Numerical simulation of scalar dispersion downstream of a square obstacle

By R. Rossi† and G. Iaccarino

1. Motivation and objectives

The analysis of scalar dispersion in turbulent flows is relevant for a broad range of applications, including investigation of hazardous releases, bio-terrorism and control of air quality. In the last 50 years, experimental and numerical investigations of canonical flows, such as turbulent boundary layers (Fackrell & Robins 1982) or grid-generated turbulence (Livescu et al. 2000), have enhanced theoretical understanding and subsequently enabled the development of simplified, semi-empirical models. Although these models have been successfully employed in simplified flow configurations (Sykes et al. 1984), prediction of scalar dispersion over complex and realistic geometries remains challenging, especially because of large-scale unsteady effects which cannot be properly accounted for in a simple phenomenological framework. On the other hand, it is generally accepted that detailed flow simulations (e.g., Large-Eddy Simulation, LES) provide accurate predictions of the turbulence dynamics and the scalar mixing rates, thus promising to enhance our ability to study turbulent dispersion in realistic environments. This, in turn, could lead to the development of better reduced order models. A recent example where LES has been applied to scalar dispersion in complex geometries is the work of Walton & Cheng (2002), but the comparison with experimental measurements was limited to mean scalar concentration.

In order to establish if detailed flow simulations are able to provide accurate predictions of scalar dispersion in complex geometries, in this preliminary study the experiment of Vinçont et al. (2000) is numerically reproduced. To the best of the authors knowledge, this is the first experimental setup where detailed measurements of turbulent scalar fluxes in a non-trivial geometry have been carried out. Moreover, the flow is characterized by low Reynolds numbers, thus allowing Direct Numerical Simulations (DNS) to be performed in the limit of large Schmidt numbers. In the first part of this research brief, we present a comprehensive RANS-based analysis of the experimental setup. We compare the predictions obtained using various one-point statistical models, namely $k - \epsilon$, $k - \omega$ and Reynolds Stress Transport, to the experimental measurements. The simulation results appear to give only a limited agreement with the experiments, both in terms of low-order (mean concentration) and high-order statistics (turbulent flux). Furthermore, no closure was able to reproduce the streamwise component of turbulent scalar fluxes. Although the resulting effect on the scalar transport equation is found to be not significant, this limitation of eddy-diffusivity-based models is more severe in the analysis of scalar dispersion over complex boundaries (i.e., strongly spatially developing flows). As a second step, we performed DNS of the same experimental setup aiming at providing a detailed analysis of the interaction between turbulence structures and scalar dispersion. Note that several examples exist in the literature where DNS have been applied to the

† Laboratorio di Termofluidodinamica Computazionale, Seconda Facoltà di Ingegneria di Forlì, Università di Bologna, Via Fontanelle 40, 47100 Forlì, Italy
analysis of scalar dispersion, but the simulations were generally limited to shearless or simple shear flows (Fackrell & Robins 1982; del Álamo & Jiménez 2002).

2. Background

In the reference experimental setup the scalar dispersion from a line source downstream of a 2-D square obstacle has been investigated. The obstacle was completely immersed in a turbulent boundary layer with an approximate ratio $\delta/h \approx 7$, where $\delta$ is the boundary layer thickness previously measured without the obstacle in place and $h$ the obstacle height. The experimental measurements were carried out in a water channel and in a wind tunnel where the flow was characterized by a Reynolds number of 700 and 1500, based on $h$ and the freestream velocity $u_\infty$, and by a Schmidt number of 2500 and $10^{-6}$, respectively. The scalar was injected in the main flow through a rectangular slot of $0.14h$ width located $1h$ downstream of the obstacle. The flow and the scalar field were subsequently measured at two different streamwise locations downstream of the obstacle: $x = 4h$ and $x = 6h$. Available measured quantities are the following: mean velocity and mean concentration, streamwise and vertical turbulence intensity, Reynolds shear stress and turbulent scalar fluxes. For details about the measurement techniques, the reader is referred to the study conducted by Vinçont et al. (2000).

