of the diffusive sublayer (a),(b), creation of a patch at the sediment-water interface (SWI) of above-average mass flux and correspondent thinning of the diffusive sublayer (mass transfer enhancement) (c),(d), creation of an elongated patch at the SWI of above-average DO concentration and local relaxation of the mass flux (e),(f), slow bacterial absorption of the excess DO transferred across the SWI (g),(h); Figures (b),(d),(f),(h) correspond to concentration profiles as observed from the respective control points in Figures (a),(c),(e),(g). The gray lines show the evolution in time of the oxygen concentration profiles, as shown by the arrow. The solid line represents the time corresponding to the animation on the left.
Figure 3.9: Contours of instantaneous wall-shear stress $\tau_w$ (left), mass flux at SWI $J_{swi}$ (middle) and DO concentration at SWI $c_{swi}$ (right) for $Re_\tau = 400$, $Sc = 400$ and $\chi^* = 100$ mg l$^{-1}$. Initial time $t = 0$ (top row), $t = 0.056 \delta/u_\tau$ (second row), $t = 0.095 \delta/u_\tau$ (third row) and $t = 0.311 \delta/u_\tau$ (forth row). Black and white arrows highlight different transport events like the one described in Figure 3.8.
developing (primarily) in the streamwise direction. At this stage the above-average DO concentration patch has not yet appeared; in this case, it will take another $\Delta t = 0.215 \delta / u_\tau$ (arriving at time $t = 0.311 \delta / u_\tau$) for it to be visible reaching its peak when the mass flux in that region is starting to relax. The same description also applies to the transport event indicated by the white arrow which is, however, captured here at a later stage of evolution.

In additional multimedia material (not included in the present thesis) we show how intense bursting events periodically ‘scar’ the diffusive sublayer, sustaining a statistically steady mass transfer. It is possible to appreciate the long time scales and the slow response of the diffusive sublayer to the overlying turbulence; this is the reason why the scalar field, in high-Schmidt-number mass-transfer simulations, takes considerably longer to reach a statistical steady state than the velocity field for the same flow as also pointed out by Bergant & Tiselj (2007). It is also shown how subsequent, but completely uncorrelated bursting events, occurring on the same location on the SWI, can prolong the spatial extension and the residence time of the same above-average patch of mass-flux developing there. A similar event is shown in Figure 3.5 where an above-average value of the mass flux, at the same location on the SWI, is sustained from $t = 1.8 \delta / u_\tau$ to $t = 3.3 \delta / u_\tau$ by subsequent peaks in the wall-shear stress. If bursting events affect the diffusive sublayer less frequently (due, for example, to the thinning of the diffusive sublayer with respect to the viscous sublayer) the streamwise extension of patches of mass flux will not be sustained to the same extent (see discussion in Section 3.5.3).

Additional simulations have been carried out with constant Neumann and Dirichlet boundary conditions (with no sediment layer), matching, respectively, the average gradient and average DO concentration at the SWI for case $Sc = 400$ and $Re_\tau = 400$. Temporal correlations at the wall (not shown) reveal a similar relationship between $\tau_w$ and $J_{swi}$ (for constant Dirichlet boundary conditions or constant $c_{swi}$) and between $\tau_w$ and $c_{swi}$ (for constant Neumann boundary conditions or constant $J_{swi}$). This suggests that the transport mechanisms described in the present work can be extended to high-Schmidt-number mass transfer in general. The effects on the transport dynamics of the absorbing sediment layer are, however, still visible but limited to the diffusive sublayer. In presence of an active sediment layer, temporal cross-correlations between $\tau_w$ and $c_{swi}$ reveal almost no correlation for zero separation in time. The instantaneous concentration at the SWI is not immediately affected by the overlying turbulence due to the inertia of the diffusive sublayer. On the other hand, for example, simulations with constant (instantaneous) scalar flux at the wall, cause every location of the diffusive sublayer to be synchronized and therefore, the concentration value at the wall, to retain a finite and positive correlation with the wall-shear stress for zero separation in time. This is also corroborated by the fact that rms profiles of scalar concentration, in the case of Neumann boundary conditions, are constant throughout the diffusive sublayer thickness.
3.7 Conclusions

We have investigated the mechanisms involved in oxygen depletion by smooth organic sediment layers interacting with a turbulent flow with focus on the mass transport occurring across the sediment-water interface (SWI). Statistically steady oxygen depletion has been simulated for different combinations of $Sc$, $Re_τ$ and $χ^*$ over typical lab-scale ranges in an open-channel configuration.

The average sediment-oxygen uptake varies with $Sc$ and $Re_τ$ in good agreement with classic heat-and-mass-transfer laws. The analysis of the instantaneous wall-shear-stress distribution, mass flux and DO concentration at the SWI has allowed for the extraction of a conceptual model for the transport which encompasses and extends many fundamental ideas on high-Schmidt-number mass transfer present in previous work. The complexity of the diffusive sublayer nature emerging from this analysis goes beyond the classic low-pass filter characterization, it also includes de-noising and amplitude filtering properties: the diffusive sublayer thickness or, equivalently, the mass flux at the wall, is modulated primarily by the intense sweeps (amplitude filter), it is not responsive to low-amplitude background fluctuations of the wall-shear stress (de-noising filter) and it exhibits an integral response to the forcing (low-pass filter) with a response delayed by fractions of an LETOT. The sediment layer oxygen content also exhibits a smoother and delayed response to the variable mass flux at the interface. The overall picture arising from this analysis of oxygen depletion identifies three distinct transport processes: turbulent transport within the viscous sublayer, molecular mass transport across the diffusive sublayer and transport within the sediment layer. Each of these processes exhibits distinct time and spatial scales and are connected through a well-defined cause-and-effect relationship.

The extracted transport model stresses the intrinsic unsteady and three-dimensional nature of the mass transport at the wall which should not be ignored when formulating semi-analytical models for the near-wall transport. The overall picture arising confirms the fundamental ideas at the basis of the surface-renewal theory brought forward by Hanratty (1956) and Pinczewski & Sideman (1974).
Chapter 4

A self-similar model for a decaying high-Schmidt-number concentration field in an oscillating boundary layer in the intermittently turbulent regime

4.1 Abstract

We performed numerical simulations of dissolved oxygen (DO) transfer from a turbulent flow, driven by periodic boundary-layer turbulence in the intermittent regime, to underlying DO-absorbing organic sediment layers. A uniform initial distribution of oxygen is left to decay (with no re-creation) as the turbulent transport supplies the sediment with oxygen from the outer layers to be absorbed. Oxygen dissolved in water acts as a high-Schmidt-number passive scalar characterized by a very thin diffusive sublayer, which limits the overall mass transfer rate, causing a very slow decay of the bulk oxygen concentration. In spite of the highly intermittent state of turbulence, the mean scalar field exhibits, after the first 6 cycles, a very regular decay pattern characterized by a monotonically decreasing component overlapped by coherent periodic oscillations. The former reveals a well-defined self-similar structure that, substituted into the governing equations, yields an exponential decay law. This result has allowed the formulation of a simple mathematical model where the instantaneous concentration field is linearly decomposed into a monotonically decaying, oscillating (with zero-average over one semicycle) and fluctuating (stochastic) component. The last two are shown to be also decaying exponentially if their periodic self-similar structure is hypothesized. Due to the interdependency
of the different components of the solution, an iterative procedure was designed for their separation. This allowed the extraction of a statistically (self-similar) periodic fluctuating field, on which phase-averaging could be applied in lieu of ensemble-averaging, providing statistics to analyze the physics of transport. These reveal that the oxygen distribution in the water column is modulated by the periodic ejection, during the deceleration phase, of negative peaks of high turbulent mass flux, generated at the edge of the diffusive sublayer towards the end of the acceleration phase and growing in intensity until the beginning of the deceleration phase (turbulent flux production stage). These fronts of high turbulent mixing then propagate away from the sediment-water interface (SWI), at approximately constant speed, in layers of low oxygen concentration. The persistence of high levels of mixing in the near-wall region during the turbulent flux production stage is responsible for the accumulation of high concentration levels in the diffusive sublayer. These cause, with a time lag of approximately a quarter of a cycle, an above-average value in the mass-flux across the SWI. The periodic forcing leaves its signature in the concentration field for a greater portion of the water column than in the velocity fluctuation field and, despite the highly intermittent state of the turbulent field, the scalar field behaves like a linear harmonically forced system.

4.2 Introduction

Oscillatory currents are frequently observed in marine environments (Trowbridge & Agrawal 1995) and are responsible for driving important transport processes which regulate the ecosystem balance. Dissolved oxygen (DO) transfer to organic sediment beds is one of these (Lorke et al. 2003). The presence of adequate DO concentrations (nominally above 2–4 mg l\(^{-1}\)) is critical for the survival of aquatic life in lakes and oceans. Agricultural runoff, the primary cause of low levels of oxygen (or ‘hypoxia’), transports excess nutrients to the water surface, spurring uncontrolled growth of microscopic aquatic plant life which then dies and sinks to the bottom where, in the sediment layer, DO-consuming bacteria feed on it, causing near-bed hypoxia and thereby harming the ecosystem. Stratification worsens this state by inhibiting mixing and reoxygenation of the bottom water layers where, as a result, the oxygen budget is largely governed by the sediment oxygen uptake (Bouldin 1968, Patterson et al. 1985). Areas affected by severe levels of hypoxia are known as ‘dead zones’ and come with severe economical and environmental consequences (Committee on Environment and Natural Resources 2010a). Dead zones can be found in highly populated coastal environments, including the Gulf of Mexico, the Pacific and the Atlantic coast of the U.S. and the Baltic Sea (Diaz & Rosenberg 2008, Rabalais et al. 2010).

Field scale, experimental and numerical studies have shown that the understanding of the DO absorption mechanisms by sediment beds can only follow from an accurate characterization of the transporting turbulent flow; the mass transfer rate across the sediment-water interface (SWI) is primarily governed by the near-wall
turbulent activity and, in particular, by velocity fluctuations affecting the viscous sublayer and diffusive sublayer structure (Hanratty 1956). The average oxygen transfer rate from a steady turbulent flow to a smooth cohesive sediment bed, as a function of the friction velocity and temperature, can be predicted with good accuracy by classic semi-empirical mass transfer models (Pinczewski & Sideman 1974, Shaw & Hanratty 1977b) as shown by Scalo et al. (2012a). In spite of this, current water-quality prediction applications still lack the implementation of sediment-oxygen-uptake models that take into account the state of the flow.

Additional modelling challenges arise in the presence of unsteady near-bed turbulence, such as the one found in oscillating currents. Lorke et al. (2003) carried out DO measurements in Lake Alpnach in an oscillating bottom boundary-layer modulated by an 18-hour-period current. They showed a phase lag between the mass flux to the sediments, the near-wall turbulent dissipation and the current intensity. Bryant et al. (2010) tracked the response of the sediment-oxygen uptake to a 12-hour seiche-induced turbulence, in the same lake, showing the occurrence of an almost complete laminarization of the near-bed region (close to flow reversal) and the subsequent retransition towards a fully turbulent state. The correspondent large excursion of the mass flux to the sediment layer is not predictable by classic steady-state mass-transfer models. Capturing this phenomenon would, therefore, require careful tuning of currently adopted Reynolds-Averaged Navier-Stokes (RANS) models for the transport. However, any tentative definition of a process-oriented model requires the preliminary understanding of the oxygen transport dynamics in transitional turbulent flows. With this objective in mind, in the present work we choose to focus on the idealized case of a periodically oscillating current in the intermittently turbulent regime, where transition effects are emphasized. This case exhibits all of the complex traits of an unsteady, transitional turbulent flow while still retaining enough simplicity to allow for a straightforward numerical and analytical investigation.

Oscillatory currents are caused by periodic pressure unbalances or body forces. The latter can occur over a wide range of frequencies and current intensities depending on the nature of the forcing. Periods of oscillation can range from 24 hours (tidal motions, basin scale seiches) to minutes (non-linear waves propagating on stratified layers), corresponding, respectively, to current intensities of the order of 1 cm s$^{-1}$ and 1 m s$^{-1}$. In the idealized case of a uniform and monochromatic forcing, in an infinite domain bounded by a flat bottom, the flow is uniquely determined only by the Reynolds number $Re_{\delta}$ based on the Stokes thickness $\delta^* = \sqrt{2\nu^*/\omega^*}$, where $\nu^*$ is the kinematic viscosity and $\omega^* = 2\pi/T^*$ where $T^*$ is the period of the forcing, $U^*_{om}$ is the free-stream current amplitude given by $U^*_\infty = U^*_{om}\sin(\phi)$ where $\phi = \omega^* t^* = \omega t$ is the phase angle. Flows driven by currents of different amplitude and period, but with the same $Re_{\delta}$, are dynamically similar. This leads to the following classification into different flow regimes: i) the fully laminar regime ($Re_{\delta} < 100$); ii) the disturbed laminar regime, where small-amplitude perturbations are visible but do not transition to turbulence ($100 < Re_{\delta} < 500$); iii) the intermittently turbulent (IT) regime,
turbulence is produced explosively and sustained mostly during the decelerating phase \((500 < Re_\delta_s < 1800)\); \(iv\) the fully turbulent (FT) regime characterized by fully developed turbulence through most \((Re_\delta_s > 1800)\), if not all \((Re_\delta_s > 3500)\) of the cycle. The Reynolds number chosen in present work is \(Re_\delta_s = 800\).

From an experimental and numerical prospective there has been great effort in the past to characterize the turbulent structure of an oscillating boundary layer. One of the first experiments was carried out by Hino, et al. (1983) in a square duct at \(Re_\delta_s \sim 900\). It was found that turbulence is generated explosively in the buffer layer towards the end of decelerating phase \((90^0 < \phi < 180^0)\) and then transported towards the center of the duct. In this phase there is a well-defined log layer and the energy spectrum deviates from the \(-5/3\) power law, tending towards steeper slopes. Turbulent activity is dissipated almost completely around \(\phi \sim 180^0\) and it is sustained by intermittent bursting events with production mechanisms similar to the ones of a steady boundary layer.

Sleath (1987) investigated Reynolds numbers up to \(Re_\delta_s = 800\) in the presence of rough beds. It was found that bursts in turbulent kinetic energy (TKE) are correlated with peaks in Reynolds shear stresses in the near-bed location \(<11\delta_s^+\). In the outer region TKE diffuses at constant velocity with no significant correlation with other quantities. Significant variations of eddy viscosity and mixing lengths are present throughout the cycle with negative time-averaged eddy viscosity near the bed.

The first direct numerical simulation (DNS) of an oscillating boundary layer has been performed by Spalart & Baldwin (1987) who investigated Reynolds numbers in the range \(Re_\delta_s = 600 - 1200\). The generated DNS data, together with a companion tentative theoretical formulation, is used to develop a new algebraic turbulence model based on previous work by Jonsson (1980) and Johnson & King (1984). Reynolds number effects are accounted for in modeled quantities, such as the phase-averaged wall-shear stress, in the form of a phase shift, with respect to the free-stream oscillating current, decreasing with \(Re_\delta_s\). Numerical investigations reveal that the flow is linearly stable up to \(Re_\delta_s = 2000\) with \(Re_\delta_s = 600\) being the lower limit for the presence of well-developed turbulence (defined by the existence of a log layer and regular Reynolds stress anisotropy). TKE budgets reveal a structure similar to the one of a steady boundary layer expect at flow reversal. Mechanisms of TKE production and diffusion found by Hino et al. (1983) and Sleath (1987) are confirmed.

Jensen et al. (1989) carried out an experimental study over smooth and rough beds covering the range \(Re_\delta_s = 100 - 3600\). Diffusion of turbulence away from the wall occurs in the acceleration phase \((0^0 < \phi < 90^0)\) while the turbulence production mechanisms are frozen due to favourable pressure gradient effects (even at very high Reynolds numbers). The establishment of the log law in the deceleration phase occurs earlier for higher Reynolds numbers. Effects of roughness are localized in the near-bed region and do not inhibit the creation of a logarithmic layer as observed in the presence of a smooth wall.

A similar range of Reynolds numbers, \(Re_\delta_s = 550 - 2000\), is covered by the experimental and numerical investigations in Akhavan, et al. (1991b) and Akhavan, et al. (1991a) for pipe flow. The same turbulent
production and dissipation mechanisms present in the channel flow case are observed. Direct numerical simulations reveal that all types of infinitesimal disturbances experience a transient growth which is not sustained by the flow. Perturbations eventually decay towards a periodic steady state. The correct transitional Reynolds number is, however, predicted by the secondary instability of two-dimensional perturbations. Lodahl, et al. (1998) investigated transition for different combinations between a steady flow in a pipe and a superimposed oscillatory one which exhibits, overall, stabilizing effects.

Verzicco & Vittori (1996) performed a DNS of transition in oscillating boundary layers perturbed by small imperfections at the wall (with roughness height of $\epsilon \sim 5 \times 10^{-3}\delta_s^*\)$. Roughness was found to be necessary to sustain turbulence under $Re_{\delta_s} = 500$ (disturbed laminar regime). For higher Reynolds numbers the flow was unaffected by it. Vittori & Verzicco (1998) and Costamagna, et al. (2003), with similar computational setups, by analyzing coherent structures dynamics, find that the regenerative cycle of TKE is the same as the one observed in steady wall-bounded flows (Jimenez & Pinelli 1999) but occurring over an entire semicycle. Roughness is found to affect the onset and end of transition but not the resulting turbulent vortex structures.

More recently, Salon, et al. (2007) performed LES with a plane-averaged dynamic mixed model (PADMM) at $Re_{\delta_s} = 1790$ where fully developed turbulence appears already at $\phi = 60^0$, and persists until $\phi = 150^0 - 160^0$, with features very similar to the ones observed in steady equilibrium flows (including TKE budgets, spectra and the presence of a log-layer). Several issues have been addressed including the nature of the disagreement on second order statistics between experiments and numerical simulations and effects of the computational domain height or bed roughness. Additional simulations have been carried out at at $Re_{\delta_s} = 990$, which have revealed the difficulty of the PADMM model in reproducing the non-equilibrium turbulence dominating the IT regime, not present at $Re_{\delta_s} = 1790$.

