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COMPARISON OF THE ACCURACY OF K-EPSILON AND K-OMEGA SST TURBULENCE MODELS IN AN UNKNOWN SOURCE PARAMETERS ESTIMATION APPLICATION

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Abstract:
The present work aims to identify the source location and the release rate of an unknown air pollutant source in an urban-like domain by implementing two different turbulence models for the calculation of the meteorological parameters via CFD simulations. The MUST wind tunnel experiment is selected for the methodology's application. The k-epsilon and the k-omega SST turbulence models have been utilized separately in a forward RANS steady-state simulation for wind field and turbulence parameters calculation purposes. The estimated meteorological parameters are used in the backward CFD simulations to resolve the adjoint equations and to calculate the adjoint concentrations. The simulations are performed using the OpenFOAM open-source CFD suite. The source location is predicted using a cost function that correlates the modelled and observed concentrations, while the release rate is estimated using a quadratic cost function. The results indicate good agreement between the estimated source parameters of the two cases and the corresponding values of the true source. Very high accuracy is achieved in source location identification in the k-omega SST case. The performance of the k-epsilon case is lower in regard to the source location estimation, but a better solution is achieved for the release rate calculation compared with the k-omega case.

Keywords:* *inverse dispersion modelling, source term estimation, computational fluid dynamics, k-epsilon technique, k-omega SST technique, point source identification

INTRODUCTION

Releases of airborne gases or agents can lead to negative impacts on the environment and on the population's health. In the case of toxic releases, the so-called Hazardous Material (HazMat) threats, either industrial accidents or malevolent actions can be the underlying cause. In many cases, the characteristics of the source of this pollutant are unknown. Such an event must be addressed immediately based on accurate information provided to the decision makers and the relevant authorities. Especially in high densely urban areas, the estimation of the unknown source parameters is crucial for the protection of the population. The characterization of the parameters of the unknown source is called Source Term Estimation (STE) and combines Atmospheric Transport and Dispersion Models (ATDM), inverse modelling techniques, and data from the sensors of a measurement network. An STE problem can be solved by applying both forward and backward approaches. In the forward approach the ATDM calculates the concentration field for specific source parameters (location, release rate) and compares this concentration to the observed concentrations of the sensors. The ATDM runs by using different values of source parameters until a good agreement between the estimated modelled concentrations and the observed concentrations is achieved. In the backward approach, the ATDM is solved once in the reverse direction from each sensor to estimate the source parameters by means of Source Receptors Functions (SRF) which describe the sensitivity of sensors concentration to the source parameters. A literature review of STE techniques is given in Hutchinson et al. (2017). In complex geometry of urban or industrial areas, the Computational Fluid Dynamics (CFD) models are used to simulate the meteorological parameters that are affected by the turbulence phenomena as a result of interaction between the wind flow and the geometry surfaces. CFD models utilize different approaches to calculate a consistent wind field, such as the Reynolds Averaged Navier Stokes (RANS) and the Large Eddy Simulation (LES). A variety of methods have been proposed in the RANS approach for the estimation of turbulence parameters. Two widely used turbulence models are the k-epsilon model that resolves the turbulence kinetic energy, k, and the turbulent kinetic energy dissipation rate, epsilon, and the k-omega SST that solves the turbulence kinetic energy, k, and the turbulence specific dissipation rate, omega.

In the presented study, the RANS approach is combined with the k-epsilon, and the k-omega SST turbulence models to resolve the airflow in an urban-like domain. Each case is utilized in an STE sensitivity application. The geometry of the Mock Urban Setting Test (MUST) wind tunnel experiment and the corresponding datasets are used for evaluating the methodology. For the STE problem, a backward approach is investigated, where the SRF are stored based on the values of the adjoint concentrations. The methodology follows the two-step approach (Efthimiou et al., 2017) to estimate the source parameters. Firstly, the source location is estimated using a correlation-based cost function. Then, the release rate is calculated in the determined source location by a quadratic cost function. The results for each turbulence model case are compared to each other. Also, the contribution of each turbulence model in the source parameters estimation is investigated. The open-source CFD model suite OpenFOAM is utilized in this investigation. The methodology has a wide range of applications, including support of rapid response to accidental or malicious substance releases and determination of emission factors of spatially ambiguous sources. In addition, the methodology will enable detection and quantification of transient emissions from shipping sources in harbour areas near dense urban fabric. To this end, a developed high-resolution modelling toolbox will support control and enforcement of shipping emission limits in harbour areas.

