The Effects of Atmospheric Turbulence on Peak-to-Mean Concentration Ratio and its Consequence on the Odour Impact Assessment Using Dispersion Models

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The present work evaluates the use of two regulatory atmospheric dispersion models (AERMOD and CALPUFF) and two CFD models (LES-Dynamic Smagorinsky and LES-Wale) to assess odour impact. Average concentration results are compared with experimental wind tunnel (WT) data. P/M concentration ratio results estimated from the regulatory models through a power law scaling factor are compared with the P/M concentration predicted by LES results. CFD/LES results showed good agreement when compared to wind tunnel results, both for the mean and fluctuating flow and concentration patterns. AERMOD and CALPUFF underestimated the highest concentration levels when compared to CFD/LES results and WT measurements. Peak to mean (P/M) concentration ratio estimated by the regulatory models through the use of a power law relating the P/M concentration ratio to short-to-large-term averaging time ratio were underestimated when compared to CFD/LES observed P/M. Results indicate CFD/LES can be a viable tool for studying fluid flow characteristics that affect odour impact assessment.

1. Introduction

Regulatory models such as AERMOD (Lee et al., 1996) and CALPUFF (Scire et al., 1990) are commonly employed to assess atmospheric dispersion of odorant compounds (Latos et al., 2011; Karageorgos et al., 2010; Capelli et al., 2011; Sironi et al., 2010). Such models are based on the Gaussian plume approach and include the effects of complex phenomena such as the presence of obstacles, wind meandering, complex terrain and other effects through the use of empiric expressions, estimating the concentration of the emitted compound averaged in periods ranging from one hour to one year. However, odour impact is commonly related to short term concentration or "peaks" lasting for a few seconds to few minutes depending on the frequency of exposure. In order to estimate concentration peaks (short term averaged concentration) or peak-to-mean (*P/M*) concentration ratio, an empirical power law scaling factor is usually employed (Schauberger et al., 2002; Mavroidis, 2009; Santos et al., 2009).

Computational fluid dynamic (CFD) technique allows for a more detailed description of the atmospheric flow and dispersion than Gaussian models and can enhance the understanding of the physical phenomena involved in these processes (Hong et al., 2011). Large Eddy Simulation (LES) is an advanced turbulence model used in dispersion models based on CFD to include the effects of atmospheric turbulence (generated by mechanical and buoyancy forces) and also the effects of the turbulence generated by the presence of obstacles either in urban (usually a group of complex shaped obstacles) or rural areas (Hong et al., 2011).

Obstacles act as sources of mechanical turbulence, affecting the dispersion of emitted compounds as the atmospheric flow is captured by the originated recirculating regions and wakes. Wind meandering also affects the flow so that the highly turbulent concentration field downwind the obstacle is characterized by large concentration peaks.

The present work evaluates the use of AERMOD, CALPUFF and CFD/LES to assess odour impact. Average concentration results are compared with experimental wind tunnel (WT) data. *P/M* concentration ratio results estimated from the regulatory models through a power law scaling factor are compared with the *P/M* concentration predicted by LES results.

2. Methods

2.1 Regulatory models

The present work employs two regulatory models, AERMOD and CALPUFF. AERMOD (Lee et al., 1996) is a steady state plume model based on the Gaussian distribution. The lowest possible averaging time is 1 hour. AERMOD does not natively include any option to address shorter concentration peaks (Latos et al., 2011), so this task must be performed by the user. AERMOD includes the effect of wind meandering. CALPUFF (Scire et al., 1990) is a lagragian model, treating the emitted plume as a series of discrete fluid particles (puffs) with dispersion inside each puff following a Gaussian distribution. The smallest value for the sampling and averaging time is 1 hour. Concentration peaks can be derived from the average concentration results through the use of a 1/5 power law applied to the average concentration results or to the dispersion parameters, before the concentration calculation.

2.2 PRIME model

AERMOD and CALPUFF include the effects of the presence of obstacles in the atmospheric flow through the PRIME model (Schulman et al., 2000). PRIME is a Gaussian based dispersion model which includes the effects of plume rise and downwash caused by obstacles (streamlines deflection). In the wake region modeled in PRIME, AERMOD switches off the wind meandering formulation (Venkatran et al., 2004).

