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Turbulence modelling using 3DVAR data assimilation in laboratory conditions

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Abstract— **The viability of turbulence parameter estimation in a numerical model using 3DVAR data assimilation technique is explored in this research. Water currents measured in a physical model are assimilated into the numerical model DIVAST in order to improve prediction skill of the model in regions where turbulent processes are of importance. The performance of two turbulence closure schemes, the standard *k*-ε model and the Prandtl mixing length model, is investigated.**
The assimilation of the model-predicted velocity and laboratory observations significantly improves model predictions for both turbulence schemes. The research further demonstrates how 3DVAR can be utilized to identify and quantify shortcomings of the numerical model and consequently to improve forecasting by correct parameterization of the turbulence models. Such improvements may greatly benefit physical oceanography in terms of understanding and monitoring of coastal systems and the engineering sector through applications in coastal structure design, marine renewable energy and pollutant transport.

Keywords—numerical modelling; turbulence modelling; data assimilation; 3DVAR

I. INTRODUCTION

Numerical modelling of coastal waterbodies is a major challenge due to the complexity of coastal marine dynamics and the correct mathematical representation of the physical processes that govern the dynamics. Inherent uncertainties in hydrodynamic modelling are the results of many factors including unknown model parameters such as those that define turbulence processes. Assumptions in turbulence modelling, resulting from closure on Reynolds equations, introduce a number of empirical inputs that often limit the robustness and accuracy of the solution. These simplifications are noticeable when complex turbulent flow is considered as in this research.

Existing turbulence models differ greatly in their complexity, adequacy and computational economy. The lower order models have the advantage of being computationally cheap but at the expense of accuracy, whilst the higher order models are more computationally expensive due to the greater number of equations but are more likely to produce an accurate solution to a general problem. Therefore, the selection of the model and its parameterization is not easy and requires a good knowledge of the model formulations and the governing processes.

Model parameterization is a computationally expensive and labour-intensive process carried out through so-called model 'tuning'. Usually, good parameter estimates obtained through tuning lead to reduced model errors and improved model performance. A correct parameterization of the turbulence model may significantly improve model performance, but only if an accurate dataset is available.

Unlike numerical models, observations do not suffer from process representation, however, they are usually too sparse, partial and/or too noisy to draw inferences about coastal dynamics. These difficulties have been overcome in recent years by a use of data assimilation, which combines observations with model results to provide an optimal solution close to true state when correctly implemented. With regards to parameterization of numerical models, data assimilation assures that the estimated parameter values are optimal such that they are most consistent with the observations subject to error estimates of both observations and parameters [1].

In this study, the 3DVAR data assimilation scheme is incorporated into the hydrodynamic model DIVAST in order to (1) improve the numerical model prediction through assimilation, (2) assess the performance of the 3DVAR assimilation technique, (3) identify and quantify shortcomings of the numerical model and ultimately to (4) optimize the performance of the numerical model by selecting an appropriate turbulence scheme and tuning its parameters.

In this context, two turbulence models, namely the Prandtl mixing length (PML) model and the *k*-ε model are coded into DIVAST. Their performance is evaluated by examining their accuracy, universality of application, complexity of solution, computational efficiency and numerical stability. A physical model of a single entrance symmetrical square harbour tested in a laboratory tidal basin is used to assess the performance of the 3DVAR assimilation technique and the numerical model for the two turbulence schemes. A significant advantage of such laboratory experiments is the fully controlled environment where domain setup and forcing are user-defined.

In the first step of this research, outputs from the numerical simulations are compared with experimental observations from the tidal basin. This is followed by details of the assimilation of laboratory data into the numerical model. Finally, the turbulence models are reparameterized to improve model performance by matching with an optimal solution obtained through data assimilation.

