Towards passive scalar reconstruction using data assimilation

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1 ABSTRACT

Reconstructing three-dimensional (3D) mean velocity fields using limited observations is valuable for studying pollutant dispersion in urban flows. Data assimilation addresses the challenge of limited experimental observations and the cost-accuracy trade-off of low-fidelity computational models. High-fidelity data is sourced from time-averaged velocity fields in a Detached Eddy Simulation (DES) of flow past a surface-mounted cube in a channel at Reynolds number 40,000. Additionally, pollutant dispersion is modelled by an upstream constant scalar source. DES results for mean scalar fields align well with experiments, validating its utility for pollutant dispersion studies. We use data assimilation to improve imperfect mean velocity predictions from Spalart-Allmaras (SA) Reynolds-Averaged Navier-Stokes (RANS) turbulence model using a single velocity data plane from DES. Improved mean velocity predictions across the domain highlight the potential of using limited observational data to correct RANS models for urban flow studies.

2 INTRODUCTION

RANS turbulence models offer a computationally efficient way of studying 3D flows despite limited accuracy in predicting flow physics in the presence of flow separation, streamline curvature and pressure gradients. Alternatively, the use of field imaging techniques such as particle image velocimetry (PIV) offer a realistic picture of the flow physics but provide only limited observations on discrete planes and not a continuous volumetric field. This paper aims to overcome the inherent limitations of CFD simulations and experimental measurements.

Data assimilation can be used to enhance low-cost simulations by RANS models by incorporating experimental measurements to increase accuracy. Unknown terms in the RANS simulation are tuned by minimizing the discrepancy between high-fidelity reference data and RANS output. This variational data assimilation has been used to assimilate full-field measurements in 2D at a low computational cost [4]. Its extension to 3D flows with limited measurement data is an opportunity that is explored in this paper.

The objective of this study is the assimilation of sparse mean velocity field from a high-fidelity simulation into a low-fidelity model for a 3D flow problem. The assimilation is done for the case of a 3D surface mounted cube in a channel. The geometry represents a simplified model of flow past an isolated tall building which is relevant for urban fluid mechanics. We then apply the variational method to enhance the accuracy of SA turbulence model predictions by integrating limited DES-obtained observations.

3 CASE SETUP

The case consists of a cube mounted on the bottom wall of a channel. The schematic of the case is shown in Figure 1a. The streamwise, vertical and cross-stream directions are along x, z and y respectively. The cube is located $x = 3.5H$ from the inlet and placed centrally between $y = 0$ and $y = 9H$ in the cross-stream direction. The Reynolds number of the flow based on the side of the cube H is $Re_H = 40,000$ which is set by fixing $H = 1m$, $U = 1m/s$ and $\nu = 2.5 \times 10^{-5} m^2 s^{-1}$. The structured 3D mesh consists of 1,216,000 cells with refinement in the wake region as shown in Figure 1b. The scalar is introduced as a source term shaped as a cube of side $0.1H$ that is located in the streamwise mid-plane of $y/H = 4.5$, at a distance of $1.5H$ upstream of the front face of the cube, $0.1H$ units above the bottom wall. The strength of the scalar source is 5 units. The simulations are performed using the open-source finite-volume CFD solver OpenFOAM.

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4 METHODOLOGY

4.1 Detached eddy simulation

The reference data is generated by performing a variant of DES (improved delayed DES or IDDES with SA as the background RANS turbulence model) and then time-averaging the velocity and scalar concentration fields. This model applies RANS in the near wall region and switches to LES to resolve the turbulent eddies in regions away from the wall. The computational details including the boundary conditions can be found in [1].