2.3 CFD/LES

LES explicitly resolves the large turbulence scales while the smaller scales are modeled by a subgrid model. This approach is based on the concept that larger scale vortices depends on geometry and boundary conditions while smaller vortices are isotropic and, therefore, easier to model (Schmidt and Thiele, 2002). The larger scales are separated from the smaller ones through the use of a space filter. Two different LES models were employed in the present work, the Dynamic Smagorinsky model (Germano et al., 1991) and the WALE model (Nicoud and Ducros, 1999) which differ in the way turbulence is modeled near solid surfaces.

2.4 Peak-to-mean ratio

This parameter is used in odour dispersion modeling in order to estimate the occurrence of concentration peaks and odour events based on the long-term average concentration results obtained from dispersion models such as AERMOD and CALPUFF. This is usually accomplished by the use of a power law (Equation 1) relating the peak-to-mean concentration ratio (C_p/C_m) to short-to-large-term averaging time ratio (t_p/t_m) (Schauberger et al., 2002; Mavroidis, 2009; Santos et al., 2009).

$$\frac{C_p}{C_m} = \left(\frac{t_p}{t_m}\right)^a \tag{1}$$

Researchers have found values for the power law exponent (a) ranging from -1 to 0 depending on atmospheric stability and also on source to receptor distance, with -0.2 being recommended by most authors (Schauberger et al., 2002; Mavroidis, 2009) and used by CALPUFF.

2.5 Case description

The present work studies the flow and dispersion around an isolated cubical obstacle using AERMOD, CALPUFF and CFD/LES. The results are compared to wind tunnel data. For details of the wind tunnel experiment the reader is referred to Sada and Sato (2002).

The AERMOD and CALPUFF domain was scaled up from the wind tunnel with a 250:1 ratio The obstacle height is H=50 m. The source is located 75 m upwind the obstacle center. The free stream velocity is U_∞= 2.0 m/s and the boundary layer height is 75 m. The same non-dimensional mean wind velocity profile is used in AERMOD, CALPUFF and CFD/LES, based on experimental wind tunnel data from Sada and Sato (2002). Atmospheric stability was neutral, and mean wind direction was constant. CFD calculation domain is 7.0 m, 1.0 m and 1.0 m for the downwind, horizontal and vertical directions (x, y and z). The cubical obstacle had its center located 4.9 m from the domain entrance. Additional details of the LES simulation are given in Dourado et al. (2011).

3. Results

AERMOD, CALPUFF, Dynamic Smagorinky model (D-LES) and the Wale model (W-LES) simulations are compared with Sada and Sato (2002) wind tunnel (WT) data regarding non-dimensional concentration results. The peak-to-mean (P/M) concentration ratio predicted by D-LES and W-LES simulations is compared to the P/M value obtained by Eq. 1.

3.1 Flow field
LES models adequately represent the wind tunnel flow field around the cube, showing the reverse flow regions observed on top and downwind the obstacle. There is good agreement between D-LES, W-LES and wind tunnel results. For a more detailed description of the flow field results the reader is referred to Dourado et. al (2011).

3.2 Concentration field
Mean non-dimensional concentration profiles are shown in Figure 1. All results exhibit the same general trend, with the highest and lowest concentration values observed at similar vertical positions.
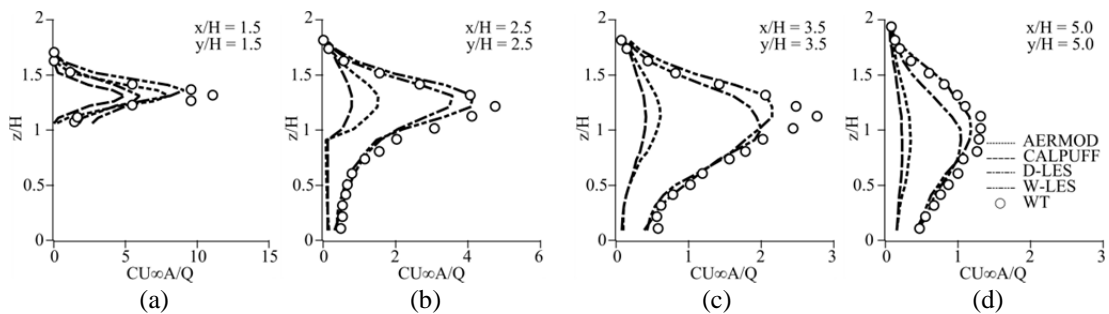