Although plenty of literature is available on the characterization of the velocity field in turbulent oscillating boundary layer, not as much attention has been devoted to heat-and-mass transport in the same flow. Previous studies appear to be limited to special cases of interest. The closest work to the present paper is the one by Wang & Lu (2004) who performed LES of heat transfer in a pulsating channel for Prandtl numbers up to $Pr = 100$. It has been found that for the high Prandtl numbers temperature fluctuations are not sustained in the core region of the channel and that the important mechanisms regulating the heat transfer occur primarily in a very thin region close to the wall (diffusive and thermal buffer layers). Overall results confirm previous findings available in the literature on the topic (Shaw & Hanratty 1977b, Campbell & Hanratty 1983b). Gayen, et al. (2010) looked at the influence of a uniform background stratification on a (zero mean) turbulent oscillating boundary layer. Stratification increases the asymmetry of turbulence between the accelerating and decelerating stages and reduces the vertical extent of the turbulent entrainment and upwards propagation of turbulence during the decelerating phase. The log-law layer thickness and persistence during the cycle is significantly shortened by the presence of stratification, however, the near-bottom layers
(the wall-shear stress in particular) are not. The thermally mixed bottom layer shows, however, a steady and very slow growth probably due to energetic eddies that overshoot the thermocline.

In the present paper we investigate the transient decay of the dissolved oxygen concentration field in an oscillating boundary layer at $Re_{\delta_s} = 800$ driving the transport towards an underlying mass-absorbing sediment layer. Re-areation from the top-boundary is prevented to simulate the oxygen evolution in the hypolimnetic layers of stratified water-bodies. An extensive overview on the issues regarding the modelling of the interaction between the turbulent transport on the water side and the one in the sediment layer, including the characterization of high-Schmidt-number heat-and-mass transfer, can be found in Boudreau & Jørgensen (2001), Scalo et al. (2012b) and Scalo et al. (2012a). In the following, we begin by describing the mathematical and numerical methods used for the transport on the water side and in the sediment layer. The transient data is then analyzed and a model for the decay is extracted which allows to investigate mixing dynamics and the structure of the concentration field via ensemble averaged statistics.

### 4.3 Problem Formulation

The equations for conservation of mass and momentum for an incompressible oscillating flow, driven by a sinusoidal freestream current of amplitude $U_{om}^*$ and period $T^* = 2\pi/\omega^*$, can be written in dimensionless form.
as

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

\[ \frac{\partial u_j}{\partial t} + \frac{\partial u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{1}{Re_{\delta_s}} \nabla^2 u_j + \frac{2}{Re_{\delta_s}} \cos(\omega t) \delta_{1j} \quad (4.2) \]

where \( x_1, x_2 \) and \( x_3 \) (or \( x, y \) and \( z \)) are, respectively, the streamwise, wall-normal and spanwise coordinates and \( u_i \) the velocity components in those directions. These equations have been made dimensionless by using \( \delta_s^* = \sqrt{2 \nu^*/\omega^*} \) as reference length scale, where \( \nu^* \) is the kinematic viscosity of water and \( U_{om}^* \) is the velocity scale. The dimensionless time is \( t = t^* U_{om}^*/\delta_s^* \). The intensity of the driving pressure gradient force is chosen so that the non-dimensional free-stream value of velocity is unitary. The Reynolds number is defined as \( Re_{\delta_s} = U_{om}^* \delta_s^*/\nu^* \).

Oxygen dissolved in water behaves like a passive scalar with low molecular diffusivity compared to the kinematic viscosity. Due to the presence of sub-Kolmogorov scales in the scalar field the subgrid-scale closure is retained. The filtered transport equation for DO is

\[ \frac{\partial c}{\partial t} + \frac{\partial u_i c}{\partial x_i} = \frac{1}{Sc Re_{\delta_s}} \frac{\partial c}{\partial x_i} - J_{i}^{sgs} \quad (4.3) \]

where \( Sc = \nu^*/D^* \) is the Schmidt number, \( D^* \) the molecular diffusivity of oxygen in water and \( \tau \) the instantaneous filtered scalar field normalized by the freestream DO concentration, \( C_{\infty}^* \), at the beginning of the simulation. The SGS scalar flux, \( J_{i}^{sgs} \), is parametrized by a dynamic eddy-diffusivity model. The extension of the dynamic model (Germano et al. 1991, Lilly 1992) to the scalar transport at high Schmidt numbers has been shown to be accurate by Zang et al. (1993), Calmet & Magnaudet (1997) and Na (2004).

The normalized instantaneous DO concentration level in the sediment layer, \( c_s \), is determined by more complex mechanisms. Dissolved oxygen is diffused but also depleted by decomposing organic matter. Advection and dispersion effects due to pore-water flow can be neglected for smooth beds (Scalo et al. 2012b). The governing equation for \( c_s \) is

\[ \frac{\partial c_s}{\partial t} + \frac{\partial c_s}{\partial x_i} \left[ \frac{F(\varphi)}{Sc Re_{\delta_s}} \right] - \dot{c}_s \quad (4.4) \]

where \( F(\varphi) \) is a function of the sediment porosity \( \varphi \) which accounts for reduction of the molecular diffusivity due to porosity and tortuosity. A commonly used approximation for this function is \( F(\varphi) = \varphi^2 \) (for \( \varphi < 0.7 \). The DO absorption by organic matter is represented by the sink term, \( \dot{c}_s \), which must be modelled.

The effective DO diffusion inside the sediment is lower than in water because molecules cannot travel along the concentration gradient direction but must follow a tortuous path around sediment grains. Also, the resulting flux must be reduced by a factor \( \varphi \) to account for the pore-space fraction available to transport in pore water. All of these factors are accounted for in \( F(\varphi) \). It is possible to retrieve the value of the sediment
porosity from the measurable slope discontinuity in the mean oxygen profiles at the SWI (Røy et al. 2004).

The parametrization for the non-linear sink term, $\dot{c}_s$, due to Higashino et al. (2008), is

$$\dot{c}_s = \chi \frac{c_s}{K_{O_2} + c_s}$$

(4.5)

where

$$\chi = \frac{\mu^* \chi^*}{Y_c U_{om} C_\infty}$$

(4.6)

The parameters used in (4.6) are $\mu^*$, maximum specific DO utilization rate (in day$^{-1}$), $K_{O_2}^*$, half-saturation coefficient for DO utilization (in mg$^{-1}$), $Y_c$ effective yield for the microbial utilization of DO and $\chi^*$, is the value of biomass concentration of oxygen absorbing organism, currently not directly measurable. The values of these constants are shown in Table 4.1. We will assume a constant and uniform value of $\chi^*$ across the sediment layer.

### 4.4 Computational Setup

The computational setup used is shown in Figure 4.1. The governing equations (4.1) and (4.2) are solved in a Cartesian domain. In the streamwise and spanwise directions, $x$ and $z$, periodic boundary conditions are used for all quantities. The velocity obeys, at the lower wall, no-slip conditions and, at the top boundary, free-slip conditions; for the scalar we use Neumann conditions, with assigned flux at the bottom wall derived from the solution of (4.4) (see (Scalo et al. 2012b)). Reareation from the top boundary is prevented where homogeneous Neumann conditions for the scalar are used.

The numerical model used to compute the flow on the water side is a well-validated finite-difference code (Keating et al. 2004), based on a staggered grid. Second-order central differences are used for both convective and diffusive terms. The time advancement scheme is a Crank-Nicolson scheme for the wall-normal diffusive term, and a low-storage third-order Runge-Kutta method for the other terms. The solution of the Poisson equation is obtained by Fourier transform of the equation in the spanwise and streamwise directions, followed by a direct solution of the resulting tridiagonal matrix, at each wavenumber. The code is parallelized using the MPI protocol. The equations in the sediment layer are solved with the same numerical approach as the one adopted for water side and have the same accuracy and stability properties. The code has been validated against results of (Moser et al. 1999a) in the channel flow configuration and (Spalart & Baldwin 1987) for
We performed DNS of the velocity field and LES for the scalar field for $Re_{\delta_s} = 800$ and $Sc = 1020$ (corresponding to water temperature of $8^\circ C$ and dissolved oxygen saturation levels of $C_\infty^* = 12 \text{ mg l}^{-1}$). Two different bacterial populations have been tested, $\chi^* = 100$ and $700 \text{ mg l}^{-1}$, resulting in two different boundary conditions for the oxygen field. In all cases, the oxygen field is initialized with a uniform distribution equal to the reference value and a completely anoxic sediment layer. The initial velocity field is taken from an independent, fully converged simulation carried out on the same grid without the scalar field. The box size has been chosen in order to accommodate the large structures, the near-wall streaks and the elongated concentration patches at the SWI (Scalo et al. 2012a). Also, a very large computational domain has the advantage of reducing the variance of plane averaged statistics, which is useful when studying transient flows. The grid size has been chosen accordingly in order to maintain a DNS resolution for the velocity field and to model exclusively the sub-Kolmogorov scales of the concentration field. The resolution in the wall-normal direction has been chosen based on the diffusive sublayer thickness. All the parameters used are summarized in Table 4.2.

Table 4.2: Simulation parameters adopted for both low and high bacterial population cases.

<table>
<thead>
<tr>
<th>$Re_{\delta_s}$</th>
<th>$L_x \times L_y \times L_z$</th>
<th>$N_x \times N_y \times N_z$</th>
<th>$\Delta x^+$</th>
<th>$\Delta y^+$</th>
<th>$\Delta y_{max}^+$</th>
<th>$Sc$</th>
</tr>
</thead>
<tbody>
<tr>
<td>800</td>
<td>$150 \times 13\pi \times 25$</td>
<td>$1024 \times 384 \times 256$</td>
<td>1 – 6</td>
<td>0.6 – 4</td>
<td>0.2 – 12</td>
<td>1020</td>
</tr>
</tbody>
</table>

Figure 4.2: Plane-averaged free-stream oxygen concentration: $\langle c(x,t) \rangle_{xz}$ at $y = L_y$ (---) for $\chi^* = 100 \text{ mg l}^{-1}$ (a) and $\chi^* = 700 \text{ mg l}^{-1}$ (b) and mean decay trend obtained by fitting over $t > 6 T$ (----) (see text).
4.5 Results

4.5.1 Formulation of self-similar decay model

Figure 4.2 shows the time series of plane-averaged oxygen concentration at the top boundary \((y = L_y)\) which is indicative of the monotonically decaying bulk concentration value. The total decay rate is approximately 2\% over 20 cycles for the highly absorbing case. At this distance from the wall the plane-averaged concentration field exhibits irregular and low-amplitude oscillations occurring over time scales comparable to the whole simulation run-time. On the other hand, the same quantity plotted at different heights in the fully mixed region, \(y < 15\) (Figure 4.3), shows the signature of the harmonic forcing driving the transporting turbulent velocity field and, therefore, the mixing. For \(y > 15\) traces of coherent oscillations are lost and the turbulent mixing can be regarded as statistically steady (shown later).

Most of the fluctuations in the scalar field are filtered out by the plane-averaging operator given the large computational box (Table 4.2) and the relatively low variance of the resolved high-Schmidt-number scalar. However, well defined low-amplitude, low-frequency deviations of the plane-averaged oxygen concentration from the (qualitatively determined) mean decay trend are also present in the fully mixed region and persist over several oscillation periods. These resemble the anomalous features observed in time series of passive scalars such as the ramp-cliff structures (Warhaft 2000), which are typically amplified in the case of a high-Schmidt-number contaminant (Antonia & Orlandi 2003). There is no apparent correlation with the periodic forcing but, rather, with the underlying, intermittent velocity field. These effects become more significant in simulations with smaller computational boxes (not shown) suggesting they belong to the non-coherent component of the turbulent scalar field.

An initial transient evolution of the oxygen levels is visible at all distances from the sediment-water interface (SWI) and, in particular, for \(y < 1\). This is due to the long time scales of adjustment of the bacterial absorption, in the initially anoxic sediment layer, to the mass flux imposed across the SWI from the water side turbulence. After approximately 6 cycles a dynamical equilibrium is reached and the oxygen distribution exhibits a well-defined decay pattern. A preliminary fitting for all \(y\) is carried out over \(t > 6 T\) revealing the following functional form for the non-oscillating decaying component of the ensemble average oxygen distribution

\[
C(y, t) = c_0(y) \, d(t)
\]  

where \(d(t)\) is a positive, dimensionless, monotonically decaying function of time obtained by fitting the plane-averaged oxygen distribution at \(y = L_y\) with a (for now) first-order polynomial in time; the fitting is carried out over equally distributed samples in time (64 per period) and obtained by imposing that the (oscillating)
Figure 4.3: Time series of plane averaged oxygen concentration for $y = 0, 0.1, 0.5, 1, 15$ and $40$ (from bottom to top) and $x^* = 100 \text{ mg/l}$ (a) and $x^* = 700 \text{ mg/l}$ (b). Non oscillating/steady transient decay and fitting over $t > 6T$ (see text). Approximate bounds for oscillating component (---) with same decay rate as mean trend.
Figure 4.4: Profiles of $c_0(y)$ for $\chi^* = 100$ mg/l (a) and $\chi^* = 700$ mg/l (b); the inset figure highlights the near-wall ($0 < y < 1$) concentration boundary layer.

residual

$$R(t) = \langle c(x,t) \rangle_{xz} - d(t), \quad \text{at} \quad y = L_y,$$

where $\langle \rangle_{xz}$ is the one-time planar-average operator, has a zero average (discrete integral in time) over 36 complete semi-periods after $t = 6T$. For a given $d(t)$, the fitting coefficient $c_0(y)$ in (4.7) (set to 1 at $y = L_y$) is calculated for every $y$ so that (4.7) returned the best fit of the plane-averaged oxygen concentration over the same time range.

In spite of the approximations made, the resulting profiles of $c_0(y)$ (Figure 4.4) closely resemble the shape of an ensemble-averaged decaying mean oxygen distribution in a statistically steady turbulent open channel flow, with zero-mass-flux conditions at the top boundary and an absorbing sediment layer at the bottom boundary. This is the first evidence supporting the possibility of the existence of a self-similar structure in the decaying mean oxygen field of which $c_0(y)$ represents only the non-oscillating component. More rigorous derivations (carried out in Section 4.5.2) will show that the linear approximation used for $d(t)$ is, actually, first-order accurate in time.

As previously mentioned, sufficiently far away from the turbulent bottom boundary layer the plane-averaged oxygen concentration loses trace of the harmonic forcing and is characterized by a low-amplitude, slowly evolving, stochastic component. The latter is especially true on large computational boxes like the
one used here where the deviation of the ensemble-averaged free-stream (decaying) oxygen concentration

\[ c_\infty(t) \equiv \langle c(x,t) \rangle, \quad (4.9) \]

where \( \langle \cdot \rangle \) is the ensemble average operator\(^1\), from the one-time plane average

\[ |c_\infty(t) - \langle c(x,t) \rangle_{xz}| \quad \text{at} \quad y = L_y \quad (4.10) \]

is negligible. Fitting the plane-averaged time-series at \( y = L_y \) with the correct functional form for \( d(t) \), over a sufficiently long time interval, will, therefore, return values very close to the true ensemble average (4.9). Also, (4.7) and (4.9) imply that

\[ c_\infty(t) = d(t) \quad (4.11) \]

over the time range of self-similar decay.

Given the pronounced signature of the statistically periodic forcing in the scalar field evolution (Figure 4.3) and the linearity of the governing equations (4.3), we hypothesize that, in the self-similar range, the concentration field contains a coherent oscillating component, \( \tilde{C} \), (linearly) overlapping the mean monotonic decay (4.7) such that

\[ \langle c(x,t) \rangle = C(y,t) + \tilde{C}(y,t). \quad (4.12) \]

Without loss of generality, \( \tilde{C}(y,t) \) can be rewritten as

\[ \tilde{C}(y,t) \equiv \tilde{d}(y,t) \tilde{c}_0(y,t) \quad (4.13) \]

where \( \tilde{d}(y,t) \) is a non-oscillating dimensionless function, modulating in time the oscillating quantity \( \tilde{c}_0(y,t) \) and chosen, for every \( y \) and \( t \), such that \( \tilde{c}_0(y,t) \) is a periodic function with period \( T/2 \) and zero average over a semi-period \( T/2 \). The latter property is, in particular, implied by the fitting procedure adopted to derive (4.7). All quantities in (4.13) and (4.12) are not stochastic and, therefore, do not include, for example, the previously discussed irregular low-amplitude fluctuations. The aforementioned properties can be formalized as follows:

\[ \begin{align*}
\tilde{c}_0(y,t) &= \tilde{c}_0(y,t + T/2) \\
\overline{\frac{\tilde{c}_0(y,t)}{T/2}} &= 0
\end{align*} \quad (4.14) \]

where \( \overline{()}^{T/2} \) is the cycle-average operator (defined over the semi-period of \( \Delta \phi = T/2 \)). With the introduction

\(^1\)Note that, for the present computational setup, the plane-average operator is absorbed by the ensemble-average one, \( \langle \cdot \rangle = \langle \langle \cdot \rangle_{xz} \rangle \), and by the phase-average one, \( \langle \cdot \rangle_\phi = \langle \langle \cdot \rangle_{xz} \rangle_\phi \), which will introduced later on.
of (4.13) we hypothesize the existence of a self-similar oscillating component of the mean-oxygen distribution, \( \tilde{c}_0(y,t) \), but, at the same time, do not exclude that the coherent oscillating component \( \tilde{C}(y,t) \) is also decaying.

A visual inspection of the data in Figure 4.3 provides no elements to anticipate the functional form of \( \tilde{d}(y,t) \). The solid lines bounding the times series suggest that there might be either no decay of \( \tilde{C}(y,t) \) (i.e. \( \tilde{d}(y,t) = \text{const} \)) or that \( \tilde{d}(y,t) \) varies with times scales similar to \( d(t) \). No further assumptions on \( \tilde{d}(y,t) \) are, however, required to proceed in our analysis.