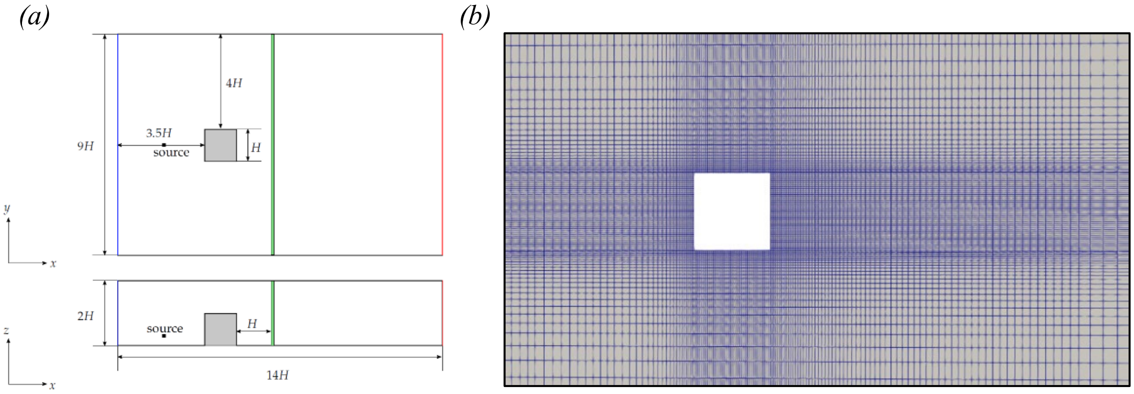

Figure 1. (a) Schematic of the test case. Inlet (—) and outlet (—) boundaries shown with location of reference data plane (—) and scalar source. (b) Close up of transverse section of the mesh at z/H = 0.5.

4.2 Reynolds-Averaged Navier-Stokes

The reference data obtained from DES is assimilated into a low-fidelity RANS turbulence model. The RANS equations are given by,

$$\overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu_{eff}\frac{\partial \overline{u}_i}{\partial x_j}\right), \tag{2}$$

where the overbar indicates Reynolds averaging, u is the velocity, P is the combined pressure and turbulent kinetic energy k and $\nu_{eff} = \nu + \nu_T$ is the effective kinematic viscosity which is the sum of molecular viscosity ν and eddy viscosity ν_T. The eddy viscosity can be obtained by solving a transport equation using SA turbulence model, the functional form of which is given by,

$$\frac{D\tilde{\nu}}{Dt} = P(\tilde{\nu}, \boldsymbol{w}) + T(\tilde{\nu}, \boldsymbol{w}) - D(\tilde{\nu}, \boldsymbol{w}), \tag{3}$$

where P, T and D are respectively production, diffusion transport and destruction terms, $\tilde{\nu}$ is the surrogate viscosity and $\boldsymbol{w}$ is the vector of state variables.

4.3 Variational data assimilation

The time-averaged DES velocity data can be used to improve the prediction of the RANS SA model. The goal is find an optimum control variable distribution that minimizes an objective function, formulated as a discrepancy between reference data and RANS model output, subject to constraints given by,

$$f(\boldsymbol{u}, \beta) = \frac{1}{2}\left\| Q(\boldsymbol{u}, \beta) - \widetilde{\boldsymbol{Q}} \right\|^2, \tag{4}$$

where β is the control/design variable of choice, Q is a projection function, $\widetilde{\boldsymbol{Q}}$ is a set of high-fidelity velocity measurements obtained from DES (can also be obtained from PLIF or DNS). The production term of the SA model is pre-multiplied by a spatially varying scalar multiplier $\beta(x, y)$. The modified transport equation for the SA model is given by,

$$\frac{D\tilde{\nu}}{Dt} = \beta P(\tilde{\nu}, \boldsymbol{w}) + T(\tilde{\nu}, \boldsymbol{w}) - D(\tilde{\nu}, \boldsymbol{w}). \tag{5}$$

The baseline SA model can be recovered by setting $\beta = 1$ throughout the domain. We use the discrete adjoint method implemented in DAFoam [3] to obtain the gradient and an interior point method with line search filter implemented in IPOPT to perform the optimization. A single plane of reference data that is located at *x/H = 5.5* or *1H* from the trailing face of the cube (as shown in Figure 1a) is supplied to the assimilation step to perform data assimilation using limited measurements.

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5 RESULTS

5.1 Mean velocity fields

The mean streamwise and vertical velocity fields from DES along planes *z/H = 0.5* and *y/H = 4.5* are presented in Figure 2. The wake recirculation region in Figure 2a is clearly delineated by the $\frac{\bar{u}}{U_\infty} = 0$ contour. Figure 2b suggests that the flow is pushed upward near the trailing face of the cube denoting the presence of recirculation. It is also observed that most of the wake recirculation is confined to a very small region in the vicinity of the cube (~1.5H from the trailing edge). These results are also supported by similar observations made in [5], albeit for a tall building.

