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ENGENHARIA AMBIENTAL

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Modelling odour dispersion in built environments

Modelagem da dispersão de odores em ambientes
urbanos

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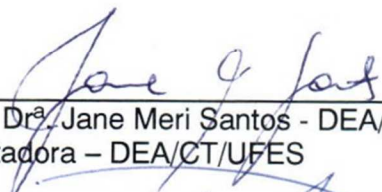


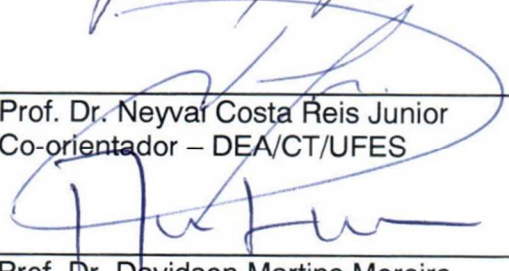
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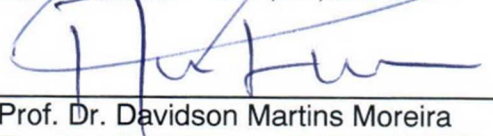
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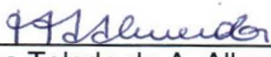
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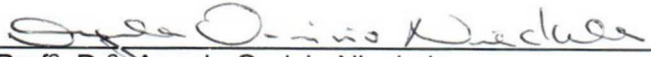
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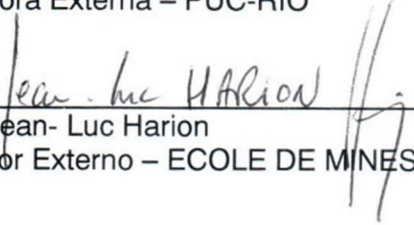

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List of symbols

A : dispersion parameter enhancement linear decay factor

A^+ : damping factor

B_L : maximum between building height and width

B_S : minimum between building height and width

c : chemical species concentration

c : parameter indicating plume reattachment at the top of the obstacle

C_d : Dynamic Smagorinsky parameter

C_F : concentration at the far wake

C_m : concentration for long averaging time t_m

C_N : concentration inside the cavity

C_p : concentration for short averaging time t_p

C_P : concentration for the non captured portion of the plume

c_p : constant pressure specific heat capacity

C_S , C_{S0} : Smagorinsky coefficient

D_m : diffusion coefficient for chemical species m

d_s : stack exhaust diameter

e_{ij} : error associated to the Smagorinsky model

F , F_C : factors modifying the ambient wind equation

f : any flow variable; frequency; maximum product of the vertical and horizontal mass distributions

f' : the modelled part of any flow variable containing the smaller scales

F_b : buoyancy flux

F_m : momentum flux

f_x : vertical mass distribution

f_y : horizontal mass distribution

F_Z : streamline inclination attenuation factor

g : gravitational acceleration

H : building height

h : height of the plume centreline

H : obstacle height, source of energy

h : specific enthalpy

H_C : cavity height

h_e : height of the elevated plume centreline

H_W : wake height

$i = 1, 2, 3$ and $j = 1, 2, 3$: x, y and z directions;

$I_{r(x,y,z)}$: intermittency at a receptor location

i_y : lateral turbulence intensity

i_z : vertical turbulence intensity

k : Von Karman constant

k_c : thermal conductivity

L : along flow projected building length

L_C : cavity length

L_e : length of virtual line source

L_{ij} : resolved turbulent stress

L_u : axial integral turbulence length scale

M : fraction of the plume captured by the near wake, source of mass

P/M : peak-to-mean

p : pressure, exponent of power law expression relating C_p and C_m

Q : rate of emission of the contaminant

R : building length scale

r : plume radius

R_0 : dilution radius

R_p : parameter characterizing radiation properties

s : distance along the plume centerline measured from the source

S_{ij} : rate of deformation tensor

$S_{uu}(f)$: longitudinal velocity spectral density

t^* : non dimensional time

T : integral time scale

T : temperature

T_a : ambient temperature

T_{ij} : stress tensor, sub grid-scale stress tensor at a scale $\{\Delta\}$

T_s : exhaust gases temperature

U_0 : free stream velocity

$U_a(z)$: ambient wind speed

U_H : mean wind speed at building height

u_i : velocity component in direction x_i

u_j : velocity component in direction x_j ,

U_{ref} : reference wind speed

u_s : wind speed at stack height

U_{SC} : velocity of the plume cross section along its centreline

$U_w(z)$: ambient wind speed profile downwind the building, as a function of height

W : along flow projected building width

W_C : cavity half-width

W_W : wake half-width

x : downwind position

y : lateral position

z : vertical position

z_0 : roughness length

z_d : plume elevation due to buoyancy and building influences

z_{ref} : reference height

α : entrainment parameter

β : entrainment parameter

β_1 : neutral capture parameter (≈ 0.6)

β_j : jet capture coefficient

δ : boundary layer height

Δ : length scale of the LES filter function

Δx , Δy and Δz : grid size in x, y and z directions

Λ : integral length scale

v_s : velocity of the gases exiting the stack;

ξ : auxiliary variable for calculating downwind distance from the building

ξ_b : obstacle reference length

ρ : fluid density

ρ : plume density

ρ_a : air density

σ_y : horizontal dispersion parameter

Σ_y : modified horizontal dispersion parameter

σ_{y0} : horizontal dispersion parameter modified due to building effects

σ_{y0}' : horizontal dispersion parameter at 3 building heights downwind the obstacle lee face

σ_{ycav} : horizontal dispersion coefficient inside the cavity

Σ_z : modified horizontal dispersion parameter

σ_z : vertical dispersion parameter

σ_z'' : vertical dispersion parameter with building downwash and buoyancy effects

σ_{z0} : vertical dispersion parameter modified due to building effects

σ_{z0}' : vertical dispersion parameter at 3 building heights downwind the obstacle lee face

σ_{zcav} : vertical dispersion parameter for the cavity source,

σ_θ : standard deviation of the wind direction

σ_v : standard deviation of the lateral wind speed

τ_{ij} : sub grid-scale stress at a scale $\Delta < \{\Delta\}$

Φ : energy dissipation function due to viscous stress

ϕ : plume centreline inclination

τ_{ij}^s : LES subgrid stress tensor

t : time

$\bar{f}$, $\bar{f}(x_i, t)$: any filtered flow variable variable containing the larger scales

$R_x'(t)$: autocorrelation function

$\bar{C}(x, y, z)$: average concentration for receptor located at point (x, y, z)

$\bar{S}_{ij}$: filtered rate of deformation tensor

$\bar{g}_{ij}$: filtered velocity gradient tensor

$\bar{\Omega}_{ij}$: filtered vorticity tensor

u_* : friction velocity

$G(x_i; x_i')$: LES filter function

$\bar{u}$: mean wind speed

$\bar{u}_H$: mean wind speed at the height of plume centreline

$\tilde{y}$: non-dimensional distance from the wall

S_{ij}^d : symmetric traceless part of the square of the filtered velocity gradient tensor ($\bar{g}_{ij}$)

μ_t : subgrid-scale eddy viscosity

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RESUMO

O presente trabalho investigou o problema da modelagem da dispersão de compostos odorantes em presença de obstáculos (cúbicos e com forma complexa) sob condição de estabilidade atmosférica neutra. Foi empregada modelagem numérica baseada nas equações de transporte (CFD¹) bem como em modelos algébricos baseados na pluma Gausseana (AERMOD², CALPUFF³ e FPM⁴). Para a validação dos resultados dos modelos e a avaliação do seu desempenho foram empregados dados de experimentos em túnel de vento e em campo. A fim de incluir os efeitos da turbulência atmosférica na dispersão, dois diferentes modelos de sub-malha associados à Simulação das Grandes Escalas (LES⁵) foram investigados (Smagorinsky dinâmico e WALE⁶) e, para a inclusão dos efeitos de obstáculos na dispersão nos modelos Gausseanos, foi empregado o modelo PRIME⁷. O uso do PRIME também foi proposto para o FPM como uma inovação. De forma geral, os resultados indicam que o uso de CFD/LES é uma ferramenta útil para a investigação da dispersão e o impacto de compostos odorantes em presença de obstáculos e também para desenvolvimento dos modelos Gausseanos. Os resultados também indicam que o modelo FPM proposto, com a inclusão dos efeitos do obstáculo baseado no PRIME também é uma ferramenta muito útil em modelagem da dispersão de odores devido à sua simplicidade e fácil configuração quando comparado a modelos mais complexos como CFD e mesmo os modelos regulatórios AERMOD e CALPUFF. A grande vantagem do FPM é a possibilidade de estimar-se o fator de intermitência e a relação pico-média (P/M), parâmetros úteis para a avaliação do impacto de odores. Os resultados obtidos no presente trabalho indicam que a determinação dos parâmetros de dispersão para os segmentos de pluma, bem como os parâmetros de tempo longo nas proximidades da fonte e do obstáculo no modelo FPM pode ser melhorada e simulações CFD podem ser usadas como uma ferramenta de desenvolvimento para este propósito.

Palavras chave: controle de odor, dispersão, fluidodinâmica computacional, modelagem matemática, modelagem gaussiana de pluma flutuante, simulação de grandes vórtices (LES).

¹ Computational Fluid Dynamics – Dinâmica dos Fluidos Computacional

² AERMIC Model – AMS/EPA Regulatory Model Improvement Committee Model

³ California Air resources Board Puff model

⁴ Fluctuating Plume Model

⁵ Large Eddy Simulation

⁶ Wall Adaptative Local Eddy-viscosity model

⁷ Plume Rise Model Enhancements

ABSTRACT

The present work investigated odour dispersion modelling in the presence of obstacles (cubical and complex-shaped buildings) under neutral atmospheric conditions employing numerical modelling based on the transport equations (CFD⁸) as well as on algebraic Gaussian-based models (AERMOD⁹, CALPUFF¹⁰ and FPM¹¹) and using field and wind tunnel data to validate the models results and evaluate the models performance. To include atmospheric turbulence effects on dispersion, two different subgrid scale models associated to the Large Eddy Simulation (LES) technique were investigated (Dynamic Smagorinsk and WALE¹²) and to include the building effects on dispersion in the Gaussian-based models, PRIME¹³ was used. The use of PRIME was also proposed for FPM as a novelty. Overall, results indicate the use of the CFD/LES might be a useful tool for assessment of odour dispersion and impact in the presence of obstacles and also for the development of Gaussian models. Results also indicate that the proposed FPM, which included the effects of the obstacle based on the PRIME model, is a very useful tool in odour dispersion modelling, due to its simplicity and easy set up if compared to the more complex CFD modelling and even regulatory models AERMOD and CALPUFF. The great advantage of FPM is the possibility of estimating intermittency and also the peak-to-mean (P/M) concentration ratio, which are useful parameters for odour impact assessment. Results obtained in the present work indicate the determination of the plume segments dispersion parameters, as well as the long term dispersion parameters in the near field of the source and obstacle in FPM might be improved and CFD could be used as development tool for this purpose.

Key words: Odour control, dispersion, computational fluid dynamics (CFD), mathematical modelling, fluctuating plume Gaussian modelling, Large Eddy Simulation (LES).

⁸ Computational Fluid Dynamics – Dinâmica dos Fluidos Computacional

⁹ AERMIC Model – AMS/EPA Regulatory Model Improvement Committee Model

¹⁰ California Air resources Board Puff model

¹¹ Fluctuating Plume Model

¹² Wall Adaptative Local Eddy-viscosity model

¹³ Plume Rise Model Enhancements

1 Introduction

The Brazilian National Environment Policy (law no. 6,938, of August 31, 1981) defines pollution as “the degradation of environmental quality resulting from activities that directly or indirectly: a) impair population health, security and well-being; b) create adverse conditions for social and economic activities; c) unfavourably affect the biota; d) affect the appearance or sanitary conditions of the environment; e) release substances or energy in disagreement of the established environment standards. The effects of unpleasant odours vary from light disturbances to physical symptoms such as nose, eyes and throat irritation, headaches, nausea, diarrhea, nasal congestion, palpitation and changes in mood (Schiffman & Williams, 2005) affecting population well-being and health, and also creating adverse conditions to social activities. Brazilian laws presently do not have any regulations to prevent the environmental impact caused by odorous gases, although CONAMA resolution no. 382 from December 26, 2006 establishes thresholds for the emission of sulphur reduced compounds (hydrogen sulphide, methyl mercaptan, dimethyl sulphide and dimethyl disulphide) for cellulose plants (pulp mill factories). The European Union (EU) has recently developed laws for maximum ambient odorant gases concentration, while some members of the EU such as Germany already have regulation for emission and ambient concentration thresholds of odorant gases. Similar laws are also found in other European countries such as England, Holland and also in the United States of America, Australia and Japan (Drew et al., 2007).

Odorant compounds are commonly generated by industrial processes, oil refinery plants, cellulose plants, animal meat processing plants, domestic and industrial sewage treatment plants and also by deposition of solid residue from residences, hospitals and industries. The composition of odorant gases varies from reduced sulphur compounds (i.e. hydrogen sulphide, ammonia), organic acids, aldehydes, ketones and volatile fatty acids to an ample range of chlorate, aromatic and aliphatic hydrocarbons also called volatile organic compounds (VOCs), all pollutants which increases health risks to workers and nuisance to the general population.

The main efforts in scientific research on the estimation of the environmental impact of odorant compounds in built environment have been based on the development of (i) sampling and measuring techniques of odorant gases (or mixtures) at the impacted

site or at the source; (ii) mathematical models, wind tunnel and field experiments in order to estimate emissions and atmospheric dispersion of compounds in built environment (meteorological micro scale) and (iii) sensorial evaluations of odours based on four characteristic dimensions: detection threshold, intensity, quality and degree of pleasantness or unpleasantness of an odour.