The decomposition (4.12) must now be extended to the instantaneous scalar field to include a stochastic component. It can be recovered as the reminder of the ensemble averaging operator

\[
C'(x,t) = c(x,t) - \langle c(x,t) \rangle,
\]

and it accounts for the previously discussed low-amplitude irregular fluctuations and, most importantly, the effects of the three-dimensional turbulent mixing, which determines the observed structure of the mean profiles (Figure 4.4) and the oscillating component \( \tilde{C}(y,t) \). The introduction of (4.15) suggest the following form of the decomposition

\[
c(x,t) = C(y,t) + \bar{C}(y,t) + C'(x,t).
\]

For the current computational setup, the statistical distribution of \( C'(x,t) \) is necessarily homogeneous in the streamwise and spanwise directions. However, there is no evidence to support that its distribution is also periodic in time. Let’s introduce another, in general, unknown function \( f(y,t) \) such that

\[
C''(x,t) = f(y,t) c'_0(x,t)
\]

where, by definition, \( c'_0(x,t) \) is random variable with a statistically periodic probability distribution (with period \( T/2 \)). While the spatial variability of \( f \) has been restricted to \( y \), being the flow statistically non-homogeneous only in the wall-normal direction (and time), to retain complete generality in the decomposition (4.17), from a statistical standpoint, \( f(y,t) \) should also be a different stochastic process, for every \( y \), unfolding in time. However, given the obvious presence of a periodic component in the scalar field evolution — which can only be the result of statistically periodic turbulent mixing events (shown later), therefore, necessarily involving \( C' \) — and the fact that the passive scalar fluctuations are created and sustained by a statistically periodic turbulent velocity field, is it safe to assume that \( C'' \) naturally contains a periodic component. This implies that \( f(y,t) \) does not need to be stochastic.
The properties of the quantities in (4.17) can be formalized as follows:

\[
\begin{align*}
\langle C'(x,t) \rangle &= \langle c'_0(x,t) \rangle = 0 \\
\langle \v' \, \tilde{c}_0(y,t) \rangle &= \langle \v' \, c_0(y) \rangle = 0 \\
\langle \v'(x,t) c'_0(x,t) \rangle &= \langle \v'(x,t+T/2)c'_0(x,t+T/2) \rangle = \langle \v'(x,t)c'_0(x,t) \rangle \phi
\end{align*}
\]  

(4.18)

where \( \langle \rangle \phi \) is the phase-averaging operator with period \( T/2 \). Substituting (4.19), (4.13), and (4.17) into (4.16) yields the final form of the self-similar decay model for the instantaneous concentration field

\[
c(x,t) = d(t) \, c_0(y) + \tilde{d}(y,t) \, \tilde{c}_0(y,t) + f(y,t) \, c'_0(x,t).
\]

(4.19)

In the following, the mathematical implications of the assumptions made so far will be explored and solutions of the form (4.19) will be tested against the governing equations and the numerical data (Section 4.5.2). Analytical constraints determining the functional forms of \( d(t) \), \( \tilde{d}(y,t) \) and \( f(y,t) \) will be derived. Statistics will then be extracted by removing the monotonically decaying component (4.7) from the total solution (Section 4.5.4) and phase-averaged quantities will be analyzed (Section 4.5.5). The low and the high absorption cases do not exhibit any significant difference and, therefore, only results for the \( \chi^* = 700 \text{ mg l}^{-1} \) case will be shown from now on, unless otherwise specified.

### 4.5.2 Implications of self-similarity

Substituting (4.19) into (4.3) yields

\[
\left( \frac{d}{dt} \right) c_0(y) + \left( \frac{\partial}{\partial t} \tilde{d}(y,t) \right) \tilde{c}_0(y,t) + \tilde{d}(y,t) \frac{\partial}{\partial y} \tilde{c}_0(y,t) + \left( \frac{\partial}{\partial y} f(y,t) \right) c'_0(x,t) +
\]

\[
f(y,t) \left( \frac{\partial}{\partial y} c'_0(x,t) \right) = \frac{1}{\text{Re}_{\delta_s} \, \text{Sc} \, dy^2} \left[ \tilde{d}(y,t) \tilde{c}_0(y,t) + f(y,t) c'_0(x,t) \right] + \frac{1}{\text{Re}_{\delta_s} \, \text{Sc} \, dy^2} \nabla^2 \left[ f(y,t) c'_0(x,t) \right].
\]

(4.20)

The subgrid-scale contribution has been omitted for the sake of simplicity as it would add unnecessary complications to the following derivations. Applying the ensemble averaging operator to (4.20) and dividing by \( d(t) \), yields

\[
\frac{d}{dt} \log (d(t)) \, c_0(y) + \frac{1}{d(t)} \left( \frac{\partial}{\partial t} \tilde{d}(y,t) \right) \tilde{c}_0(y,t) + \frac{\tilde{d}(y,t)}{d(t)} \frac{\partial}{\partial y} \tilde{c}_0(y,t) =
\]

\[
- \frac{\partial}{\partial y} \left( \frac{f(y,t)}{d(t)} \left( \frac{\v' \, c'_0 \phi}{T/2} \right) \right) - \frac{\partial}{\partial y} \left( \frac{f(y,t)}{d(t)} \left( \frac{\v' \, c'_0 \phi}{T/2} \right) \right)
\]

\[
+ \frac{1}{\text{Re}_{\delta_s} \, \text{Sc} \, dy^2} \left[ \tilde{d}(y,t) \tilde{c}_0(y,t) + \frac{1}{\text{Re}_{\delta_s} \, \text{Sc} \, dy^2} \nabla^2 \left[ f(y,t) c'_0(x,t) \right] \right]
\]

(4.21)
where the cycle-average operator has been used to decompose the resulting turbulent flux into a constant and a zero-mean periodic component

$$\langle v'c'_0 \rangle = \langle v'c'_0 \rangle_\phi = \langle (v'c'_0)^{T/2} \rangle + \langle (v'c'_0) \rangle_\phi. \quad (4.22)$$

In the new form (4.21), it is possible to discriminate the contributions to the overall mean concentration budget deriving from the different components in (4.19). For example, the steady self-similar diffusion term (third term on the right-hand-side) can only be balanced by other constant, non-oscillating terms. Moreover, the terms in (4.21) containing the periodic functions $\tilde{c}_0(y,t)$ and $\langle v'c'_0 \rangle_\phi$ cannot add up to a constant function of time but, rather, to (at most) a modulated periodic signal. Therefore, the only terms that could balance the steady diffusion term are the first term on the left-hand-side, representing the steady, non-oscillating decay of oxygen concentration occurring at every $y$, and the first term on the right-hand-side, representing the redistribution of mass within the water-column due to the mean cycle-averaged turbulent mass flux. This allows to extract from (4.21) the budget for the non-oscillating component of the mean oxygen distribution that reads

$$\frac{d}{dt} \log (d(t)) c_0(y) = -\frac{\partial}{\partial y} \left( \frac{f(y,t)}{d(t)} \langle v'c'_0 \rangle_\phi^{T/2} \right) + \frac{1}{Re \delta \ Sc} \frac{d^2}{dy^2} c_0(y). \quad (4.23)$$

The exact decay law for $d(t)$ can be extracted regardless of the functional form of $f(y,t)$ by integrating (4.23) in the wall-normal direction, yielding

$$\frac{d}{dt} \log (d(t)) = -\frac{1}{Re \delta \ Sc \ C_{0,B}} \frac{d}{dy} c_0(y) \bigg|_{y=0} \quad (4.24)$$

where

$$C_{0,B} = \int_0^{L_y} c_0(y)dy \quad (4.25)$$

and no-slip and symmetry the boundary conditions

$$\langle v'c'_0(x,t) \rangle_{y=0} = 0, \quad \langle v'c'_0(x,t) \rangle_{y=L_y} = 0 \quad (4.26)$$

respectively, have been used. By introducing the mean rate of decay

$$k = \frac{1}{C_{0,B}} J_{swi,0} \quad (4.27)$$

where

$$J_{swi,0} = (Re \delta \ Sc)^{-1} \frac{d}{dy} c_0(y) \bigg|_{y=0} \quad (4.28)$$
the final expression for \( d(t) \) (or \( c_\infty(t) \)) becomes

\[
c_\infty(t) = d(t) = d_0 \, e^{-kt}
\]

(4.29)

where \( d_0 \) is the normalized free-stream value of the steadily decaying component of oxygen concentration at \( t = 0 \) which will be defined, for convenience, the virtual origin of the concentration decay. The relations (4.27) and (4.28) are an important analytical constraint between \( c_\infty(t) \) and \( c_0(y) \), allowing us to confirm the interpretation of \( c_0(y) \) as the self-similar steady component of the mean oxygen distribution responsible for the mean bulk rate of decay (with time constant \( k^{-1} \)) and (4.28) as the corresponding flux across the SWI. This result leads to an improved iterative fitting strategy to determine \( d(t) \) described in the following.

The constraint in (4.27) is a direct consequence of self-similarity and leads to a new iterative strategy to determine \( d(t) \) and \( c_0(y) \). A first guess for the constants \( d_0 \) and \( k \) in (4.29) is obtained by performing a least-square fit of the plane-averaged scalar at the top-boundary. The following iterative procedure is then carried out until convergence is reached on (4.27):

1. The current estimates for \( k^{(i)} \) and \( d_0^{(i)} \) (i-th tentative form for \( d(t) \)) allow to calculate \( c_0^{(i)}(y) \) (i-th guess for the \( c_0(y) \) profile) by fitting (4.7) to \( \langle c(x, t) \rangle_{xz} \), over an integer number of semi-periods at all \( y \) locations.
2. The newly calculated \( c_0^{(i)}(y) \) allows to update \( k^{(i)} \) to \( k^{(i+1)} \) via (4.27).
3. The new guess for \( k \) allows to update \( d_0^{(i)} \) to \( d_0^{(i+1)} \) by the fitting \( \langle c(x, t) \rangle_{xz} \) at the top boundary for \( k \) fixed to \( k^{(i+1)} \).
4. If the condition (4.27) is not satisfied, return to (a).

The iterative procedure converges to machine precision after 4 steps. The first error is of the order to 10% and is reduced with longer time-series. Note that the mean decay rate \( d(t) \) is not influenced by \( \tilde{d}(y, t) \) or \( f(y, t) \).

Given the very slow decay rate (\( k << T^{-1} \)), due to the limiting effects on the overall mass transfer rate of the high Schmidt number scalar, a Taylor expansion of (4.29) about \( t = 0 \) is possible, which, truncated to first-order, becomes

\[
d(t) = d_0 \, e^{-kt} \simeq d_0 \, (1 - k \, t) .
\]

(4.30)

This explains why the linear fitting used in the preliminary analysis carried out in Section 4.5.1 to calculate \( d(t) \) provides a very accurate approximation. Moreover, due to the limited time span covered by the numerical results (with respect to the very long time scales of decay of the scalar field) it is not possible to appreciate in Figures 4.2 and 4.3 the difference between a linear and an exponential fit of the time series.
In the present derivation an initial, empirically based, formulation of the self-similar form of (part of) the solution (4.7) has lead, via mathematical manipulation of the governing partial-differential equations, to the exact definition of the decay law (solution scaling parameter in time), derived from the integration of an ordinary-differential equation (4.24); this is consistent with a commonly accepted approach in the study of self-similarly decaying flows (Pope 2000).

By substituting (4.29) into (4.23)

$$-k \ c_0(y) = -\frac{\partial}{\partial y} \left( \frac{f(y, t)e^{k \ t}}{d_0 \langle v' c'_0 \rangle_0} \right) + \frac{1}{Re_s \ Sc \ d_0^2} c_0(y).$$

(4.31)

it follows, necessarily, that the term in square brackets must be a constant function of time, therefore, in general, only a function of $y$, say, $g(y)$, such that

$$f(y, t) = g(y) d_0 e^{-k \ t}. \tag{4.32}$$

At this point we can extract the budget for the oscillating component of the oxygen distribution by substracting (4.23) to (4.21) and using (4.32), yielding

$$\frac{1}{d(t)} \left( \frac{\partial}{\partial t} \tilde{d}(y, t) \right) \tilde{c}_0(y, t) + \frac{\tilde{d}(y, t)}{d(t)} \frac{\partial}{\partial t} \tilde{c}_0(y, t) = -\frac{\partial}{\partial y} \left( g(y) \langle v' c'_0 \rangle_0 \right)$$

$$+ \frac{1}{Re_s \ Sc \ d_0^2} \left[ \frac{\tilde{d}(y, t)}{d(t)} \tilde{c}_0(y, t) \right]. \tag{4.33}$$

The presence of a non-zero, periodic turbulent forcing term (first term on the right-hand-side) implies that $\tilde{d}(y, t)$ cannot be a constant function of time and, in particular, that at least one of the other terms in (4.33) must be periodic. This implies either that

$$\frac{\tilde{d}(y, t)}{d(t)} = h(y) \tag{4.34}$$

where $h(y)$ is some function of $y$, and, therefore

$$\frac{1}{d(t)} \frac{\partial}{\partial t} \tilde{d}(y, t) = -k \ h(y), \tag{4.35}$$

where $d(t)$ is given by (4.29), or viceversa. The function $h(y)$ can be, in this case, arbitrary since the only assumption made when defining $\tilde{d}(y, t)$, according to the rationale behind the formulation of (4.13), is that $\tilde{c}_0(y, t)$ must be periodic in time. It is has been shown that this condition is already satisfied by $d(t)$ in (4.34), regardless of the functional form of $h(y)$. For the sake of simplicity we will, therefore, take $h(y) = 1$.

The last unknown function left to determine is $g(y)$. The result (4.32) already states that the decay rate of the amplitude of the fluctuating field scales, in time, with the same law as the steady and oscillating
component. This can be physically explained noting that scalar variance production for $C'$, originally defined in (4.15), must decay, in time, as $d(t)^2$ since it is proportional to the product of the mean scalar gradient and the turbulent flux, both scaling independently with $d(t)$. Equivalently, the scalar variance budget of the statistically steady self-similar stochastic component $c'_0(x, t)$,

$$-k g(y) \langle c'_0(x, t)^2 \rangle + g(y) \frac{\partial}{\partial t} \frac{1}{2} \langle (c'_0(x, t))^2 \rangle = -\langle c'_0 v' \rangle + \frac{d}{dy} c_0(y) - \frac{1}{Re_\delta Sc} \langle c'_0 \Delta^2 (g(y)c'_0(x, t)) \rangle$$

(4.36)

reveals three non-decaying, periodic, production terms which are, also, unaffected by the choice of $g(y)$. The latter simply determines a redistribution of the variance in $y$ due to a redistribution of the turbulent diffusion and dissipation intensities, which has no physical relevance. Therefore, analogously to $h(y)$, we will pose $g(y) = 1$.

### 4.5.3 Final form of the decomposition

The final functional form of the decomposition (4.19) is

$$c(x, t) = [c_0(y) + \bar{c}_0(y, t) + c'_0(x, t)] c_{\infty}(t).$$

(4.37)

The budget for the steady component, $c_0(y)$, is

$$-k c_0(y) = \frac{d}{dy} \left[ J_0(y) - \langle v' c'_0 \rangle \right]$$

(4.38)

where

$$J_0(y) = \frac{1}{Re_\delta Sc} \frac{d}{dy} c_0(y).$$

(4.39)

The budget of the oscillating component, $\bar{c}_0(y, t)$,

$$-k \bar{c}_0(y, t) + \frac{\partial}{\partial t} \bar{c}_0(y, t) = \frac{\partial}{\partial y} \left[ \bar{J}(y) - \langle \bar{c}'_0 v' \rangle \right],$$

(4.40)

where

$$\bar{J}(y) = \frac{1}{Re_\delta Sc} \frac{\partial}{\partial y} \bar{c}_0(y, t).$$

(4.41)

is a set of ODEs (one for every $y$) each describing a linear system subject to a zero-mean harmonic forcing (turbulent flux term).

Equation (4.38) highlights how the non-zero divergence on the right-hand-side, caused by the vertical unbalance of the total cycle-averaged mass flux, is responsible for the constant mean decay rate, on the
left-hand-side, originating from the unsteady term in (4.20). On the other hand, equation (4.40) suggests the interpretation of the periodic component of the concentration field as the solution to a linear system harmonically forced by the oscillating component of the total mass flux.

The final form for the budget of the scalar variance is

\[-k \langle c'_0(x,t)^2 \rangle_\phi + \frac{\partial}{\partial t} \frac{1}{2} \langle c'_0(x,t)^2 \rangle_\phi = -\langle c'_0 v'_0 \rangle_\phi \frac{d}{dy} c_0(y) - \langle c'_0 v'_0 \rangle_\phi ^T \frac{\partial}{\partial y} c_0(y, t)\]

\[-\langle c'_0 v'_0 \rangle_\phi \frac{\partial}{\partial y} \tilde{c}_0(y, t) - \frac{\partial}{\partial y} \langle v'_1 \frac{1}{2} c'_0^2 \rangle_\phi + \frac{1}{Re_\delta} \frac{Sc}{Sc} \left( \langle c'_0 \nabla^2 c'_0(x, t) \rangle_\phi \right)\]

where a similar structure as in (4.40) is present, with the addition of turbulent and molecular diffusion and dissipation terms.

### 4.5.4 Extraction of phase-averaged statistics

The extraction of the three components in (4.37) requires an iterative procedure since \(c_\infty(t)\) and \(c_0(y)\) are interdependent via (4.27). Once \(c_\infty(t)\) and \(c_0(y)\) are determined, the instantaneous data, \(c(x, t)\), could be reprocessed as

\[\tilde{c}_0(y, t) + c'_0(x, t) = \frac{c(x, t)}{c_\infty(t)} - c_0(y)\]

and, by means of phase averaging, any statistic could be evaluated. However, this would require to load the instantaneous data twice: once to calculate the time series of plane-averaged quantities, used to calculate \(c_\infty(t)\) and \(c_0(y)\), and, a second time, to reprocess the data via (4.43). Fortunately, the decomposition (4.37) can also be exploited to evaluate statistics directly from the plane-averaged quantities of the instantaneous...
Figure 4.6: Profiles of turbulent mass flux $\langle c'v' \rangle_\phi$ (a) for different phases shown in the inset figure; cycle-averaged mass flux $\langle c'v' \rangle_\phi^T$ (---) and steady component of the diffusive flux (——) (b).

transient data, without the need to reprocess the whole dataset via (4.43). For example, the variance of $c'_0(x,t)$ can be calculated by solving (4.37) for $c'_0(x,t)$, squaring both sides and taking the phase-average, resulting in

$$\langle c'_0 \rangle^2_\phi = \langle \frac{1}{c'_\infty(t)} (c(x,t))^2 \rangle_{xz} \rangle_\phi + \left[ c_0(y) + \bar{c}_0(y,t) \right]^2$$

$$- 2 \left[ \bar{c}_0(y,t) + c_0(y) \right] \langle \frac{1}{c'_\infty(t)} \langle c(x,t) \rangle_{xz} \rangle_{xz} \rangle_\phi.$$  (4.44)

The statistically periodic turbulent flux can, also, be more simply extracted by multiplying both sides of (4.43) by $v'(x,t)$, taking the plane average, and, finally, the phase average, resulting in

$$\langle v'c'_0 \rangle_\phi = \langle \frac{v'(x,t)c(x,t)}{c'_\infty(t)} \rangle_{xz} \rangle_\phi.$$  (4.45)

where $\langle v'(x,t) \rangle_{xz}$ vanishes at every time due to continuity and the no-slip conditions at the bottom wall.
4.5.5 Transport dynamics

High-Schmidt-number mass transfer problems are characterized by highly concentrated scalar gradients at the wall. As a result, molecular diffusion effects become important in a very thin layer of fluid (typically $Sc^{1/3}$ times thinner than the viscous sublayer) renewed only by rare and intense bursting events (Pinczewski & Sideman 1974, Scalo et al. 2012a). Figure 4.6 shows the very rapid transition, across the diffusive sublayer, between purely molecular and fully turbulent transport, occurring in approximately 0.2 Stokes thicknesses from the wall. This allows to identify a near-wall region, of the order of one Stokes thickness or less, $y < 1$, where both mechanisms of transport are present, and an outer region, $y > 1$, characterized by purely turbulent transport for the scalar field.