3. Reynolds-averaged Navier-Stokes simulations

This section summarizes the Reynolds-averaged Navier-Stokes (RANS) simulations of the experimental test case. The objective of these initial computations is twofold: first, to evaluate the capabilities of one-point turbulence models for the analysis of scalar dispersion in complex geometries. The second goal is to provide suitable inlet boundary conditions for LES and DNS of the same experimental setup. A Newtonian fluid with constant properties is assumed in the computations and the scalar advection is approximated to a passive mechanism. The RANS governing equations thus read as follows:

$$ \frac{\partial U_i}{\partial x_i} = 0 $$

$$ U_j \frac{\partial U_i}{\partial x_j} = \frac{1}{\rho} \frac{\partial \rho}{\partial x_j} + \frac{\nu}{\rho} \frac{\partial^2 U_i}{\partial x_j^2} - \frac{\partial}{\partial x_j} \left( \overline{u_i u_j} \right) $$

$$ U_j \frac{\partial C}{\partial x_j} = D \frac{\partial^2 C}{\partial x_j^2} - \frac{\partial}{\partial x_j} \left( \overline{u_j C} \right), $$

where uppercase and lowercase letters denote mean and fluctuating variables, respectively.

The flowfield governing equations (3.1)–(3.2) are solved with the help of the finite-volume code FLUENT and further employing three different turbulence models: the standard $k-\epsilon$ model (Launder & Spalding 1972), the standard $k-\omega$ model of Wilcox (1998) and a Reynolds Stress Transport (RST) model (Launder 1975). The one-equation model of Wolfstein (1969) is used to resolve the viscosity-affected near-wall region of the flow, along with the $k-\epsilon$ and the RST closures. On the other hand, the $k-\omega$ model already incorporates modifications for low-Reynolds-number effects and is therefore adopted in the outer flow as well as in the near-wall region. The “frozen” velocity field is then employed in the finite-volume code PS-SOLVER (Rossi 2008), designed to
solve the scalar transport equation in complex geometries. The closure model for the averaged scalar transport equation (3.3) relies on the gradient-diffusion hypothesis, where turbulent scalar fluxes $\overline{u_jc}$ are assumed proportional to the mean scalar gradient, as follows:

$$\overline{u_jc} = -\nu_t \frac{\partial C}{\partial x_j},$$

(3.4)

where the turbulent Schmidt number $Sc_t = \nu_t/D_t$ denotes the ratio of the eddy-viscosity $\nu_t$ to the eddy-diffusivity $D_t$. It is worth noting that scalar dispersion at very large molecular Schmidt number $Sc = \nu/D$ is dominated by the turbulent transport. Therefore, adopted values of $Sc_t$ greatly affect the numerical predictions. Although it is known that $Sc_t$ depends upon underlying transport phenomena, for the present case a constant value of 0.85 appears to be a reasonable hypothesis (Koeltzsch 2000).

3.1. Numerical setup

The numerical model employed in the computations is based on a 2-D block-structured hexahedral mesh. The overall grid size is $394 \times 160$ in the streamwise and spanwise directions, respectively, while $64 \times 64$ cells are placed around the obstacle. Note that the grid resolution at the wall is such that $y^+ \leq 1$ and several cells lie within the viscous sublayer. A second-order accurate discretization is adopted for the flowfield and scalar governing equations, based on the upwind-biased reconstruction of advective terms (Barth & Jespersen 1989).

In order to match the desired boundary-layer thickness at the obstacle location, the boundary condition at the inflow has been obtained by computing a zero-pressure gradient boundary layer over a flat plate using the $k-\omega$ model. In this case, the same computational settings and the same grid resolution adopted with the obstacle in place are employed, while the computational domain extends up to $130h$ upstream of the obstacle location and $150h$ downstream. Computed mean streamwise velocity and Reynolds stress profiles at $x = 150h$ are shown in Fig. 1 and compared with the DNS of Spalart (1988). The agreement with the reference data for the velocity profile in Fig. 1(a) is excellent up to the buffer region, while a slightly different slope in the log region is obtained. As it can be noted from Fig. 1(b), this is determined by the under-predicted Reynolds
stress. However, the overall agreement can be considered satisfactory thus mean velocity, turbulent kinetic energy and energy dissipation profiles are employed as the inflow boundary condition with the obstacle in place. At the upper domain boundary a slip condition is applied, while a convective boundary condition is adopted at the outlet section. A uniform scalar concentration is finally specified at the slot while the zero-flux condition is applied at the remaining boundary surfaces.