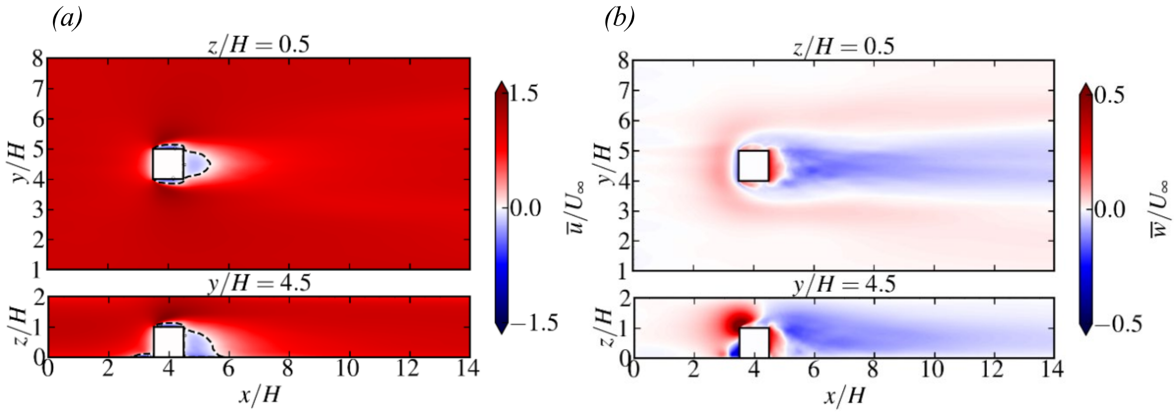

Figure 2. Velocity contours of (a) streamwise (b) wall-normal mean velocity along planes z/H = 0.5 (top) and y/H = 4.5 (bottom). The dashed line is contour of $\frac{\bar{u}}{U_\infty} = 0$.

An interesting point to note is the location of the stagnation point in Figure 2b (the location where the vertical velocity magnitude changes from negative to positive). This is located at *z/H ~ 0.58* which agrees well with [5]. Placing a scalar source below this stagnation point affects the manner in which it diffuses which will become clear upon examining the mean scalar concentration field.

5.2 Mean scalar fields

The mean scalar concentration on two cross-stream planes is presented in Figure 3a. The double peak structure is visible on both planes. The scalar is confined to a region close to the bottom wall with a limited spread in the cross-stream direction. The double peak observation agrees well with experiments performed in [5] where they speculate the distribution to be a result of entrainment in the horseshoe vortex. This is a result of placing the scalar source below the stagnation point of the cube which discourages scalar dispersion over the cube.

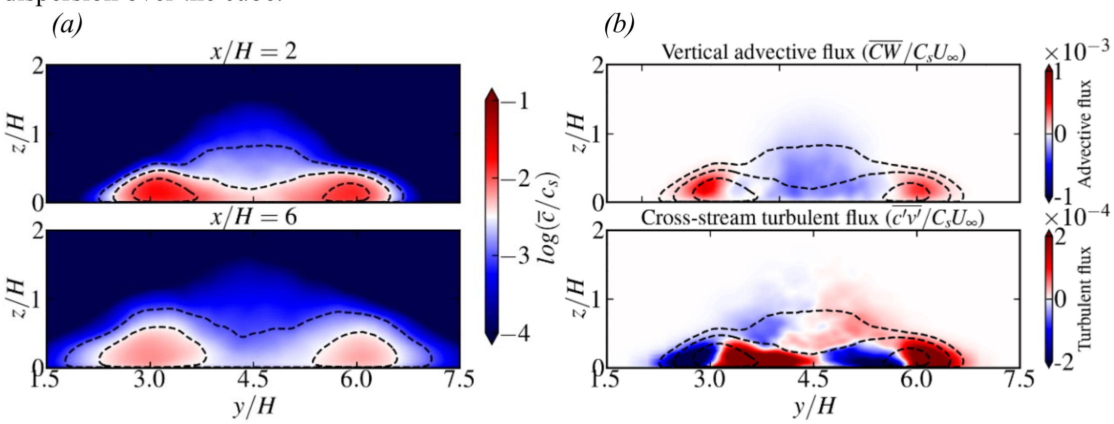

Figure 3. (a) Mean scalar concentration along two cross-stream planes at x/H = 2 and x/H = 6 from the cube trailing face. Dashed contour lines indicate scaled logarithmic scalar concentrations of -3, -2.5 and -2 (b) advective and turbulent fluxes along cross-stream plane at x/H = 2.