The same structure is present in the case of statistically steady mass transfer from one wall to another in a channel flow. The outer region is fully mixed with a constant value of the turbulent flux (Scalo et al. 2012b). In the case of an oscillating boundary layer, however, the mixing is confined in a region close to the wall and the cycle-average turbulent flux $\langle c_0 v' \phi \rangle T/2$ decreases linearly with $y$ (Figure 4.7 (a), 4.6 (b)). At this Reynolds number, the periodic modulation of the oscillating component of the turbulent flux dominates the transport for $y < 15$ (phase averaged quantities exhibit periodic variations), while, for $y > 15$, the turbulent mixing tends towards a statistically steady state, where all phase-averaged profiles collapse onto the cycle-average value.

Turbulent mass flux is generated in the near-wall region (Figure 4.6 (a)) where it exhibits the greatest variability (over more than one order of magnitude) particularly at the edge of the diffusive sublayer. Here, a peak in the turbulent flux starts to appear towards the end of the acceleration phase, $\phi = 70^\circ$, and rapidly grows in intensity until $\phi = 120^\circ$, persisting at approximately the same distance from the wall. It then propagates in the outer layer while diffusing for most of the deceleration phase and the first part of the acceleration phase. The signature of the periodic forcing is evident in the cyclic evolution of the mixing front for the scalar and momentum field in the outer region (Figure 4.7).

The oscillating component of the turbulent flux in the water column modulates, via (4.42) and (4.40), the oscillating and fluctuating term of the instantaneous scalar field while the mean rate of decay, $k$, is only determined by the cycle-average value via (4.38). Despite the remarkable linear structure of the concentration field suggested by (4.37), the overall turbulent mixing process is, however, characterized by strong non-linearities. These enter the transport dynamics via production mechanisms feeding energy into the scalar variance (4.42), and, therefore, the turbulent mass flux, which then sustains via (4.42) and (4.40), the mean oscillating and steady concentration profiles, respectively, by providing the background concentration gradient to generate production of scalar variance.

The evolution pattern of the turbulent mass flux in the outer region follows closely the Reynolds shear
Figure 4.7: Profiles of turbulent mass flux $\langle c'_0 v' \rangle_\phi$ (a) and momentum flux $\langle u' v' \rangle_\phi$ (b) for semi-cycle $\phi = 0^\circ - 180^\circ$. Corresponding phases shown in the inset figure. Semi-cycle-averaged mass flux $\langle c'_0 v' \rangle_{T/2}$ and momentum flux $\langle u' v' \rangle_{T/2}$ are plotted against the phase angle. The propagation of the maximum Reynolds shear-stress stops being significant towards the middle of the acceleration phase, while the scalar mixing front is still propagating upwards, modulating the concentration field distribution by entraining fluid layers richer in oxygen and gradually loosing phase coherence. At around $\phi = 40^\circ$ the growth of the near-wall Reynolds shear stress peak triggers the build-up of the peak in turbulent mass flux with a phase lag of $\phi = 30^\circ$. Ejection occurs around $\phi = 120^\circ$ for both quantities however the scalar mixing front propagates faster into the outer region.
Figure 4.8: Location of maximum turbulent mass flux, $y_1(\phi)$ (—) and of maximum Reynolds shear-stress, $y_2(\phi)$ (---) as a function of the phase angle. The loss of coherence of phase-averaged statistics is evident after $y > 10$.

The propagation speed of below ($\bar{c}_0(y,t) < 0$) and above-average ($\bar{c}_0(y,t) > 0$) concentration layers follows closely the mixing front. This is shown in Figure 4.9 (a) where $y_1(\phi)$ is overlapped to contours of $\bar{c}_0(y,t)$, normalized at every $y$ by

$$\text{rms}(\bar{c}_0)(y) = \sqrt{\frac{1}{T} \int_{0}^{T} \bar{c}_0^2(y,t) \, dt} \quad (4.48)$$

shown in Figure 4.9 (b). Layers of above-average concentration at a certain $y$ only appear after a peak in turbulent mass flux has occurred at the same $y$ approximately $\phi \sim 100^\circ$ earlier. Very close to the wall, the persistence of a growing peak in the turbulent mass flux from $\phi = 90^\circ$ to $\phi = 120^\circ$ creates a long lasting above-average concentration layer very close to the wall, from $\phi = 135^\circ$ to $\phi = 180^\circ$. When the mixing front propagates outwards it loses intensity and it progressively leaves shorter-lasting above-average concentration layers. The signature of the periodic forcing in $\bar{c}(y,t)$ disappears after $y > 14$ (not shown). Here a statistically steady intermittent entrainment of high-in-oxygen irrotational fluid governs the transport.

The frequency response analysis of (4.40) confirms the dynamics observed in Figure 4.9. For a given Fourier component its forcing term with angular frequency $\omega$, the transfer function is

$$G(\omega) = \frac{1}{j \omega - k} \quad (4.49)$$

where base angular frequency is $\omega T/2 = 1$. For our calculation we have that $k T/2$ is $1 \times 10^{-4}$ and $6 \times 10^{-4}$ for, respectively, the low and high absorption cases. This means that the transfer function can be approximated by $G(\omega) \approx 1/j \omega$, confirming that $\bar{c}_0(y,t)$ is delayed by $\sim 90^\circ$ with respect to the forcing turbulent mass flux.

Figure 4.10 shows the time response of the diffusive sublayer and viscous sublayer, represented by the
ensemble-averaged wall-shear stress \( \tau_w(\phi) \) and the periodic component of the mass flux at the SWI,

\[
\tilde{J}_{swi,0}(\phi) = (Re_{\delta_s}Sc)^{-1} \left. \frac{\partial}{\partial y} \tilde{c}_0(y, t) \right|_{y=0}
\]  

(4.50)

to the overlying turbulent transport events. The peak in mass flux at the SWI is delayed with respect to the one in wall-shear stress although the maximum Reynolds shear-stress and turbulent mass flux occur at the same time (around \( \phi = 120^\circ \)). The wall-shear stress exhibits an extended plateau from \( \phi = 45^\circ \) to \( \phi = 120^\circ \) (also visible in Figure 4.8) corresponding to the residence time of the Reynolds stress peak, in the same phase range, at \( y \approx 1 \). The peak in \( \tilde{J}_{swi0}(\phi) \) is delayed by \( \sim 50^\circ \) and its shorter due to the relatively short residence of the turbulent mass flux peak in the near-wall region at \( y = 0.2 \). The peak in \( \tilde{J}_{swi0}(\phi) \) occurs only when above-average value of oxygen concentration is accumulated in the layers between \( y = 0 \) and \( y = 0.2 \) (from \( \phi = 135^\circ \) to \( \phi = 180^\circ \) in Figure 4.9).
4.6 Conclusions

We carried out direct-numerical simulation of the velocity field and large-eddy simulation of the scalar field to investigate the transient decay of oxygen concentration due to sediment absorption in an oscillating boundary layer in the intermittently turbulent regime. A Reynolds number of $Re_{δ} = 800$ was chosen to maximize the asymmetry of turbulence between the acceleration and deceleration phases and investigate its effects on the sediment oxygen absorption rate. A uniform initial distribution of oxygen is left to decay (with no re-creation from the top boundary) in a fully developed statistically periodic turbulent velocity field. The bulk oxygen concentration exhibits a very slow decay rate, with characteristic time scales very large compared to the oscillation period $(k^{-1} >> T)$, due to the limiting effect for the mass transfer of the very thin diffusive sublayer at the sediment-water interface (SWI).

Despite the highly intermittent state of the turbulent velocity field, after the first 6 cycles, the plane-averaged scalar field exhibits a surprisingly regular pattern of decay in which is possible to identify a monotonically decaying component (linearly) overlapped by coherent oscillations (with a fundamental period of $T/2$ and zero mean over a semi-cycle). The former reveals a distinct self-similar structure, which, tested against the governing conservation equations for the scalar field, implies an exponential decay of the total ensemble averaged scalar field (including the oscillating component). A linear decomposition of the instantaneous concentration field is then proposed, where self-similarity is extended to the fluctuating component, also shown to decay exponentially.

The monotonically decaying and oscillating component of the ensemble-averaged scalar field could be
interpreted as the solution of two different transient mass transfer problems. The first is the transient decay
of oxygen in a statistically steady open channel flow with no reareation from the top boundary and an
absorbing sediment layer at the bottom. The second is a harmonically forced mass transfer problem, by
oscillating boundary layer turbulence, with alternating flux at the wall and zero cycle-average bulk value.

The assumptions made in the derivation of the decomposition and the analytical implications of the
existence of self-similarity are partly verified in a separate set of transient simulations performed on a smaller
box size (minimal channel simulations), to achieve longer time-series while still simulating a physically relevant
flow. These have allowed to empirically confirm the predicted exponential decay for the mean and oscillating
component, especially in the lower Schmidt number cases (with no sediment layer), which exhibited a faster
decay. The small box size emphasizes the anomalous nature of the fluctuating component in the plane-
averaged time series (confirming the presence of ramp-cliff-like structures and low-frequency variations) and
limits the size of the larger structures, which govern the entrainment in the outer region, delaying the start
of the scalar decay at the top boundary. The speed at which the mixing front propagates in the outer
region is reduced, while turbulent mixing of momentum is confined in a well-defined region ($y < 25$ for
$Re_\delta = 800$). Schmidt number effects have also been investigated, showing that in the high-Schmidt-number
limit, the overall decay rate (determined by the monotonically decaying component of the scalar field) scales
like $Sc^{-0.704}$, consistently with empirical parametrizations for statistically steady high-Schmidt-number mass
transfer and the physical interpretation of $c_0(y)$ as the solution of a steady state mass transfer problem.

Due to the interdependency of the components of the solution, the extraction of the three distinct contribu-
tions requires an ad-hoc iterative procedure. The thus calculated transient decaying component has been
removed from the instantaneous concentration field in order to isolate a statistically periodic component (the
self-similar state), allowing for the evaluation of phase averaged statistics in lieu of ensemble average ones.
These have allowed to investigate the physical transport mechanisms associated with each component of the
solution. It is shown that the oxygen distribution in the water column is modulated by the periodic ejection,
during the deceleration phase, of negative peaks of high turbulent mass flux, generated at the edge of the
diffusive sublayer towards the end of the acceleration phase and growing in intensity until the beginning of
the deceleration phase (turbulent flux production stage). Ejection of the near-wall streaks occurs at this
stage. The resulting highly turbulent mixing front propagate away from the SWI in the outer region, at
approximately constant speed, in layers of low oxygen concentration and faster than the Reynolds shear-
stresses. The periodic forcing leaves its signature in the concentration field for a shorter portion of the water
column than in the velocity fluctuation field and, despite the highly intermittent state of the turbulent field,
the average oscillating component of the scalar field behaves like a linear harmonically forced system.

The persistence of high values of mass flux at the edge of the diffusive sublayer during the turbulent flux
production stage (at $y \sim 0.2$ between $\phi = 70^\circ$ and $\phi = 120^\circ$) is responsible for the accumulation of high
concentration levels in the diffusive sub-layer. This causes a significant overshoot of oxygen concentration very close to the wall (after 90°), which is responsible for modulating the mass transfer across the SWI. The intensity of such overshoot exceeds by an order of magnitude the one of fluid layers of above-average concentration propagating in the outer field.
Chapter 5

Large-eddy simulation of variable sediment oxygen uptake in a transitional oscillatory flow

5.1 Abstract

We have tested an oxygen transport model based on the large-eddy simulation (LES) technique, in a transitional oscillatory flow observed in the bottom boundary layer of lake Alpnach. The highly variable state of turbulence and the very small scales associated with oxygen transport, raise questions on the suitability of a Reynolds-Averaged Navier-Stokes Equation (RANSE) model in predicting the essential features of this flow; by directly resolving the full range of governing transport processes, LES provides a reliable prediction of the sediment-oxygen uptake (or demand, SOD), even in non-equilibrium conditions. The simulation parameters have been calibrated against the first available set of published in-situ DO measurements. The thus-obtained fully developed flow is used as an initial condition for the imposed oscillatory forcing. The turbulent momentum and mass transport in the outer layer is in equilibrium with the main current throughout most of the cycle. Numerical predictions reveal non-equilibrium effects limited to the diffusive sublayer response to the external forcing. During flow deceleration the concentration boundary layer slowly expands as the overlying turbulence is left to decay; later, during re-transition, turbulent transport is restored by intense turbulent production events which enhance the SOD with a well-defined time lag. A simple model for the SOD is proposed, for eventual inclusion in RANSE biogeochemical management-type models, building on parametrizations used in turbulent mass transfer, and with the support of published numerical data and the present simulation. The only input parameters required are the sediment oxidation rate, bulk temperature and oxygen concentration, and friction velocity.
5.2 Introduction

The prediction of dissolved oxygen (DO) concentrations is critical for managing and monitoring marine ecosystems. Oxygen evolves in water bodies as a high-Schmidt-number passive scalar with saturation levels highly dependent on temperature. It is entrained at the surface and transported down the water column by turbulent motions. Many natural factors can interfere with this mixing process such as stratification, which damps the turbulence, reducing the supply of oxygen to the near-bed region. Here, in the sediment layer, decomposition of dead organic matter (resulting from eutrophication, i.e. the ecosystem response to the introduction of excess artificial or natural nutrients) by oxygen-consuming bacteria can cause the DO concentration to drop to unsustainable levels for aquatic life making the sediment-oxygen uptake the most important factor affecting oxygen depletion in the hypolimnetic layers (below the thermocline) of stratified water bodies (Patterson et al. 1985, Scalo et al. 2012c, Bouffard, et al. 2012).

Despite the considerable environmental and economical impacts of oxygen depletion (Committee on Environment and Natural Resources 2010b) the interaction among all the processes involved in oxygen transport across the sediment-water interface (SWI) and absorption by an organic sediment bed is still not well understood, with obvious consequences on the quality of modelling. The prediction of the different components of the oxygen budget throughout the water column still suffers from many deficiencies, including incomplete large-scale turbulence modelling (which includes obvious computational limits and narrow range of applicability of Reynolds-Averaged Navier-Stokes Equations (RANSE) models) and imperfect (or missing) parametrization of the biogeochemical transport processes occurring at or below the sediment-water interface, in the porous bed. Numerical studies have shown that fully understanding the biological responses to physical variability requires models that couple hydrodynamics and the dynamics of water quality and aquatic organisms (Koseff et al. 1993, Boegman et al. 2008a). The broad spectrum of physical processes leading to oxygen depletion can be grouped into water-side and sediment-side transport (Grant & Marusic 2011); in general, the problem of solute transport in the environment involves up to 41 principal diffusive and advective transport processes (Thibodeaux & Mackay 2011).

Transport on the water side is governed by hydrodynamics. In the presence of turbulence, resolving and/or modeling the broad range of spatial and temporal scales is the first challenge. The velocity spectrum extends from basin-scale waves (order of kilometers) down to the Kolmogorov length scale, \( \eta \) (order of centimeters or less); a high-Schmidt-number scalar, such as oxygen and many other biolimiting contaminants dissolved in water, will also exhibit sub-Kolmogorov scales, extending down to the Batchelor scale, \( \eta_B \) (of the order of \( \eta/30 \) for DO), and a very thin diffusive sublayer at sediment-water interface (of the order of millimeters) (Wiest & Lorke 2003). Its thickness is regulated by the near-wall coherent turbulent structures and is inversely proportional to the instantaneous mass flux. Hanratty (1956) was perhaps the first to identify and model...
the high unsteadiness of a high-Schmidt-number diffusive sublayer. Further work on its characterization has been carried out by Reiss & Hanratty (1962), Sirkar & Hanratty (1970), Pinczewski & Sideman (1974) and Campbell & Hanratty (1983b) who concluded that high-Schmidt-number mass transfer is controlled only by the low frequency component of the near-wall turbulent vortical structures and that its intensity (in steady state mass transfer problems) is correlated to the mean wall-shear stress. Scalo et al. (2012a) extended this analysis to the case of a statistically steady-state oxygen transfer to flat organic sediment beds, showing how the mass transfer is sustained by intense bursting events that leave their signature in the sediment layer over time scales typical of bacterial absorption. The presence of roughness can add further complications by altering the structure of the near-wall transport, changing the overall rate of mass and momentum transport, depending on its characteristic size. The latter can span a wide range of scales, from the single sediment grain to the large-scale roughness, characterized by the wavelength and amplitude of the bedform shape (van Rijn 1984).

On the sediment side a wide range of processes occur, including biochemical reactions and hyporheic transport, defined as the exchange of solutes and fluid, between a flow and the sediment immediately adjacent to it, by means of advection (Grant et al. 2012). Due to their inherent complexity, diversity and multi-scale nature, an empirical approach is often inevitable. The most important biochemical process governing oxygen depletion is bacterial absorption via organic matter decomposition, currently modeled as a non-linear sink term whose intensity is proportional to the average bacterial population density \( \chi \) (which is not directly measurable (Higashino et al. 2008)). Other chemical processes that can affect the DO oxygen concentration in the sediment layer include (but are not limited to) denitrification, manganese- and ferric-oxide reduction, sulfate reduction and methane production (Boudreau & Jørgensen 2001). In general, every solute dissolved in the pore water is transported by means of molecular diffusion, governed by porosity, \( \varphi \), mean advection and dispersion by pore water flow, governed by permeability, \( K \). Depending on the sediment’s properties the transport can be diffusion- or advection-dominated and, in the latter case, significant momentum exchange with the flow can occur. Pore water flow is driven by a non-uniform pressure distribution at the interface which is due, for example, to pressure waves generate by traveling waves (Riedl, et al. 1972), fluctuating pressure distributions due to a turbulent boundary layer, or persistent pressure differences due to an uneven bed form (Boudreau & Jørgensen 2001). In presence of a sharp interface, oxygen transfer from the fluid to sediments across the interface occurs by means of direct diffusion (driven by concentration gradient) and advection (driven by the normal-to-interface velocity component). However, if sediment resuspension and bi-phasic flow are present (typically due to high values of bed-shear stresses and fine particle sizes) the nature of these mechanisms may be more complex and requires careful modeling (Higashino & Stefan 2012).