II. Methods

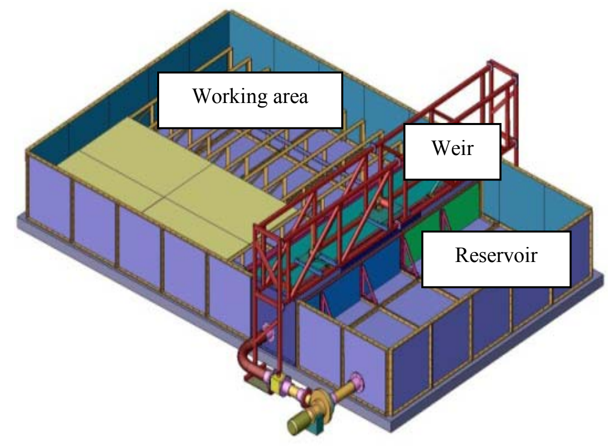
A. Tidal basin

The observational dataset of hydrodynamic flows, required for data assimilation and assessment of turbulence schemes, was obtained from the tidal basin experiment. A tidal basin is a physical model designed to generate tides and tidally-induced water circulation that can represent flow features of a prototype when appropriate scaling relationships are adopted. In horizontal plan the basin consists of a 8.0x5.0 m tank divided into three sections: (1) the reservoir that stores the excess of water, (2) the manifold chamber with pumping apparatus and weir, and (3) the working area separated from the manifold chamber by a porous baffle which promotes uniform flow within the working area and reduces swirl. The working area, with horizontal dimensions 4.75x5.0m, is the experimental part of the basin where measurements of flow fields and water elevations are performed. A schematic illustration of the tidal basin is shown in Fig. 1a. More details of the tidal basin design and functionality can be found in [2].

Tides are produced by a variable elevation weir that moves in the vertical direction according to a predetermined motion controlled by a computer-based control system. Upward and downward movement of the weir cause filling and emptying of the working area of the tank; these motions reflect flood and ebb flow conditions, respectively.

In this research, a simple square harbour with flat bottom, four vertical walls and one centrally located entrance was selected as a test case. The 1.0x1.0 m harbour of mean depth 0.27m is located in the middle of the working area of the tidal basin. For simplicity, the tidal spectrum consists of only one constituent characterized by a sinusoidal shape of amplitude 0.05 m and period 789 s. Harbour dimensions and all relevant flow parameters are shown in Fig. 1b. Flow measurements were sampled at 10 equidistant points along four axes A-D shown in Fig. 1b.

(a)



(b)

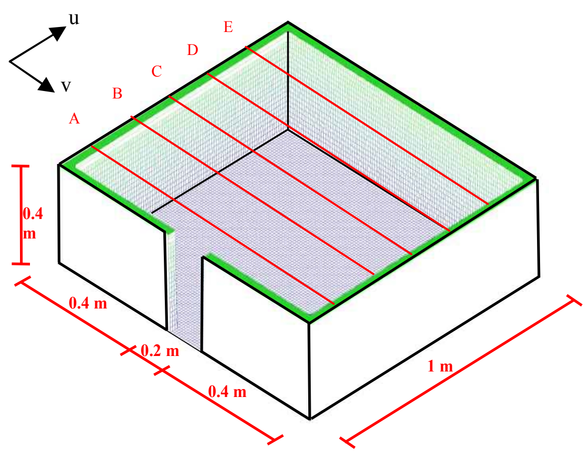


Fig. 1. Schematic illustration of tidal basin (a) and harbour dimensions with locations of axes A-E (b).

B. Numerical model

The numerical model adopted for this study is DIVAST (Depth Integrated Velocity and Solute Transport), a two-dimensional, depth-integrated, finite difference model. The hydrodynamic module is based on continuity and Reynolds-averaged Navier-Stokes equations, and includes the effects of local and advective accelerations, the rotation of the earth, barotropic pressure gradients and bed resistance. The mathematical formulation, technical details and the parameterization of the DIVAST model can be found in [3] and [4].

The model domain covers the entire working area of the tidal basin. Computations are carried out on a horizontal rectangular mesh consisting of 200x190 grid cells, each of which has dimensions 0.025x0.025 m. Tidal flows in the working area are driven by a variable surface elevation due to tides. At the open boundary a radiation condition relates the normal component of currents to the sea surface elevation accounting for tidal input. The numerical model setup represents exactly the same conditions as the physical model.

The dimensions and flow regime in the harbour, although partly a result of tidal basin capacity, reflect real-world tidal conditions and harbour configurations when scaled up using the Froude scaling law.

C. Turbulence models

In the scope of turbulence modelling, zero-equation Prandtl mixing length (PML) model and two-equation *k*-ε model are employed to verify a turbulence solution and its effect on complex hydrodynamic regimes. The PML model, commonly representing this group of models, determines eddy viscosity from the characteristic dimension given by the size of energy-containing eddies and the velocity of the flow itself. The depth-averaged form of the PML model correlates eddy viscosity for the horizontal transport $\overline{\nu_t}$ with friction velocity U_* and water depth H as follows:

$$\overline{\nu_t} = aU_*H \quad (1)$$

where α is a dimensionless coefficient to be determined. In general, α is smaller for open channels and where secondary motions are insignificant. Values in the range 0.13-0.15 have been reported for such domains by [5], [6], [7] and [8]. For natural channels and/or varying cross-section flows, α tends to be greater and may vary from 0.2-0.27 for straight natural channels and floodplains [9] to 0.6 in rivers [8] and up to 1.0 in channel bends [10].