3.2. Flowfield analysis
The profiles of mean streamwise velocity are presented in Fig. 2. The results show that the mean flow is fairly well-predicted by the RST model for both the water and the air setup. Moreover, while in both cases the $k - \epsilon$ closure gives a strong under-estimation of the separated region downstream of the obstacle, the profiles predicted by the $k - \omega$ model are in better agreement with the experimental measurements. The reattachment lengths given by the three different turbulence closures are summarized in Table 1. As suggested by mean velocity profiles, the RST model leads to the best agreement with the experimental results. It is worth noting that although the air setup is characterized by a higher Reynolds number compared to the water setup, the same value of reattachment length has been reported in the experiments.

The significant changes in predicted reattachment lengths can be partly explained by analyzing the turbulent kinetic energy field shown in Fig. 3. As suggested in the study of the flow past a surface-mounted cube performed by Lakehal & Rodi (1997), the size of the separated region is largely influenced by the estimated level of turbulent kinetic energy produced in the separated shear layer. In the present case, the $k - \epsilon$ model gives the highest level of $k$, with the peak located very close to the obstacle. Therefore, the flow rapidly reattaches after the obstacle leading to a significant under-estimation of the reattachment length. The intensity of turbulent fluctuations is found to be reduced using the RST closure, while in the case of the $k - \omega$ model, the turbulent kinetic energy almost vanishes in the flow region up to $x = 2h$ downstream of the obstacle, leading to a significant over-estimation of the reattachment length. The turbulence intensity is further investigated in Fig. 4 by comparing the streamwise and vertical components to the reference data. Although the two components are not independently computed by the $k - \epsilon$ and $k - \omega$ models, the profiles given by the Boussinesq’s assumption $u_i^2 = 2/3k$ are reported for the sake of comparison. It is interesting to note that while the RST model is able to predict the Reynolds stress anisotropy fairly well, the profile shape for both the water and air setup is overall better reproduced by the $k - \omega$ model. The computed vertical component given by the $k - \epsilon$ and the RST closures is also found very similar in the case of the air setup.

The vertical profiles of Reynolds stress are shown in Fig. 5. For the water setup, an excellent agreement with the experimental measurements is found for the $k - \omega$ model, while both the $k - \epsilon$ and the RST closures yield a significant over-estimation of computed profiles. A similar scenario is found in the case of the air setup, but here the $k - \omega$ model
Figure 2. Profiles of mean streamwise velocity, (a,b) water setup at $x = 4h$ and $x = 6h$, (c,d) air setup at $x = 4h$ and $x = 6h$; (---) $k - \epsilon$, (—) $k - \omega$, (——) RST, (◦) Vinçon et al. (2000).

shows a larger departure from the experiments and it also gives a similar prediction to the $k - \epsilon$ model at $x = 6h$.

3.3. Scalar dispersion analysis

The computed vertical profiles of mean scalar concentration are shown in Fig. 6. The most interesting result is that an accurate prediction of local mean velocity profiles does not guarantee a satisfactory prediction of the scalar concentration; the key component is indeed the turbulent scalar diffusivity $D_t$. This is clearly shown by the comparison of predicted mean concentration profiles given by the $k - \epsilon$ and the RST closures, which have a different shape but are almost equivalent in terms of average concentration. The
resulting profiles are largely under-estimated in the water setup, while a closer agreement with the experiments is found at $x = 6h$. Although the $k-\omega$ model gives a better overall agreement with measurements, the results for the air setup suggest a significant influence of the Reynolds number on the prediction capability of adopted turbulence closures.