Mathematical modelling of atmospheric dispersion can be based on empirical formulations, analytical or numerical solutions of the fundamental transport equations, depending on the simplifying hypothesis employed. Algebraic models are largely employed by environment agencies and industries due to their low cost and fast results which provide information used in (i) environment impact studies for new industrial sites, (ii) determination of source apportionment of pollutants, (iii) evaluation of emission control techniques or (iv) urban occupation planning.

Those models are, in general, based on the Gaussian approximation of vertical and horizontal profiles of concentration and include empirical expressions in order to model complex phenomena such as the presence of obstacles, wind direction oscillation due to low frequency turbulent eddies, chemical reactions, transient emissions, complex terrain, etc. Gaussian models commonly recommended by environment agencies for urban and rural regions are the ones originally proposed by Lee *et al.* (1996) (AERMOD), Scire *et al.* (1990) (CALPUFF) and by Carruthers *et al.* (1994) (ADMS).

Another model reported in the literature is the Fluctuating Plume Model (FPM), originally proposed by Gifford (1959) and developed by Murray *et al.* (1978). This model is capable of providing the percentage of time during which concentration remains above or below a defined threshold. This characteristic turns the FPM a valuable tool for odorant compounds dispersion modelling. Mussio *et al.* (2001) evaluated FPM performance and obtained better results for maximum odour concentration than a Gaussian model adapted to account for odour perception average time by a constant factor. De Melo Lisboa *et al.* (2006) modelled odour dispersion using the FPM and obtained good agreement with field data. The use of FPM with different formulations to include the effects of the presence of a complex geometry obstacle on dispersion was investigated by Dourado (2007). The author pointed out that the formulations proposed by Gifford (1960), Gifford (1968), Turner (1969), Huber and Snyder (1976), Johnson *et al.* (1975) and Scire *et al.* (2000) did not adequately reproduced wind tunnel results.

A more recent tool to include the effects of building on dispersion in Gaussian-based models was developed by Schulman *et al.* (2000) and named PRIME (Plume Rise Model Enhancement). This model incorporates the effect of plume elevation and downwash due to buoyancy and the presence of obstacles by enhancing the plume dispersion coefficients and accounting for the streamline deflection effect on plume rise. PRIME is included in AERMOD (Lee *et al.*, 1996; Cimorelli *et al.*, 2005) and CALPUFF (Scire *et al.*, 1990; Scire *et al.*, 2000) models.

AERMOD, CALPUFF and ADMS (Carruthers *et al.*, 1994; McHugh *et al.*, 1997; Carruthers *et al.*, 2000) include in their formulation the state-of-the-art in the development of Gaussian models (Section 3.4). Several studies have been conducted in order to validate these models using experimental data for different situations (e.g., Carruthers *et al.*, 1994b, Perry *et al.*, 2005, Kumar *et al.*, 2006, Isakov *et al.*, 2007 e Drew *et al.*, 2007) and also to compare the results obtained by different models and identify the most appropriate one for specific situations (Caputo *et al.*, 2003, Spanton *et al.*, 2005 and Wang *et al.*, 2006, among others).

All of the above mentioned models are based on the Gaussian plume equation, obtained from the solution for the chemical species mass conservation under idealized conditions. Gaussian modelling depends on several empirical parameters which restrict its generality. Therefore, many studies employing models based on the complete solutions of the fundamental transport equations have been undertaken (e.g., Brown & Flecher, 2005, Hanna *et al.* 2006). The main motivation is to improve the accuracy of estimations by using a more complex mathematical modelling, with fewer simplifications. In this sense, computational fluid dynamics (CFD) is a great deal as it supplies a detailed description of atmospheric flow and dispersion, allowing for the comprehension of the physical phenomena involved (e.g., Riddle *et al.*, 2004 and Li & Guo, 2006). These more complex models can be used to improve analytical models or for field and laboratory experiment planning.

Studies show that turbulence models based on the Large Eddy Simulation (LES) technique have obtained better results than other models when compared to experimental data for dispersion in the presence of obstacles (Murakami *et al.* (1996), Sada & Sato, 2002, Brown & Fletcher, 2005, Hu *et al.*, 2011, Moonen *et al.*, 2011, Salim *et al.*, 2011, among others). However, compared to algebraic models, CFD simulations are

more complex to set up and require more computer processing. A fundamental aspect of LES is the separation of the solved (large) turbulence scales from the modelled (smaller) scales. The effect of these smaller scales is included through a sub grid model. The most common sub grid models used in engineering applications are the Smagorinsky (Smagorinsky, 1963) and the Dynamic Smagorinsky (Germano *et al.*, 1991) models (Su *et al.*, 2001). Another sub grid model is the Wall Adaptative Local Eddy-viscosity model (WALE), proposed by Nicoud and Ducros (1999). The Dynamic Smagorinsky and WALE models better represent flow behaviour near solid walls.

Odorant gases dispersion modelling presents an additional challenge as besides the effect of turbulent diffusion, the effect of low frequency turbulent eddies (which promotes oscillations in wind direction) and the presence of obstacles (odour emission and dispersion usually occurs in built environment), which causes the appearance of intense recirculation regions, where turbulence is highly three-dimensional and anisotropic, must be included. These phenomena are related to the impact caused by the odour during the time of a single breath (1 to 5 seconds) as well as to the frequency of occurrence of odour perception. The obstacles are represented by buildings found near the emission point or area sources, or they can be volume sources themselves.

Computer fluid dynamics simulations using Large Eddy simulation to model atmospheric turbulence is an interesting tool to model odorant compounds dispersion, especially in the presence of obstacles.

This work aims to investigate odour dispersion modelling in the presence of obstacle under neutral atmospheric conditions using computational fluid dynamics associated to Large eddy Simulation to include the effects of atmospheric turbulence as well as algebraic Gaussian-based models (AERMOD and CALPUFF) associated with PRIME to include the building effects on dispersion. In addition, an improvement in the fluctuating Gaussian plume model was proposed by also including the use of PRIME in this Gaussian-based model.

During the development of the present work, the obtained results allowed for the submission of three articles on international conferences and the further publication of two papers on scientific journals, as shown in Table 1-1.

The present work is divided into six chapters. After this brief introduction (Chapter 1), the objectives of the present work are explained in Chapter 2. Chapter 3

covers the background information related to odour dispersion modelling, while Chapter 4 describes the recent works on the subject presented in scientific journals. Chapter 5 explains the methodology employed in the present work, as well as a description of the proposed Fluctuating Plume Model which includes the building effects by coupling PRIME. Results are presented in Chapter 6 and the conclusions as well as suggestions for future works are presented in Chapter 7.

Table 1-1: List of publications.

Paper no.	Title	Presented/published at
1	Numerical modelling of odour dispersion around a cubical obstacle using large eddy simulation.	Presented at the 4th IWA specialized conference on odours and VOCs, Vitória, Brazil, 17-21 October, 2011. Published as a full article in Water Science and Technology, Volume: 66, Issue: 7, Pages: 1549-1557. DOI: 10.2166/wst.2012.369. Published: 2012
2	The Effects of Atmospheric Turbulence on Peak-to-Mean Concentration Ratio and its Consequence on the Odour Impact Assessment Using Dispersion Models	NOSE 2012 - 3rd International Conference on Environmental Odour Monitoring and Control; Palermo, Italy, 23-26 September, 2012. Published as a full article in Chemical Engineering Transactions - vol.30. DOI:10.3303/CET1230028 Published: 2012
3	Validation of gaussian models using wind tunnel experiments and numerical simulation	HARMO 15: 15th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. Madrid, Spain, 6-9 May 2013.

2 Objectives

2.1 Main goal

To investigate odour dispersion modelling in the presence of obstacles under neutral atmospheric conditions.

2.2 Aims of this study

This study aims to:

- Evaluate the use of two sub grid scale models of LES (Dynamic Smagorinsky and WALE) to simulate wind flow and dispersion in the presence of obstacles under neutral atmospheric conditions;
- Verify the capacity of LES to estimate odorant gas concentration and concentration fluctuation in atmospheric flows affected by in the presence of isolated obstacles (cubical and complex shaped geometries) under neutral atmospheric conditions by comparing the numerical results with wind tunnel and field experimental data;
- Assess the performance of regulatory models AERMOD and CALPUFF including PRIME by comparing these Gaussian-based models results with LES, wind tunnel and field data;
- Propose the use of the Fluctuating Plume Model (FPM) including the effects of obstacles on dispersion by coupling PRIME for odour dispersion modelling, validate the obtained results of average concentration and concentration fluctuation with wind tunnel and field experimental data and compare FPM performance with LES, AERMOD-PRIME and CALPUFF-PRIME;
- Evaluate AERMOD-PRIME and CALPUFF-PRIME predictions of short period peak concentration in comparison with LES and FPM-PRIME.

3 Background Information

The use of mathematical models for the study of atmospheric dispersion of pollutants has been a constant practice since the second half of the 20th century, especially for atomic energy researches that aimed to investigate the impact of accidental releases. Currently, the use of mathematical models is facilitated by the large availability of computer processing power and includes different applications such as research, planning and regulation. The study of the impact of the release odorant gases is a recent application of such models.

The present chapter aims to present the relevant issues concerning atmospheric odour dispersion modelling and the different approaches to this problem as presented in the literature.

3.1 Atmospheric dispersion in the planetary boundary layer

Atmospheric dispersion, as considered in the present work, is the transport and spreading of material by the wind flow as it happens in the lower layer of the atmosphere, called the Troposphere, which extends from the earth surface up to 10-15 km altitude, and is characterized by decreasing temperature with height and by rapid processes of vertical mixing (Seinfeld and Pandis, 2006). The lower region of the Troposphere, in which the influence of the ground is exerted in the atmospheric flow, is called the planetary boundary layer (PBL) (Hanna et al., 1982). The majority of pollutant sources is situated inside the PBL and this is the region where human life is developed. Any pollutant released in the PBL will have its transport influenced by mechanically or thermally generated turbulence, a direct result of the presence of obstacles, complex terrain, earth surface heating and cooling, and by wind speed (Turner, 1984).

The PBL height varies during day time as a direct result of surface heating and its depth may extend on a range from 0.2-5km, with the highest depth attained in the late afternoon (Arya, 2001). This period is characterized by buoyant convection. During night time, when the ground surface cools, turbulent mixing is weakened or even suppressed, bringing the PBL height to the range of approximately 20-500 m (Arya, 2001). The stability condition of the atmosphere gives an indication of how vertical motions

are enhanced or inhibited. When the atmosphere is unstable, vertical motions are enhanced by buoyancy and the mixing of pollutants is rapid, whereas in neutral atmosphere vertical movements are not affected by buoyancy forces; when the atmosphere is stable, vertical movement is damped and pollutants tend to spread horizontally (Seinfeld and Pandis, 2006). The determination of the atmosphere stability condition is based on the determination of parameters such as the flux Richardson number (R_f), the Monin-Obukhov length (L) and also Pasquill stability classes. The flux Richardson number is equal to the ratio of turbulent kinetic energy produced by buoyancy and to the shear stresses; the Monin-Obukhov length is the height where production of turbulence by mechanical forces and buoyant forces are equal (Seinfeld and Pandis, 2006). Determination of R_f and L require measurements of turbulent fluxes as well as determination of the friction velocity. Until recently these parameters were not easily determined (Wyngaard, 2010) and atmospheric stability was determined by a classification proposed by Pasquill (1961) and modified by Turner (1969), which is based on wind velocity measurements (at 10 m height), solar radiation and cloud cover. The Pasquill stability classes (SC) are shown in table 3-1, where stability classes are identified by a letter (A-F) or a number (1-6). These classes are defined based on a set of meteorological conditions shown in table 3-2. These conditions rely on wind speed values, daytime incoming solar radiation and night time cloud cover.

Table 3-1 : The Pasquill stability classes

Stability class	Definition
A (1)	Very unstable
B (2)	Unstable
C (3)	Slightly unstable
D (4)	Neutral
E (5)	Slightly stable
F (6)	Stable

(Adapted from: Seinfeld and Pandis, 2002)

Table 3-2 : Estimation of Pasquill Stability Classes

Wind speed		Daytime incoming solar radiation			Nighttime cloud cover	
m/s	mph	Strong	Moderate	Slight	>50%	<50%
< 2	< 5	A	A – B	B	E	F
2 – 3	5 – 7	A – B	B	C	E	F
3 – 5	7 – 11	B	B – C	C	D	E
5 – 6	11 – 13	C	C – D	D	D	D
> 6	> 13	C	D	D	D	D

Class D applies to heavily overcast skies, at any wind speed day or night.

(Adapted from: Seinfeld and Pandis, 2002)

Wind speed is measured at 10 m height above ground. According to Wark and Warner (1981, cited by De Melo Lisboa, 1996), strong daytime incoming solar radiation ($\geq 600 \text{ W/m}^2$) corresponds to clear sky condition, typical of a sunny afternoon and highly convective atmosphere; moderate radiation (300 to 600 W/m^2) is typical of a summer day with sparse clouds; slight incoming solar radiation ($\geq 300 \text{ W/m}^2$) is normally found at the end of a typical sunny summer day with sparse clouds; > 50% nighttime cloud cover can be used in a typical (northern hemisphere) winter day.

3.2 Atmospheric dispersion modelling based on the transport equations

The transport of contaminants in the atmosphere is a combination of diffusion and advection (Stockie, 2011). The set of equations describing fluid flow and transport of its properties are based on the conservation laws of physics – conservation of mass (Equation 3-1) Newton's second law, or conservation of momentum (Equation 3-2), the first law of thermodynamics (Equation 3-5) and the chemical species conservation (Equation 3-7), a set of six partial differential equations shown below for a Newtonian fluid in Cartesian coordinates (using index notation). This system of equation can only be solved analytically for very simple cases (Ferziger and Perić, 2002) For atmospheric flows, characterized by high Reynolds numbers and a chaotic and random state of motion (Versteeg and Malalasekera, 2007), the system of transport equations does not have

a complete analytical solution and usually calls for numerical methods to obtain its solution.