The two-equation model selected for this research is the standard *k*-ε model [11] which employs a transport equation for the kinetic energy of turbulence *k* and a transport equation for the dissipation of turbulent energy ε. *k* is a direct measure of the intensity of turbulence fluctuations while ε represents the rate at which this energy dissipates. When the local depth-averaged state of turbulence is characterized by $\overline{k}$ and $\overline{\varepsilon}$, and the depth-averaged turbulent stresses are related to the depth-averaged velocity gradients, the depth-averaged form of the *k*-ε equation becomes [12]:

$$\frac{\partial \overline{k}}{\partial t} + U_i \frac{\partial \overline{k}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\overline{\nu_t}}{\sigma_k}\frac{\partial \overline{k}}{\partial x_i}\right) + P_h + P_{kv} - \overline{\varepsilon} \quad (2)$$

$$\frac{\partial \overline{\varepsilon}}{\partial t} + U_i \frac{\partial \overline{\varepsilon}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\overline{\nu_t}}{\sigma_\varepsilon}\frac{\partial \overline{\varepsilon}}{\partial x_i}\right) + c_{1\varepsilon}\frac{\overline{\varepsilon}}{\overline{k}}P_h + P_{\varepsilon v} - c_{2\varepsilon}\frac{\overline{\varepsilon}}{\overline{k}} \quad (3)$$

where depth-averaged horizontal production is related to depth-averaged velocity gradients through

$$P_h = \overline{\nu_t}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\frac{\partial U_i}{\partial x_j} \quad (4)$$

P_{kv} and $P_{\varepsilon v}$ are vertical production terms that absorb non-uniformity of vertical profiles and therefore strongly depend on bottom roughness. These terms are related to bottom shear stress through the friction velocity U_* as:

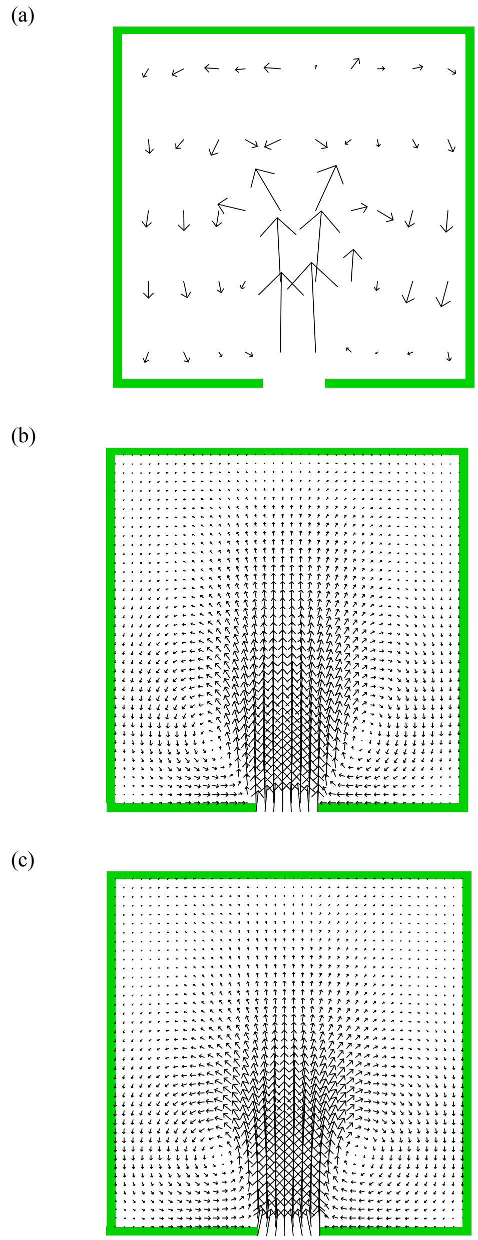


Fig. 2. Flow pattern in the harbour: observations (a), PML model (b) and *k*-ε model (c).

$$P_{kv} = c_k \frac{{U_*}^3}{H} \quad (5)$$

$$P_{\varepsilon v} = c_\varepsilon \frac{{U_*}^4}{H^2} \quad (6)$$

where the empirical coefficients c_k and c_ε are related to the friction coefficient C_f through $c_k = \frac{1}{\sqrt{C_f}}$ and