Complete (water and sediment) measurements have been carried out in a laboratory recirculating flume by O’Connor & Hondzo (2008). A few numerical attempts, to our knowledge, have been made to reproduce
these experimental results, primarily with Reynolds-Averaged Navier-Stokes Equations (RANSE) (Higashino et al. 2008) and LES (Scalo et al. 2012b). Good agreement was found in general for low current intensities. The calibrated bacterial population returned, in both cases, values that exceeded the expected maximum by a factor of 3 and 2, respectively. Discrepancies were observed for higher current intensities (exceeding 7 - 8 cm s\(^{-1}\)) and attributed, by Higashino et al. (2008), to pore-water-flow-induced transport in the sediment layer which had not been taken into account. This has been extensively investigated by Scalo et al. (2012b) in the case of a statistically steady turbulent flow evolving over a flat sediment bed; they showed that building on the solute exchange models developed by Higashino et al. (2009) and Higashino & Stefan (2011), dispersion effects can become dominant for high permeabilities, whereas mean advection (driven by small-scale turbulent pressure fluctuations) is always negligible. Moreover, the inclusion of the dispersion and advection in the model did not remove the observed discrepancies and the question of how to correctly couple eddy resolving methods such as LES with lower-order hyporheic exchange models still deserves further consideration.

The above mentioned lab-scale work focuses on transport dynamics in the near-wall and sediment regions. Strong assumptions are made to extrapolate the results of such investigations to field scale, for which extensive data is very onerous to collect. In Bryant et al. (2010) turbulence induced by oscillatory fluid motions and the vertical distribution of DO above and within the sediments were measured and analyzed in Lake Alpnach, a lake in central Switzerland that exhibits pronounced seiching (i.e. presence of basin-scale standing waves characterized by very long oscillation periods). The transient nature of the sediment oxygen uptake is stressed, as well as its correlation with the near-wall turbulent intensity. This is the first attempt to correlate sediment oxygen demand to the large-scale dynamics, and is a natural extension of the earlier work by Lorke et al. (2003) who focused on the near sediment region. Brand, et al. (2008) has also investigated, for the same lake, turbulent oxygen transport dynamics in the outer region with the eddy-correlation (EC) technique, revealing a highly intermittent behaviour of the vertical oxygen turbulent flux sometimes exceeding (therefore not in equilibrium with) the sedimentary oxygen uptake. This is confirmed by the turbulent transport mechanisms found in the numerical study by Scalo et al. (2012c) of the transient oxygen uptake driven by a low-speed oscillating turbulent boundary layer.

All of the aforementioned processes are only some of the physical processes occurring in aquatic environments that need to be taken into account when attempting to predict DO levels in realistic configurations. However, for field scale applications, there is no process-oriented model for the sediment oxygen uptake that can take advantage of all the resolved quantities in currently adopted RANSE models. The most advanced aquatic ecosystem model, to our knowledge, is the Computational Aquatic Ecosystem Dynamics Model (CAEDYM) (Hipsey & Hamilton 2008). Here, a simple sediment oxygen flux model is available, called static sediment oxygen demand model, where the DO flux to the sediments is simply a function of the near-bed water temperature and dissolved oxygen concentration, bounded by an assigned maximum value. Other
(minor) contributions to the dissolved oxygen in the sediment pore water include photosynthesis, respiration and production caused by macrophytes, seagrass and macroalgae. A more sophisticated model for the sediment oxygen flux, referred to as the dynamic model, is also available and incorporates a comprehensive characterization of the sediment geochemistry and the organic matter diagenesis. Although the dynamic model already includes a Fickian-based model for the solute flux (from the water side) at the SWI, there is no explicit dependency, in its formulation, on near-wall flow parameters such as wall-shear stress or turbulent dissipation. As the literature shows, the DO flux to the sediment layer depends heavily on the fluid-dynamic conditions (Bryant et al. 2010, O’Connor & Hondzo 2008); if the flow is laminar or turbulent mixing is not fully established or is inhibited by other factors, the DO flux to the sediments can become negligible, given the low diffusivity of dissolved oxygen in water.

At present the flux is typically a tune-able parameter, fixed in time (and often in space) chosen over an order of magnitude scale so that water-quality models can reproduce observations. In Trolle et al. (2008), for example, the DO flux to the sediments is fixed to 0.7 g m$^{-2}$ day$^{-1}$ as a calibration parameter for the one-dimensional water-quality model DYRESM-CAEDYM to match data for Lake Ravn, a deep lake in Denmark. This model couples a one-dimensional hydrodynamic model (DYRESM), which resolves the vertical distribution of temperature, salinity and density in a lake (or reservoir), with the water-quality model CAEDYM. The three-dimensional hydrodynamic model ELCOM driving the CAEDYM model is adopted in the work by Leon, et al. (2006), where good agreement with measured DO profiles in Lake Erie was found. A static model for the SOD is used with a maximum value of 0.6 g m$^{-2}$ day$^{-1}$ (Leon, et al. 2012). A two-dimensional coupled hydrodynamic and water-quality reservoir model, CE-QUAL-W2 was adopted by Boegman et al. (2008b) for Lake Erie’s western basin with the same purpose. Here an SOD coefficient of 0.55 g m$^{-2}$ day$^{-1}$ was used. Based on the formulation in Zhang, et al. (2008) (similar to the static CAEDYM model) Conroy, et al. (2011), for the same lake, used a maximum SOD of 0.23 g m$^{-2}$ day$^{-1}$. Patterson et al. (1985) used 0.39 g m$^{-2}$ day$^{-1}$, obtained from Burns & Ross (1972) for central Lake Erie in August. These models simulated different years and used validation data from different sites, which perhaps explains the differences. The tuning of the SOD is, however, year-dependent and modeled values differ from the observations. Matisoff & Neeson (2005), for example, report values for the SOD in Lake Erie exhibiting more than an order of magnitude difference (from 0.1 to 5.5 g m$^{-2}$ day$^{-1}$) due to seasonal and spatial variations. This variability is not captured in the CE-QUAL-W2 and CAEDYM models where SOD is fixed in time and space (except for the temperature dependence in CAEDYM). The variation between observed and model-adopted values motivates the need to develop a time-space variable predictive model for SOD that may be included in a RANSE code.

In the present work we adopt the eddy-resolving oxygen transport model developed by Scalo et al. (2012b) to numerically investigate the processes leading to the unsteady sediment-oxygen uptake observed in Bryant
et al. (2010) by accurately resolving the near-wall turbulent velocity field and concentration distribution across the SWI. The goal is to understand the limitations of the adopted modeling approach and test the validity of commonly used assumptions, in a realistic geophysical environment.

In the following, we briefly describe the complete transport model and the problem setup. Results are then presented describing the initial conditions used at the beginning of the 8-hr seiche cycle and then the transient response of the near-wall region is analyzed and compared to field scale measurements. The observed flow physics are discussed and compared to previous related field-scale work. Finally, a simple parametrization of the sediment-oxygen uptake for field scale (wall-modeled) LES or RANSE applications is also derived based on the understanding of the fundamental near-wall mass transport mechanisms and with the support of the observed data.

5.3 Methodology

The choice of large-eddy simulation— RANSE models provide accurate predictions of mean profiles of velocity and other transported quantities in fully developed, high-Reynolds-number flows in simple configurations. However, in the presence of non-equilibrium turbulence, fully three-dimensional mean velocity fields or complex geometries, they fail to provide the required level of accuracy. Moreover, a RANSE approach does not allow the estimation of higher-order turbulent statistics or the interpretation of mixing dynamics, which are entirely modeled. Large-eddy simulations (LES), on the other hand, are a well established approach in the field of turbulent simulations allowing the estimation of turbulence characteristics for a wide variety of flows. The main idea is to adopt grids fine enough to resolve directly the evolution of those large turbulent scales that are strongly dependent on the initial and boundary conditions, while modeling the residual mixing and dissipation occurring in the unresolved subgrid scales, which are supposed to exhibit universal characteristics (Richardson 1922, Kolmogorov 1941b). Depending on the adopted model, LES can provide three-dimensional, time-dependent solutions of the filtered Navier-Stokes equations with the same accuracy of direct numerical simulations (DNS) at the large scales, but, at a significantly lower cost. The resolution of all the turbulent scales in the presence of dissolved oxygen would require a grid that is approximately 30 times finer in each direction than a simulation without a transported contaminant. This makes DNS of high-Schmidt-number scalars, like dissolved oxygen, prohibitive, especially for field-scale applications. LES can be a feasible alternative since the scalar field and the velocity field share the same integral scale (Tennekes & Lumley 1972), and the effect of all subgrid scales (sub-Kolmorogorov and not) are accounted for in the model, explained in the following.
The mathematical model—The governing equations on the water side for the velocity field are the filtered continuity and Navier-Stokes equations (Leonard 1974):

\[
\frac{\partial \pi_i}{\partial x_i} = 0, \quad \text{(5.1)}
\]

\[
\frac{\partial \pi_j}{\partial t} + \frac{\partial \pi_i \pi_j}{\partial x_i} = - \frac{1}{\rho} \frac{\partial p}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_i} - f_1 \delta_{ij} - f_3 \delta_{ij} + \nu \nabla^2 \pi_j \quad \text{(5.2)}
\]

where \(x_1, x_2, x_3\) (or \(x, y, z\)) are, respectively, the west-to-east, wall-normal and north-to-south directions, \(\bar{u}_i\) the filtered velocity components in those directions, and \(\rho\) and \(\nu\) are the fluid density and kinematic viscosity, \(\delta_{ij}\) the Kronecker delta. The forcing terms \(f_1\) and \(f_3\) are the two mean pressure gradient components adjusted to achieve the desired flow rate in the \(x\) and \(z\) directions.

The filter used is a top-hat filter composed of three one-dimensional 3-point discrete filters. The subgrid scale (SGS) stresses \(\tau_{ij} = \pi_i \pi_j - \pi_i \pi_j\) are parametrized by an eddy-viscosity model:

\[
\tau_{ij} - \delta_{ij} \tau_{kk}/3 = -2 \nu_T \bar{S}_{ij} \quad \nu_T = C \Delta^2 |\bar{S}| \quad \text{(5.3)}
\]

where

\[
\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \pi_i}{\partial x_j} + \frac{\partial \pi_j}{\partial x_i} \right) \quad \text{(5.4)}
\]

is the filtered strain-rate tensor and \(|\bar{S}| = (2\bar{S}_{ij}\bar{S}_{ij})^{1/2}\) is its magnitude; \(\Delta = (\Delta_x \Delta_y \Delta_z)^{1/3}\) is the filter width. The coefficient \(C\) is evaluated using the dynamic procedure (Germano et al. 1991, Lilly 1992), and averaged over directions of statistical homogeneity (in this case, planes parallel to the sediment-water interface). In this technique, information from the smallest resolved turbulent eddies is used to model the residual mixing due to the unresolved ones. By construction, the subgrid-scale contribution in the model automatically vanishes when turbulent fluctuations are suppressed in case of, for example, flow laminarization (Piomelli & Liu 1995, Piomelli & Scalo 2010).

The oxygen concentration field is modeled as a high-Schmidt-number passive scalar where the Schmidt number, \(Sc = \nu/D\), is the ratio between the kinematic viscosity of water and the molecular diffusivity of dissolved oxygen. The same SGS closure for the velocity field is used for the modelling of the unresolved turbulent scales of the dissolved oxygen field. The filtered conservation equation for DO is

\[
\frac{\partial c}{\partial t} + \frac{\partial \pi_i c}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ D \frac{\partial c}{\partial x_i} - J_{gs} \right]\quad \text{(5.5)}
\]

which is absorbed across the sediment-water interface (SWI) by an organic sediment layer. Here the instantaneous DO concentration is transported by means of diffusion, advection and dispersion but also depleted
exclusively by decomposing organic matter according to

\[
\frac{\partial c_s}{\partial t} + \frac{\partial u_{si} c_s}{\partial x_i} = \frac{\partial}{\partial x_i} \left( [F(\phi)D + D_e] \frac{\partial c_s}{\partial x_i} \right) - \dot{c}_s
\]

(5.6)

Here the effects of porosity and tortuosity on diffusion in the pore water are accounted for in \( F(\phi) \) (which can be approximated by \( \phi^3 \) for high porosities, \( \phi > 0.7 \)), whereas dispersion effects are modelled by an effective diffusivity, \( D_e \), calculated based on the parametrization proposed by Higashino & Stefan (2011) and, later on, extended to instantaneous quantities by Scalo et al. (2012b), resulting in

\[
D_e = \phi^2 d_s (u_{si} u_{sj})^{1/2}
\]

(5.7)

where \( d_s \) is the sediment grain size, proportional to the square root of permeability via the Kozeny-Carmen relationship (Bear 1972), and \( u_{si} \) is the \( i \)-th component of the interstitial velocity vector given by Darcy’s Law

\[
 u_{si} = -\frac{K}{\mu_w} \frac{\partial p_s}{\partial x_i}
\]

(5.8)

where \( \mu_w \) is the dynamic viscosity of water and \( p_s \) is the pore-water pressure that satisfies a Laplace equation in the sediment layer (Scalo et al. 2012b) enforcing the continuity condition (incompressible pore water). The parametrization for the non-linear sink term, \( \dot{c}_s \), is

\[
\dot{c}_s = \mu c_s \frac{c_s}{K_{O_2} + c_s}
\]

(5.9)

where \( \mu \) is the maximum oxidation rate that can be expressed as (Higashino et al. 2008),

\[
\mu = \frac{\mu_0}{Y_c} \chi
\]

(5.10)

where \( \mu_0 \) is maximum specific DO utilization rate (in day\(^{-1}\)), \( K_{O_2} \) is the half-saturation coefficient for DO utilization (in mg L\(^{-1}\)), \( Y_c \) is the effective yield for the microbial utilization of DO and \( \chi \) (in mg L\(^{-1}\)), is the value of biomass concentration of oxygen absorbing organisms, currently not directly measurable. The values of these constants are shown in Table 5.1. We will assume a constant and uniform value of \( \chi \) in the sediment layer. While the overall SOD is approximately proportional to this quantity, the oxygen concentration at the sediment-water interface exhibits a reduced sensitivity to \( \chi \), varying less than 10% for changes of 100% in the bacterial population (Scalo et al. 2012b).

The complete model has been validated by reproducing fluid dynamic conditions for different flow rates and temperatures in a laboratory flume where complete (water and sediment) DO measurements were obtained from micro-sensor data by O’Connor & Hondzo (2008). The numerical predictions show good agreement with
Table 5.1: Bio-geochemical parameters for oxygen absorption model (5.9) and transport (5.6), (5.8) in the sediment layer. Maximum oxidation rate, $\mu$, (5.10); maximum specific DO utilization rate, $\mu_0$; Biomass concentration of oxygen absorbing organism, $\chi$; effective yield for the microbial utilization of DO, $Y_c$; half-saturation coefficient for DO utilization, $K_{O_2}$; sediment layer porosity, $\varphi$, and intrinsic permeability, $K$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>240 mg L$^{-1}$ day$^{-1}$</td>
</tr>
<tr>
<td>$\mu_0$</td>
<td>2.4 day$^{-1}$</td>
</tr>
<tr>
<td>$\chi$</td>
<td>100 mg L$^{-1}$</td>
</tr>
<tr>
<td>$Y_c$</td>
<td>1 mg$_{DO}$ mg$^{-1}$</td>
</tr>
<tr>
<td>$K_{O_2}$</td>
<td>0.6112 mg L$^{-1}$</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>0.94</td>
</tr>
<tr>
<td>$K$</td>
<td>$2 \times 10^{-7}$ cm$^2$</td>
</tr>
</tbody>
</table>

Figure 5.1: Sketch of three-dimensional doubly-periodic open channel with an oxygen absorbing sediment layer (a); time series of mean current velocity at 10 cm from the SWI (b), west-to-east, $\langle u \rangle$ (---), and south-to-north, $-\langle w \rangle$ (---), components predicted by LES and corresponding measurements by Bryant et al. (2010) (○) via acoustic Doppler velocimeter (ADV).

5.4 Computational setup

Boundary conditions — The computational setup used is a turbulent open channel driven by two components of the pressure gradient (along $x$ and $z$) with an underlying DO absorbing organic sediment bed (Figure 5.1 (a)). The boundary conditions are periodic in the west-to-east ($x$) and south-to-north ($-z$) directions for all quantities. Homogeneous Neumann conditions are applied to the DO field at the bottom of the sediment layer ($y = -\delta_s$) and at the top boundary ($y = L_y$) on the water side; the fluctuating DO flux at the sediment-water interface (SWI) is dynamically assigned to the water side by solving at every time step equation (5.6) in the sediment layer with the coupling strategy developed by Scalo et al. (2012b). Free-slip conditions are applied to the velocity field at the top boundary whereas, at the SWI, the assigned velocities match the ones calculated by the pore-water-flow solver (5.8) in the sediment layer (negligible with respect to the friction.
velocity).

Initializing large-eddy and direct numerical simulations— In eddy resolving methods such as direct numerical simulations (DNS) or LES it is common practice to use instantaneous flow fields, stored from previously converged simulations on the same grid, as initial conditions to start a transient calculation. In the case of statistically steady flows, if other realizations of the same flow field are not available, simulations are typically initiated on coarse grids, with random noise or by interpolating the solution of a previous (similar) simulation. Simulations are carried out initially by deactivating the subgrid scale model. This prevents dissipation (not resolvable on the grid but still modelable) from damping turbulent fluctuations being generated by production mechanisms (occurring at large scales, thus resolvable even on coarse grids). The flow field is then integrated in time until a physical, statistically steady state is reached, losing memory of the unphysical initial conditions. The thus-obtained converged solution is then interpolated on a refined grid at the desired resolution and the model is added if needed. On the other hand, in unsteady and transitional flows like the one analyzed in this work the flow is highly dependent on the turbulent field used as an initial condition. Also, the prediction of transition can be affected by the grid-size, particularly in LES. By starting the simulations with a previously developed fully turbulent and statistically steady flow we insure that the simulated flow in time range of interest (between \( t = 0 \) h and \( t = 11 \) h) is always physical. ‘Real world’ flows take on a wide range of additional complexities and knowing the actual initial conditions and boundary conditions to an accuracy required for a realistic LES is impossible.