The conservation equations for a newtonian fluid in cartesian coordinates using index notation are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (3-1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \frac{\partial T_{ij}}{\partial x_j} - \rho g_i \quad (3-2)$$

where:

$$T_{ij} = 2\mu S_{ij} - \left(p + \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (3-3)$$

and:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3-4)$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial}{\partial x_i} \left(k_c \frac{\partial T}{\partial x_i} \right) + \Phi + \left(\frac{\partial p}{\partial t} + u_i \frac{\partial \rho}{\partial x_i} \right) + H \quad (3-5)$$

with (for a perfect gas):

$$\frac{\partial h}{\partial x_i} = c_p \frac{\partial T}{\partial x_i} \quad (3-6)$$

$$\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u_i c}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D_m \frac{\partial c}{\partial x_i} \right) + M \quad (3-7)$$

where ρ is fluid density, t is time, u_i and u_j are the flow velocity component in directions x_i and x_j , with $i = 1, 2, 3$ and $j = 1, 2, 3$ corresponding to x, y and z directions; T_{ij} is stress tensor, S_{ij} is rate of deformation tensor; h is the fluid specific enthalpy, k_c is the fluid thermal conductivity, T is the temperature; Φ is energy dissipation function due to viscous stress, p is the pressure, c_p is the fluid constant pressure specific heat capacity; c is the chemical species concentration, D_m is diffusion coefficient for chemical species m ; H and M are sources of energy and mass.

3.3 Turbulence modelling

Turbulence is a condition of the flow in which “fluid velocity field varies significantly and irregularly in both position and time” (Pope, 2000). The majority of engineering flows are turbulent such as the flow around vehicles, aircrafts, ships, flow inside pumps, reactors, etc. The same thing happens with atmospheric flows.

The basic characteristics of turbulent flows are (Tennekes and Lumley, 1972; Davidson 2003; Tsinober, 2004):

- *Irregularity, randomness in space and time*: this is an intrinsic property, i.e., this condition arrives without the need of an external random forcing, as long as the Reynolds number is sufficient large; the flow is described as chaotic;
- *Large Reynolds number*: transition from laminar to turbulent motion happens at large Reynolds numbers (e.g., for boundary layer flows, the critical Reynold Number is about 10^5)
- *Wide range of scales*: with eddy sizes as large as the flow geometry (such as boundary layer thickness, size of obstacles, etc.) and ranging down to fractions of millimeters, turbulent motion present a wide spectrum;
- *Loss of predictability*: different realization of “the same” flow will exhibit completely different values of its properties at each instant although they will present the same statistical properties;
- *Three dimensional and rotational*: Turbulent flows are always three dimensional and presents random fields of vorticity;
- *Diffusivity*: as turbulence increases the exchange of momentum, its spreading rate augments, leading to the increase of diffusivity;
- *Dissipation*: there is a continuous flow of energy as the largest and more energetic eddies divide up onto progressively smaller and less energetic eddies – the small eddies receive energy from the larger ones and the largest eddies receive energy from the mean flow; the smallest eddies are finally damped due to viscous effects this process is called the energy cascade (Figure 3-1);

- *Continuum*: although the smaller scales are damped due to viscous action, their sizes are much larger than the molecular scales so the basic assumption of fluid as a continuum media still holds.

Figure 3-1 shows a general representation of the turbulent spectrum of a turbulent flow. One can notice three main regions (I, II and III) with different levels of energy. The first region (I) is where the largest eddies interact with the main flow and turbulent energy is at its highest levels. Region III is called the dissipation range, where the smallest eddies are found. In this region, eddies are isotropic and does not depend on flow geometry. Region III is called the Kolmogorov scales. Region II is called the inertial subrange. It is where the transport of energy happens, with eddies independent to both the larger scale and the smallest scale eddies. The Kolmogorov spectrum law (the -5/3 law) states that the energy spectrum of a turbulent flow will exhibit a -5/3 decay.

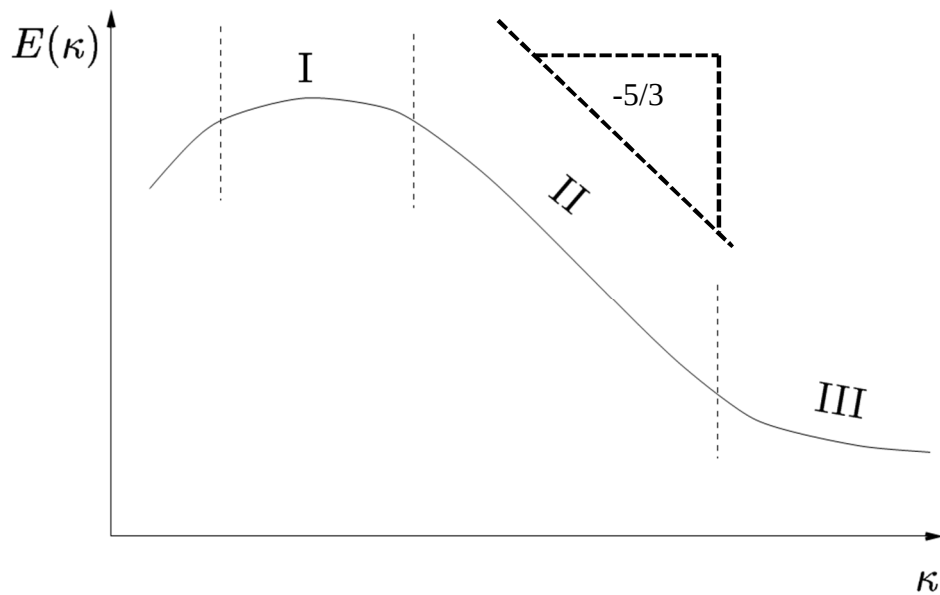


Figure 3-1: energy spectrum of a turbulent flow as a function of the wavenumber. Region I contains the largest eddies which interact with the main flow, region II is the inertial subrange, where energy is transported onto region III, where energy is finally dissipated into the smallest eddies. Region II presents a -5/3 decay. (Adapted from Davidson, 2003)

As mentioned above, although turbulence has an intrinsic randomness, the statistical description of the properties of a turbulent flow allows for the identification of a similar behaviour in different realizations of the same flow (Tsinober, 2004), so the common procedure is to treat turbulent flow statistically. It is interesting to note that, in spite of its apparently randomness, Panofsky and Dutton (1983) state that statistical de-

scription of turbulence might be a consequence of human limitation in terms of knowledge of all initial conditions that trigger turbulence and also the limitation in available computer power, which would eliminate randomness.

There are three basic forms of solving the transport equations through numerical modelling: (i) direct numeric simulation, (ii) time averaged equations and (iii) space averaged equations (Vesteeg and Malalasekera, 2007). In direct numeric simulation (DNS), transport equations are solved including all scales of turbulence. This method requires a huge amount of computer power as sufficient fine grids and sufficient small time steps are necessary to solve the Kolmogorov scales and therefore is not used in engineering daily work. Time averaged equation models (or RANS models) focus its attention on the mean flow and the effect of turbulence on the mean flow parameters while the space averaged (or space filtered) equation models, also called Large Eddy Simulation (LES) models, solve the larger scales and models the effect of the smaller scales.

3.3.1.1 LES models

Large eddy simulation technique is based on the theory by Kolmogorov (1941) where the large eddies of a turbulent flow are dependent on the flow geometry and the smaller scales are more universal and isotropic. As the larger scales are more energetic (see Figure 3-1), their influence on the flow will be more important so LES models solve the larger scales and models the smaller ones, as can be observed in Figure 3-2. Smaller scales are accounted through the use of a sub grid-scale model. The turbulent field is thus divided into a resolved part and a sub grid modelled part. The separation is accomplished through a spatial filter. If f is any of the flow variables then:

$$f = \bar{f} + f' \quad (3-8)$$

where $\bar{f}$ is the filtered variable containing the larger scales and f' is the modelled part containing the smaller scales. The filter function is represented by:

$$\overline{f}(x_i, t) = \int_{VOL} G(x_i; x_{i'}) f(x_{i'}, t) dx_{i'} , i = 1, 2, 3 \quad (3-9)$$

where: $G(x_i; x_{i'})$ is the filter function applied to $f(x_{i'}, t)$ within a volume element with the order of magnitude of the computational grid, usually taken as (Ferziger and Perić, 2002; Berselli et al., 2006; Versteeg and Malalasekera, 2007; Jiang and Lai, 2009):

$$\Delta = (\Delta x \Delta y \Delta z)^{1/3} \quad (3-10)$$

where Δx , Δy and Δz are the grid size in x, y and z directions.

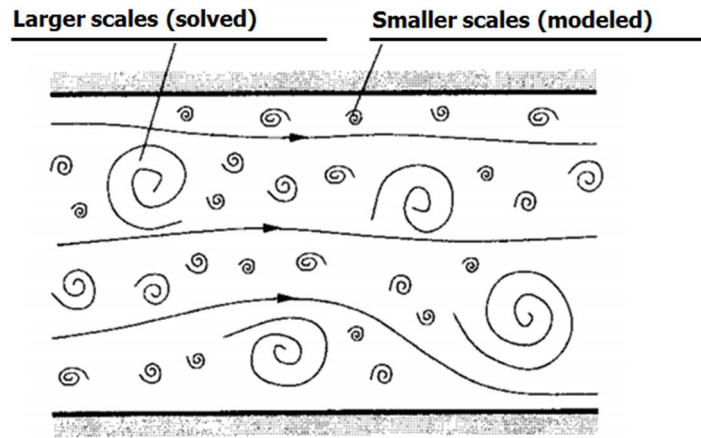


Figure 3-2: Representation of the large and small turbulent scales on the flow. Note how the flow trajectory is influenced by the larger scales. (Adapted from Ferziger e Perić, 2002)

Being a low-pass filter, the effect of the spatial filtering is to smooth out the small scales fluctuations on the flow properties (Figure 3-3), where the unfiltered velocity field (thin trace) and the correspondent fluctuations are compared to the filtered field (bold trace) and its fluctuations.

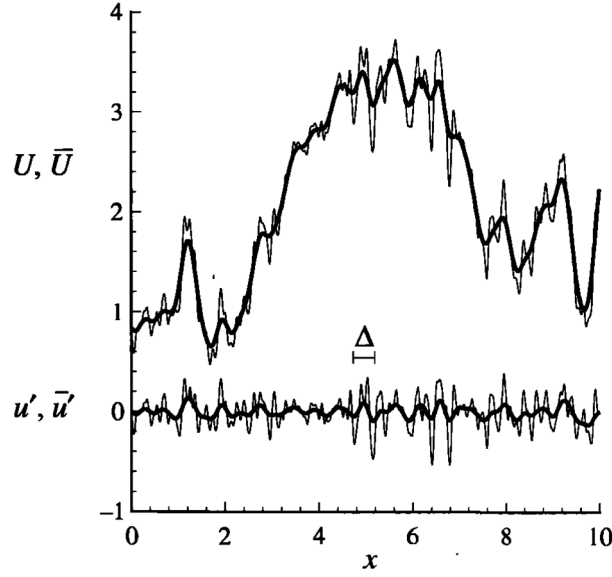


Figure 3-3: Comparison of unfiltered (thin line) and filtered (bold line) velocity field $U(x)$: upper curves show velocity magnitude and lower curves show velocity fluctuation (Source: Pope, 2000).

Equation 3-11 is the filtered momentum equation. Although it has the basic form of the unfiltered equation (Equation 3-2) there is the addition of a new unknown term, relating to the small scales, the sub grid scale stress tensor:

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right) - \frac{\partial p}{\partial x_i} + \rho g_i - \frac{\partial}{\partial x_j} (\tau_{ij}^s) \quad (3-11)$$

where τ_{ij}^s is the sub grid stress tensor.

3.3.1.1.1 Smagorinsky LES

Smagorinsky (1963) provided an eddy viscosity model relating the subgrid tensor to the flow solved scales. It is based on the assumption that the main effects of the subgrid stress is to increase transport and dissipation, which in turn is related to viscosity in laminar flows (Ferziger and Perić, 2002). The proposed model is (Equation 3-12):

$$\tau_{ij}^s = -2\mu_t \bar{S}_{ij} + \frac{1}{3}\tau_{kk}^s \delta_{ij} = -\mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) + \frac{1}{3}\tau_{kk}^s \delta_{ij} \quad (3-12)$$

where μ_t is the sub grid-scale eddy viscosity, and $\bar{S}_{ij}$ is the rate of deformation tensor, or strain rate tensor (Equation 3-4).

The sub grid eddy viscosity is related to the solved scales by (Equation 3-13):

$$\mu_t = C_s^2 \rho \Delta^2 |\bar{S}| \quad (3-13)$$

where C_s is a model parameter; and $|\bar{S}| = (\bar{S}_{ij} \bar{S}_{ij})^{1/2}$, is the characteristic filtered strain rate.

C_s , also called the “Smagorinsky coefficient” (Pope, 2000) is a flow dependent parameter, and although 0.2 is the often used value, other values are also employed in the literature, such as 0,17 – 0,21 (Lilly, 1966, 1967); 0,19 – 0,24 (Rogallo & Moin, 1984) and 0,1 (Deardoff, 1970). The reason for varying the value of C_s is to correctly model the shear flow behaviour, for instance in regions near walls, where the relation expressed by Equation 3-13, leads to high values of the eddy viscosity due to the high strain rates in those regions. On the other hand, a value of C_s that is adequate to near wall regions would not correctly model the effect of subgrid scales in other regions of the flow. This issue can be dealt with the use of special damping functions to attenuate C_s near walls (a practice commonly used with RANS models) or by dynamically varying C_s along the flow domain.