The overall effect of the estimated level of turbulent scalar diffusivity is also suggested by the contour plots of mean scalar concentration downstream of the obstacle in Fig. 7. A similar scenario to the one described in the work of Vinçon et al. (2000) is predicted, where the scalar is first convected upstream and in the vertical direction within the flow reversal region to fill the separation bubble over the top of the body, before being convected downstream by the primary flow. Therefore, each one of the adopted turbulence models is able to capture the salient features of the mean flow: the large flow-reversal region behind the body and the smaller separation bubble above the obstacle. However, a different size of the scalar wake is highlighted in the contour plots. As expected, the $k-\epsilon$ and the RST closures yield a larger wake, suggesting a stronger diffusive flux across the wake boundary. Moreover, although the RST model gives a better representation of the wake development, both turbulence closures give rise to a sharp decrease of the scalar concentration after the injection into the main flow. It is clear when considering the results in Figs. 7(b) and (e) that this is not the case when the $k-\omega$ model is employed, where the scalar concentration is almost uniform in the region of flow reversal close to
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The profiles of turbulent scalar fluxes are presented in Fig. 8. A reasonable agreement with the experimental data is found for the $k-\omega$ model, which is able to partially match the body. Furthermore, a higher concentration is predicted in the shear layer above the obstacle, which finally results in the development of a confined scalar wake.

Figure 4. Profiles of turbulence intensity, (a,b) streamwise component of water setup at $x = 4h$ and $x = 6h$, (c,d) vertical component of water setup at $x = 4h$ and $x = 6h$, (e,f) streamwise component of air setup at $x = 4h$ and $x = 6h$, (g,h) vertical component of air setup at $x = 4h$ and $x = 6h$; (—) $k-\epsilon$, (••••) $k-\omega$, (——) RST, (◦) Vinçont et al. (2000).
the location and magnitude of local extrema of the vertical component, while no one of the adopted turbulence closures is able to predict the streamwise flux. Since it has been shown that the \( k - \omega \) model gives a reliable estimation of mean scalar concentration, it is therefore expected that the net contribution of the streamwise component in the scalar transport equation is negligible. Note that the experiments show a very strong negative streamwise flux within the shear layer at \( y/h \approx 2 \). This region does not correspond to a positive streamwise scalar gradient (the scalar concentration is monotonically decreasing between \( x = 4h \) and \( x = 6h \)) and therefore corresponds to an actual \textit{anti-diffusion} mechanism.
4. Direct numerical simulations

Direct numerical simulations of the experimental setup are carried out aiming at providing a comprehensive understanding of the interaction between turbulent structures and scalar dispersion and to highlight the limits of semi-empirical models. The solution of the flow and scalar governing equations is obtained using second-order accurate finite-volume techniques. The computations are performed using the CDP code (Mahesh et al. 2004) and the code FLUENT, to test specific inflow turbulence-generation techniques. In this case the scalar transport equation is solved by the code PS-SOLVER (Rossi 2008). A passive scalar transport of the contaminant is considered in the computations, while the
Schmidt number of the flow is limited to a value of 10 in order to relax the requirement of a finer grid resolution dictated by the Batchelor length scale (Warhaft 2000). In spite of this constraint, the use of upwind-biased schemes has been required to guarantee the numerical stability for the solution of the scalar transport equation. On the contrary, the adoption of low-order central schemes for the momentum equation leads to stable numerical solutions and they are therefore employed to compute the flowfield.

4.1. Numerical setup

The numerical solution of the Navier-Stokes and scalar transport equations is obtained using second-order accurate finite-volume techniques and a block-hexahedral grid. In this framework, the presence of the obstacle is easily managed by employing an unstructured grid connectivity. However, the most critical issue in the modeling of spatially developing flows using DNS and LES is represented by inflow and outflow boundary conditions. While it is generally accepted that convective boundary conditions at the outlet of the computational domain are suitable to the analysis of incompressible flows, it has been clearly established that inflow conditions can strongly affect the downstream development of the flowfield (Le & Moin 1992). Therefore, two different boundary settings have been tested in the computations: a constant velocity profile with zero fluctuations (uniform inflow) and a boundary-layer profile using superimposed fluctuations (turbulent inflow).

