ARISTOTLE UNIVERSITY OF THESSALONIKI

KIT Karlsruher Institut für Technologie

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

Panagiotis Gkirmpas, Nicolas Moussiopoulos, Lenidas Ntziachristos

Sustainability Engineering Laboratory, Department of Mechanical Engineering,
Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

Aims and Objectives

Aim:

- To identify the location and the release rate of an unknown air pollutant source in an urban-like domain.

Objectives:

- To utilize two different turbulence models (k-epsilon and k-omega SST).
- To compare the accuracy of the two models in a Source Term Estimation (STE) application.
- To evaluate each model’s accuracy in estimating source term.
- To utilize the Mock Urban Setting Test (MUST) wind tunnel experiment dataset.

Methodology

Wind field calculation – CFD forward simulation

Adjoint advection – diffusion equations resolving – CFD backward simulations

Source Receptors Functions (SRF) storing

Calculation – minimization of the cost function

Source location – release rate estimation

Wind field simulations

Forward simulation

- Steady-state
- Reynolds Averaged Navier Stokes (RANS) approach
- Two different turbulence models
  - k-epsilon
  - k-omega SST
- simpleFoam solver

Inlet boundary conditions

- $u(z) = \frac{u^*}{\kappa} ln\left(\frac{z-z_0}{z_0}\right)$
- $k = \frac{(u^*)^2}{\sqrt{C_\mu}}$
- $epsilon = \frac{(u^*)^3}{\kappa(z+z_0)}$
- $omega = \frac{(u^*)^3}{\kappa(z+z_0)\sqrt{C_\mu}}$

Implementation: OpenFOAM CFD tool

Backward simulations

- Steady-state
- Modified ScalarTransportFoam solver
- Wind field of forward simulation is used reversed
- Calculation of the adjoint concentrations c_n^*:
    - Adjoint advection-diffusion equation (Marchuk, 1982; 1996)

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

- Number of simulations = Number of sensors

Implementation: OpenFOAM CFD tool

Source term estimation

Estimation of location and release rate --> Two step methodology (Efthimiou et al., 2017)

- Cost function for location estimation:

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

  - *Where* c^c *is concentration calculated by SRF:*

$$c^c = q_s c^*$$

- Release rate calculation equation:

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

Evaluation of the SRF

1. Solve forward dispersion problem with true source location and release rate
2. Calculate SRF based on adjoint concentrations at the true source location
3. The SRF calculated concentrations are compared with the forward concentrations at sensors
4. Scatter plot
   Validation metrics
5. Evaluate the SRF

Validation Metrics (Schatzmann et al., 2010)

- Hit rate - HR
- Factor of two observations - FAC2
- Fractional bias - FB
- Geometric mean bias - MG
- Normalised mean square error - NMSE
- Geometric variance - VG
- Mean absolute error - MAE

Case study - Mesh

- ***Geometry***

➢ MUST wind tunnel experiment

➢ 120 shipping containers

➢ 45 degrees wind direction

➢ (X, Y, Z): $(340m, 300m, 21$ m)