Moin and Kim (1982) proposed the use of the Van Driest damping function in order to adapt the value of C_s near walls (Equation 3-14):

$$C_s = C_{s0} \left(1 - e^{-\tilde{y}/A^+} \right)^2 \quad (3-14)$$

where C_{s0} is the Smagorinsky coefficient, $\tilde{y} (= yu_*/\nu)$ is the non-dimensional distance from the wall, $u_* (= \sqrt{\tau_w/\rho})$ is the friction velocity, τ_w is the shear stress at the wall and A^+ is a constant damping factor (≈ 25).

Ferziger and Perić (2002) criticize this approach by stating that an SGS should only depend on the flow local properties and that the parameter distance from the wall does not qualifies as a local property of the flow.

3.3.1.1.2 Dynamic Smagorinsky LES

Dynamic Smagorinsky sub-grid model was proposed by Germano et al. (1991). This approach is based on a scale similarity model, where the smallest resolved scales of the flow are related to the largest subgrid scales. By sampling the smallest resolved scales, the subgrid scales are modelled, exhibiting the correct behavior near solid surfaces. The model employs a double filtering process, with two different subgrid scales.

The model is based on the identity

$$L_{ij} = T_{ij} - \{\tau_{ij}\} \quad (3-15)$$

where: L_{ij} is the resolved turbulent stress, T_{ij} is the subgrid-scale stress at a scale $\{\Delta\}$ (the test filter scale), τ_{ij} is the subgrid-scale stress at a scale $\Delta < \{\Delta\}$.

The Smagorinsky model is then employed for both the test scale and subgrid-scale:

$$\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = C_d \left(-2\Delta^2 \left| \bar{S}_{ij} \right| \bar{S}_{ij} \right) = C_d m_{ij}^{sgs} \quad (3-16)$$

$$T_{ij} - \frac{\delta_{ij}}{3} T_{kk} = C_d \left(-2\{\Delta\}^2 \left| \{\bar{S}_{ij}\} \right| \{\bar{S}_{ij}\} \right) = C_d m_{ij}^{test} \quad (3-17)$$

Using the Germano identity (Equation 3-15) in Equations 3-16 and 3-17:

$$L_{ij}^a = L_{ij} - \frac{\delta_{ij}}{3} L_{kk} = C_d m_{ij}^{test} - \{C_d m_{ij}^{sgs}\} \quad (3-18)$$

In order to solve the over-determined system of Equation 3-18, the error associated with the Smagorinsky model, e_{ij} , is defined as:

$$e_{ij} = L_{ij}^a - \left[C_d m_{ij}^{test} - \{ C_d m_{ij}^{sgs} \} \right] \quad (3-19)$$

Lilly (1992), applied a least square approach in order to minimize e_{ij} , and C_d is then taken out of the filtering procedure:

$$C_d = \frac{L_{ij}^a M_{ij}}{M_{ij} M_{ij}} \quad (3-20)$$

$$M_{ij} = m_{ij}^{test} - \{ m_{ij}^{sgs} \} \quad (3-21)$$

Now, the eddy viscosity is obtained (Equation 3-22):

$$\mu_{sgs} = C_d \rho \Delta^2 \left| \overline{S_{ij}} \right| \quad (3-22)$$

The value of C_d is then dynamically adjusted as a function of the flow local properties, eliminating the need for damping functions near walls. In order to avoid instability due to negative or over large values of C_d , a lower bound of 0.0 and an upper bound ranging from 0.04 to 0.09 might be employed (ANSYS, 2010)

3.3.1.1.3 The Wall Adaptative Local Eddy-viscosity (WALE) model

This approach was proposed by Nicoud and Ducros (1999). The WALE subgrid-scale is based both on the resolved rate of strain tensor and on the resolved vorticity tensor. The idea behind the model is that the flow energy dissipation is concentrated in turbulent eddies and convergence zones, where vorticity is more influent than strain.

In the WALE model, the eddy-viscosity is obtained by (Equation 3-23):

$$\nu_T = (C_w \Delta)^2 \frac{\left(S_{ij}^d S_{ij}^d \right)^{3/2}}{\left(\overline{S_{ij}} \overline{S_{ij}} \right)^{5/2} + \left(S_{ij}^d S_{ij}^d \right)^{5/4}} \quad (3-23)$$

where: $S_{ij}^d = \frac{1}{2}(\bar{g}_{ij}^{-2})$ is the symmetric traceless part of the square of the filtered velocity gradient tensor ($\bar{g}_{ij}$);

$$\bar{g}_{ij} = \bar{S}_{ij} + \bar{\Omega}_{ij} \quad \text{and} \quad \bar{g}_{ij}^{-2} = \frac{\partial \bar{u}_i}{\partial x_k} \frac{\partial \bar{u}_k}{\partial x_j}$$

$$\bar{S}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) \quad \text{is the filtered rate of deformation tensor;}$$

$$\bar{\Omega}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{U}_i}{\partial x_j} - \frac{\partial \bar{U}_j}{\partial x_i} \right) \quad \text{is the filtered vorticity tensor;}$$

then, S_{ij}^d is written as:

$$S_{ij}^d = \bar{S}_{ik} \bar{S}_{kj} + \bar{\Omega}_{ik} \bar{\Omega}_{kj} - \frac{1}{3} \delta_{ij} (\bar{S}_{mn} \bar{S}_{mn} - \bar{\Omega}_{mn} \bar{\Omega}_{mn}) \quad (3-24)$$

The advantages of the model are (Nicoud and Ducros, 1999; Ansys, 2010):

- Invariant for any coordinate translation or rotation;
- Easily employed with any kind of computational mesh;
- Depends on both rate of deformation and rate of rotation tensors;
- Eddy viscosity naturally tends to zero near walls, reproducing the no slip condition;
- The model correctly reproduces the asymptotic variation of the eddy viscosity near walls, $O(y^3)$;
- The model is capable of reproducing the transition from laminar to turbulent regime;
- As the model does not requires double filtering, it requires less computational resources than the Dynamic Smagorinsky model.

3.3.1.1.4 Other sub grid scale models

The previously described sub grid models are included in commercial CFD packages such as ANSYS CFX and Fluent, but the literature reports other types of sub grid scale models. A review of the several sub grid models was presented by Meneveau and Katz (2000). Su *et al.* (2001) stated that most of the proposed models use the Bous-

sinesq hypothesis to calculate eddy viscosity, with the most popular models being the Smagorinsky and the dynamic models.

3.3.1.2 The Detached Eddy Simulation (DES) model

The detached eddy simulation (DES) model is a hybrid formulation, combining LES and Reynolds Averaged Navier-Stokes (RANS) models. In regions of boundary layer flow RANS (where the effect of all turbulent scales are modelled) is employed and in separated regions LES is employed.

Although the recent literature shows a variety of application of the DES model in areas such as naval engineering (Forrest and Owen, 2010), geomorphology (Keylock et al, 2012), and in the study of particle dispersion in enclosed spaces (Wang et al., 2011), use of DES models in atmospheric flows is still on the horizon (Cochran and Derickson, 2011).

3.4 Gaussian models

As already mentioned, atmospheric transport phenomena is usually described through algebraic or numerical solutions of the fundamental transport equations. The most commonly employed models are algebraic, usually derived from the original Gaussian dispersion model, based on original work from Sutton (1932), Pasquill (1961, 1974) and Gifford (1961, 1968). Its basic formulation can be obtained as a solution for the transport equations through Eulerian or Lagrangian approaches, as described by Arya (1999), Seinfeld and Pandis (2006), and recently, by Stockie (2011), considering some simplifying hypothesis:

- Constant rate of emission (Q), from a single point source, located at the origin of the coordinate system $(0, 0, H)$ at height H above the ground;
- Constant positive wind speed aligned with the x -axis;
- Steady state flow;
- Eddy diffusivities are functions of the downwind (x -axis) distance only, and diffusion is isotropic;
- Wind velocity value is sufficiently high so that x -direction diffusion can be neglected when compared with advection;
- The terrain is flat, i.e., the ground always correspond to $z = 0$;

- The contaminant does not penetrate the ground.

The Gaussian plume equation is shown below (Equation 3-25):

$$\bar{C}(x, y, z) = \frac{Q}{2\pi \bar{u}_H \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot \left[\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right) \right] \quad (3-25)$$

where (with typical units of measurement): $\bar{C}(x, y, z)$ is the average concentration for receptor located at point (x, y, z) ; Q is the rate of emission of the contaminant; $\bar{u}_H$ is the mean wind speed at the height of plume centreline; σ_y is the horizontal dispersion parameter; σ_z is the vertical dispersion parameter; h is the height of the plume centreline.

The plume is modelled as an infinite number of overlapping of discrete packets of pollutant traveling in space (or “puffs”) emitted from a fixed point (Gifford, 1959). Pollutant dispersion is then the combined effect of diffusion and turbulent transport. The contaminant concentration follows a Gaussian distribution laterally and vertically, where the dispersion parameters σ_y and σ_z are the standard deviations of the Gaussian distribution. The obtained concentration corresponds to the ensemble average of a set of average concentrations obtained from infinite repeated measurements. This concept is illustrated at Figure 3-4, where the concentration distribution is shown at two different downwind locations. The plume cross-section has the form of an ellipse that grows with of downwind distance increase. The dispersion parameters also grow with downwind distance and represent the effect of atmospheric turbulence promoting contaminant spread. Gifford (1961) proposed correlations between the value of σ_y and σ_z and the Pasquill stability classes which became known as the Pasquill-Gifford (P-G) curves, shown in figures Figure 3-4 and Figure 3-5. Several empirical analytical expressions have been developed to represent the P-G curves (Seinfeld and Pandis, 2002). Briggs (1973) have proposed a set of expressions for the dispersion parameters for rural and urban areas, shown in table 3-3.

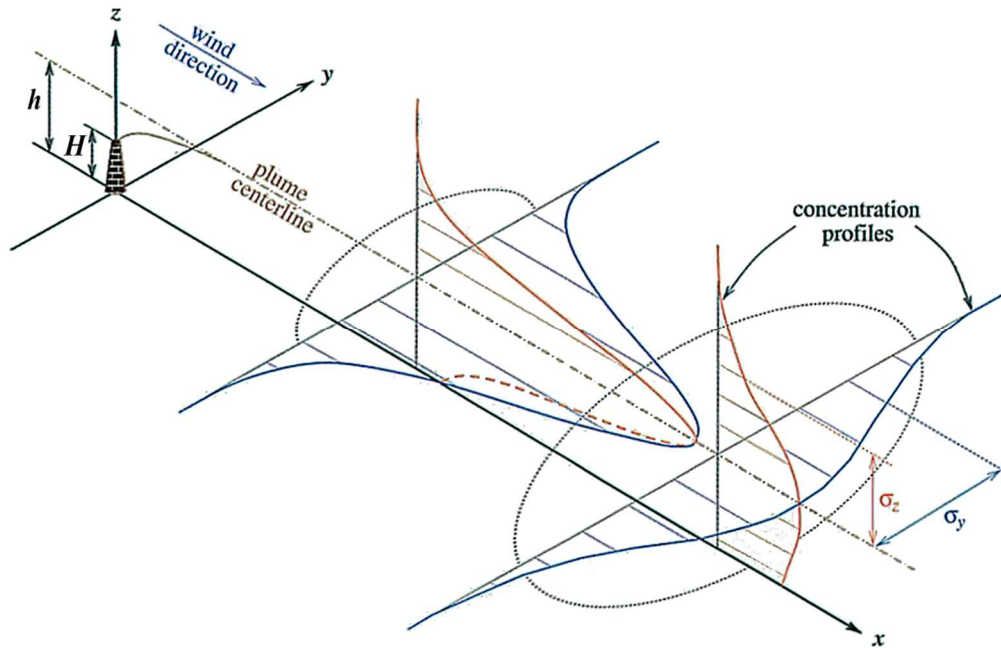
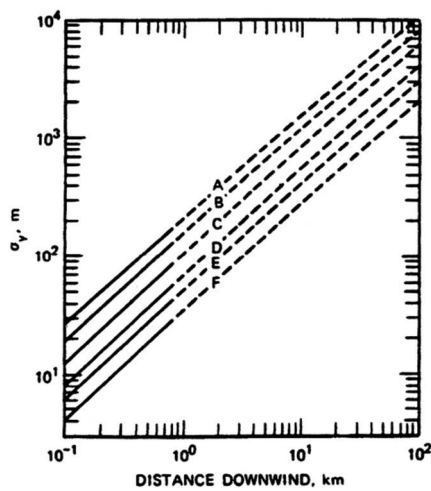
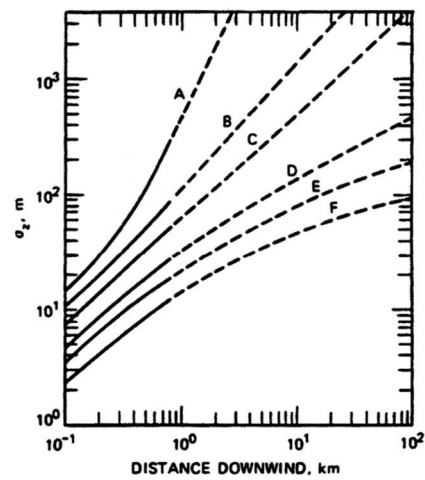


Figure 3-4: representation of the gaussian plume, with concentration distribution at two different downwind distances, notice with the elliptical shape of the plume cross-section (Adapted from Stockie, 2011).



(a)



(b)

Figure 3-5: Pasquill-Gifford curves correlating horizontal and vertical dispersion parameters and stability classes (Source: Hanna, Briggs and Hosker Jr., 1982).