$c_\varepsilon = \dfrac{c_{2\varepsilon} {c_\mu}^{1/2}}{(e^* \sigma_\emptyset) {C_f}^{3/4}}$. Other empirical coefficients are $c_\mu = 0.09$, $c_{1\varepsilon} = 1.44$, $c_{2\varepsilon} = 1.92$, $\sigma_k = 1.0$, and $\sigma_\varepsilon = 1.3$, $\sigma_\emptyset = 0.5$. Dimensionless diffusivity e^* is more problematic to determine and ranges between 0.15-1.1 based on experimental studies. Finally, the depth-averaged eddy viscosity is calculated as:

$$\overline{v_t} = c_\mu \frac{\overline{k}^2}{\overline{\varepsilon}} \tag{7}$$

D. 3DVAR data assimilation

The data assimilation method implemented and evaluated in this research is the three-dimensional variational data assimilation (3DVAR) method [13]. This multi-step algorithm finds an optimal solution of the model by minimizing the following cost function

$$J(x) = \frac{1}{2}(x - x_b)^T B^{-1} (x - x_b) + \frac{1}{2}(H(x) - y)^T R^{-1} (H(x) - y) \tag{8}$$

where x is the analysis state vector, x_b is the background state vector, B is the background error covariance matrix weighting the misfit between analysis and background state, R is the observational error covariance matrix weighing the misfit between analysis state and observation and H is the non-linear observational operator. The first and the second terms in (8) are referred to as background and observational cost functions. The quadratic and positive definite $J(\delta x)$ guarantees a unique minimum in the process of minimization. A conjugate gradient solver [14] is employed to minimize the cost function. The ultimate analysis solution of the incremental 3DVAR is :

$$x_a = x_b + \delta x_a \tag{9}$$

where the analysis increment δx_a minimizes $J(\delta x)$.

Model and observation error variances are computed according to method described in [15]. Background error covariance matrices are stationary and explicitly modelled from their covariance structure and background error variances predetermined at the beginning of the assimilation. Three exponential correlation functions, (1) Gaussian, (2) first-order auto regressive and (3) second-order autoregressive models were examined. The ultimate selection of the function and the tuning of function parameters such as correlation length scale was made using a cross-validation of RMSEs.

In parallel to the analysis of the performance of data assimilation system, computational efficiency was assessed by testing various algorithms for data interpolation and matrix inversion. Ultimately, the bilinear interpolation algorithm of [16] was employed to map the first guess velocity vectors from model grid into observation space. With regards to the matrix inversion required for the minimization of cost function, three methods, (1) Gauss, (2) LU and (3) Choleski decomposition, were examined prior to their application to the data assimilation system in order to explore common problems with matrix inversion. The quality control method of [17] is adopted to improve analysis of the solution by judging the quality of data.

The effectiveness of the data assimilation scheme is evaluated by statistically comparing non-assimilated and assimilated model solutions with observations. The RMSE, as a standard model verification measure, and the data assimilation skill, based on mean square error (*mse*) given by expression [18]

$$DA_{skill} = 1 - \frac{mse_a}{mse_b} \tag{10}$$

are ultimately used in the verification process. mse_a (mse_b) is the mean square error between assimilated (non-assimilated) model solution and observation. A DA_{skill} in the range 0-1 indicates improvement in the model performance as a result of assimilation.

III. RESULTS AND DISCUSSION

A. Flows in square harbour

An assessment of the predictive abilities of the hydrodynamic model and the accuracy of turbulence schemes was the first stage of this investigation. The length of recirculation cell and the velocity magnitude predicted by the model using the two turbulence schemes are examined and compared with physical model records.

Fig. 2 compares experimental results of velocity fields at mid flood with modelled fields simulated by the numerical model using two different turbulence schemes. Flow patterns are generally comparable in all three cases and are as would be expected for such a harbour configuration. Velocity distribution in the vicinity to the harbour entrance represents a jet-sink type circulation. On the flood tide the flow entering through the harbour inlet takes the form of a jet while on the ebb tide the water leaving from the harbour has a sink-like shape. The highest velocity magnitudes are observed at mid flood in the vicinity of the entrance. Strong angular momentum of the flood flow separates water entering the harbour into two counter-rotating gyres. These symmetrical eddies persist over a full tidal cycle, though their location, size and strength alter throughout.

Velocity magnitudes and profiles along four axes, A-D, are shown in Fig. 3 (see Fig. 1b for location of axes). In general, the strength of inflow jet simulated by both turbulence models is underpredicted in the front part of the harbour when compared to observations from the same region. This underestimation of advective currents is likely to result from overgeneration of turbulence because higher turbulent shear stress causes stronger reduction of advective flow. As shown in Fig. 4, eddy viscosity fields at the entrance to the harbour predicted by both models are high; in particular when