Figure 1: Mean non-dimensional concentration profiles around the obstacle at y/H =0 and x/H = 1.5 (top of the obstacle), x/H = 2.5 (recirculation zone), x/H = 3.5 (beginning of the obstacle wake) and x/H = 5.0 (far wake)

D-LES and W-LES show better agreement with WT measurements while AERMOD and CALPUFF clearly underestimate the concentration in all locations examined (x/H = 1.5, x/H = 2.5, x/H = 3.5 and x/H = 5.0). AERMOD and CALPUFF results were closer to WT results at x/H = 1.5 (top of the obstacle) than at the other locations, with AERMOD results agreeing better to WT than CALPUFF. Both models employ PRIME to estimate the dispersion in the obstacle vicinity so the observed behavior is possibly attributed to the way the PRIME code is implemented in each model, as AERMOD is a steady state model. AERMOD results at x/H = 1.5 also presented better agreement than D-LES.

Overall, W-LES agreed better to WT than D-LES. Both LES models overestimated the lower concentration levels at x/H = 1.5. At receiver positions close to the ground, where the average concentration (predicted and observed) is lower, AERMOD and CALPUFF results are closer to WT and LES. Figures 2 and 3 scatter plots compares each model mean concentration with the experimental data for x/H = 1.5 and x/H = 5.0.

3.3 Assessment of the peak to mean (*P/M*) concentration ratio

The use of the concentration time series obtained from the LES simulation allows the calculation of the *P/M* concentration ratio and also the exponent (*a*) of Eq. 1. This is accomplished by splitting the concentration time series into smaller time intervals and calculating the respective mean concentrations. The value of a is calculated for x/H = 3.5, at y/H = 0.0 and z/H = 1.0. Intervals (tp/tm) varied from 0.0012 to 1.00, with the larger number meaning an average time corresponding to the full simulation time. If compared to the commonly used 1-hour averaging time this range would indicate a shortest interval of about 5 s. Table 1 summarizes these results.
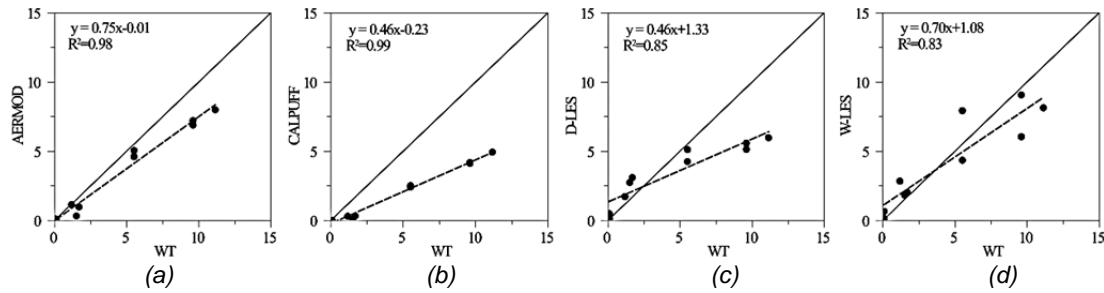