➢ 248 sensors

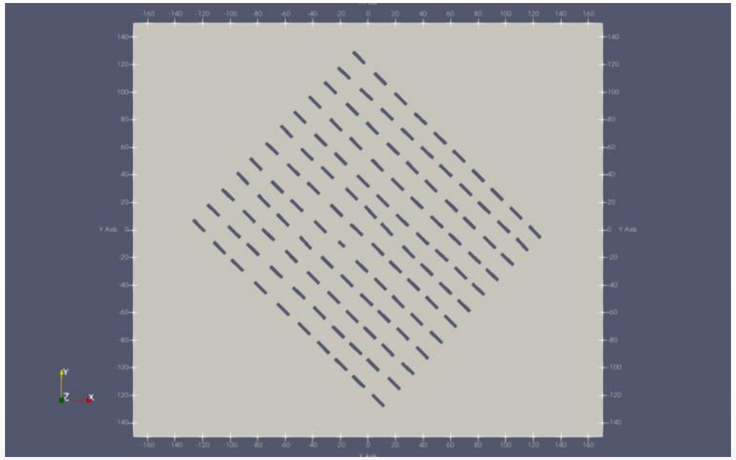


Figure 1: Computational domain in x - y level

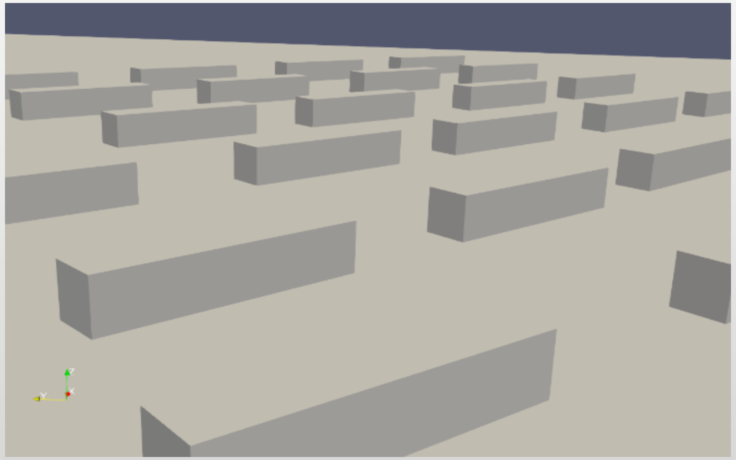


Figure 2: Computational domain's buildings view

- ***Mesh***

➢ Unstructured - Tetrahedral

➢ 1.024.119 cells

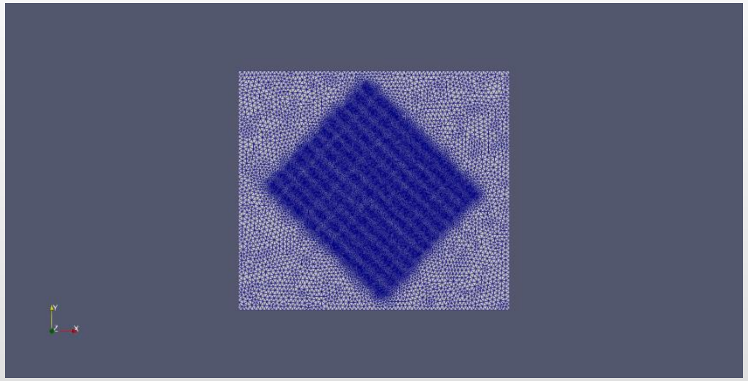


Figure 3: Computational mesh in x – y level

Results of wind field

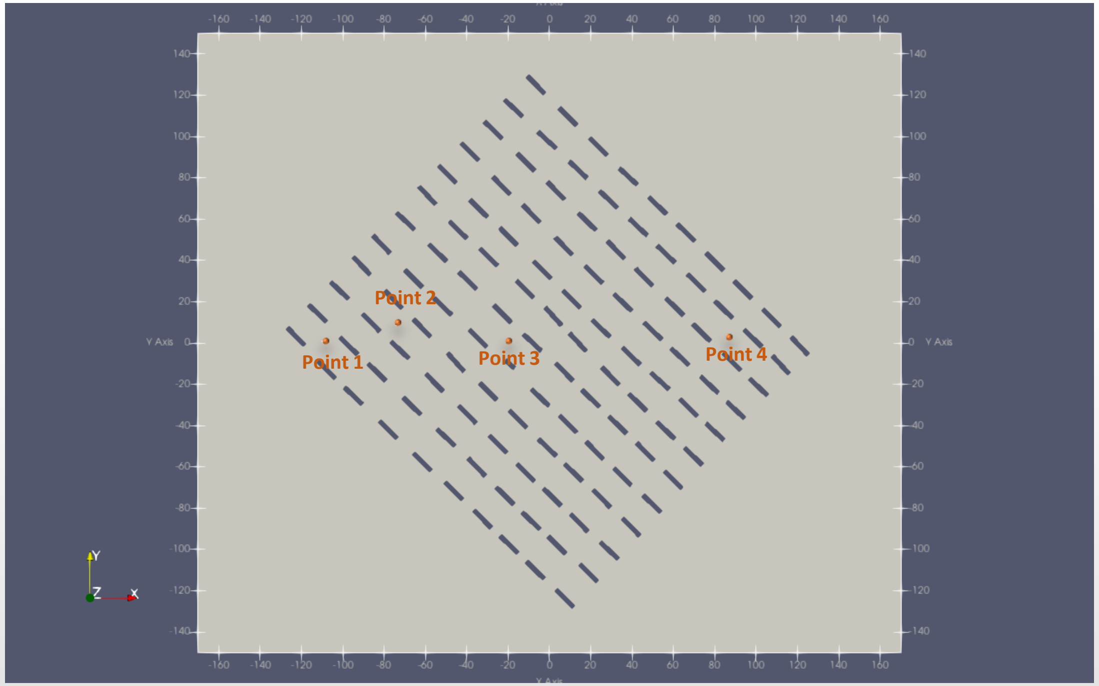


Figure 4: Selected points for comparison of wind tunnel and calculated values of the three velocity components