Figure 7. Mean scalar concentration downstream of the obstacle, (left column) water setup, (right column) air setup; (a,b) $k - \epsilon$, (c,d) $k - \omega$, (e,f) RST; contours range is 0.001–0.9.
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Figure 8. Profiles of turbulent scalar fluxes, (a,b) streamwise component of water setup at $x = 4h$ and $x = 6h$, (c,d) vertical component of water setup at $x = 4h$ and $x = 6h$, (e,f) streamwise component of air setup at $x = 4h$ and $x = 6h$, (g,h) vertical component of air setup at $x = 4h$ and $x = 6h$: (----) $k - \epsilon$, (---) $k - \omega$, (----) RST, (⊙) Vinçont et al. (2000).

In both cases the flow is supposed to be homogeneous in the spanwise direction, where a periodic condition has been applied, while a slip condition is employed at the upper boundary of the computational domain. The extent of the computational domain and the
overall grid resolution in wall units† are reported in Table 2. Although the computations are limited to very low Reynolds numbers, it must be noted that both the streamwise resolution far away from the obstacle and the resolution in the spanwise direction are such that the dissipative range cannot be properly resolved. However, preliminary tests performed by changing both the domain extent and the number of cells in the spanwise direction highlighted that the results are not strongly affected by the resulting modified grid resolution.

The code CDP (Mahesh et al. 2004) is adopted in the analysis of the uniform inflow condition while the turbulent inflow simulation is performed using the FLUENT code along with the code PS-SOL VER (Rossi 2008) for the solution of the scalar transport equation. The specification of the turbulent inflow is based on the random flow generation technique originally proposed by Kraichnan (1970) and later modified by Smirnov et al. (2001). This technique allows the generation of nearly divergence-free time-dependent flowfields with prescribed turbulent length/time scales which can be superimposed to a specified mean velocity profile. In the present analysis both the velocity profile and turbulent scales are obtained from the computation of the flow over a flat plate using the $k – \omega$ model, which has been previously performed to extract the set of inflow conditions adopted in the RANS-based analysis. A summary of numerical techniques for the Navier-Stokes equations adopted in the two different codes is presented in Table 3. Note that a low-order central interpolation scheme (LO-CD) is employed in both cases in order to guarantee the conservation of kinetic energy and therefore the numerical stability (Mahesh et al. 2004; Felten & Lund 2006).

At each time step, the continuity-satisfying mass flow rates are employed at cell faces

† The wall units are determined using the friction velocity obtained from RANS-based computations without the obstacle in place.

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Table 3. Summary of numerical techniques for the solution of governing equations.
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4.2. Uniform inflow analysis

In this section the results obtained from the analysis of the uniform inflow condition are presented. For the sake of completeness, the computations have been carried out using both the CDP code and the FLUENT/PS-SOLVER package, while the results previously obtained using the \( k - \omega \) model are also reported to allow a direct comparison. Note that the RANS-based analysis has been performed by specifying a boundary-layer profile at the inflow.

An illustration of the instantaneous flow structure is presented in Fig. 9, where turbulent coherent structures are identified using the \( \lambda_2 \) method of Jeong & Hussain (1995). In the same figure, an iso surface of scalar concentration is also reported to show where the mixing occurs. The flow is mainly characterized by the shear layer developing at the leading edge of the obstacle. The scalar plume emanating from the line source downstream of the obstacle is first convected up to the top of the square bar and then downstream in the wake. It is also clear that the shear layer development is strongly affected by the bulk Reynolds number of the flow. At the lower Reynolds number, corresponding to the water setup, the flow is characterized by large and intermittent structures close to the obstacle,
indicating a transitional flow; on the other hand, at the higher Reynolds number of the air setup, small-scale turbulent eddies are clearly evident in the wake.