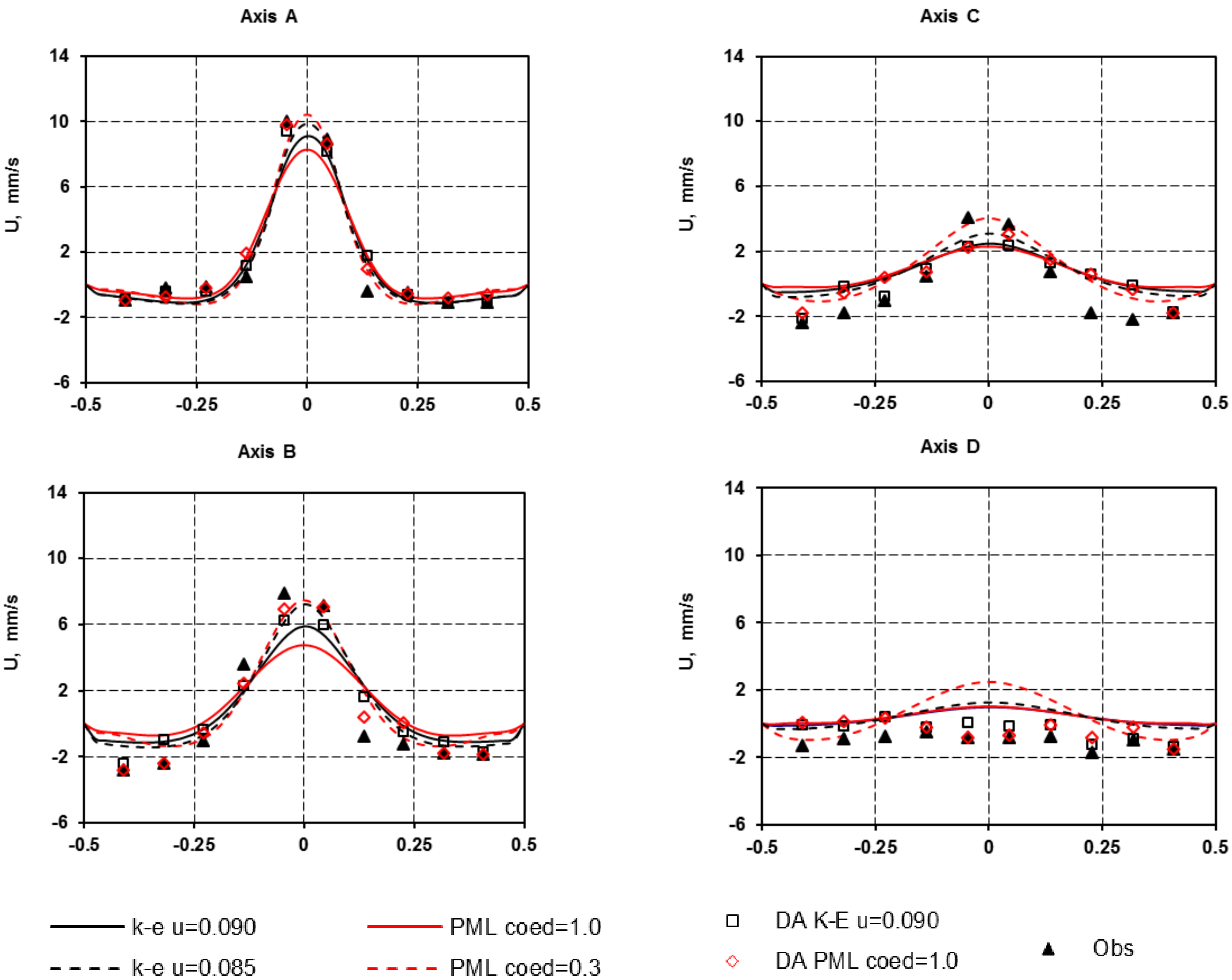


Fig. 3. Observed, assimilated and non-assimilated velocity magnitudes along axes A, B, C and D in the harbour.

simulated by the PML model with a predefined default diffusion coefficient of 1.0. This model simply relates eddy viscosity to local mean flow and bottom friction only (bed-generated turbulence) while ignoring the effect of horizontal shear stresses. As a result, spatial distributions of eddy viscosity follow the trends and patterns of velocity fields. Unlike the PML model, the *k*-ε model accounts for the transport of turbulence quantities and time history, and therefore exhibits more uniform distributions and over-predicts turbulence to a lesser degree. This over-prediction stems from the model assumption of equilibrium between generation and dissipation of turbulence which for strong mean-strain flows such as the recirculating flows investigated in this research is invalid. A modification to the dissipation equation would be needed in the form of an extra production term, or parameter retuning, to account for increased production when mean strain is significant.

In summary, the standard *k*-ε model is in better agreement with observations and is therefore superior to the simpler PML model which due to simplification of the empirical formula has limited universality and lower accuracy of solution. The superior ability of the technically advanced *k*-ε model to simulate complex flow features is balanced, however, by its higher computational cost, c. 55% higher than in the case of the PML model.

B. Data assimilation in square harbour

Taking into account that observations in the tidal basin contain a portion of instrumental error (particularly for relatively small velocities) the assumption that observations represent a true state of the hydrodynamics in the harbour is incorrect. The practical solution to finding an optimal value that is as close as possible to the true state is to assimilate velocity observations into a numerical model. This has been achieved by incorporating the 3DVAR assimilation scheme into DIVAST.