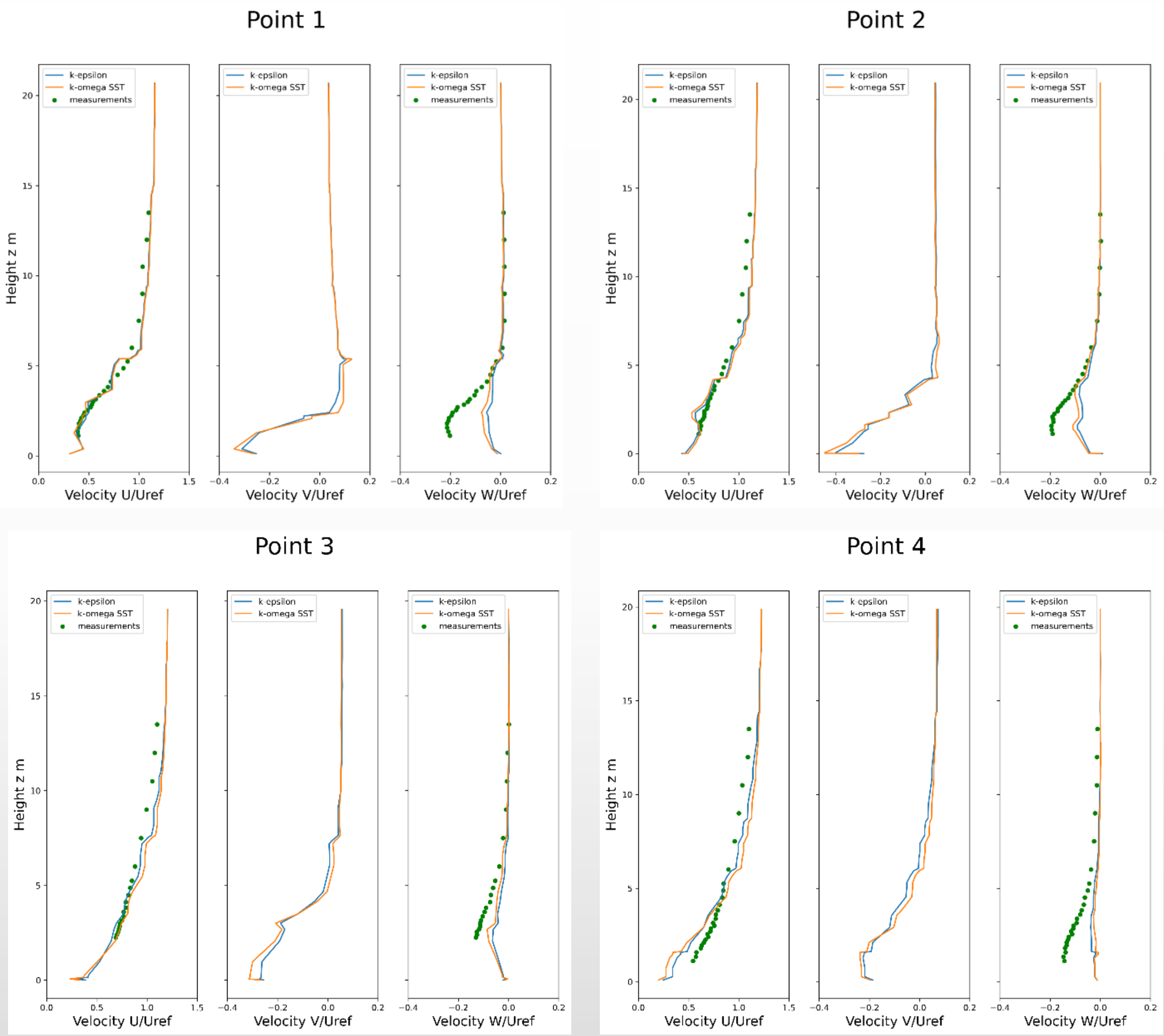


Figure 5: Comparison of vertical values of the three velocity components of k-epsilon and k-omega SST forward simulations and wind tunnel measurements in four points