4.2.1. Flowfield

The vertical profiles of mean streamwise velocity are shown in Fig. 10. Although the separated regions are clearly over-estimated in both the numerical experiments, in the case of the water setup the profile’s shape is also very different from measurements: at \( x = 4h \) the flow is nearly stagnant within the recirculating region, while at \( x = 6h \) the backflow velocity is almost constant up to the location of the shear layer \( (y \approx 1.5h) \). The results obtained by the CDP and the FLUENT code are almost identical. The situation is considerably different in the air setup, where the backflow velocity is not consistently computed using the two codes. This result indicates that the different numerical techniques adopted in CDP and FLUENT affect the prediction of the turbulent structures. It is also interesting to note that the velocity at the edge of the profile is largely affected by the uniform inflow, being strongly over-predicted compared to both the reference datasets.

The analysis of computed streamwise and vertical turbulence intensity profiles for the water setup in Fig. 11 shows that the region close to the obstacle is characterized by a lower level of turbulent fluctuations compared to the experimental measurements. Therefore, the prediction of a flat velocity profile in Fig. 10(a) corresponds to a nearly laminar separated region. The comparisons between the simulations and the measurements are clearly unsatisfactory. The turbulence intensity profiles for the air setup show that velocity fluctuations are very large compared to the measurements. However, although the turbulence intensity indicates a very energetic flow, the separated region is very large and the reattachment length significantly over-estimated.

4.2.2. Scalar dispersion

The computed mean scalar profiles are presented in Fig. 12. It is clear from the analysis of the water setup in Figs. 12(a) and (b) that turbulent dispersion is nearly absent at both streamwise locations. This is suggested by the local peak of scalar concentration within the shear layer \( (y \approx 1.5h - 2h) \), which is very similar to the laminar profile that would be obtained in the limit of \( Sc, Sc_t \to \infty \) using RANS models. Therefore, in the case of the water setup, the scalar dispersion is dominated by the mean flow transport. This is also confirmed by the constant scalar concentration within the obstacle height \( (y < 1h) \) where the flow is nearly stagnant (see Figs. 10(a) and (b)). The concentration profiles also show the more diffusive character of the upwind discretization adopted in the code PS-SOLVER compared to the QUICK scheme employed in the CDP code. In the air setup, the concentration is under-predicted (see Figs. 12(c) and (d)) and the absence of high concentration in the shear layer indicates a stronger turbulent scalar flux in the vertical direction compared to the water setup.

4.3. Turbulent inflow analysis

The analysis of the results obtained by adopting the uniform inflow clearly suggests a strong influence on the development of the scalar wake, determined by the onset of transition in the shear layer developing from the leading edge of the square obstacle. Therefore, in this section the analysis is focused on the effect of the turbulent inflow condition described in Sect. 4.1. The computations are performed using the FLUENT/PS-SOLVER package and the results will be directly compared to those obtained from the uniform
inflow analysis. Furthermore, in this case the profile of Reynolds stress and turbulent scalar fluxes are also discussed and compared to the experimental measurements.

An initial insight into the effect of introducing randomly generated turbulent fluctuations at the inflow is given in Fig. 13. In the case of the water setup, the breakdown of the shear layer occurs closer to the obstacle when the turbulent inflow is adopted; the region above the scalar source is characterized by larger fluctuations. In the air setup, the opposite behavior is observed, with the shear layer becoming more regular. In the water setup, the boundary layer approaching the obstacle changes the inception of the shear layer and, as it has been shown by Zhuang (1999), produces an increased streamlines
curvature which is destabilizing. In the air setup, the velocity profile at the inlet results in a lower velocity at the obstacle height, and therefore in a more stable shear layer.
4.3.1. Flowfield

In order to provide a more detailed analysis of the mean field predicted by the present computations, in this section both turbulence intensity and Reynolds stress profiles are presented. The relationship between the mean velocity field and the turbulent transport can be highlighted by writing explicitly the terms arising from the Reynolds stress tensor.
in the momentum equation for the mean field as follows\footnote{Here the uppercase and lowercase letters are used to denote the mean and fluctuating velocity components, respectively.}: \[\text{NS}(U) = -\frac{\partial}{\partial x}(\overline{u^2}) - \frac{\partial}{\partial y}(\overline{uv}) \] \[\text{NS}(V) = -\frac{\partial}{\partial x}(\overline{uv}) - \frac{\partial}{\partial y}(\overline{v^2}),\] where NS is the Navier-Stokes operator applied to the streamwise and vertical mean velocity components \(U, V\).