METHODOLOGY

Overall, the methodology for the estimation of the unknown source parameters is summarized in the following computational steps:

1. A forward steady-state CFD simulation runs to calculate the wind field.
2. The above wind field is used "reversed" in backward steady-state CFD simulations. The adjoint advection-diffusion equations are solved by considering every sensor as a source.
3. The SRFs are stored based on the values of adjoint concentrations.
4. The correlation-based cost function is calculated in every cell of the computational domain. The cell with the minimum value indicates the location of the source.
5. The quadratic cost function is solved for the estimated source location to calculate the release rate.

The methodology is applied in two cases, using two turbulence techniques to calculate the wind field during the forward simulation. Each turbulence model is combined with the RANS steady-state approach. In the first case, the two-equation turbulence k-epsilon model is applied. The turbulent quantities that k-epsilon solves are the turbulence kinetic energy k (m^2s^{-2}) and the turbulent kinetic energy dissipation rate epsilon (m^2s^{-3}). In the second case, the turbulence effect is estimated using the two-equation model k-omega SST, which solves the turbulence kinetic energy k (m^2s^{-2}), and the turbulence-specific dissipation rate omega (s^{-1}).

The solution of the wind field is used (inversed) for resolving the adjoint advection-diffusion equation (Marchuk, 1982; 1996). The adjoint equation is solved for every sensor of the measurement network to calculate the adjoint concentrations based on the relation:

$$-\frac{\partial c_n^*}{\partial t} - u_i\frac{\partial c_n^*}{\partial x_i} - \frac{\partial}{\partial x_i}\left(Dc + \frac{v_t}{Sc_t}\right)\frac{\partial c_n^*}{\partial x_i} = p_n \tag{1}$$

where u_i are the three velocity components in the Cartesian coordinate system ($i = (x, y, z)$), c_n^* is the adjoint concentration at measurement point n, Dc is the diffusion coefficient, v_t is the turbulent viscosity, Sc_t is the turbulent Schmidt number, and p_n is the scalar product that describes the source term in each sensor's location. Note that the term $-\partial c_n^*/\partial t$ is defined in transient conditions and is neglected for the steady-state solution.

The SRF can be stored based on the values of the adjoint concentrations c_n^*. The SRF expresses the sensitivity of sensors concentrations to the source parameters and can estimate the calculated concentration of the forward dispersion solution at the sensors based on the adjoint concentration via the relationship (Kovalets et al., 2011):

$$c_n^c = q_s c_n^* \quad (2)$$

where q_s is the source release rate. The total number of SRF is equal to the number of sensors. The location can be estimated by solving the correlation-based cost function from the relationship:

$$J = -\frac{\langle (c^c - \langle c^c \rangle)(c^o - \langle c^o \rangle) \rangle}{\sqrt{\langle (c^c - \langle c^c \rangle)^2 \rangle}\sqrt{\langle (c^o - \langle c^o \rangle)^2 \rangle}} \quad (3)$$

where c^o is the observed concentration measured in the n sensor and c^c is calculated by equation (2) for an arbitrary release rate q_s. As shown in Efthimiou et al. (2017) study, the value of the cost function J does not depend on the value of the release rate q_s. Note that the angled brackets indicate the average values over all sensors. The cost function J is calculated in every cell of the computational domain, and the source location is estimated to the coordinates of the cell center with the minimum value of J. The release rate is calculated, for the estimated location, by the following relationship:

$$q_s = \frac{\sum_{n=1}^{K} c_{n,k}^* c_n^o}{\sum_{n=1}^{K} \left(c_{n,k}^*\right)^2} \quad (4)$$

where k is the cell of the estimated source location.