Evaluation of forward dispersion model

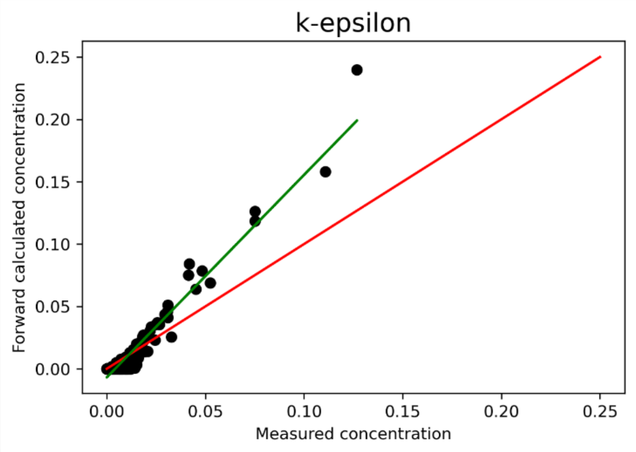


Figure 6: Scatter plot of the forward and the measured concentrations calculated by the k-epsilon model

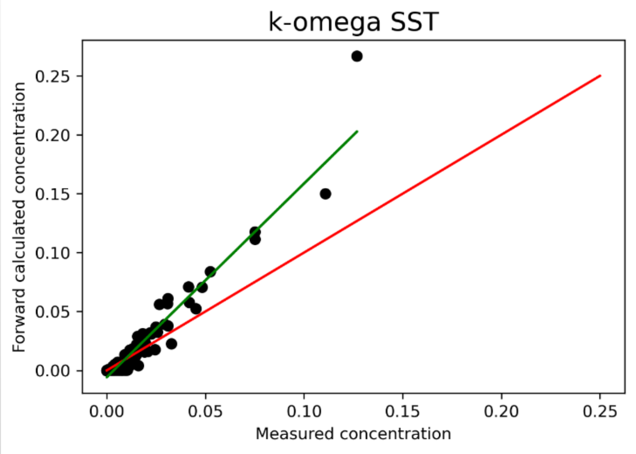


Figure 7`: Scatter plot of the forward and the measured concentrations calculated by the k-omega SST model

Validation metrics	k-epsilon	k-omega SST	Ideal model
HIT RATE	0.516	0.621	1
FAC2	0.641	0.750	1
FB	0.106	-0.037	0
MG	1.373	1.196	1
NMSE	1.557	1.443	0
VG	1.423	1.244	1
MAE	0.654	0.476	0

Table 1: Validation metrics factors for the forward and the measured concentrations comparison

Evaluation of the SRF

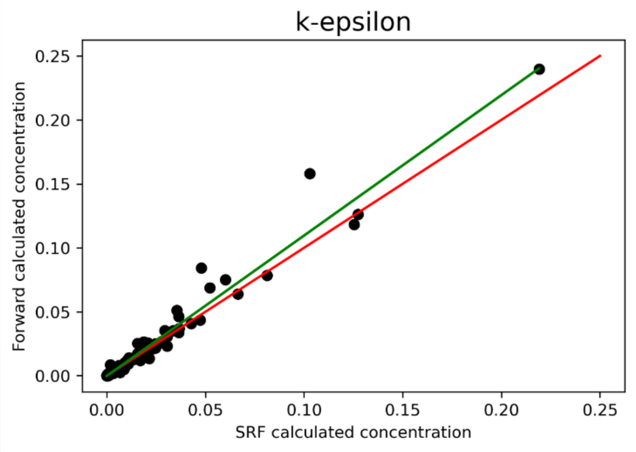


Figure 8: Scatter plot of the forward and the SRF concentrations calculated by the k-epsilon model