Spatial maps of analysis solutions on an observational grid for the *k*-ε and PML models are shown in Fig. 5c along with maps of observations (Fig. 5a) and background values (Fig.

(a)

(b)

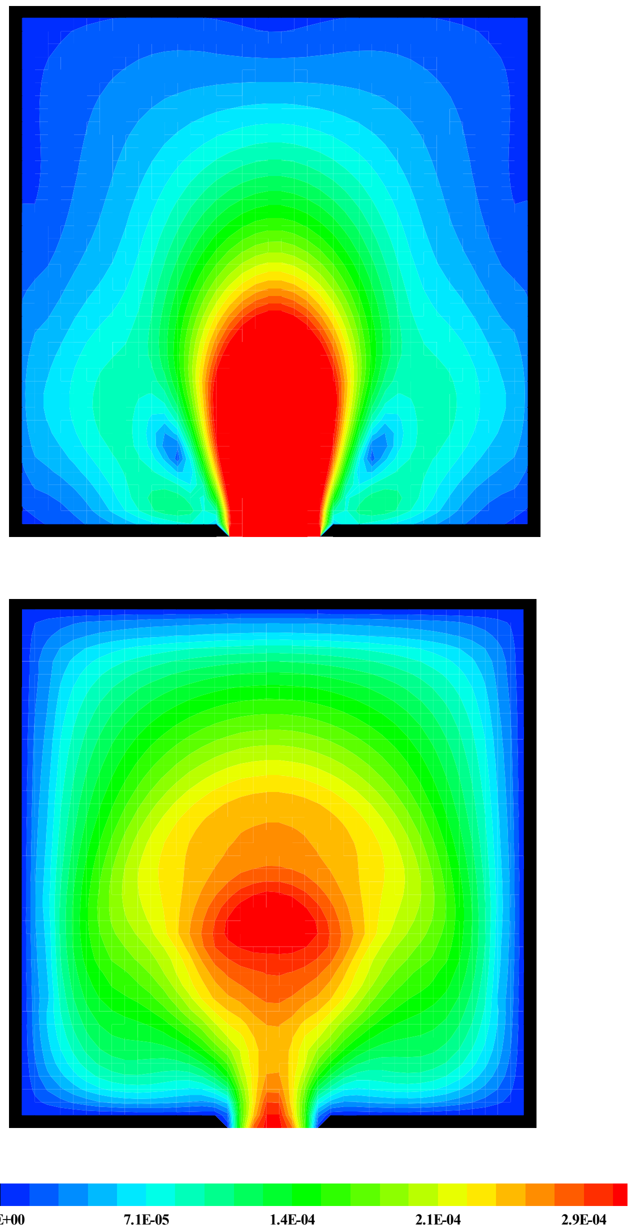


Fig. 4. Eddy viscosity (m^2/s) predicted by DIVAST with PML (a) and k-ε model (b).

5b). Patterns of assimilated flow fields are similar to those modelled and observed though velocity magnitudes differ from those modelled and observed (Fig. 3). The analysis values are generally greater than those simulated by the models, yet smaller than the observations. This is particularly evident at the inflow region characterized by strong velocities, where data force greater flow magnitudes.

Interestingly, despite marked discrepancies in the flow magnitudes between the two turbulence models (particularly in the inflow region) the assimilated products are in close agreement. This indicates that the analysis product is an optimal solution towards which the turbulence models should be tuned. The 3DVAR scheme is assessed statistically by comparing differences between the model results and observations for assimilated and non-assimilated experiments.

In the case of both turbulence schemes, the model performance measured by the RMSE reduction is shown to be significantly improved at every point of data assimilation. The effectiveness of the data assimilation scheme is also verified by the DA skill (10). As shown in Fig. 6 a and b, all values are in the range 0-1, implying overall improvement of the simulation by data assimilation. The closer the DA skill value to unity, as in the case of the PML model, the greater the improvement.

C. Parametrization of turbulence models

Since there is no true state available to assess the accuracy of parameter estimation, the turbulence models are reparameterized to fit the data assimilation optimal product. In the case of the PML model a number of values for the diffusion coefficient were examined; the tested range was 0.1-1.0 at 0.1 intervals. Coefficients closer to 1.0 tend to overestimate turbulence yielding underestimation of advective currents. In contrast, very small coefficients significantly underpredict turbulence processes. The smallest RMSE between the data assimilation analysis and the model was found for a diffusion coefficient of 0.3. The improvement, however, is only regional and while the modelled velocities along the front axes A-B are significantly increased giving an overall improvement in model performance, the velocities towards the rear are also increased resulting in significant over-prediction of velocities in that region. This exercise shows that the model cannot be applied to cases of complex flow fields, such as rapidly developing flows or recirculating flows, by simply applying one universal empirical constant. It is clear that for different parts of the flow, characterized by different states of turbulence, different empirical solutions are needed.