The methodology is applied using MUST wind tunnel experiment test case. The wind tunnel experiment took place in the WOTAN wind tunnel at the Hamburg university to simulate the corresponding field experiment in a scale of 1:75. The field and wind tunnel experiments provide datasets for the study of the airflow and the dispersion in a simplified urban-like area. The geometry of the MUST field experiment consisted of 120 shipping containers placed in 12 rows of 10 containers. Each container has a 2.42 m length, 12.2 m width, and 2.54 m height. The concentrations in the wind tunnel experiment were measured from 256 sensors placed between containers at 1.275 m height.

In this work, the geometry of the MUST experiment is used to configure the computational domain (Figure 1). The shipping container arrangement is rotated at 45 degrees to the inlet of air flow to simulate a -45 degrees approaching wind flow. The computational domain dimensions are 340 m at the x-axis, 300 m at the y–axis, and 21 m at the z-axis. An unstructured tetrahedral computational mesh was constructed using the Ansys Fluent tool. The total number of computational cells is 1024119. Furthermore, 248 pollutant concentration receptor points are used to extract the appropriate data for the STE application.

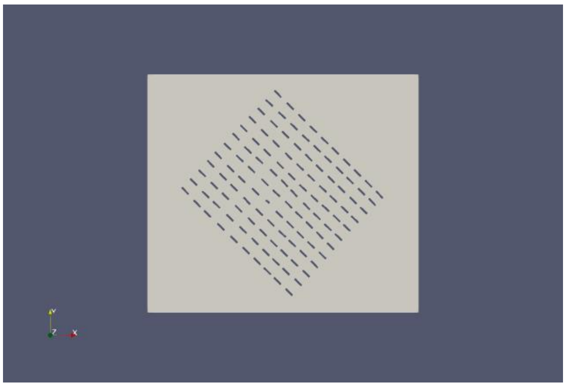

Figure 1. The structure of computational domain in x-y level

The forward simulation is implemented for the steady-state using the SimpleFoam solver. To determine the Atmospheric Boundary Layer (ABL) conditions for the velocity and the turbulence quantities at the inlet boundary, the equations of OpenFOAM class atmBoundaryLayer are used. The reference velocity is u_{ref} = 5 ms^{-1} at a height of z_{ref} = 7.29 m. The other two velocity components are kept equal to zero. Each forward simulation runs for 4000 seconds with a timestep equal to 1 second.

For the backward simulations, the solver ScalarTransportFoam was modified to accommodate the steady-state condition. The total number of simulations for each case is equal to the number of receptor points (248). Every backward simulation runs for 2000 sec with a timestep of 1 sec. The value of Schmidt number was selected equal to 0.7. The wind speed and turbulent viscosity fields were exported by the final timestep of the forward simulations.

RESULTS

Figure 1 presents the vertical profile of the three velocity (u/u_{ref}, v/v_{ref}, w/w_{ref}) components at x = -109.95 m and y = 0.825 m for two turbulence models (k-epsilon and k-omega SST). The specific point is located in the shipping containers area. The simulated velocities are compared to the corresponding wind tunnel measurements. Note that observations are available only for the two velocity components (u, w). The results show that the profiles of the two simulations are similar for the u and v velocity components, while there is a divergence below 5 m height in the w component. In the v component, both model profiles follow the distribution of the corresponding measurements. This agreement between modeled and measured velocities is apparent very near the ground surface and lower than the shipping container's height. On the other hand, a high bias is evident for the w velocity below the 5 m height. In this case, the k-omega SST models reduce the variance between modeled and measured w velocity. The explanation of this bias has to take into account the height of the shipping containers (2.54 m). As a result, the existence of obstacles appears to affect the model's accuracy.