The vertical advective and cross-stream turbulent fluxes along a cross-stream plane at *x/H = 2* from the cube trailing face are show in Figure 3b. The advective fluxes are greater than the turbulent fluxes by an order of magnitude. Since the scalar concentration is positive, a negative vertical advective flux indicates a downward transport of the scalar just behind the cube. The positive advective flux shows a double peak

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that coincides with the region of maximum scalar concentration (shown as dashed contours in Figure 3b). The cross-stream turbulent flux shows structures alternating in sign that accumulate the scalar towards the two peaks as can be seen in the dashed isocontours of scalar concentration. In general, these show good agreement with the advective and turbulent fluxes from [5]. The complex flow physics that involve wake recirculation, presence of horseshoe vortex and leading edge flow separation with a shear layer present a good case for data assimilation since they cannot be captured accurately by RANS models.

5.3 Assimilated mean velocity

The comparison of the mean velocity field from baseline SA model with the reference DES result is offered in Figures 4a. The baseline model over predicts the extent of the recirculation bubble as can be seen in Figure 4a. The assimilated mean velocity fields show a very good improvement over the baseline when compared to the reference DES result (Figure 4b). While the reference data was supplied along one cross-stream plane (Figure 1a), the improvement in mean velocity can be observed across other planes in Figure 4b. This encouraging result is particularly beneficial for experiments where it is expensive to image volumetric fields. This result shows that limited planar measurements can be incorporated into RANS models to improve the accuracy of mean flow predictions of 3D flows in the entire domain.

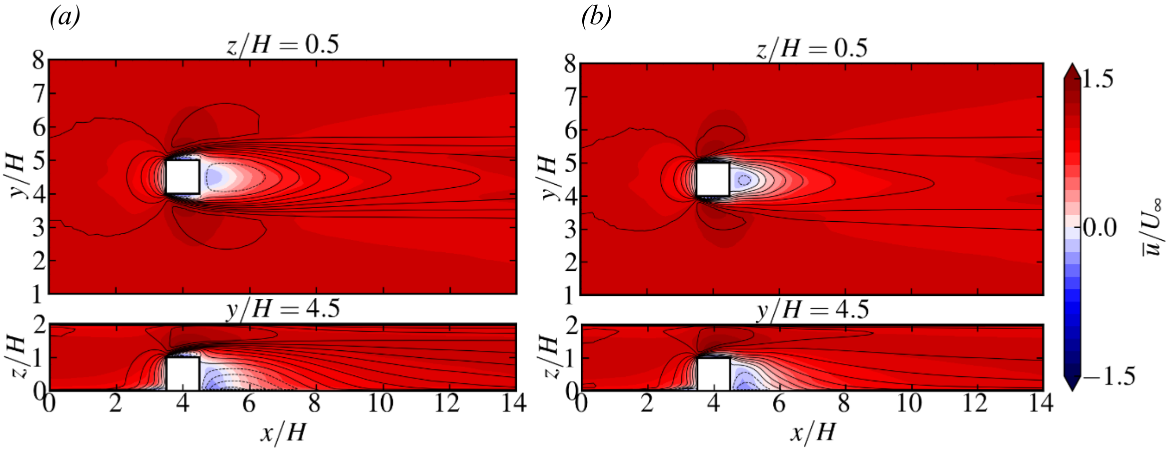

Figure 4. Mean streamwise and vertical components of velocity from (a) baseline RANS SA model and (b) assimilated RANS SA model (solid contours show reference DES velocity field and contour lines show the results from RANS).

6 CONCLUSION AND FUTURE WORK

We performed a DES of a 3D surface mounted cube in a channel with a fixed strength passive scalar source at Re_H = 40, 000. The mean scalar concentration fields, and the advective and turbulent fluxes show good agreement with experiments. Data assimilation using the variational method was performed by supplying a single plane of reference data generated by time-averaging the DES velocity field. The improvement in mean velocity field of a baseline RANS SA model demonstrates the utility of using limited measurements in 3D data assimilation using the variational method. Future work includes scalar source location identification and assimilation of the turbulent scalar flux term (which is typically modelled in RANS models) using reference scalar concentration and mean velocity field from volumetric experimental measurements.

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