Limitations of the PML model are partially overcome by the k-ε turbulence model which takes better account of changes in turbulence structure. The standard model, however, assumes equilibrium in local turbulence so that the rate of turbulence production and dissipation are in approximate balance. In complex shear flows, as in the square harbour, production differs from ε and so, to account for this difference, the dissipation equation needs to be reparameterized. Reference [12] relates P and ε through an empirical function $c_\mu = f(P/\varepsilon)$ where $c_\mu = 0.09$ for $P = \varepsilon$ and $c_\mu < 0.09$ for $P > \varepsilon$. A number of values for c_μ was tested in this research and $c_\mu = 0.085$ yields the best model performance against analysis solution; thus, this is number is recommended for shear turbulent flows. Retuning changes the rate of P to ε from 1.0 to approximately 1.2. Fig. 3 confirms a significant improvement of model prediction when the turbulence processes are optimized by an accurate parameterization of the k-ε model. This accuracy coupled with the complexity of the numerical solution results, however, in a high cost of simulation, which when compared to the PML model is approximately 55% higher.

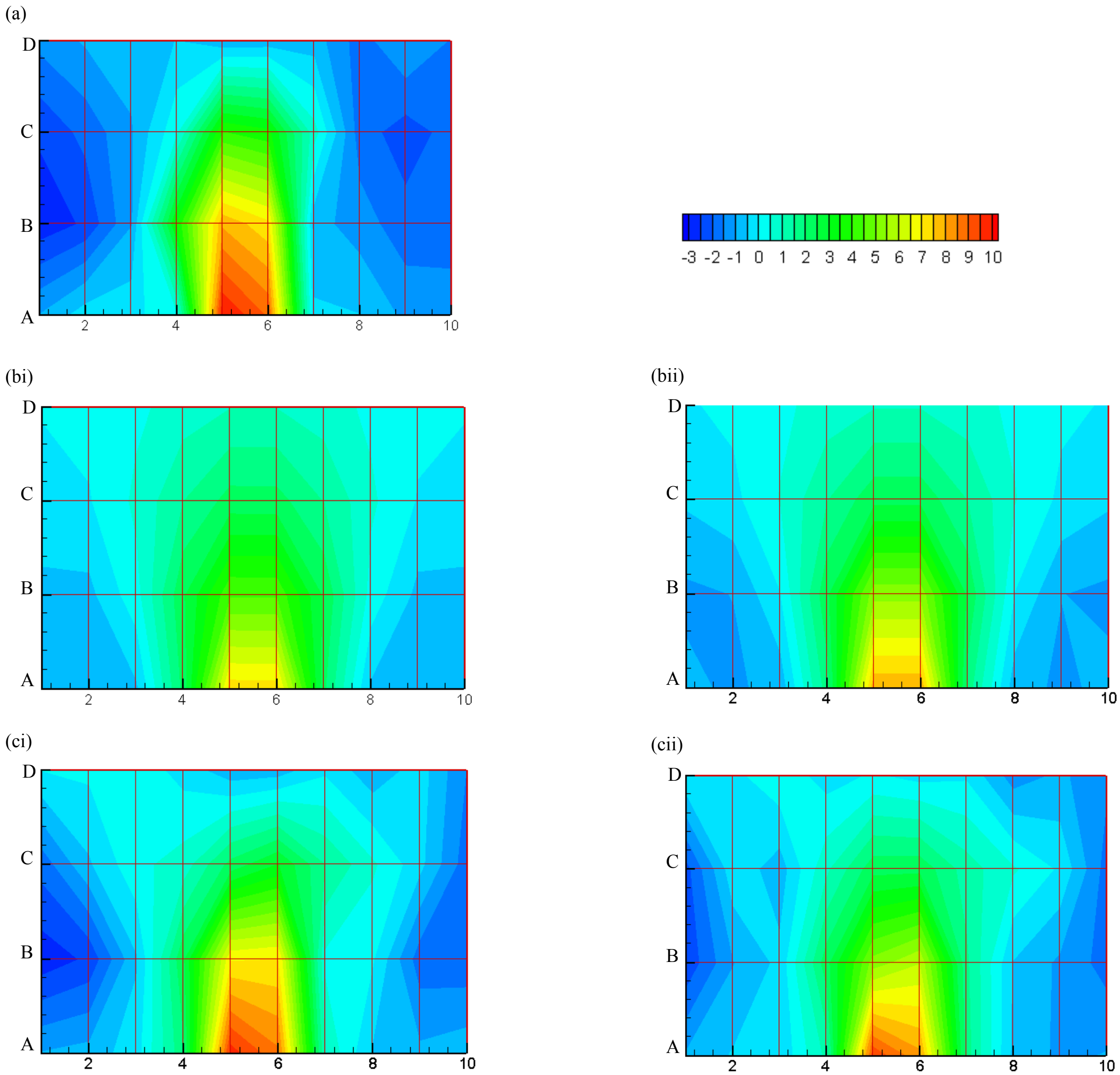


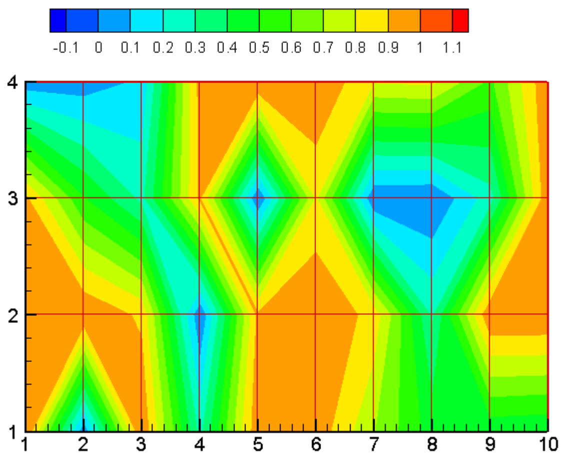
Fig. 5. U-velocity magnitudes (mm/s) along axes A-D: observations (a), model simulations (b) and 3DVAR analysis (c). PML model (i), *k*-ε model (ii).

I. CONCLUSIONS

In this research the 3DVAR data assimilation scheme is implemented in the numerical model DIVAST in order to optimize the performance of the numerical model by selecting an appropriate turbulence scheme and tuning its parameters. With regard to turbulence modelling the first conclusion is that both turbulence models, with default parameterization predefined according to literature recommendations, overestimate eddy viscosity which in turn results in a significant underestimation of velocity magnitudes in the harbour.