Table 3-3: Briggs recommended formulas for σ_y and σ_z

Stability class	Dispersion coefficients	
	Rural conditions	
	σ_y (m)	σ_z (m)
A	$0.22x(1 + 0.0001x)^{-1/2}$	$0.20x$
B	$0.16x(1 + 0.0001x)^{-1/2}$	$0.12x$
C	$0.11x(1 + 0.0001x)^{-1/2}$	$0.08x(1 + 0.0002x)^{-1/2}$
D	$0.08x(1 + 0.0001x)^{-1/2}$	$0.06x(1 + 0.0015x)^{-1/2}$
E	$0.06x(1 + 0.0001x)^{-1/2}$	$0.03x(1 + 0.0003x)^{-1/2}$
F	$0.04x(1 + 0.0001x)^{-1/2}$	$0.016x(1 + 0.0003x)^{-1/2}$
	Urban conditions	
A – B	$0.32x(1 + 0.0004x)^{-1/2}$	$0.24x(1 + 0.001x)^{-1/2}$
C	$0.22x(1 + 0.0004x)^{-1/2}$	$0.20x$
D	$0.16x(1 + 0.0004x)^{-1/2}$	$0.14x(1 + 0.0003x)^{-1/2}$
E – F	$0.11x(1 + 0.0004x)^{-1/2}$	$0.08x(1 + 0.0015x)^{-1/2}$

(Source: Hanna, Briggs and Hosker Jr., 1982)

Researches developed in the 1970's and 1980's led to an understanding of the behavior of the convective boundary layer structure (CBL), the stable boundary layer (SBL) as well as the effect of complex terrain. As a result, improved versions of the Gaussian model started to appear (Cimorelli et al., 2005), addressing issues not covered in the original formulations due to above cited simplifications. The Gaussian model was also adapted to cover line, area and volume sources (Seinfeld and Pandis, 2006). The effect of the presence of obstacles was also addressed (Hosker Jr., 1981; Schulman et al., 2000).

There are several Regulatory Agencies approved models derived from the original Gaussian plume formulation such as ISC3 (EPA, 1995), AERMOD (Lee *et al.*,

1996; Cimorelli *et al.*, 2005), CALPUFF (Scire *et al.*, 1990; Scire *et al.*, 2000) and ADMS (Carruthers *et al.*, 1994; McHugh *et al.*, 1997; Carruthers *et al.*, 2000).

3.4.1 AERMOD model

AERMOD model was developed as a replacement for the ISC3 model, including the advancements for treating dispersion of pollutants in the PBL both in convective and stable conditions acquired as a result of late 70's and 80's researches (US-EPA, 2004). It is a steady-state dispersion model and includes in its formulation the effects of variations in the PBL on pollutant dispersion (Cimorelli *et al.*, 2005). The emitted plume is treated as updrafts and downdrafts sections moving with main wind, with vertical and lateral velocities represented by random variables (Figure 3-6); also included is the effect of quasi-reflection of the plume at the top of the mixing layer and the effect of plumes penetrating stable layer above the CBL and reentering it afterwards (US-EPA, 2004). The effect of plume reflection at the top of the mixing layer, as well as the penetration in the stable layer above it is represented by virtual plumes (Figure 3-7). Horizontal and vertical concentration distribution is Gaussian in neutral and stable conditions; however, in convective conditions, lateral concentration is Gaussian and vertical concentration is described by a bi-Gaussian distribution. The effect of the presence of obstacles is included through the PRIME model (section 3.6.7).

AERMOD system is divided in three modules: the AERMOD module and the AERMET and AERMAP pre-processors. AERMET reads meteorological data input by the user based on field measurements and generates vertical profiles of wind direction, wind speed, temperature, vertical potential temperature gradient, vertical turbulence and lateral turbulence representing the PBL. AERMAP processes terrain, sources and receptor data. The complete AERMOD package is publicly available on the United States Environmental Protecting Agency (US-EPA) website.

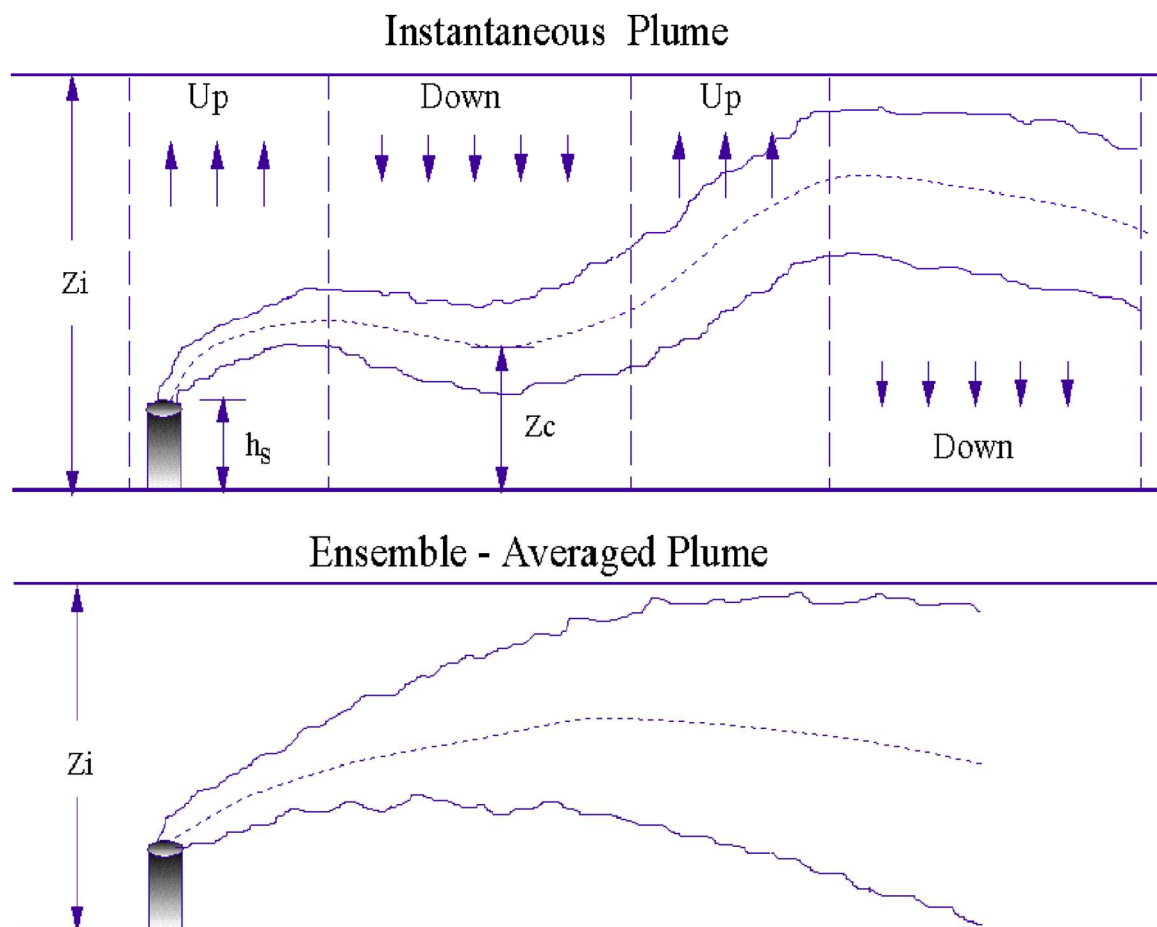


Figure 3-6: AERMOD representation of the instantaneous plume and the resulting ensemble-averaged in convective conditions (source: US-EPA, 2004).

The performance of AERMOD against 17 field study databases was described by Perry et al., 2005. In general, AERMOD was more successful in predicting the concentration distributions for tall-stack buoyant releases in moderate to complex terrain, as well as the upper end of the concentration distribution for similar releases in flat terrain. This performance was attributed to the characterization of the vertical structure of the PBL as well as for the treatment of complex terrain employed in AERMOD. Performance in urban situation was also considered good. On the other hand, performance in building wake situations presented some contrasting results, highlighting the influence of local meteorological behaviour and building geometry on atmospheric dispersion under such conditions.

For more information, the reader is referred to EPA (2004a).

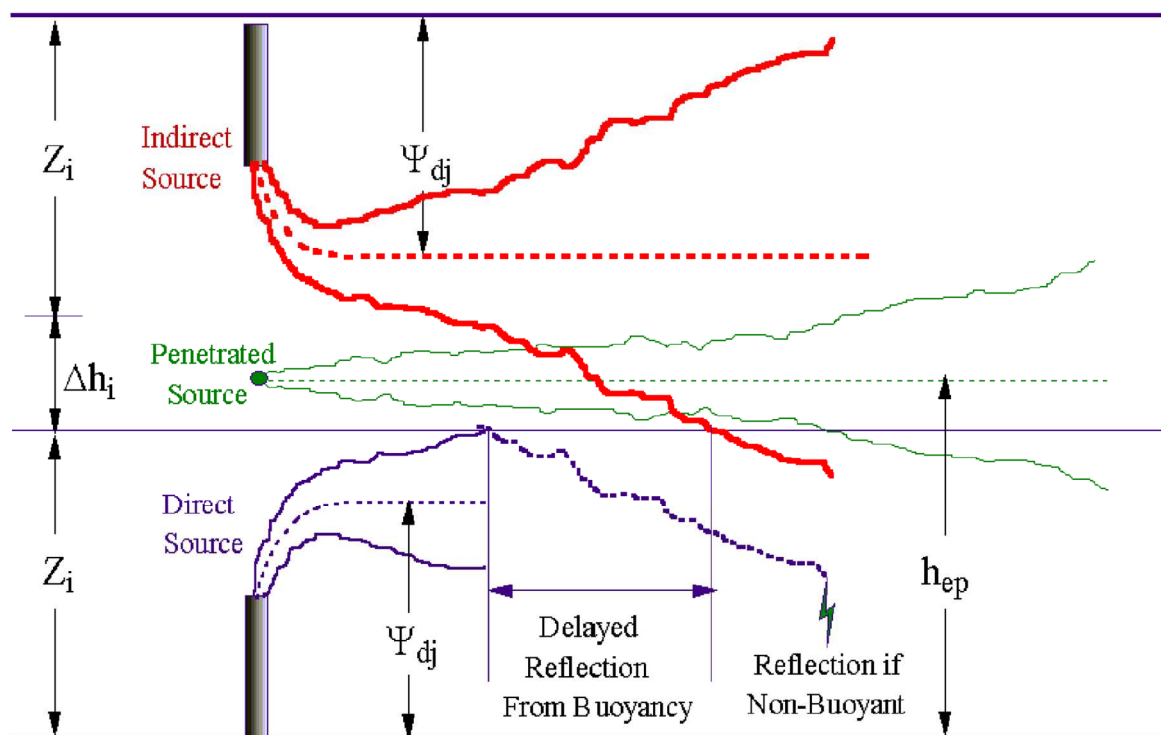


Figure 3-7: Virtual plumes used in AERMOD to represent the effects of quasi-reflection at the top of the mixing layer and penetration on the stable layer (US-EPA, 2004).

3.4.2 CALPUFF model

CALPUFF (Californian Puff Model) is an US-EPA approved model for use in near-field as well as domains with hundreds of kilometres from a source (Scire et al., 2000), especially in situations where non-steady effects are important (US EPA, 2013). Pollutant emissions are treated as a series of pollutant puffs which are dispersed and transformed during advection. Temporal and spatial variations of meteorological conditions are included in the simulation, with averaging times ranging from 1 hour to 1 year.

The CALPUFF system is composed of three main modules, CALMET, CALPUFF and CALPOST. CALMET is the meteorological pre-processor in which data from field measurements or meteorological models such as MM4, MM5 or CSUMM are read and processed. CALPUFF is the non-steady state Lagrangian Gaussian puff model which estimates concentrations under different meteorological and terrain conditions. CALPOST is the postprocessor module, used to compute the time averaged concentrations.

CALPUFF include effects of plume rise, partial plume penetration in the stable layer, chemical transformation, pollutant removal, overwater transport, vertical wind shear and building downwash. Originally, CALPUFF dealt with the presence of obstacles with two different approaches, the Huber-Snyder model (Huber and Snyder, 1976; Huber, 1977) and the Schulman-Scire model (Scire and Schulman, 1980; Schulman and Hanna, 1986), depending on stack height and building dimensions. Later on it was upgraded with the option of using the PRIME model (described in section 3.6.7).

CALPUFF represents the continuous plume as a series of puffs of pollutant traveling in space. The sampling period is divided in sampling steps with each puff changing position and size at each sampling step, corresponding to a “snapshot” of the plume at that particular sampling step (Figure 3-8). Dispersion of the pollutant inside each puff follows a Gaussian distribution. The total concentration at a receptor point is the sum of the contributions of all puffs that are located near it, averaged for all sampling steps within the averaging period. The Sampling period is always equal or higher than the sampling step. In CALPUFF the sampling step is one hour. The main limitation of this kind of model is the large quantity of emitted puffs necessary to adequately represent a continuous emission. The maximum distance between two consecutive puffs must be equal to the horizontal dispersion parameter, σ_y , depending on atmospheric stability and wind speed.

Cui et al. (2011) evaluated the application of CALPUFF to simulate short-term emission in a near-field application. Results showed CALPUFF could adequately predict the plume the trajectory and shape of the emitted plume, but underestimated the horizontal extent of the plume and also the higher values of concentrations.

For more information, the reader is referred to Scire et al. (2000).