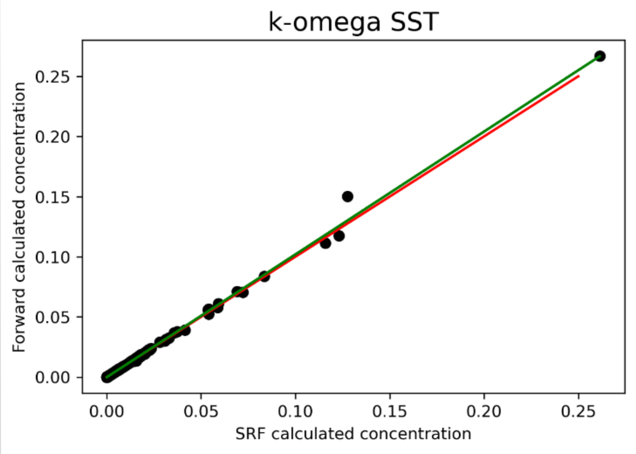


Figure 9: Scatter plot of the forward and the SRF concentrations calculated by the k-omega SST model

Validation metrics	k-epsilon	k-omega SST	Ideal model
HIT RATE	0.948	1	1
FAC2	0.988	1	1
FB	-0.075	-0.007	0
MG	0.991	1.001	1
NMSE	0.370	0.026	0
VG	1.021	1	1
MAE	0.153	0.033	0

Table 2: Validation metrics factors for the forward and the SRF concentrations comparison

Results – evaluation of source parameters estimation

Case	Location – Domain coordinates			Release rate
	X (m)	*Y* (m)	*Z* (m)	*q* (kg/s)
True source	-102.48	-7.06	0.00	$1.35 \cdot 10^{-5}$
Estimated k-epsilon	-97.22	-12.03	3.20	$0.94 \cdot 10^{-5}$
Estimated k-omega SST	-102.28	-7.39	1.22	$0.72 \cdot 10^{-5}$
Divergence k-epsilon	5.26	4.97	3.20	$0.41 \cdot 10^{-5}$
Divergence k-omega SST	0.20	0.33	1.22	$0.63 \cdot 10^{-5}$

Table 3: Source parameters estimation results

Evaluation criteria (Kovalets et al., 2011)

- $R_H = \sqrt{(x_e - x_t)^2 + (y_e - y_t)^2} \leq 15\ m$
- $R_V = |z_e - z_t| \leq 1.5\ m$
- $\Delta q = \max[(q_e/q_t), (q_t/q_e)] \leq 4$

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

Table 4: Horizontal and vertical distances and release rate ratio results

Conclusions - Future work (1/3)

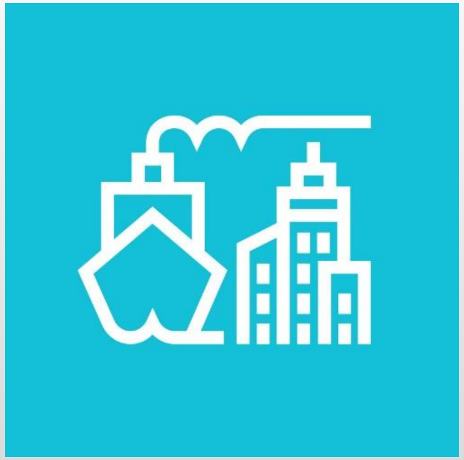
- Both models provided accurate solutions in the location estimation at the horizontal level and release rate
- k-epsilon failed to achieve the criteria in the vertical distance
- k-omega SST estimated the source location very accurately
- k-epsilon calculated more accurately the release rate
- k-omega SST had higher achievement in the calculation of the forward dispersion model
- The SRF were solved more correctly by k-omega SST

Conclusions - Future work (2/3)

- A sensitivity analysis for the number of sensors is under investigation
- The methodology will be tested in transient conditions (unsteady RANS, Large Eddy Simulation)
- Investigate a complex geometry case

Conclusions - Future work (3/3)

- The utilization of methodology in cases of shipping sources in harbour areas in order to detect and quantify the shipping emissions