This research further demonstrates that the data assimilation of the model-predicted velocity and laboratory observations significantly improves model predictions for both turbulence models by adjusting modelled flows in the harbour to match de-errored observations. Such analysis gives an optimal solution based on which numerical model parameters can be estimated. The process of turbulence model optimization by reparameterization and tuning towards optimal state led to new constants that may be potentially applied to complex turbulent flows, such as rapidly developing flows or recirculating flows.

(a)



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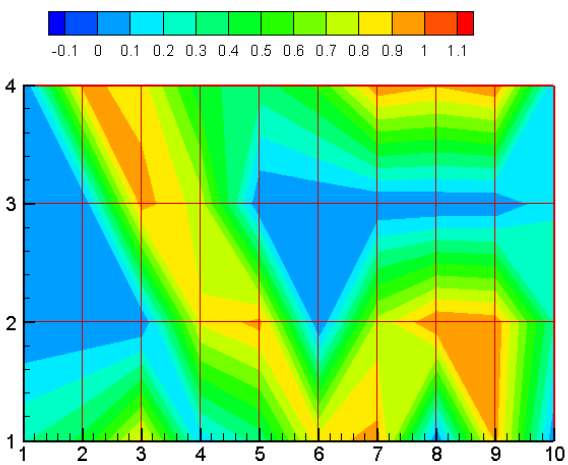

Fig. 6. Data assimilation skill assessment based on Equation 10 for PML model (a) and k-ε model (b).

The new diffusion coefficient for the PML model alleviates the problem in regions of strong turbulence but simultaneously deteriorates results at the back of the harbour characterized by weak turbulence. The method cannot be used in its current form (a single constant throughout the full domain) where the state of turbulence changes across the flow. One feasible solution is to update the parameter spatially by utilizing various constants to various sections of the flow based on predetermined regional assessment of turbulence regimes. Such modification would improve model performance across the flow while making its application universal, simple and, most importantly, computationally inexpensive.

With regard to the standard k-ε model, tuning the production-dissipation parameter c_μ to account for strong mean-strain flows, where production of turbulence is not in equilibrium with dissipation, greatly improves the model solution across the flow. The method is demonstrably superior to the simple PML model due to its universality and accuracy. Nonetheless, its numerical complexity and associated high computational cost are fundamental drawbacks.

Although, the estimation of numerical model parameters is an important and useful aim of data assimilation, it has not to date been much explored and utilized in hydrodynamic modelling. This research demonstrates that data assimilation can be a useful tool not only for improving numerical prediction though assimilation but also for identifying and quantifying shortcomings of a numerical model and consequently parameterizing a model in order to improve forecasts. Such applications of data assimilation may greatly benefit both oceanographers and coastal engineering communities.

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