Figure 2: mean concentration observed in the wind tunnel and estimated by (a) AERMOD, (b) CALPUFF, (c) D-LES and (d) W-LES, at x/H=1.5 and y/H=0.
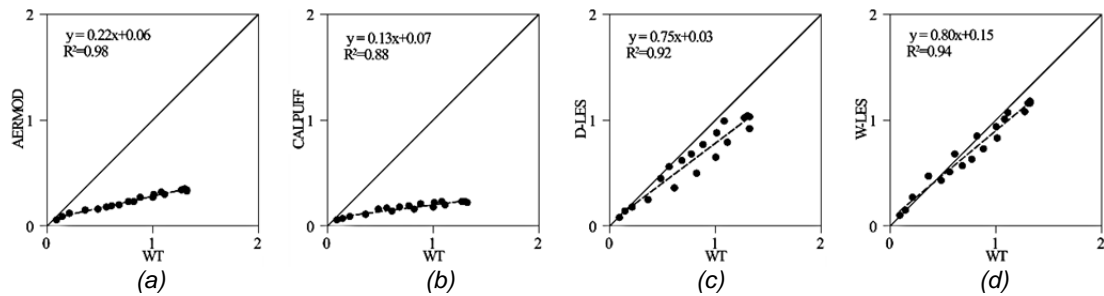

Figure 3: mean concentration observed in the wind tunnel and estimated by (a) AERMOD, (b) CALPUFF, (c) D-LES and (d) W-LES, at x/H = 5.0 and y/H = 0

Table 1: peak-to-mean concentration ratio (P/M) observed in LES simulations and calculated value for the power law exponent (a) relating the peak-to-mean concentration ratio to the short to long-term averaging times at y/H = 0.0, z/H = 1.0 for x/H = 1.5, x/H = 2.5 and x/H = 3.5

| | y/H = 0 and z/H = 1.0 | | |
	x/H = 1.5	x/H = 2.5	x/H = 3.5
D-LES	*P/M* = 10.05, *a* = -0.37	*P/M* = 7.906, *a* = -0.31	*P/M* = 6.092, *a* = -0.28
W-LES	*P/M* = 11.75, *a* = -0.39	*P/M* = 7.730, *a* = -0.32	*P/M* = 6.833, *a* = -0.28

D-LES and W-LES results were similar, within 5.4 % of difference. As expected, the *P/M* concentration ratio and the absolute value of *a* become lower as the distance from the obstacle is increased. This is due to the lower concentration peaks observed further downwind the obstacle. The calculated values of a (absolute values) were higher than the value used in CALPUFF and AERMOD (a = -0.2) which gives a P/M concentration ratio of 3.73. LES results indicate a = -0.2 would probably be obtained further downwind the obstacle far wake. Santos et al. (2009) found values of a ranging from -0.22 to -0.34 close to the walls of a complex shaped building for neutral atmospheric conditions in a field experiment. Present results also indicate that the use of different values of a depending on receptor to source distance with AERMOD and CALPUFF would give better estimates of the *P/M* concentration ratio.

Another alternative would be the use of an attenuation function for the *P/M* results (Schauberger et al., 2002).

4. Conclusion

The present work evaluated the use of AERMOD, CALPUFF and CFD/LES to odour impact assessment in which *P/M* concentration ratio and frequency of exposure are strongly affected by turbulence. Average concentration results were compared with experimental wind tunnel data. *P/M* concentration ratio results estimated from the Gaussian models through the use of a scale factor were compared with the *P/M* concentration predicted by LES results. CFD/LES results showed good agreement when compared to wind tunnel results, both for the mean and fluctuating flow and concentration patterns. AERMOD and CALPUFF also showed the same trend for mean concentration but the highest concentration levels were underestimated. AERMOD and CALPUFF concentration results were underestimated when compared to CFD/LES and wind tunnel data but were closer to LES results close to the ground. The calculated power law exponent (*a*) relating P/M concentration ratio to short-to-long averaging time of CFD/LES was higher than the one employed by CALPUFF – which was also employed to AERMOD results – resulting in lower values for *P/M* concentration ratio estimated by the regulatory models. The calculated value of *a* of CFD/LES was also found to depend on the distance to the obstacle, with values becoming lower with the increasing distance from the obstacle. The *P/M* concentration ratio predicted by CALPUFF and obtained from AERMOD results tends to approach CFD/LES results downwind in the obstacle far wake.

Results indicate CFD/LES can provide good estimates of the concentration field, its fluctuation intensity and thus, the peak-to-mean concentration ratio, making it a viable tool for studying fluid flow characteristics for odour impact assessment. Further investigations should be undertaken, comparing CFD/LES, CALPUFF and AERMOD estimations to field data.

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