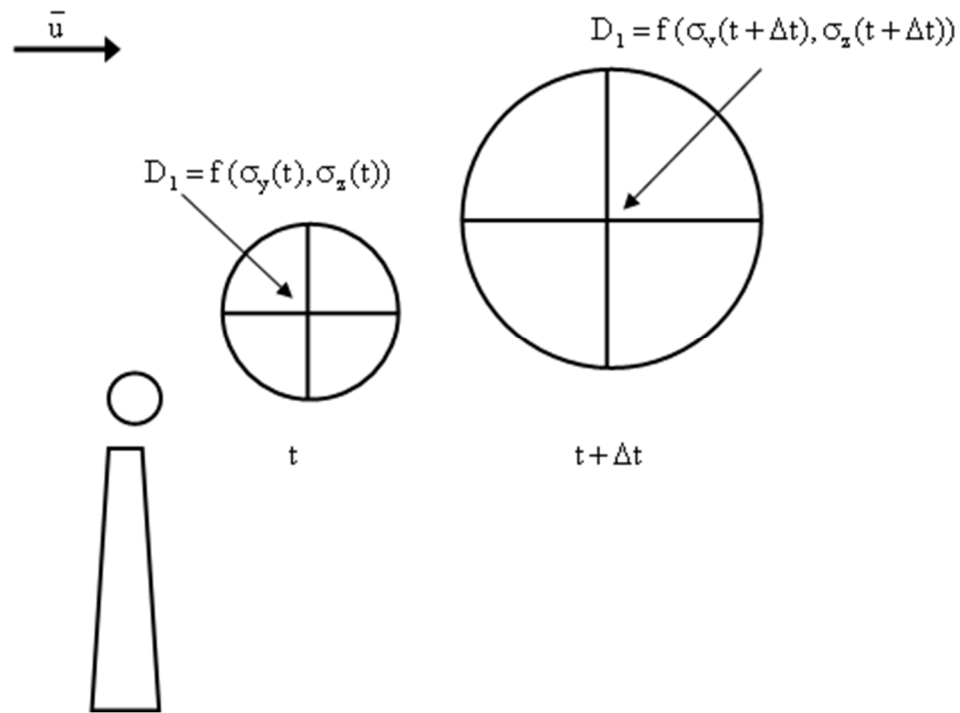


Figure 3-8: An emitted puff shown in two different instants (t and $t + \Delta t$), with puff size as function of time. (Melo, 2011).

3.4.3 Fluctuating Plume Model (FPM)

Gifford (1959) proposed the concept of the fluctuating plume model. Based on observations of emitted plumes and on the puff superposition theory, the author stated that the apparent irregular spreading of plumes is a consequence of material dispersion inside each puff and its movement around the plume centreline (meandering). The plume is described as a series of plume elements that grow as a function of the distance from the source. During a certain averaging time (eg., 60 minutes), the plume mean trajectory is obtained as the average position of the centroid of each plume element which fluctuates laterally and vertically, as shown in Figure 3-9, where the long term (for instance, 60 minutes) averaged plume, represented by the red lines, is the result of the fluctuation, during the averaging time, of the smaller plume elements around the plume mean trajectory. Concentration inside each plume element, as well as the lateral and vertical positions of the plume elements follow a Gaussian distribution whose standard deviations are related to the mean plume long term dispersion parameter. The fluctuating plume model equations are presented in details in section 5.4.1.

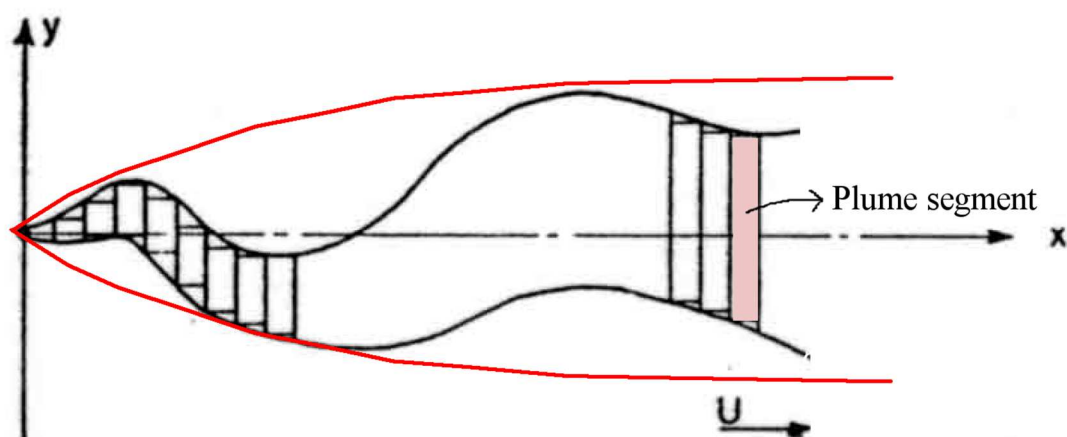


Figure 3-9: The fluctuating plume concept by Gifford (1959): the long term average plume (shown in red) is the result of the fluctuation of the plume segments (shown in light red) around the plume mean trajectory. Adapted from Gifford (1959).

3.5 The influence of the presence of obstacles on wind flow and dispersion

The presence of obstacles has a direct influence on the atmospheric flow and on the dispersion of emitted pollutants. The induced mechanical turbulence increases the mixing and dilution of the pollutant as the plume width is enhanced as it contours the obstacle. A classic figure produced by Hosker (1981) shows the main vortex structures created by the obstacle (Figure 3-10): on the roof as well as on the sides there are separation zones due to the high pressures observed on the walls; downwind the obstacle, just after the lee face, is the cavity, recirculation zone or near wake, where the flow presents higher turbulence levels and lower velocity; downwind the obstacle the flow is still affected – the region called the far wake – where turbulence levels gradually decay to the unaffected ambient observed levels. Obstacle geometry influences not only the extent but also the number of near wakes which may appear not only after the lee wall but also on the top of the obstacle.

If a pollutant plume is captured by the near wake, high levels of concentration may be observed at ground level, as shown in Figure 3-11. Other factors influencing downwind concentrations are stack/source location and pollutant characteristics (Schulman et al., 2000).

Turbulence is characterized by fluctuations of the instant value of the flow properties (such as velocity, energy and concentration) around their mean values. These fluctuations play an important role on the dispersion of odorant compounds, as the impact of odours are related to short bursts of concentration or concentration peaks. A direct consequence is the possibility of an odour being detected by a receptor even when the average concentration level is below the detection threshold, a concept illustrated in Figure 3-12 (Högström, 1972). As the obstacle is a source of mechanical turbulence, odorant compounds emitted near an obstacle have higher probability of causing impact on nearby receptors.

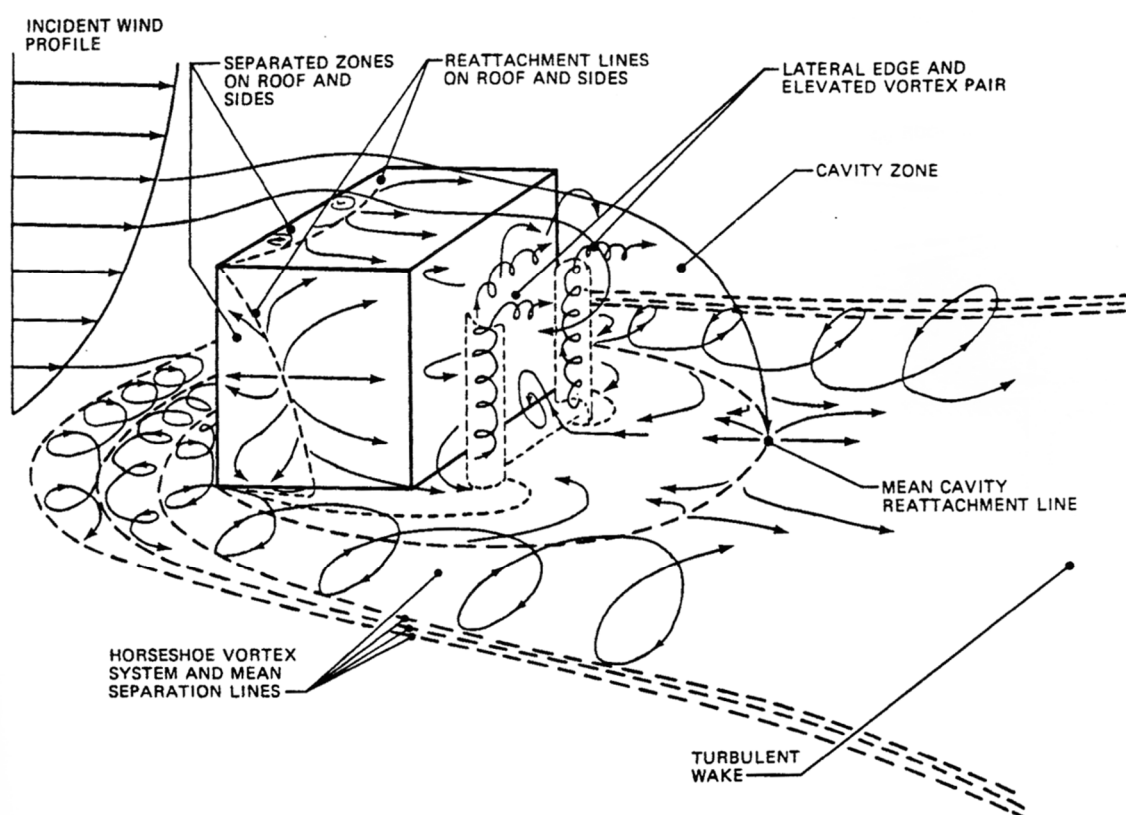


Figure 3-10: aerodynamic effects of the presence of a cubical obstacle in the atmospheric flow. (Hosker, 1981)

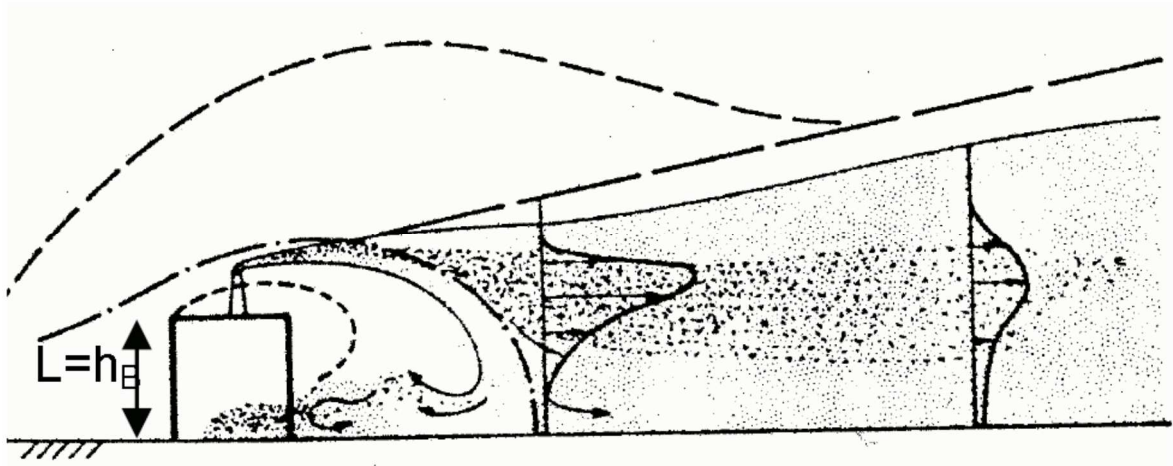


Figure 3-11: Effect of the building near and far wakes on the flow and dispersion of a pollutant (Schaubergger and Piringer, 2004).

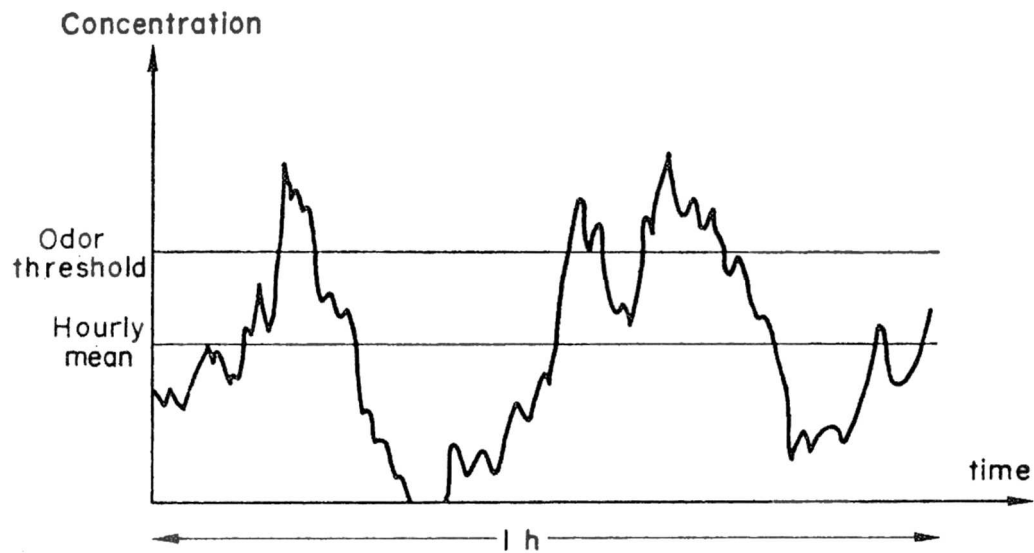


Figure 3-12: Fluctuation of the concentration value of an emitted odorant compound triggering odour events even when the average concentration is below the detection level (Högström, 1972).

3.6 Accounting for obstacle effects in Gaussian models

As the obstacle acts as a source of mechanical turbulence, the inclusion of the effects of the obstacle in Gaussian models basically involves a modification on the dispersion parameters σ_y and σ_z . There has been several techniques proposed in order to account for the effect of the building discussed below.

3.6.1 Turner (1969) approach

Turner (1969) employs a virtual source located downwind of the real source. The virtual plume dispersion parameters are initially calculated based on the obstacle height (H) and width (W) as:

$$\sigma_{y0} = 2W / 4.3 \text{ and } \sigma_{z0} = 2H / 2.15 \text{ [for } L / H < 1] \quad (3-26)$$

$$\sigma_{y0} = W / 4.3 \text{ and } \sigma_{z0} = H / 2.15 \text{ [for } L / H > 1] \quad (3-27)$$

By making $\sigma_y(x_{y0}) = \sigma_{y0}$ and $\sigma_z(x_{z0}) = \sigma_{z0}$, the position of the virtual source is determined as $\sigma_y = \sigma_y(x + x_{y0})$ and $\sigma_z = \sigma_z(x + x_{z0})$, with x measured from the building lee face.