Seiche forcing and initial velocity field— A statistically steady turbulent velocity field is first obtained by running the numerical model until convergence with fluid dynamics conditions corresponding to the ones observed at 10 pm in Bryant et al. (2010), which is time \( t = 0 \) h in the present calculation. In particular, the two velocity components measured at \( y = 10 \) cm, in the west-to-east and south-to-north directions, at this time (Figure (b)), were matched by imposing a flow rate, in both directions, calculated by analytical integration of an approximate velocity profile reconstructed assuming equilibrium conditions (i.e. velocity profiles are well approximated by the classic log-law). The resulting total friction velocity at time \( t = 0 \) h is

\[
\tau_{x,0} = \sqrt{\tau_{w,0}/\rho} \tag{5.11}
\]

where \( \tau_{w,0} = \sqrt{\tau_{w,0x}^2 + \tau_{w,0z}^2} \) is the magnitude of the total wall-shear stress where, at this time, \( \tau_{w,0z} \) is negligible with respect to \( \tau_{w,0x} \). The thus-obtained flow rates in both directions, imposed at time \( t = 0 \) h, are then varied (for \( t > 0 \) h) proportionally to the measured velocities at \( y = 10 \) cm by dynamically adjusting the pressure gradient terms \( f_1 \) and \( f_3 \) in (5.2). In spite of the approximations made, the two components of the velocity at \( y = 10 \) cm predicted by the LES (Figure 5.1 (b)) return a very good agreement with the observations.
Sediment layer parameters and initial DO distribution— The initial turbulent DO distribution is obtained from the same statistically steady simulation used to initialize the velocity field; in particular, the sediment layer maximum oxidation rate, $\mu$, and permeability $K$, have been adjusted in order to match the DO measurements at 10 pm (Profile 2 in the paper). A Schmidt number of $Sc = 1024$, consistent with a water temperature of $T \sim 8 ^\circ C$, and a porosity of $\varphi = 0.94$ (as suggested in Bryant et al. (2010)) have been adopted. A free stream dissolved oxygen concentration of $C_{\infty} = 3.84 \text{ mg L}^{-1}$ is used at $t = 0$. For these parameters, a bacterial population of $\chi = 100 \text{ mg L}^{-1}$ returned the best match inside the sediment layer at the initial time $t = 0$ under steady-state conditions. Also, a permeability of $K = 2 \times 10^{-7} \text{ cm}^2$ has been chosen to account for the gradient discontinuity in measured oxygen profiles which is, in some cases, not present (or visible) and in other cases inverse, that is to say, consistent with an overall diffusivity in the pore water higher than the one on the water side (see Results). This can only be explained by a dispersive behaviour of the sediment layer (Scalo et al. 2012b), due to the relatively high value of porosity. After time $t = 0$ h the initial concentration field is left to decay, with no top-boundary re-aeration and with an instantaneous absorption rate modulated by the transient flow. The bulk oxygen value will decay by only 3% over 10 hours.

Domain size— The vertical extent of the computational domain $L_y$ has been chosen so that $Re_{\tau,0} = u_{\tau,0}L_y/\nu = 400$ at $t = 0$ h. This results in $L_y = 52$ cm. Simulating a shorter water-column would have the effect of reducing the size of the outer scales, introducing low Reynolds numbers effects. A taller domain would increase the size of largest eddies in the outer layers, increasing the overall computational cost (more points would be needed in $y$), without any significant benefit for the present calculation. Although the outer layer structures would be better resolved (in $x$ and $z$), they typically exhibit a mild influence on the near-wall turbulence which, for $Re_{\tau,0} > 400$, starts to exhibit Reynolds number invariance (Moser, et al. 1999b); the near-wall structures, if normalized by $u_{\tau,0}$ and $\nu$ (fixed quantities in our problem), exhibit universal characteristics that are (approximately) unchanged by the Reynolds number, i.e. unchanged by the domain height, in this case. Moreover, the near-wall transport events are the only ones that need to be accurately reproduced in order to predict the DO flux across the SWI (Scalo et al. 2012b). The extension of the computational domain in the other two directions, $L_x$ and $L_z$, is chosen to accommodate the largest scales and the near-wall structures.

Numerical Model— The numerical model used to compute the flow on the water side is a well-validated finite-difference code (Keating et al. 2004), based on a three-dimensional Cartesian staggered grid. Second-order central differences are used for both convective and diffusive terms. The time advancement scheme is a Crank-Nicolson scheme for the wall-normal diffusive term, and a low-storage third-order Runge-Kutta method for the other terms. The solution of the Poisson equation is obtained by Fourier transform of the equation in the spanwise and streamwise directions, followed by a direct solution of the resulting tridiagonal matrix, at each wavenumber. The code is parallelized using the MPI protocol. The equations in the sediment layer
Table 5.2: LES parameters. Water side computational box extension in the west-to-east, $L_x$, south-to-north, $L_z$, and vertical, $L_y$, direction. Thickness of sediment layer, $\delta_s$. Grid points in the respective directions $N_x, N_z, N_y$ and $N_{y,s}$. Kinematic viscosity of water $\nu$ and molecular diffusivity of oxygen, $D$.

<table>
<thead>
<tr>
<th>$L_x$ (cm)</th>
<th>$L_z$ (cm)</th>
<th>$L_y$ (cm)</th>
<th>$\delta_s$ (cm)</th>
<th>$N_x$</th>
<th>$N_z$</th>
<th>$N_{y,s}$</th>
<th>$\nu$ (cm$^2$/s)</th>
<th>$D$ (cm$^2$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>150</td>
<td>52</td>
<td>1</td>
<td>128</td>
<td>48</td>
<td>192</td>
<td>$1.39 \times 10^{-2}$</td>
<td>$1.36 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Figure 5.2: Profiles of mean (——) and resolved RMS (— —) for west-to-east velocity component (a) and dissolved oxygen (b) at time $t = 0$ h. Oxygen measurements obtained via microprofiling by Bryant et al. (2010) (symbols) at 10 pm.

are solved with the same numerical approach as the one adopted for water side and have the same accuracy and stability properties.

Spatial and temporal resolution— The grid resolution at time $t = 0$ h is $\Delta x^+ = 18$ and $\Delta z^+ = 11$ where ($^+$) are wall units, i.e. lengths normalized by $\nu/u_\tau$. A high resolution is used to account for the effects of the seiche-induced high variability of the wall-shear stress (resulting in a highly variable turbulent spectrum, and the presence of turbulence decay and re-transition), to reduce the numerical dissipation due to a mean current not aligned with the grid lines and, finally, to accurately resolve the high-Schmidt-number passive scalar field. This results in a grid size of approximately $\Delta x = 2.3$ cm and $\Delta z = 0.8$ cm. A grid convergence test has been carried out by progressively refining the solution from coarser grids. No significant difference in the statistics has been observed in the last grid refinement step leading to the present resolution. The grid resolution in the wall-normal direction $\Delta y$ at the SWI (in the diffusive sublayer) is one tenth of a millimeter. The Navier-Stokes solver time step varied in the range of 0.01- 0.1 seconds.

5.5 Results

Steady state: initial conditions — The RMS and mean profiles of the statistically steady velocity and concentration field, used as initial conditions, have been averaged over 2 hours and are shown in Figure 5.2. The flow rate was adjusted so that the mean velocity at $y = 10$ cm, approximately $1.65$ cm s$^{-1}$, matches the
Figure 5.3: Oxygen concentration profiles before flow reversal ($t < 6$ h) (a), (b), (c) and (d); after flow reversal ($t > 6$ h) (e), (f), (g) and (h); oxygen measurements obtained via microprofiling by Bryant et al. (2010). Top panel: magnitude of mean velocity vector, $V$, at 10 cm from the SWI.
measured one at time $t = 0 \ h$ (Figure 5.1 (b)). For these flow conditions, the RMS peak in the streamwise component of the velocity is located at $y = 1.8 \ \text{cm}$ from the SWI, where buffer-layer turbulent transport events occur. These are responsible for governing the high-Schmidt-number mass transfer across the SWI and sustaining the scalar variance profile that peaks at $y = 1.4 \ \text{mm}$, approximately the edge of the diffusive sublayer. The gradient of the corresponding oxygen distribution appears to be continuous across the SWI; in reality, the enhanced diffusivity due to dispersion effects, which tend to reduce the overall DO gradient (increase the mixing) in the sediment layer, for a given flux at the SWI, are compensated by the reduced molecular diffusion in pore water due to porosity. The diffusive sublayer predicted by the calibrated LES is slightly thicker than the one observed in the measurements. A better agreement with the oxygen measurements on the water side could be obtained by decreasing the bacterial population, $\chi$, increasing the Reynolds number or increasing the permeability, $K$. In the first case, the oxygen levels in the sediment layer would be significantly overestimated, given the relatively reduced sensitivity of the oxygen distribution on the water side to variations in $\chi$ (Scalo et al. 2012b). Increasing the Reynolds number would improve the agreement, for $0 < y < 1 \ \text{mm}$, by reducing the diffusive sublayer thickness. This would, however, require the adoption of physical parameters (water temperature, viscosity, current velocity, etc.) not consistent with the flow conditions in Bryant et al. (2010) and, therefore, not justifiable. Increasing the permeability would increase the DO penetration depth in the sediment layer by increasing the effective diffusivity of the sediment layer; this would increase the overall absorption and, therefore, increase the DO flux from the water side and improving, only here, the agreement. This would, however, also result in severe discrepancies in the pore water DO distribution. For the particular flow investigated, the observations reveal a well defined structure of the diffusive sublayer and, despite the presence of dispersive effects in the measured oxygen profiles, their influence on the transport dynamics are of secondary importance, as shown later.

An interesting feature of the measured oxygen profiles, also observed in lab-scale measurements (O’Connor & Hondzo 2008) but not reproduced in our numerical model at this stage, is the noticeable gradient discontinuity visible, on the water side, at $y \simeq 1 \ \text{mm}$. This is present in many measured profiles (for example at $t=0.8, 3.2, 9.0, 10.5 \ \text{h}$ in Figure 5.3). This discontinuity could be explained with an abrupt variation in the eddy diffusivity (from zero, for $y < 1 \ \text{mm}$, to a finite value, for $y > 1 \ \text{mm}$) which, however, cannot be found in fully developed turbulent concentration boundary layers. For example, the modeled subgrid shear stress in a channel flow varies smoothly as the cube of the distance from the wall (Piomelli, et al. 1988). A possibility is that the concentration boundary layer is at its early stages of spatial development and the sharp variation in the mean gradient is actually determined by the upwardly propagating front of concentration defect. This issue requires further investigation.

**Transient evolution of DO profiles**— The complete evolution of the oxygen concentration for $t > 0$ is shown in Figures 5.3 (a) to (h). The effects of the flow acceleration (from $t=0$ to $t = 2 \ \text{h}$) are visible in
the thinning of the diffusive sub-layer (resulting from the enhanced buffer-layer turbulent mixing, discussed later). In this phase, the LES follows closely the observations.

During the initial stage of the deceleration phase \((2 \, h < t < 4 \, h)\) the diffusive sublayer thickness predicted by the numerical model undergoes a more rapid increase, with respect to the observations, following closely the reduced intensity of the overlying turbulent transport (shown later). Good agreement is recovered at \(t = 4.8 \, h\) where the observed and predicted DO flux across the DO match. At this stage, the DO profiles start to exhibit a laminar-like shape. Although the observed diffusive sublayer starts to expand later than in the model predictions, it does so more rapidly and steadily, until the end of the deceleration phase (up to \(t = 6 \, h\), right before flow reversal). On the other hand, the concentration boundary layer predicted by the LES exhibits a very slow expansion (from \(t = 4 \, h\) to \(t = 6 \, h\)) retaining a higher value of the DO flux across the SWI. The low molecular diffusivity of dissolved oxygen becomes an important limiting factor for the rate of expansion of the diffusive sublayer.

Complete re-transition is evident from the DO profiles for \(t > 6 \, h\), when the current is reaccelerating towards south (Figure 5.1 \((b)\)), and good agreement with the field measurements is observed. However, understanding the mechanisms leading towards the restoration of a fully developed turbulent mass transport requires a better characterization of the hydrodynamics in the near-wall portion of the water column Scalo et al. (2012a).

Near-wall turbulence governing the sediment-oxygen uptake—A reliable prediction of the DO profiles can only follow from the correct prediction of the near-wall turbulent activity. The latter is entirely modeled in a RANSE computation and, also, highly dependent from the particular adopted method. Figure 5.4 shows the correlation between the intensity of the near-wall turbulent mixing, measured by the near-wall volume-averaged mean velocity fluctuation intensity,

\[
q' = \sqrt{\frac{1}{2} \int_{0}^{y_1} (u'^2 + v'^2 + w'^2) \, dy}, \quad y_1 = 1 \, cm \tag{5.12}
\]

and the DO flux across the SWI, \(J_{swi}\). As the flow decelerates with characteristic time-scales longer than that of turbulence, the turbulent kinetic energy decreases accordingly, approaching zero around \(t = 4.5 \, h\). At the same time, the sediment layer approaches an anoxic state, due to the reduced mass flux across the SWI (Figure 5.4 \((b)\)). However, while the total wall-shear stress (or momentum flux) follows \(q'\) closely, the DO flux to the sediment layer exhibits a delay in its response to the turbulent forcing of \(\sim 20 \, mins\), which is visible during the two abrupt acceleration events occurring after flow reversal, around \(t=6.6 \, h\) and \(7.6 \, h\). A slower response to variations in \(q'\) is present during the deceleration phase.

The predicted wall-shear stress in the west-to-east and south-to-north directions (Figure 5.4 \((a)\)) follows very closely the current velocities at \(y=10 \, cm\) (Figure 5.1 \((b)\)). This confirms the validity of the equilibrium
assumptions made on the velocity field when deriving the initial conditions for the present work and verified by Bryant et al. (2010). Moreover, non-equilibrium effects typically present in oscillating currents in the intermittently turbulent regime (Spalart & Baldwin 1987, Hino et al. 1983), such as violent production of turbulent kinetic energy at the end of the deceleration phase, break down of the validity of the log-law during the acceleration phase and visible phase lags between dissipation and the current, are not present in this case (shown later).

\[ u_\tau = \sqrt{\epsilon(y) k y} \]  
\[ (5.13) \]

where \( k \) is the Von Kármán constant (\( k = 0.41 \)), to dissipation measurements at \( y = 10 \text{ cm} \), extracted with the inertial dissipation method. The measured dissipation (Figure 5.5) is systematically lower than the value calculated directly from the resolved flow (including the modeled subgrid scale contribution) in our LES. The measured values (within the range \( 10^{-11} - 10^{-8} \text{ W kg}^{-1} \)) are, inexplicably, very close to analogous

Figure 5.4: Time-series of near-wall volume averaged (for \( y < 1 \text{ cm} \)) mean velocity fluctuation intensity \( q' \) (---), total friction velocity \( u_\tau \) (-----), west-to-east friction velocity (with sign) (----), south-to-north friction velocity (-----) (with sign), estimates of wall-shear stress using log-law of the wall by Bryant et al. (2010) (o) (a); oxygen concentration level at the SWI, \( c_{swi} \) (----), and sediment oxygen uptake, \( J_{swi} \) (----) (b).

Dissipation and wall-shear stress measurements vs LES—The corresponding total friction velocity estimated by Bryant et al. (2010) (Figure 5.4 (a)) does not follow the variations in the measured current velocity at \( y=10 \text{ cm} \) to the same extent of the numerical model. It was estimated by applying the law-of-the-wall,
measurements taken by Lorke, et al. (2002) in the same lake, for a lower-Reynolds-number flow, at \( y = 4 \) m from the SWI with local current intensities of \( \sim 3 \text{ cm s}^{-1} \). The present flow has current intensity of the same amplitude but observed at \( y = 10 \) cm, therefore, it should be much more energetic than what suggested by the dissipation measurements. Moreover, the observations in Bryant et al. (2010) show no sign of a significant stratification at \( y = 10 \) cm (possibly responsible for partial turbulent kinetic energy transfer to irreversible diapycnal mixing), or non-equilibrium, low-Reynolds-number effects (which are, instead, apparent in the observations of Lorke et al. (2002)), that could justify this apparent underestimation of the turbulent viscous dissipation. The predicted dissipation at \( y = 10 \) cm by our LES is consistent, via (5.13) (valid close to the wall and/or in high-speed flows), with the directly calculated total wall-shear stress (shown later, in Figure 5.9 (a)). In spite of the self-consistency of our results, also supported by the comparison with Lorke et al. (2002), the source of the observed discrepancy could still lie in the (idealized) adopted computational setup via, for example, an improper definition of boundary and/or initial conditions, and requires further investigation.

Turbulent transport dynamics— Figures 5.6 and 5.7 reveal the different features of the turbulent transport events that govern the mass transfer to the sediment layer, ultimately leading to oxygen depletion. The energy required for sustaining turbulent mixing and transport across the water column is provided by the mean current which is initially directed eastward, decelerates almost completely between \( t = 4 \) h and \( t = 6 \) h, and then reaccelerates by changing direction (heading south). Production mechanisms will, therefore, inject energy, from the large scales, into (primarily) the \( u' \) and \( w' \) velocity fluctuating components, respectively, before and after flow reversal as shown by the distributions of Reynolds shear stresses (Figures 5.6 (a) and (b)), RMS of turbulent velocity fluctuations (Figure 5.6 (c), and Figures 5.7 (a), (b), (c)) and turbulent kinetic energy production (Figure 5.7 (d)).

The gradual compression of the viscous sublayer for \( 0 \) h < \( t < 2 \) h is visible in the \( \langle u'v' \rangle \) Reynolds stress distribution, reaching the maximum intensity closest to the SWI between \( t = 1.5 \) h and \( t = 2 \) h, and in the RMS of velocity fluctuations. The signature of the milder accelerating crossflow (towards north) (Figure 5.1 (b)) is present in the \( \langle w'v' \rangle \) Reynolds stress distribution and RMS of \( w' \). The overall enhanced Reynolds shear stresses increase the rate of exchange of momentum with the no-slip boundary and, via the same transport mechanisms, increase the overall turbulent mixing and mass transfer rate, \( \langle c'v' \rangle \) (Figure 5.6 (d)), in the water column. The latter causes high-in-oxygen fluid to be ‘pumped’ towards the SWI more rapidly resulting in the thinning of the diffusive sublayer, visible in the oxygen concentration contours (Figure 5.6 (e)) and RMS of concentration fluctuations \( c' \) (Figures 5.7 (f)).

At this stage, there is no visible phase lag between the seiche-induced forcing, the enhanced turbulent activity across the water depth and the evolution of the near-wall concentration boundary layer. The turbulent and molecular momentum and mass fluxes are, approximately, in equilibrium at every time with the main current. During the deceleration stage (2 \( h < t < 6 \) h), the effects of turbulent transport have almost
Figure 5.5: Turbulent kinetic energy viscous dissipation at $y = 10$ cm; measurements by Bryant et al. (2010) (○) obtained by inertial dissipation method using longitudinal, planar, and vertical velocity data as measured via acoustic Doppler velocimeter (ADV), total (—), resolved (---) and modeled (……) dissipation directly calculated from LES.

completely vanished already at $t = 3$ h, remaining negligible, throughout the water column, until $t = 6$ h. During the whole period of ceased turbulent activity, the diffusive sublayer exhibits a slow but steady expansion, starting between $t = 2$ h and $t = 3$ h, limited by the long diffusive time scales of oxygen. This is consistent with the conceptual model for the near-wall transport described by Scalo et al. (2012a) where the same behaviour is observed at an instantaneous level in the case of a fully developed turbulent mass transfer problem.