The analysis of mean velocity profiles in Fig. 14 shows that the turbulent inflow condition has a dominant effect on computed first-order statistical moments for the water setup. The early stage of transition occurring closer to the obstacle causes a significant change in the profiles shape, particularly at \(x = 6h\). Furthermore, the adoption of the boundary layer profile at the inlet of the computational domain yields a very large velocity reduction at the edge of the boundary layer, giving a closer agreement with the experiments. However, the region of flow reversal is still strongly over-estimated. In the case of the air setup, the profiles confirm the early transition of the shear layer even in the absence of superimposed fluctuations at the inlet section, the profile’s shape being very similar between the uniform and turbulent inflow conditions. This suggests that the turbulent transport is active in both cases. Note that as in the case of the water setup, the outer velocity in Figs. 14(c) and (d) is significantly reduced by adopting the boundary-layer profile at the inflow, but the separated region is still over-predicted.

The streamwise and vertical turbulence intensity profiles for the water setup are presented in Fig. 15. At the streamwise position \(x = 4h\) the most evident effect resulting from the turbulent inflow is the local maximum located roughly at \(y \approx 1h - 1.5h\), i.e., within the shear layer. The same peak is found in the experimental measurements for the streamwise component while it is not evident in the vertical direction. However, up to the obstacle height the computed profiles are fairly similar, in agreement with the results for the mean velocity shown in Fig. 14(a). This is not the case of turbulence-intensity

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Figure 14. Profiles of mean streamwise velocity, (a,b) water setup at \( x = 4h \) and \( x = 6h \), (c,d) air setup at \( x = 4h \) and \( x = 6h \); (---) uniform inflow, (----) turbulent inflow, (◦) Vinçont et al. (2000).

Profiles at \( x = 6h \), where the vertical component shown in Fig. 15(d) is greatly enhanced within the height of the obstacle by the turbulent inflow condition. Moreover, although the streamwise component is still under-predicted in this region (see Fig. 15(b)), the overall agreement with the reference dataset is significantly improved in the presence of superimposed fluctuations at the inlet. The profiles of turbulence intensity for the air setup clearly show the unexpected enhancement of turbulent fluctuations when the uniform inflow is employed. In the case of the turbulent inflow, the damping effect is evident in both the streamwise and vertical components and the agreement with the experimental measurements is greatly improved. It must be noted that a slower reattachment of the flow downstream of the obstacle could be expected owing to the lower
level of turbulence intensity. Although this is in contrast with the mean velocity profile at $x = 4h$ shown in Fig. 14(c), the reduced flow reversal can also be a consequence of the low-momentum fluid across the shear layer determined by the boundary-layer profile specified at the inflow.

The analysis of the Reynolds stress $\overline{uv}$ in Fig. 16 shows that the profiles are consistent
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with the scenario depicted for the mean velocity field and turbulence intensity. In the case of the water setup the turbulent transport at $x = 4h$ is practically absent when the uniform inflow is employed, indicating that streamwise and vertical turbulent fluctuations are not correlated. If the turbulent inflow is activated, a significant contribution is present across the shear layer, while it is nearly zero up to the obstacle height. This is again in agreement with the small change in the mean velocity profile shown in Fig. 14(a). The flow conditions at $x = 6h$ are similar; the turbulent transport is significantly larger in the case of the turbulent inflow within the obstacle size, resulting in the different shape of the velocity profile in Fig. 14(b). The Reynolds stress profiles for the air setup in Figs. 16(c) and (b) suggest once again the damping effect following from the boundary-layer profile with superimposed fluctuations at the inlet. At both streamwise locations, a significant reduction of the correlation between velocity fluctuations is found.

4.3.2. Scalar dispersion

As in the case of the flowfield, the relationship between the mean scalar field and the turbulent transport can be highlighted by writing explicitly the contributions arising from turbulent scalar fluxes in the mean scalar transport equation as follows:

$$ST(C) = -\frac{\partial}{\partial x}(\bar{u}c) - \frac{\partial}{\partial y}(\bar{v}c),$$

(4.3)

where $ST$ denotes the transport operator for the mean scalar concentration $C$. Since the flowfield analysis highlighted a weak development of the wake downstream of the obstacle, the vertical component of turbulent scalar fluxes in Eq. (4.3) should give the most relevant contribution to the scalar dispersion.