3.6.2 Gifford (1960) approach

Gifford (1960) directly modified the Gaussian plume equation based on the obstacle dimensions, considering it causes a rapid dilution of the emitted material in a volume proportional to the frontal area of the obstacle, projected in the flow direction (A_p):

$$\bar{C}(x, y, z) = \frac{Q}{2\bar{u}_H(\pi\sigma_y\sigma_z + cA_p)} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot \left[\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right) \right] \quad (3-28)$$

Where $c = 1.0$ if $L / H \leq 1$ (flow reattaches to the obstacle roof) or $c = 3.0$ (no reattachment). Again, dispersion parameters are then determined as a function of the obstacle lee face.

3.6.3 Gifford (1968) approach

Gifford (1968), introduces the “total dispersion parameters”, Σ_y and Σ_z , which replace σ_y and σ_z in the Gaussian plume equation, and are calculated as:

$$\Sigma_y = [\sigma_y^2 + cA_p/\pi]^{1/2} \quad (3-29)$$

$$\Sigma_z = [\sigma_z^2 + cA_p/\pi]^{1/2} \quad (3-30)$$

With c assuming the same values as above mentioned.

3.6.4 Huber and Snyder (1976) and Huber (1977) approach

Huber and Snyder (1976) and Huber (1977) proposed their enhanced expressions for σ_y and σ_z , the Huber-Snyder model, suggesting formulations based on the obstacle aspect ratio and receptor position. An obstacle reference length ξ_b is defined as $\xi_b = H$ (for $W > H$) or $\xi_b = W$ (for $H \geq W$). The enhanced dispersion are obtained with the following expressions:

$$\sigma_z' = 0.7\xi_b + 0.067(x - 3\xi_b) \quad (3-31)$$

$$\sigma_y' = 0.35W + 0.067(x - 3\xi_b) \quad [\text{for } W/H \leq 5] \quad (3-32)$$

$$\sigma_y' = 0.35W + 0.067(x - 3\xi_b) \quad [\text{for } W/H > 5] \quad (3-33)$$

$$\sigma_y' = 1.755\xi_b + 0.067(x - 3\xi_b) \quad [\text{for } W/H > 5] \quad (3-34)$$

Equation 3-33 is recommended for use if the source is located within $2.5H$ of the end of the obstacle and Equation 3-34 for sources located near the center of the obstacle; however, Equation 3-33 is generally used for regulatory applications (Scire et al., 2000). The above equations are employed for receptors located at $3\xi_b < x < 10\xi_b$.

3.6.5 Johnson et al. (1975) approach

Johnson et al. (1975) assuming that, sometimes, the plume is not always fully captured by the obstacle near wake, proposed a dual plume model called split-h. The non-captured portion of the plume is emitted at source height while the captured fraction is emitted by a virtual source located at ground level. The fraction (M) of the plume

captured by the near wake will depend on v_s/u_s , where v_s is the velocity of the gases exiting the stack and u_s is the wind speed at stack height:

- If $v_s/u_s \leq 0.9$, the plume is completely captured and $M = 1$;
- If $0.9 \leq v_s/u_s \leq 1.5$, partial capture occurs and $M = 2.2 - 1.33(v_s/u_s)$;
- If $1.5 \leq v_s/u_s \leq 5.0$, partial capture occurs and $M = 0.286 - 0.0571(v_s/u_s)$;
- If $v_s/u_s \geq 5.0$, the plume is not captured and $M = 0$.

The virtual plume (represented the captured fraction) is calculated using the Σ_y and Σ_z parameters proposed by Gifford (1968) (Equations 3-29 and 3-30).

3.6.6 The Schulman-Scire model

Scire and Schulman (1980) and Schulman and Hanna (1986) (Schulman-Scire model) propose the use of a linear decay factor for the building-enhanced the vertical dispersion coefficient, while accounting for downwash and plume rise (Scire et al., 2000). The first step consists in the determination of the enhanced dispersion coefficients at 3 building heights downwind the obstacle lee face (σ_{y0}' and σ_{z0}') using the Snyder-Huber model. If $\sigma_{y0}' \leq \sigma_{z0}'$, then:

$$z_d^3 + (3R_0 z_d / \beta_1 + 3R_0^2 / \beta_1^2) z_d = 3F_m x / (\beta_j^2 u_s^2) + 3F_b x^2 / (2\beta_1^2 u_s^3) \quad (\text{neutral/unstable}) \quad (3-35)$$

$$z_d^3 + (3R_0 z_d / \beta_2 + 3R_0^2 / \beta_2^2) z_d = 3F_m / (\beta_j^2 u_s S^{1/2}) + 6F / (\beta_2^2 u_s S) \quad (\text{stable}) \quad (3-36)$$

And if $\sigma_{y0}' > \sigma_{z0}'$, then the plume will have an elongated shape and is represented as a finite line source with length L_e :

$$z_d^3 + [3L_e / (\pi\beta_1)] z_d^2 + [3R_0 z_d / \beta_1 + 6R_0 L_e / (\pi\beta_1^2) + 3R_0^2 / \beta_1^2] z_d = \text{(neutral/unstable)} \quad (3-37)$$

$$3F_m x / (\beta_j^2 u_s^2) + 3Fx^2 / (2\beta_1^2 u_s^3)$$

$$z_d^3 + [3L_e / (\pi\beta_2)] z_d^2 + [3R_0 z_d / \beta_2 + 6R_0 L_e / (\pi\beta_2^2) + 3R_0^2 / \beta_2^2] z_d = \text{(stable)} \quad (3-38)$$

$$3F_m / (\beta_j^2 u_s S^{1/2}) + 6F / (\beta_2^2 u_s S)$$

where: z_d is the plume elevation due to buoyancy and building influences, β_1 is a neutral capture parameter (≈ 0.6), β_j is the jet capture coefficient (Equation 3-39), R_0 is the dilution radius (Equation 3-40), F_m is the momentum flux (Equation 3-41), F_b is the buoyancy flux (Equation 3-42), v_s is the stack exhaust velocity, d_s is the stack exhaust diameter, T_a is the ambient temperature and T_s is the exhaust gases temperature.

$$\beta_j = 1/3 + u_s / v_s \quad (3-39)$$

$$R_0 = 2^{1/2} \sigma_{z0} \quad (3-40)$$

$$F_m = v_s^2 d_s / 4 \quad (3-41)$$

$$F_b = g d_s v_s (T_s - T_a) / 4T_s \quad (3-42)$$

The effective line length (L_e) is:

$$L_e = (2\pi)^{1/2} (\sigma_{y0} - \sigma_{z0}) \quad [\text{if } \sigma_{y0} > \sigma_{z0}] \quad (3-43)$$

$$L_e = 0 \quad [\text{if } \sigma_{y0} \leq \sigma_{z0}] \quad (3-44)$$

The plume height affected by buoyancy and/or building downwash is then the sum of the original plume height and the calculated plume elevation:

$$h_e = h + z_d \quad (3-45)$$

After determining buoyancy and building downwash, the vertical dispersion parameter is then calculated as:

$$\sigma''_z = A\sigma'_z \quad (3-46)$$

With σ'_z obtained from the Huber-Snyder model and the linear decay factor obtained as:

$$A = 1 \quad [\text{For } H_e \leq H_b] \quad (3-47)$$

$$A = \frac{H_b - H_e}{2L_b} + 1 \quad [\text{For } H_b < H_e \leq H_b + 2L_b] \quad (3-48)$$

$$A = 0 \quad [\text{For } H_b + 2L_b < H_e] \quad (3-49)$$

The Huber-Snyder and the Sculman-Scire models were the original options used in ISC3 and CALPUFF models for accounting for building effects before the PRIME model (generally described in section 3.6.7 and detailed in section 5.3) was implemented.

3.6.7 PRIME

PRIME (Plume Rise Model Enhancements) was developed by Schulman et al. (2000), to incorporate the effect of plume elevation and downwash due to buoyancy and the presence of obstacles. It was developed based on experimental observations of field and wind tunnel experiments and was first added to the ISC3 Gaussian-based regulatory model and is currently used both in AERMOD and CALPUFF models (Cimorelli et al., 2005; Scire et al., 2000).

The basic premise is to incorporate the enhanced plume dispersion coefficients due to the obstacle wake influence and also the effect of streamline deflection on plume rise and downwash as the flow passes through the obstacle, as shown in Figure 3-13, where the plume released from the top of the building is much more influenced by streamline deflection than the plume released downwind the obstacle. PRIME equations are described in detail in section 5.3.

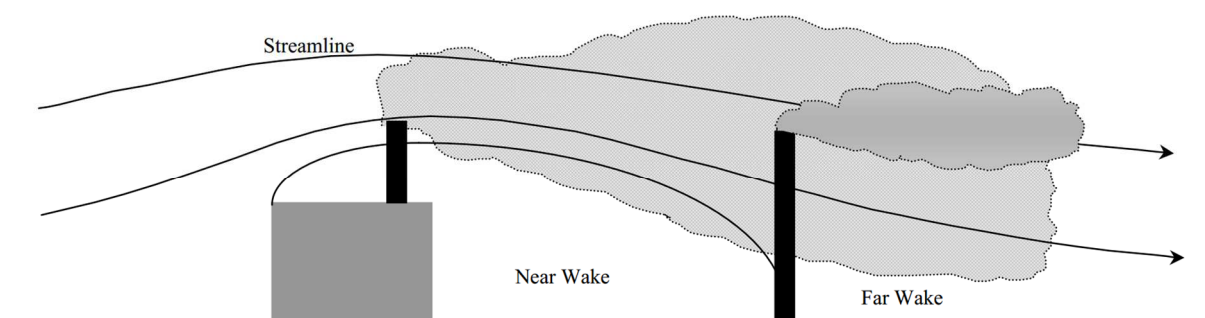


Figure 3-13: Schematic representation of the influence of a cubical obstacle in plumes released from two different locations: the plume released from the top of the obstacle is more influenced by the disturbed flow than the downwind released plume. (Source: Schulman et al., 2000)

3.7 Odour dispersion modelling

The dispersion of odorous compounds in the atmosphere is similar to other pollutants. However, the nature of odour impact is related to concentration peaks during short periods of exposure and its frequency of exposure, thus it requires the calculation of some parameters described in the sections 3.7.1, 3.7.2 and 3.7.3.

3.7.1 The peak-to-mean concentration ratio

As odours events are associated with concentration peaks, the peak-to-mean (P/M) concentration ratio is an important parameter in the study of atmospheric odour dispersion. In fact, odour safety regulations may consider a period of time as “odour polluted” if the mean concentration measured during this period is higher than 10% of the odour detection threshold for a specific compound (Boeker et al., 2000). However, Simms et al. (2000) demonstrated that this approach may be limited as higher peak-to-mean ratios may be observed depending on meteorological conditions and locations.

Atmospheric dispersion models based on the Gaussian approach in general estimate concentration levels for periods ranging from 30 minutes to one year and odour impact estimation requires much shorter averaging times, of the order of a single breath cycle (~ 5 seconds). A common procedure for estimating the peak-to-mean ratio employs a power-law expression relating the average concentration of a large period of time to the average concentration corresponding to a shorter period, as presented by

Smith (1973, cited by Schaubberger et al., 2002), following Singer et al. (1963) (Equation 3-50):

$$\frac{C_p}{C_m} = \left(\frac{t_p}{t_m} \right)^p \quad (3-50)$$

where: C_m is the mean concentration for the longer integration time t_m , C_p is the mean concentration for shorter integration time t_p and p is exponent dependent on atmospheric stability.

Smith (1973) recommends the following values for p : -0.35 (SC = 4), -0.52 (SC = 3) and -0.65 (SC = 2). Venkatram (2002) indicate a range from -0.5 to -0.2 and for elevated sources, Bartzis et al. indicate a range from -0.7 to -0.12. Schaubberger et al. (2002), pointed out that the P/M concentration ratios obtained by equation 3-50 are only valid close to the source and suggested the use of an exponential attenuation function based on distance from the source, wind speed and a Lagrangian time scale, resulting in progressively smaller values for the the P/M ratio . Equation 3-50 is used by CALPUFF when concentrations for shorter periods are needed. It is important to notice that the peak concentration predicted by Equation 3-50 corresponds to the average concentration observed during a short sampling time, which differs from much higher instantaneous peak concentration (Santos et al., 2009).

3.7.2 Frequency of occurrence

As already mentioned, odour impact is related to concentration fluctuation and, as a consequence, Högström (1972) proposes a statistical treatment of the resulting concentration field, by determining the frequency of occurrence of odour events through mathematical modelling. A similar approach was employed by Murray et al. (1978), Beaman (1980), Mussio et al. (2001), De Melo Lisboa et al. (2006) and Yu et al. (2011). All cited authors employed fluctuating Gaussian plume models. Högstrom (1972), Beaman (1980) and Yu et al.(2011) approaches were based on directly solving equations for the probability of odour concentrations above a defined threshold (detectable

odours), while the other authors used the generated frequency series for each receptor in order to calculate the frequency of occurrence. Murray et al. (1978) and De Melo Lisboa et al. (2006) expressed the frequency of occurrence of different odour concentrations with a histogram of the distribution of odour events of different intensities at a defined receptor point. This approach allows the identification of the most frequent estimated odour concentrations and also the order of magnitude of the peak concentration (by observation of the cumulative frequency). Murray et al. (1978) defined 20 different odour concentration classes, the first eight classes ranging from an upper level of 0.01 odour units (OU) to 1.00 OU, corresponding to the non-detectable odour concentrations and twelve classes, ranging from upper levels of 2.00 OU to 1000 OU, corresponding to detectable odour concentrations. This classification was also adopted by De Melo Lisboa et al. (2006).