The re-acceleration phase occurring for $t > 6$ h is, in this particular case, characterized by a less regular evolution. Most of the energy for mixing is, this time, provided by the main current directed south, (Figure 5.6 (b) and 5.7 (c)); accordingly, the near-wall turbulent structures responsible for mixing are now being re-oriented towards $-z$, feeding energy into the RMS of $w'$. The flow does not exhibit the same degree of equilibrium as observed before, which results in pronounced phase lags among the different transport processes involved, discussed in the following.

Two abrupt turbulent production events, leading to a rapid enhancement of the mixing in the water column, can be observed around $t = 6.9$ h and $t = 8.1$ h in Figure 5.6 (c) and (d) and Figure 5.7 (d) and (e). Although the acceleration stage of the background, 8-hour period oscillation, is slowly re-energizing the flow and, therefore, sustaining the overall turbulent transport, the two observed mixing events, in the present case, appear to be triggered, rather, by a two-hour-period mode, visible after flow reversal (Figure 5.1 (b)),

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from $t = 6$ h to $t = 9$ h. The time scales and current amplitude associated with it are consistent with a higher alongshore longitudinal mode 3 surface seiche (Boegman 2009).

The abrupt turbulent production mechanisms associated with them occur, however, only towards the end of the rapid acceleration phases, from $t = 6$ h to $t = 7$ h and from $t = 7.5$ h to $t = 8.2$ h, primarily in the north-to-south direction (Figure 5.1 (b)). The fact that the wall-shear stress level exhibits no visible delay (Figure 5.4) with respect to the current evolution suggests that turbulent kinetic energy is produced with the same mechanisms observed in oscillating turbulent boundary layers in the intermittent regime (short oscillating periods with respect to the free stream current intensity, see Literature Review of Chapter 4. The viscous sublayer is immediately compressed during the acceleration phase (affecting the wall-shear stress) at the end of which near-wall low-and-high speed streaks appear. These streaks then undergo instability which results in production and an upward propagation of turbulence at the beginning of the deceleration phase (Jimenez & Pinelli 1999, Costamagna et al. 2003). This also causes violent ejection of scalar variance from the edge of the diffusive sublayer, visible both in the scalar variance production (Figure 5.7 (e)) and intensity (Figure 5.7 (f)) distributions, leading to a sudden increase in the water column flux.

The resulting enhanced turbulent mass flux causes the thinning of the diffusive sublayer, and therefore, the enhancement of the mass flux at the SWI. This occurs with a delay of $\sim 20$ min (compare Figure 5.1 (b) or Figure 5.4 (a) to Figure 5.4 (b)), corresponding to a phase lag of $\phi \sim 60^\circ$ for a 2 h period oscillation. The same mechanisms observed here causing abrupt turbulent production events and sustaining the mass transfer in the time window between $t = 6$ h and $t = 9$ h, are the ones characterizing the transport dynamics in the oxygen transfer problem driven by an idealized, monochromatic oscillating current in the intermittent/non-equilibrium regime studied by Scalo et al. (2012c). The flow reverts, after $t = 8.5$ h, to a state very similar to the initial conditions used at $t = 0$ h, with fully sustained, quasi-steady, turbulent mixing and mass transfer across the SWI.
Figure 5.6: Contour plots showing history (from top to bottom) of Reynolds shear stresses $-\langle u'v' \rangle$ and $-\langle w'v' \rangle$, turbulent kinetic energy $q^2/2$, turbulent mass flux $-\langle c'v' \rangle$ and mean oxygen concentration $\langle c \rangle$. Transient simulation ($t > 0$ h) and steady state simulation used for initial condition ($t < 0$ h). Isolines of oxygen concentration in the bottom panel are for 1, 2 and 3 mg L$^{-1}$. 
Figure 5.7: Contour plots showing history (from top to bottom) of RMS of $u'$, $v'$, $w'$, production of turbulent kinetic energy, $P_k = -2\langle u'_i u'_j \rangle \partial \langle u_i \rangle / \partial x_j$, production of scalar variance $P_c = -2\langle c' u'_j \rangle \partial \langle c \rangle / \partial x_j$, and RMS of $c'$. Transient simulation ($t > 0$ h) and steady state simulation used for initial condition ($t < 0$ h).
5.6 A simple model for the sediment-oxygen uptake

In our LES calculation, the oxygen flux to the sediment layer is an output of the model and it can be directly calculated by considering the gradient of the instantaneous concentration and the velocities at the interface. In RANSE models used at field scale, the sediment-oxygen uptake is an input parameter (a boundary condition for the concentration field) and very little information on the state of the near-wall turbulence (or the bed morphology) is available to accurately model it; often a Reynolds stress, dissipation or eddy viscosity computed as an average over a time step and grid cell of the order of minutes and kilometers, respectively. Spatial resolution is also an issue. The vertical extent of the first computational cell from the SWI used in field-scale numerical models is comparable to (if not larger than) the entire height of the computational domain used here ($L_y = 52$ cm). The resolution required to accurately resolve the high-Schmidt-number transport mechanisms in such a limited domain (Table 5.2) makes a wall-resolved LES an unfeasible option for field-scale applications, given that the computational grid would also have to resolve large-scale motions such as basin-scale waves, determined by the lake bathymetry. The adoption of a RANSE (or wall-modeled LES) approach is, therefore, warranted and a simple algebraic model to estimate the SOD needs to be developed by using the few near-wall volume-average quantities available at run-time together with some biogeochemical information of the sediment layer, often very difficult to obtain. These include the bulk velocities in the two directions parallel to the bottom wall, $U_B$ and $W_B$, temperature, $T_B$, and oxygen concentration $C_\infty$, and the maximum oxidation rate, $\mu$.

Premise of the model—The following derivation will focus essentially on the water-side, diffusion-limited, component of the oxygen flux across the interface by using the present and previously published data based on LES. Although the effects of hyporheic exchange enter the model via Equation (5.7) and the velocity-matching condition at the interface (Scalo et al. 2012b), the available data does not allow a proper inclusion of these effects, due to the restricted range of permeabilities investigated, also limited to flat interfaces. Brennen and Imberger (pers. comm.) have shown that mass transport can be exclusively limited by the diffusive sublayer thickness, for example, in the deeper waters, away from the shoreline, and that a purely advective component to the flux across the SWI (in their case, induced by wave transport) can be linearly superimposed onto the molecular component. Also, a more robust hyporheic exchange parametrization, such as the one proposed by Grant et al. (2012) (sharing a similar functional form as (5.7)) could be incorporated in the present model, although strong assumptions regarding the resulting formulation of the parametrized flux, especially at the interface, would have to be made (Thibodeaux, et al. 2012).

Flux formulation—Building on parametrizations available in literature for high-Schmidt-number mass transfer (Boudreau & Jørgensen 2001), mostly valid under equilibrium conditions, we propose the following
model for the diffusive component of the DO flux across the SWI, \( J_{SWI} \), to be used in field scale simulations:

\[
J_{SWI} = \beta \Delta C
\]  

(5.14)

where \( \beta \) is a mass transfer coefficient multiplied by the oxygen concentration defect at the SWI

\[
\Delta C = (C_\infty - c_{SWI})
\]  

(5.15)

where \( c_{SWI} \) is the mean oxygen concentration at the SWI. The normalization for the DO implied by (5.14) is consistent with the linearity of the transport equation for the scalar field. Both the terms on the right-hand-side of (5.14) need to be modelled with parameters dynamically resolved in the simulation and some sediment-specific information.

Model for the mass transfer coefficient \( \beta \)—Scalo et al. (2012a) have shown that, for fixed fluid dynamic conditions, the dependency of the sediment-oxygen uptake (5.14) on the sediment’s characteristics (in particular, from the maximum oxidation rate, \( \mu \)) can be removed if normalizing it with the concentration difference, \( \Delta C \). The quantity \( J_{SWI}/\Delta C \) is, in fact, the mass transfer coefficient \( \beta \) which is typically only modeled based on the state of the flow parameters (discussed later). This suggests that \( \Delta C \) is the only term in (5.14) that contains the effects of the mass-absorbing sediment layer.

Due to the passive nature of the transported scalar, the same turbulent flow, with different underlying sediment layers, for example, one with low and one with high oxidations rates (low and high values of \( \Delta C \), respectively), will exhibit identical instantaneous mixing dynamics (determined uniquely by the velocity field). In the high absorbing case, the same mixing events lead to a higher flux simply due to the presence of a stronger background concentration gradient (higher \( \Delta C \)). From a mathematical perspective, changing the oxidation rate simply changes the boundary conditions (changing \( \Delta C \)) to the Reynolds-Averaged scalar transport equations whose solutions collapse into one if normalized by \( \Delta C \), given their linearity and homogeneity. The (dimensional) flux at the SWI will, therefore, (for the same turbulent field) simply be proportional to \( \Delta C \).

From a physical perspective, this can also be interpreted according to Fick’s law based approximation of the SOD, leading to another possible definition of the diffusive sublayer thickness, \( \delta_{DBL} \) (Lorke et al. 2003)

\[
\beta = D/\delta_{DBL}
\]  

(5.16)

For a given molecular diffusivity, \( D \), if the turbulent flow is the same, \( \delta_{DBL} \) will be the same, and changing \( \Delta C \) only (without changing the flow) changes (linearly) the gradient magnitude or the SOD, by not changing the physical transport processes leading to it, parametrized, instead, by \( \beta \). In conclusion, the formulation (5.14) is consistent with the interpretation of \( \beta \) as a measure of the efficiency of the turbulent mixing, working
against a given background concentration difference $\Delta C$.

From the aforementioned discussion it follows that $\beta$ should incorporate all of the near-wall turbulent mixing effects, which depend on the Schmidt number, $Sc$, and scale with the total friction velocity, $u_\tau$, as shown in Table 5.3 reporting some of the available parametrizations for the mass-transfer coefficient, $\beta$. The Schmidt number can be easily calculated from the near-wall average water temperature, $T_B$ (Yuan-Hui & Gregory 1974), the friction velocity can be calculated either from the bulk or free stream velocities, via the bottom-drag coefficient (Wuest & Lorke 2003) or, if possible, by using a log-law fit of the mean velocity profile. These approximations for the wall-shear stress have been tested for this particular flow (Figure 5.9 (a)) and provide very accurate estimates. A bottom-drag coefficient of $C_B = 0.0036$ has been calculated based on the bulk mean total velocity and is defined as

$$u_\tau = \sqrt{C_B \sqrt{U_B^2 + W_B^2}}$$

(5.17)

The estimates based on the law-of-the-wall (5.13) and the bottom-drag coefficient (5.17) exhibit the greatest discrepancies, especially after re-transition.

**Simplified model for $\Delta C$**— Although $\beta$ depends solely, based on approximations made, on flow parameters, the concentration difference $\Delta C$ is still, in general, dependent on all the governing parameters of the problem. It is a measure of the oxygen content of the sediment layer and is primarily determined by the equilibrium between the rate of absorption in the sediment layer and the rate of DO supply from the water side, controlled by the near-wall turbulence. These considerations lead to the following simplified functional form for the concentration difference at the SWI

$$\Delta C = C_\infty f(\mu^+, Sc, \varphi, K^*)$$

(5.18)

where

$$\mu^+ = \frac{\mu \nu}{C_\infty u_\tau^2}$$

(5.19)

is the ratio between the characteristic near-wall (viscous) time scale, $t_\nu = \nu/u_\tau^2$, and the bacterial absorption time scale, $t_{\mu} = C_\infty/\mu$ and $K^*$ is the normalized permeability with some reference length scale. The Schmidt number dependency is formally retained in (5.18) to account for its effects on the diffusive sublayer thickness, limiting the mass transfer rate from the water side. There are very few elements, at this stage of the model development, to also be able to explicitly account for the dependency from porosity and permeability. Their effects on $\Delta C$ can, however, still be deduced (shown later).

Figure 5.9 (b) shows data from the numerical study on oxygen depletion by Scalo et al. (2012a), in a steady, open-channel configuration, and the present one, overall covering a wide range (over 4 orders of magnitude) of $\mu^+$. These data are also consistent with unpublished data collected in central Lake Erie
(D. Bouffard, pers. comm.). The natural numerical bounds for \( f \) in (5.18) are,

\[
f(\mu^+ \to 0) = 0, \quad f(\mu^+ \to +\infty) = 1	ag{5.20}
\]

for every \( Sc, \varphi \) and \( K \). Moreover, the trend of the data in the semilog plot, suggest an asymptotic behaviour for \( f \) in the two extreme cases. This leads to the approximate functional form

\[
\Delta C/C_\infty = \frac{1}{2} \left[ \tanh \left( \alpha_1 \left[ \log_{10}(\mu^+) + \alpha_2 \right] \right) + 1 \right]
\]

where \( \alpha_1 \) and \( \alpha_2 \) are dimensionless fitting constants dependent, in general, from \( Sc, \varphi, \) and \( K \). This assumption is also supported by the observed asymptotic tendency of \( c_{swi} \) towards \( C_\infty \) for increasing wall-shear stress in laboratory and numerical experiments (Higashino et al. 2008, Scalo et al. 2012b), for fixed sediment layer parameters. In the case of more complex sediment biochemistry, the maximum oxidation rate in (5.19) can be replaced with an effective overall absorption rate.

While the present data set is for one value of porosity (\( \varphi = 0.95 \)) and permeability (\( K = 2 \times 10^{-7} \) cm\(^2\)), Schmidt number (\( Sc \sim 1000 \)) and oxidation rate (\( \mu = 240 \) mg L\(^{-1}\) day\(^{-1}\)), but in non-equilibrium conditions for the mass transfer, the data from Scalo et al. (2012a) covers three different Schmidt numbers (\( Sc = 400, 690, \) and 1000, respectively for water temperatures of 25°C, 15°C and 8°C), two different oxidation rates (\( \mu = 240 \) and 1680 mg L\(^{-1}\) day\(^{-1}\)), a wide range of current intensities (\( U_B = 2.5 - 27 \) cm s\(^{-1}\)) and porosity of \( \varphi = 0.55 \), but all in statistically steady conditions and for \( K = 0 \). This explains why the latter data set exhibits a clearer trend, in which Schmidt number effects are also very distinguishable. Despite the (moderate) scatter in the data from the present simulation, resulting from memory effects, the sensitivity of \( f \) with respect to \( \mu^+ \) appears to be dominant over the other parameters in (5.18). This motivates us to adopt further simplifications in the model by giving more weight in the fitting to data in equilibrium and for colder temperatures (\( Sc \sim 1000 \)) which are more representative of conditions found in bottom layers of oceans and lakes. This results in values of \( \alpha_1 = 0.7 \) and \( \alpha_2 = 3.4 \) which also captures most of the data of the present transitional flow. The higher values of \( \Delta C \) are due to the higher \( \varphi \) and \( K \) of the present case, as shown in Scalo et al. (2012b) and Higashino & Stefan (2011) and illustrated in Figure 5.8. Although we believe that the assumptions made so far lead to errors within acceptable bounds, they are, for now, only heuristic and require further empirical confirmation.

**Comparison with measurements**— Finally, the predictions of the proposed model have been compared against Bryant et al.’s (2010) SOD measurements and the sediment-oxygen uptake directly calculated from the LES (Figure 5.10). The mass-transfer coefficient was calculated using the parametrization by Shaw &
Figure 5.8: Effects of sediment porosity, $\varphi$, and dispersivity (controlled by permeability $K$) on oxygen profiles. Purely diffusive sediment layer with low porosity (profile 1), porosity approaching 1, no dispersive effects (profile 2), dispersive-dominated transport (profile 3). The effects are exaggerated for visualization purposes.

Hanratty (1977b) (the closest to the SOD predictions in Scalo et al. (2012a)), together with the bottom-drag-coefficient approximation of the total friction velocity (5.17). Despite the simplicity of the adopted model, the overall variability of the SOD during the entire cycle is correctly captured. The observable discrepancies are primarily due to the equilibrium assumptions made in the model formulation and the difference in the transporting turbulent velocity fields (Figure 5.5). Time lags with respect to the overlying turbulence (or $u_\tau$) due to long time scales of the transient growth and compression of the diffusive sublayer cannot be accounted for in the model. For example, Figure 5.10 shows how during the deceleration phase, from $t = 3$ h to $t = 6$ h, the SOD model predicts more rapid expansion of the diffusive sublayer (decrease in the mass flux), following closely, by construction (Table 5.3 and Equation (5.19)) the evolution of the wall-shear stress. The LES results, on the other hand, show a well-defined inertia in the evolution of the diffusive sublayer, retaining a higher value of the flux for a longer time, despite the low $u_\tau$, at this phase. Similarly, the delay of $\sim 20-30$ min, in the SOD enhancement, following the mixing events in the water-column at $t = 6.8$ h and $t = 8$ h, is not captured by the SOD model which predicts a DO flux across the SWI in equilibrium (synchronized) with the external forcing.
Table 5.3: Different models for high-Schmidt-number mass-transfer coefficients $\beta$ from a steady turbulent flow to a smooth wall (Boudreau & Jørgensen 2001). Alternative parametrizations taking into account porosity, permeability and surface roughness can be found in Grant et al. (2012).

<table>
<thead>
<tr>
<th>Model</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Pinczewski &amp; Sideman 1974)</td>
<td>$0.0671 u_\tau Sc^{-2/3}$</td>
</tr>
<tr>
<td>(Wood &amp; Petty 1983)</td>
<td>$0.0927 u_\tau Sc^{-1/10}$</td>
</tr>
<tr>
<td>(Steinberger &amp; Hondzo 1999), (Hondzo 1998)</td>
<td>$0.0558 u_\tau Sc^{-2/3}$</td>
</tr>
<tr>
<td>(Shaw &amp; Hanratty 1977b)</td>
<td>$0.0889 u_\tau Sc^{-0.704}$</td>
</tr>
</tbody>
</table>

Figure 5.9: Comparison of different methods to evaluate the total friction velocity $u_\tau$ (a): direct calculation from LES (□), log-law fit of mean velocity magnitude profile (---), bulk velocity bottom-drag coefficient (5.17) (-----), law-of-the-wall estimate (5.13) applied to total dissipation calculated at $y = 10$ cm (- - -); Normalized oxygen difference $\Delta C = C_\infty - c_{swi}$ at SWI as a function of $\mu^+$ (5.19) (b), data from Scalo et al. (2012a) for $Sc = 400, 690$ and $1000$, different current intensities $U_B = 2.5 - 27$ cm s$^{-1}$ and bacterial populations, $\chi = 100 - 700$ mg L$^{-1}$ (○) and corresponding fit for each $Sc$ (---), transient data from current LES (○), parametrization (5.21) for $\alpha_1 = 0.7$ and $\alpha_2 = 3.4$ (- - -).