The results for the mean scalar concentration are presented in Fig. 17. The shape of profiles for the water setup is closely related to the mean velocity field shown in Figs. 14(a) and (b). At $x = 4h$ the effect of the turbulent inflow is not particularly evident and the profile is just shifted downward in the vertical direction. Moreover, a sharp increase of the scalar concentration close to $y \approx 1.5h$ is found unchanged using both inflow conditions. In spite of that, the earlier onset of transition in the case of the turbulent inflow can be noted at $x = 6h$, where the mean scalar profile is in closer agreement with the reference dataset. On the other hand, as noted in Figs. 17(c) and (d), the overall effect of the superimposed fluctuations at the inlet is clear at both the streamwise locations for the air setup. The predicted profiles are consistent with the reduced level of turbulent velocity fluctuations, resulting in the higher scalar concentration compared to the uniform inflow results. However, while the agreement with the experimental measurements is satisfactory at $x = 4h$, the profile obtained at $x = 6h$ is over-estimated.

The analysis of turbulent scalar fluxes for the water setup in Fig. 18 shows a significant improvement in computed profiles when the turbulent inflow is employed, particularly at $x = 4h$. Moreover, while a vanishing streamwise component has been predicted by the RANS-based analysis, both the magnitude and location of the negative peak in Figs. 18(a) and (b) are correctly reproduced by the present computations. Nonetheless, the weak positive peak is over-predicted and shifted upward in the vertical direction compared to the experimental measurements. The results also show that the vertical component at $x = 4h$ is far from the reference dataset, in agreement with the results for the mean scalar profile at the same streamwise location. The prediction is improved to some extent at $x = 6h$, but the comparison with the experiments is again far from being satisfactory. A better agreement for turbulent scalar fluxes is found for the air setup. In this case, the prediction of both the streamwise and vertical components is in agreement.
Figure 16. Profiles of Reynolds stress, (a,b) water setup at $x = 4h$ and $x = 6h$, (c,d) air setup at $x = 4h$ and $x = 6h$; (---) uniform inflow, (—) turbulent inflow, (◦) Vinçont et al. (2000).

with the experiments at $x = 4h$, while this is not as satisfactory at $x = 6h$. This is again in agreement with the results for the mean scalar profile presented in Figs. 17(c) and (d), showing that accurate predictions of turbulent transport are needed for high-fidelity simulations of scalar dispersion.

5. Conclusions and future work

A preliminary study of scalar dispersion in the wake of an obstacle using RANS and DNS techniques has been presented. The comprehensive comparison with experimental measurements at two different Reynolds numbers has shown that RANS predictions are significantly affected by the modeling of turbulent scalar fluxes using the standard
isotropic eddy-diffusivity assumption. Although the $k-\omega$ model has shown good agreement with measurements for the water setup, the predicted scalar concentration at the higher Reynolds number characterizing the air setup revealed a significant departure from the reference dataset. Moreover, no one of the adopted turbulence closures has been able to predict the streamwise component of the turbulent scalar flux. The evaluation of high-order scalar flux modeling based on the generalized gradient-diffusion hypothesis has therefore been planned to overcome these limits.

As a result of the interaction between the scalar plume and the dynamics of the shear layer emanating from the leading surface of the obstacle, the results from direct numerical simulations have been found significantly affected by inflow boundary conditions. The
use of randomly generated perturbations at the inflow anticipated the transition of the shear layer in the water setup, thus considerably enhancing the turbulent transport in the region above the scalar source. The results for the air setup also suggest that the effect of inflow conditions should become weaker as the Reynolds number increases. Although further analyses should be performed in order to clarify the issue of the inflow conditions,
the discretization techniques adopted in the computations are found to be promising for high-fidelity simulations of turbulent scalar dispersion in complex geometries.

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