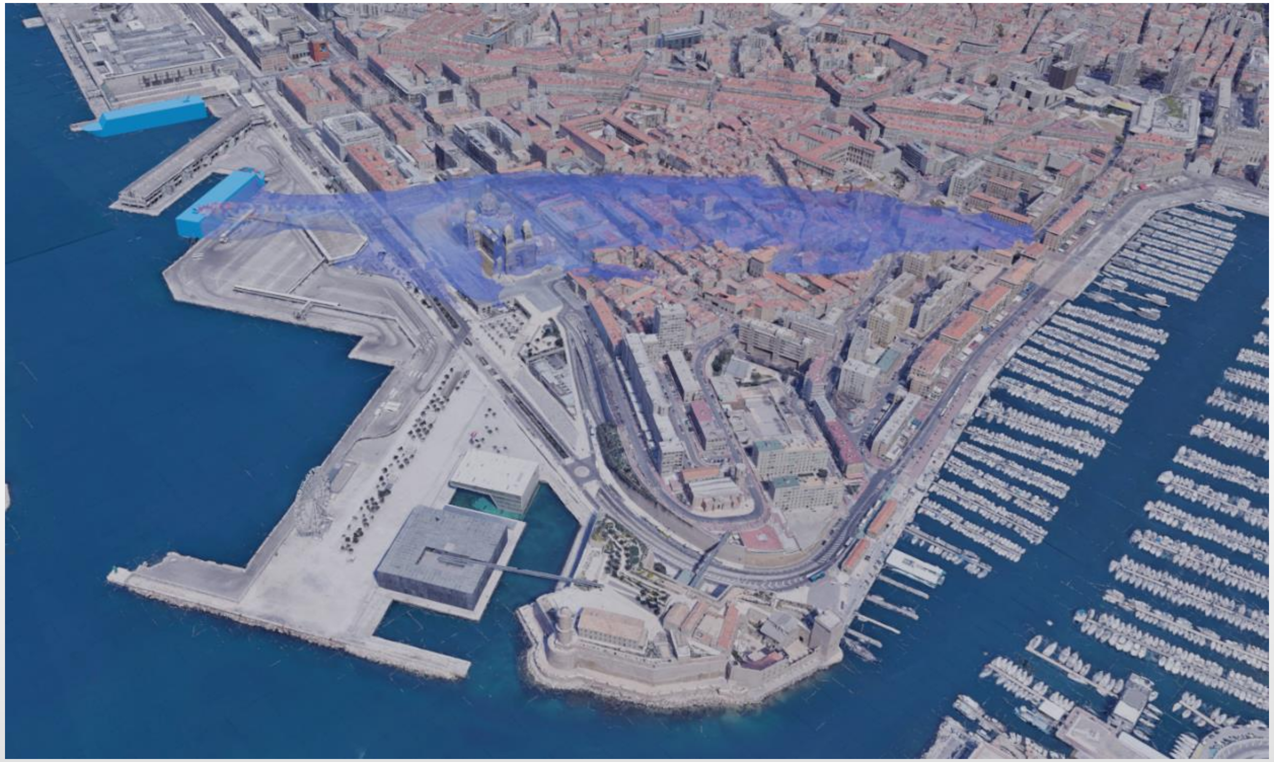


Figure 7: Numerical simulation (CFD model) to estimate pollutant dispersion in Marseille harbour– SCIPPER project

Acknowledgements

- P. Gkirmpas acknowledges the Helmholtz Association of German Research Centers for funding the doctoral dissertation through the European program Helmholtz European Partnership for Technological Advancement (HEPTA).
- Also, he acknowledges the Graduate School of the Centre for Climate and Environment (GRACE) at the Karlsruhe Institute of Technology (KIT) for financial support.
- The authors would like to acknowledge the SCIPPER Project (project that has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 814893) for financial support.

References

- Efthimiou G. C, I. V. Kovalets, A. Venetsanos, S. Andronopoulos, C. D. Argyropoulos and K. Kakosimos, 2017: An optimized inverse modelling method for determining the location and strength of a point source releasing airborne material in urban environment, *Atmospheric Environment*, **170**, 118-129.
- Kovalets, I. V, S. Andronopoulos, A. G. Venetsanos, J. G. Bartzis, 2011: Identification of strength and location of stationary point source of atmospheric pollutant in urban conditions using computational fluid dynamics model, *Mathematics and Computers in Simulation*, **82**, 244-257.
- Marchuk, G, 1982: Mathematical Modelling in the Environmental Problems, Nauka, Moscow.
- Marchuk, G, 1996: Adjoint Equations and Analysis of Complex Systems, Kluwer Academic Publishers, Dordrecht, Netherlands
- Schatzmann, M, H. Olesen, J. Franke, 2010: COST 732 model evaluation case studies: approach and results

Thank you for your attention!