Figure 5.10: DO flux across the sediment-water interface. Directly computed from LES (---), proposed parametrization (5.14) based on (5.17), (5.21) with mass transfer coefficient $\beta$ by Shaw & Hanratty (1977b) (-----), measurements by Bryant et al. (2010) (○).
5.7 Discussion and Conclusions

The nature of momentum and contaminant transport in geophysical flows is characterized by a multiplicity of temporal and spatial-scales, ranging from the large-scale forcing (e.g. basin-scale waves) to small-scale processes (e.g. oxygen transport in the sediment layer). The complete spectrum of physical processes can be conceptually modeled as a cascade or chain of events connected by a cause-and-effect relationship. Broadly speaking, global equilibrium is present when the time scales of each leading process (cause) are very long with respect to the following one (effect). Defining and understanding the limits of validity for equilibrium is crucial when developing modeling and prediction strategies.

The validity of equilibrium assumptions in field scale studies have been discussed in Lorke et al. (2002) and Lorke et al. (2003), who looked at low-speed oscillating currents in Lake Alpnach. They observe, in fact, current amplitudes of the same order of the ones observed by Bryant et al. (2010) at \( y = 10 \) cm, with oscillation periods within the same range (from \( \sim 8 \) to \( 20 \) h), but at \( y = 4 \) m. Relatively low current intensities determine longer turbulent integral time scales, and, therefore, longer response and propagation times of the turbulent mixing, generated in the near-wall region, throughout the water column (enhanced by turbulent production mechanisms occurring in the near-wall region). This results, for example, in the current intensity leading turbulent dissipation, as observed by Lorke et al. (2003) at \( y = 1 \) m, with a systematic phase lag of 1-2 h. This is not present in the flow analyzed here which can be regarded in equilibrium, as far as the momentum transport is concerned. This explains the accuracy of the agreement of the log-law fit and the law-of-the-wall (5.13) in predicting the total wall-shear stress (Figure 5.9(a)). The latter is also valid in low-Reynolds-number flows but in a region very close to the wall, which, for the particular case investigated by Lorke et al. (2002), was \( y < 0.5 \) m. An imbalance between dissipation and production is, however, observed in many other experimental and numerical studies of low-speed (or intermittently turbulent) oscillating currents (Hino et al. 1983, Spalart & Baldwin 1987, Jensen et al. 1989, Costamagna et al. 2003, Scalo et al. 2012c).

Equilibrium conditions for the scalar transport are observed in our case away from the SWI where the predicted turbulent mass flux follows closely the Reynolds stresses and turbulent kinetic energy distribution, with, however, a remarkably higher variance (Figure 5.6(d)). This is consistent with the intrinsic intermittent nature of a passively advected quantity in a turbulent flow (Warhaft 2000), which is enhanced in the case of a high-Schmidt-number contaminant (Antonia & Orlandi 2003), and has also been observed in the eddy-correlation measurements by Brand et al. (2008), who studied oxygen transport in the same lake for an oscillating flow with similar current amplitude and period. Particular care needs to be taken to verify the convergence of any (higher-order) statistic involving a fluctuating passively advected scalar field.

Although Bryant et al. (2010) has not observed any delay between the near-wall turbulent activity and the SOD response, Lorke et al. (2003) has shown a well defined time lag between the Batchelor scale (extrapolated
at the SWI from dissipation measurements taken at \( y = 0.5 \) m, representative of the state of the near-wall turbulent mixing) and the estimated diffusive sublayer thickness. It has been observed that an abrupt reduction of the near-wall turbulent activity is followed by a gradual relaxation of the diffusive sub-layer, while abrupt increases in turbulent activity can lead by more than an hour the corresponding enhancement of the SOD, depending on the time scale and intensity of the driving current. The same behaviour has been observed in the present numerical experiments (Figures 5.6, 5.7 and 5.10) and in the ones by Scalo et al. (2012c) in an oscillating boundary layer in the intermittently turbulent regime.

We have shown that the present numerical model, based on large-eddy simulation technique, correctly reproduces the essential transport mechanisms involved in dissolved oxygen transfer to organic sediment beds in the transitional oscillatory flow observed by Bryant et al. (2010) in Lake Alpnach. Despite the idealized computational setup, the effects of turbulent decay and re-transition on the SOD are correctly captured; the complete spectrum of governing transport processes involved in oxygen depletion has been accurately resolved, from the seiche-induced turbulent transport, to diffusion and absorption in the pore water.

This study has highlighted in particular the challenges that non-equilibrium conditions pose to modelling, especially in the case of high-Schmidt-number mass transfer. Moreover, the prediction of transition and turbulence decay for the velocity field alone is rather sensitive to boundary conditions and residual fluctuation levels, which are not known to the level of accuracy required by the model, for the flow under investigation. This lack of information is, most likely, the cause for the observed discrepancies between the LES predictions and observations. Overall, the high variability of the turbulent state results in non-equilibrium effects which manifest themselves in the form of phase lags; for this particular flow phase lags with respect to the main oscillatory current were only observed in the diffusive sublayer dynamics. They could, in general, also occur between the main current, the turbulent dissipation and the turbulent mixing intensity and their extent is highly flow-dependent and impossible to account for in simple algebraic RANSE models.

Despite the assumptions made in deriving the proposed SOD parametrization, the overall agreement with the observed and directly calculated SOD is remarkable. The model should, however, also be tested in flows such as the one investigated by Lorke et al. (2003) where non-equilibrium effects are present in all stages of transport. Limitations include the non-explicit definition of permeability and porosity effects, which can affect both the mass transfer coefficient \( \beta \) and the oxygen difference \( \Delta C \) at the SWI. This can be achieved by including more sophisticated hyporheic exchange laws. More careful numerical and experimental investigations, systematically covering a wide range of \( \varphi \) and \( K \), and different bed forms (with small-scale and large-scale roughnesses) need to be carried out to provide accurate data to validate the implementation of such models. We believe, however, that the proposed parametrization based on the turbulent inner-region scaling of the oxidation rate, can provide a first step towards the definition of simple process-oriented models for the SOD to be used in water-quality management applications.
Chapter 6

Discussion and Future Work

A detailed conclusion section is already provided in each of the preceding chapters. In this chapter we will rather discuss the implications of the most important findings of this thesis, by partially reiterating them in a more general and (very) critical perspective, in an attempt to outline a path for future numerical and experimental work in this field.

In Chapter 2 we have discussed the details of the development of a model for dissolved oxygen (DO) transfer, from water to underlying organic sediment beds that, for the first time, directly couples Large-Eddy Simulation (LES) of turbulent transport on the water side with existing biogeochemical models for the transport and the DO bacterial absorption in the sediment bed. The work required the investigation of the interaction between turbulence and biogeochemistry. The latter involves two well-defined problems: modelling the DO absorption due to organic matter decomposition (biochemistry) and modelling the transport processes present in a porous sediment layer (including hyporheic exchange). In the first case, the adopted modeling for the oxygen absorption is based on well-established Michaelis-Menten kinetics, adopted by many authors at field scale and lab scale, which is quite robust in reproducing the observations. Most of the uncertainties in the model, however, lie in the second aspect of the problem, specifically, in modelling the interaction across the sediment-water interface (SWI) between the turbulent flow and the different transport processes occurring in the sediment layer. The greatest challenge lies, in fact, to reconcile the different levels of modelling adopted for the water side and the sediment side. In most of the results, highly resolved LES/DNS for the water side transport were adopted, in which the amount of modelling is very minimal. On the sediment side, only volume-averaged (macroscopic) quantities are directly resolved such as the mean-pore-water flow velocity and the dispersivity. This raises fundamental questions regarding coupling strategies similar to the one involved in LES/RANSE coupling in detached eddy simulations. The SWI is modeled as a sharp and flat interface with no intermediate layer accounting for the transition from full Navier-Stokes equations (solved at an instantaneous level) to Darcy’s Law and low-order models for chemical kinetics (volume-averaged).
This layer is often referred to as the Brinkmann layer. For the cases investigated its thickness (scaling as the square of the intrinsic permeability) is, however, negligible. Taking into account complex geometries for the SWI would emphasize this issue and require the explicit implementation of a new set of governing equations to model the aforementioned transition. For high friction velocities sediment resuspension can also occur. A thin layer of stably suspended/homogeneous bi-phasic flow may exists changing completely the nature of the interaction with the turbulent transport and the modeling strategies to account for solute and momentum fluxes across the layer. Numerical simulations with resolved near-wall (small or large scale) roughness and careful companion laboratory experiments are needed to adequately tackle this problem. Improving the modelling of the exchange of momentum and solutes across the SWI should, therefore, be the priority of future work.

The aforementioned outlined research path would provide a significant contribution to the vast field of hyporheic exchange modelling, which is currently one of the main focuses of environmental fluid mechanics. For the specific problem of oxygen depletion, sediments are typically flat and composed primarily of dead organic matter, resulting in cohesive muddy layers such as clayey sand (low permeabilities). As a matter of fact, the results presented so far, and their comparison to lab-scale and field-scale measurements, do not reveal a particular need to further complicate the model when applied to DO transport.

Another promising research path leading to substantial improvement of the model is to incorporate turbulent mixing of multiple bio-limiting contaminants, leading to a direct resolution of the interaction between turbulence and the dominant diagenetic processes (the complete set of transport processes and chemical reactions occurring in the sediment layer). This includes, for example, the extension of the sediment nutrient cycle (which strongly relies on dissolved oxygen) to oxic respiration, denitrification, Manganese-oxide and Ferric-oxide reduction, Sulfate reduction and Methane production. The implementation of these processes is rather straightforward (given the computational structure of the model) and would allow for a substantial contribution to the development of the dynamic model in CAEDYM (see Introduction in Chapter 5). All of this calls for a more direct collaboration among numerical modellers, limnologists, biologists, and experimentalists, as invoked in Chapter 4.

An important aspect of our contribution as turbulence modellers has been exploring new water-side mass transport dynamics, which, we believe, are accurately reproduced by the current level of complexity of the sediment biogeochemical model. The general approach was to test different fluid dynamic conditions, starting from simple lab-scale studies, working our way up to realistic geophysical applications. Chapter 3 is the first step along this path where a range of Reynolds numbers, Schmidt numbers, and bacterial populations (reproducible in laboratory experiments) has been tested. This work is centred around the peculiarities that high-Schmidt-number mass transport dynamics exhibit with respect to momentum transport. These are due to the orders of magnitude of difference between the respective diffusivities and the highly intermittent nature
of the passive scalar. For example, the relevant mass transport events for the scalar field are (primarily) the ones occurring in the diffusive sublayer, a very thin layer close to the wall (approximately $y^+ = 5 Sc^{-1/3}$ thick). In spite of the infrequent occurrence (with respect to the bursting cycle) of turbulent transport events that reach such regions of the viscous sublayer, their intensity and structure is responsible for the observed complexity of the diffusive sublayer regeneration cycle. We have shown that its features go beyond a (simplistic) zero-dimensional low-pass filter, but, rather, include de-noising and amplitude filtering properties and a strong three-dimensionality. In particular, we have shown that the diffusive sublayer thickness or, equivalently, the mass flux at the wall, is modulated only by the intense sweeps (amplitude filter), it is not responsive to low-amplitude background fluctuations of the wall-shear stress (de-noising filter) and it exhibits an integral response to the forcing (low-pass filter) with a response delayed by fractions of an large-eddy turnover time (LETOT). Three different transport processes are identified leading to oxygen depletion: turbulent transport, diffusive transport across the SWI and absorption in the sediment layer. Each of these exhibit well-defined characteristic time scales. Time-resolution constraints (e.g. CFL condition) limit the time step of the solver allowing for rapidly evolving transport processes to be resolved. However, this creates problems in computations of statistically steady oxygen transport since, even if starting from a fully converged turbulent velocity field, hundreds of flow-through times might be necessary to reach full equilibrium in the diffusive sublayer structure (due to its aforementioned properties) and between the mass transfer across the SWI and the sediment oxygen absorption (especially for low bacterial populations). Although this is not an intrinsic limitation of the adopted computational method, but, rather, an issue inherent to the physics of the problem, a full LES approach allows to considerably increase the physical time span covered by the simulation and to yield more converged results than higher resolution hybrid simulations (DNS for velocity field and LES only for the scalar field), severely limited by the CFL condition.

The aforementioned convergence issues call for the need, in future work, to develop ad-hoc subgrid-scale models for the passive scale in the low diffusivity limit. However, this raises questions on the effects and importance of the sub-Kolmogorov scales on the large scales (see Introduction). The very high computational costs associated with a full DNS (resolving down to the Batchelor scale) and the fact that both the scalar and the velocity field share the same integral scale, makes LES an ideal prediction tool for this problem. Moreover, there has been no evidence in literature and in the present work of the dynamic relevance of sub-Kolomogorov scales in turbulent mass transport to a solid wall. On the contrary, careful grid convergence tests (shown in Chapter 2 and others, not shown, reproducing simulations of Calmet & Magnaudet (1997)) prove how high-Schmidt-number scalar fields in wall-bounded flows reach grid convergence sooner than unitary-Schmidt-number scalars fields for the same boundary conditions. This is confirmed by other works cited in the literature review in Chapter 3. We speculate that this is due to the more rapid grid convergence.
of the velocity field in the near-wall (than in the outer region), the only one truly governing high-Schmidt-number mass transfer. This requires further investigations where careful grid convergence tests are carried out monitoring the evolution of the velocity-scalar co-spectrum and the resolved near-wall turbulent structures as the mesh is refined. We are confident that an adequate solution is to adopt a hybrid approach (DNS for velocity and LES for scalar), first introduced by Bergant & Tiselj (2007), and adopted in Chapter 3 and 4. However to ideally take into account all of the effects of the sub-Kolmogorov scales (i.e., resolving the Batchelor scale), a hierarchical grid approach should be implemented, as in Schwertfirm & Manhart (2007). This, however, only allowed (at the time) the direct resolution of the scalar field up to $Sc = 49$ and cannot be applied in geophysical flows. We have shown in Chapter 3 that a classic LES can reproduce the value of the mass-flux very accurately at this Schmidt number, matching the full DNS lower-order statistics, making it the ideal approach, especially for field scale applications.

In Chapter 3 we focused on the unsteady small scale mass transport dynamics in the presence of a large scale steady forcing (constant mass flux). However, in geophysical applications, the effects of an unsteady free-stream current can have significant effects on the mass transport, leading to non-equilibrium conditions in the flow. The computational setup adopted in Chapter 4, where mixing is driven by an oscillating boundary layer in the intermittently turbulent regime, emphasizes these effects, while retaining an idealized configuration (statistically periodic turbulent velocity field). For these computations, we have chosen to prevent re-areation from the top-boundary, to model the reduced turbulent mass flux across the thermocline (stratified layer), simulating hypolimnetic oxygen depletion. The concentration field exhibits a well-defined decay pattern which has allowed the decomposition of the instantaneous solution into a monotonically steady decaying component, a coherent oscillating one and a stochastic one. The results lead to the identification of a self-similar structure in each one of them. The development of the mathematical model and the resulting analytical constraints deriving from the manipulation of the governing equations do not include, in any form, assumptions related to any aspect of oxygen transport. The potential for the application of the decay model as a prediction tool is considerable, however, its validity should be explored and verified against field scale or lab scale data.

The formulation of a simple mathematical model for the decaying oxygen concentration has lead to the possibility to use phase averaging instead of ensemble averaging to extract statistics from the flow, and to, therefore, explore the transport dynamics in an turbulent flow governed by an oscillating current. This has lead to the conclusion that oxygen distribution in the water column is modulated by the periodic ejection, during the deceleration phase, of negative peaks of high turbulent mass flux, generated at the edge of the diffusive sublayer towards the end of the acceleration phase and growing in intensity until the beginning of the deceleration phase (turbulent flux production stage). These fronts of high turbulent mixing then propagate away from the sediment-water interface (SWI), at approximately constant speed, in layers of low oxygen concentration. The persistence of high levels of mixing in the near-wall region during the turbulent
flux production stage is responsible for the accumulation of high concentration levels in the diffusive sublayer. These will cause, with a time lag of approximately a quarter of a cycle, a peak in the mean mass-flux across the SWI, towards the end of the deceleration phase. The periodic forcing leaves its signature in the concentration field for a greater portion of the water column than in the momentum field. Despite the highly intermittent state of the turbulent field, the scalar field behaves like a linear harmonically forced system. In field scale studies (Chapter 5) similar dynamics have been observed but more work needs to be done to confirm that these are the dominant transport processes in oscillating currents in realistic geophysical flows and not just an artifact of the idealized computational/physical problem setup.

In Chapter 5 we extended the computational setup adopted in Chapter 4 to the transitional oscillatory flow observed by Bryant et al. (2010) in the southwest region of Lake Alpnach in July of 2007. The effects of turbulent decay and re-transition on the SOD are correctly captured; the complete spectrum of transport processes involved in oxygen depletion has been accurately resolved, from the seiche-induced turbulent transport, to diffusion and absorption in the pore water. The high variability of the turbulent state results in non-equilibrium effects which manifest themselves in the form of phase lags; for this particular flow phase lags with respect to the main oscillatory current were observed only in the diffusive sublayer dynamics. An algebraic parametrization for the diffusive component of the SOD has been developed strictly assuming equilibrium conditions and its predictions compare well against the directly estimated oxygen flux from the LES, with phase lags of \( \sim 20-30 \) minutes. The model is currently being implemented in the latest version of CEADYM for water-quality management applications.

The model should be tested in flows such as the one investigated by Lorke et al. (2003) where non-equilibrium effects are present at all stages of transport (also in the water column transport dynamics). Other potential limitations of the model include the non-explicit definition of permeability and porosity effects, which will affect both the mass transfer coefficient \( \beta \) and the oxygen difference \( \Delta C \) at the SWI. In conclusion, the complete numerical model needs to incorporate more sophisticated hyporheic exchange models; more ad-hoc numerical and experimental investigations (systematically covering a wide range of \( \phi \) and \( K \)) need to be carried out on complex geometries for the SWI, to correctly account for these effects in lower-order algebraic models for field-scale applications.
Bibliography