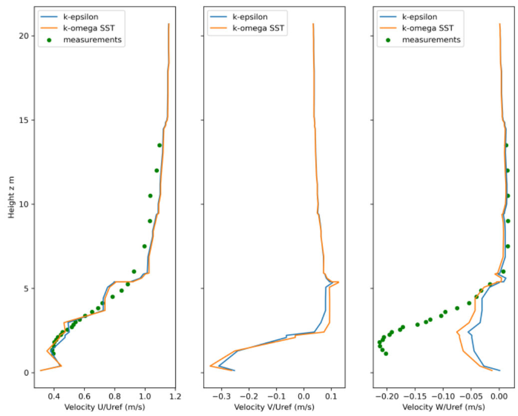

Figure 2. Comparison between modeled and measured velocity components profile (u/u_{ref}, v/v_{ref}, w/w_{ref}) at x = -109.95 m and y = 0.825 m

Table 1 presents the results of source parameters estimation (source location and release rate) in the two investigated cases, k-epsilon and k-omega SST. In the k-omega SST case, the distance between the cell of the estimated location and the true location is negligible. Specifically, the distance between the point that is located in the true source and the corresponding predicted point is 1.28 m in the k-omega SST case, while for k-epsilon it is 7.91 m. On the other hand, the k-epsilon implementation provides better results in the release rate estimation. The divergence between the estimated and the corresponding true release rate is $0.41\cdot10^{-5}$ kg s^{-1} in the k-epsilon, and $0.63\cdot10^{-5}$ kg s^{-1} in the k-omega SST case.

Table 1. Source parameters estimation results

Case	Location – Domain coordinates			Release rate
	***X* (m)**	***Y* (m)**	***Z* (m)**	***q* (kg/s)**
True source	-102,48	-7.06	0.00	$1.35\cdot10^{-5}$
Estimated source k-epsilon	-97.22	-12.03	3.20	$0.94\cdot10^{-5}$
Estimated source k-omega SST	-102.28	-7.39	1.22	$0.72\cdot10^{-5}$
Divergence true - estimated (k-epsilon)	5.26	4.97	3.20	$0.41\cdot10^{-5}$
Divergence true - estimated (k-omega SST)	0.20	0.33	1.22	$0.63\cdot10^{-5}$

To quantify the quality of the solution, the quantities $R_H = \sqrt{(x_e - x_t)^2 + (y_e - y_t)^2}$ for the horizontal and $R_V = |z_e - z_t|$ for the vertical distance are calculated. Respectively, for the release rate ratio, $\Delta q = \max[(q_e/q_t), (q_t/q_e)]$, is used as a bias estimator, where (x_e, y_e, z_e, q_e) are the estimated source parameters and (x_t, y_t, z_t, q_t) are the true source parameters. The estimated source parameters results are evaluated based using the criteria of Kovalets et al. (2011), where a good solution is considered to be achieved for $R_H \leq 15$ m, $R_V \leq 1.5$ m and $\Delta_q \leq 4$. Table 2 presents the results for the horizontal and vertical distances and the release rate ratio. The low bias in horizontal and vertical distances indicates a good solution for the source location estimation in the k-omega SST implementation. On the other hand, in the k-epsilon case, the vertical criteria are not met. In both cases, good results are provided for the release rate calculation.

Table 2. Horizontal and vertical distances and release rate ratio results

Case	R_H (m)	R_V (m)	Δq (-)
k-epsilon	7.24	3.20	1.44
k-omega SST	0.39	1.22	1.88

CONCLUSIONS

The CFD models can accurately estimate the meteorological parameters and the pollutant dispersion over complex geometry such as a dense urban area, taking into account the small-scale turbulence effects. The STE methods can successfully use CFD models to estimate the parameters of an unknown source. In this work, two turbulence models (k-epsilon and k-omega SST) are investigated in an STE application using the computational domain and measurement set of the MUST wind tunnel experiment. The methodology solves a correlation-based cost function to estimate the source location. The release rate is calculated for the predicted source location by solving a quadratic cost function. Results indicate very high accuracy in the location estimation by the k-omega SST case. The horizontal uncertainty of the location estimation is insignificant, while the vertical one is very low. In the k-epsilon case, a higher bias is found at both horizontal and vertical levels. On the other hand, a better solution is achieved regarding the release rate calculation using k-epsilon implementation. Both cases provide good results in release rate prediction. The foreseen applications of the methodology include support of rapid response to accidental or malicious substance releases as well as detection and quantification of transient emissions from shipping sources in harbour areas in support of control and enforcement of emission limits.

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