In order to express odour concentration in odour units (OU) it is first necessary to relate the odorant pollutant concentration expressed in usual units of mass per unit of volume (i.e., $\mu\text{g}/\text{m}^3$) to concentration expressed in OU through olfactometric tests. The model concentration result expressed in units of mass per volume is then converted to odour units. If the model is programed to accept the odour units at the source and the source volumetric flow rate in place of the emission rate, the output results will be expressed in OU instead of mass per unit of volume.

3.7.3 The Intermittency factor

Another important parameter for odour impact studies is the intermittency factor. Different definitions appear in the literature (Chatwin and Sullivan, 1989), with studies of flow and dispersion of compounds emitted in the presence of obstacles defining it as the percentage of the averaging time during which the concentration value is at or below a given threshold value (Higson et al., 1994; Mavroidis and Griffiths, 2001; Santos et al., 2009). On the other hand, Aubrun and Leitzl (2004) employed the term intermittency to express the percentage of time during which the concentration stayed above a given threshold. Any of the two definitions considered, the importance of this parameter for odour impact studies is that humans are sensitive to the intermittent characteristic of odours: although the human olfactory system can adapt to odour sensation during continued exposure, sensitivity is rapidly recovered after exposure interruption (Aubrun and

Leitl, 2004). The increased turbulence levels observed in the obstacle wake directly influence concentration fluctuation and thus, the intermittency factor (Mavroidis et al., 2003).

The sum of the frequency of occurrence of non-detectable odours is equivalent to the intermittency as defined by Higson et al. (1994), Mavroidis and Griffiths (2001) and Santos et al. (2009), while the sum of the frequency of occurrence of detectable odours is equivalent to the intermittency as defined by Aubrun and Leitl (2004). Frequency of occurrence of detectable odours as expressed by Högstrom (1972), Beaman (1980), Mussio et al. (2001), and Yu et al. (2011) corresponds to the intermittency factor, as per Aubrun and Leitl (2004) definition.

4 Literature Review on dispersion modelling in the presence of obstacles

This section presents some recent relevant scientific works on dispersion modelling and/or odour dispersion modelling in the presence of obstacles using numerical simulation techniques to solve the transport equations which describes the turbulent atmospheric flow and dispersion of gases, and Gaussian-based models (AERMOD, CALPUFF and FPM).

4.1 AERMOD

AERMOD has been employed to study dispersion in urban regions, but building effects are not always investigated. Hanna et al. (2001) and Kumar et al. (2006) compared AERMOD results with different field experiments without using PRIME and found out that AERMOD underestimated concentration levels. Venkatram et al. (2004) compared AERMOD-PRIME results with wind tunnel observations and indicated that concentration results were overestimated near the source and the obstacle.

Dispersion in the presence of complex geometry obstacles was investigated by Petersen and Carter (2006). These authors revealed that ground level concentrations predicted by AERMOD were underestimated in comparison to wind tunnel experiments.

Even when the obstacle does not have complex geometry, its aspect ratio (H/W) is still an important factor according to the results obtained by Olesen et al. (2009) using AERMOD-PRIME. Comparison with experimental data showed dependency on aspect ratio and source height, and slightly underestimated results for wide buildings; for sources higher than building height (1.5 times), results were overestimated near a cubic obstacle and highly overestimated near a wide building.

Odour dispersion modelling using AERMOD was done by Latos et al. (2010) and Karageorgos et al. (2010) in order to estimate hydrogen sulfide and ammonia concentrations due to emission from a pig farm in Crete (Greece). These authors proposed some changes in the model in order to apply AERMOD to odour dispersion modelling, such as the determination of the peak-to-mean (P/M) concentration ratio (using equation 3-50) and relationships between annoyance and exposure time, using expressions

suggested by Nicell (2003). The model results are then given in terms of probability of annoyance, instead of hourly mean concentration.

Barclay and Borissova (2013) pointed out that although AERMOD is the US-EPA preferred model for predicting air quality in the near field, it presents limitations for odour impact assessment, which include the model inability to handle calm and stagnation conditions, lack of 3-dimensional meteorology and its steady state assumption. Comparison of estimates of concentration emitted by a fictitious waste water treatment plant from AERMOD and CALPUFF showed that the later model better reproduced the effect of complex terrain and its influence on the wind field.

4.2 CALPUFF model

CALPUFF model has been used to assess odour dispersion in urban regions or in the presence of obstacles, although there were no mention of the use of PRIME. Wang et al. (2006) evaluated CALPUFF and ISCST3 for estimations of daily odour concentration and emission rates from area sources (commercial beef cattle feedlots). No obstacle effects were included. Both models failed to estimate the peak concentrations measured in the field. Elbir et al. (2007) employed CALPUFF in order to estimate odour intensities downwind a meat processing plant. Results showed good agreement to field data obtained by olfactometric tests at two different receptor locations (250 m and 500 m from the source), with odour intensities valid a 10-minute averaging time, but no details were given on obstacle effect inclusion. Similarly, Yu et al. (2009) employed CALPUFF to study odour dispersion from a pig farm but did not give any details on obstacle treatment. The aims were to explore odour dispersion using steady-state and annual hourly weather conditions using CALPUFF and to identify the equivalent odour criteria (such as odour concentration and frequency of occurrence) for determining setback distance for each type of weather conditions used.

Capelli et al. (2010) and Sironi et al. (2011) used CALPUFF in a study of urban odour impact in the north of Italy. Meteorological data and concentrations estimations were based on 1 hour periods. Odour impact was estimated by multiplying the hourly concentrations by a fixed P/M factor ($=2.3$), according to local regulatory norms. There was no mention of the inclusion of obstacles effects.

4.3 Fluctuating Plume Model

Murray et al. (1978) developed the TRC (The Research Corporation of New England) model, essentially a Gaussian plume model based on Gifford (1959) theory (Equation 5-51) and Högström formulations to assess odour dispersion impact. Obstacle effects were included by Gifford (1968) formulations (Equations 3-29 and 3-30). Mean concentration at distances of 1,500 ft from the source were underestimated, while the peak concentration at 2,750 ft from the source was overestimated in comparison with field measurements. The work of Murray (1978) was further developed by Mussio et al. (2001), who studied odour dispersion in an industrial area. Obstacle effects were identically included as in the TRC model, with the addition of Johnson et al. (1975) methodology. Results showed best agreement near the source, and were overestimated at distances higher than 500 m. The model performed better in predicting the highest values of mean concentration and frequency of occurrence when compared to field measurements.

Vrieling and Nieuwstadt (2003) developed a FPM model based on Gifford (1959) theory to study dispersion from nearby line sources within a channel based on DNS simulation results. There was no obstacle effects included. Similarly, the problem of interference of two plumes originated from nearby point sources was studied by Yee et al (2003) using a FPM. No obstacle effects were included. In these both studies FPM agreed qualitatively with experimental data.

De Melo Lisboa et al. (2006) developed a model for odour dispersion which included formulations from the TRC model and compared their results with field measurements. Model results showed good agreement with field measurements of mean concentrations. There were no obstacle effects included.

Dourado (2007) used a FPM to study different methods (Turner, 1969; Gifford, 1960, 1968; Huber and Snyder, 1976; Johnson et al., 1975 and Scire and Schulman 1980/Schulman and Hanna, 1986), for including building effects. Although the best agreement for average concentration was found for Johnson et al (1975) and Gifford (1968) approaches, all methods failed to represent the intermittency levels found in the near wake (underestimation) and far wake (overestimation).

Recently, Yu et al. (2011a, 2011b) employed a FPM in order to estimate concentration of odorant gases emitted by a livestock building. Building effect was included

using Turner (1969) method (Equations 3-26 and 3-27). Results showed higher agreement with field measurement data at longer distances than at close range.

4.3.1 CFD Techniques

The increase on computational power and its availability has favoured the use of numerical modelling. The literature reports several studies over the last decade in which CFD based models were used to study flow in the presence of obstacles, with different turbulence models, such as Schmidt and Thiele (2002), Izuka and Condo (2004), Gao and Chow (2005), Tominaga et al. (2008), Xie et al. (2008), Lim et al. (2009). Gousseau et al. (2012) pointed out that although most studies use RANS approach to include turbulence effects, there is a consensus that LES is a more accurate technique for modelling wind flow and dispersion, having performed better than RANS in situations of flow around buildings.

Similarly, dispersion of gases emitted nearby obstacles has also been intensively investigated, again using different turbulence models, such as Sada and Sato (2002), Pospisil et al. (2004), Diehl et al. (2006), Hanna et al. (2006), Mazzoldi et al. (2008), Cai et al. (2008), Oliveira et al. (2008), Diego et al. (2009), Tominaga and Stathopoulos (2007, 2010, 2011), Gousseau et al. (2011a, 2011b, 2012), among others.

More closely, CFD-based models of odorous compounds dispersion have been the object of few recent studies. Brown and Fletcher (2005) studied odour dispersion inside an industrial complex, but did not include obstacles; Lin et al. (2007) used numerical modelling to study the effectiveness of windbreaks in attenuating odour impact; Maïzi et al. (2010) used CFD technique to study dispersion of odorant gases emitted by a sewage treatment plant. All cited studies employed RANS-based models (κ - ϵ and κ - ω).

The use of LES to estimate odour dispersion in the presence of obstacles has just begun to be an object of research. Li and Guo (2006) simulated dispersion of odorant compounds emitted by a pig farm using CALPUFF and LES. They used the Smagorinsky sub grid model and the inlet boundary conditions were set as random generated velocity fluctuations. Concentration fluctuation or frequency of odour events data were not published. Li and Guo (2007), assessed the influence of the averaging time (applied to meteorological data used as inlet boundary conditions) on ambient odour

concentration from a 3000-sow farrowing operation. Results showed that the use of 1-hour time steps implicate in overestimating concentrations and also plume travel distance, while time steps of 1 minute provide more accurate instantaneous odour plume predictions as variations in wind direction are better represented. Finally, Hong et al. (2011a, 2011b) employed LES to study dispersion of odorant gases emitted by livestock over complex terrain. Obstacles were not included. Meteorological boundary conditions (wind speed and direction) were variable and based on field measurements. The authors used commercial package Fluent, with the kinetic energy transport sub grid model. Computational time step was 10 seconds and concentration results were for a 5000 seconds averaging time. Although “instantaneous concentration” results were given at instants 1000 s, 2000 s, 3000 s, 4000 s and 5000 s, no information on intermittency was given.

4.4 Remarks

Odour dispersion modelling using Gaussian-based regulatory models such as AERMOD and CALPUFF are often reported in the literature. These models present a relatively simple implementation but are not fully capable to accurately estimate odour impact, which is mainly related to short concentration peaks while Gaussian models generally give results for 1 hour or longer periods. However, this characteristic does not prevent the use of such models for odour impact assessment, as they can be useful tools for preliminary analysis. Both models employ the PRIME model, which is the current state-of-the-art in modelling the effects of the presence of obstacles in Gaussian modelling.

The concept of the fluctuating plume model can be a viable tool for odour impact studies as it makes possible the estimate concentration fluctuation parameters such as the peak to mean concentration ratio and intermittency factor. However, the inclusion of building effects on the simulation presents an interesting field of research, especially the inclusion of the recent techniques in modelling these effects, such as the PRIME model.

Computational fluid dynamics is a useful tool for the study of atmospheric dispersion. Results are much more accurate than Gaussian models but at a much higher computer processing cost and with increased complexity. Among the several techniques

to solve the transport governing equations including turbulence effects, LES presents itself as an interesting tool for odour dispersion studies. Due to its transient nature, it is possible to obtain information about peak concentrations and intermittency from LES results, a useful information to estimate odour impact. However, the use of LES as a tool for odour impact studies has just begun; a literature research revealed few studies on the subject, and only one work assessing intermittency, albeit without comparison to wind tunnel or field experiments.

5 Methodology

This chapter presents the methodology employed in the present work, describing the set of wind tunnel and field experimental data used to validate the mathematical modelling of odour dispersion around cubical and complex-shaped obstacles. Also described are the transport equation of mass, momentum and mass of a chemical species which represents the wind flow and dispersion of odorant gases and Large Eddy Simulation models used to include the atmospheric turbulence effects. Finally, the PRIME used to include the building effects into Gaussian-based dispersion models, the proposed FPM-PRIME model and the inlet boundary conditions for FPM, AERMOD and CALPUFF are addressed.

5.1 Experimental data for model validation

The FPM-PRIME and LES simulations, along with AERMOD and CALPUFF simulations are validated using experimental results. Three different set of experimental data were selected: Wind tunnel experiments (Experiment A, section 5.1.1) performed by Sada and Sato (2002) and full-scale field experiments (Experiment C, section 5.1.3) performed by Mavroidis et al. (2003) were chosen to investigate flow and dispersion of odorant gases around a cubical building under neutral atmospheric conditions. Wind tunnel experiments (Experiment B, section 5.1.2) performed by Aubrun and Leiti (2004) to investigate flow and dispersion of odorant gases around a complex shaped obstacle under neutral atmospheric conditions. This set of experiment was chosen to allow for the analyses of the building shape influence on dispersion.

5.1.1 Wind tunnel experiment on wind flow and dispersion around a cubical obstacle (Sada and Sato, 2002): Experiment A

Sada and Sato (2002) compared LES using the Smagorinsky subgrid scale model with a wind tunnel experiment of the flow around a cubic obstacle. The case of an isolated cubic obstacle has been a benchmark for validation of dispersion models, including LES. Several authors have compared the results of LES with wind tunnel (WT) data of flow and dispersion around an isolated obstacle, showing good agreement between

results of mean quantities (i.e, Lim and Castro, 2009; Tominaga and Stathopoulos, 2010).

The wind tunnel experiment was performed on a test section with 3 m, 1.5 m, 20m (width, height and length), using a free stream velocity of $U_0 = 2.0$ m/s, with the modelled boundary layer height $\delta = 30$ cm. A cubical obstacle with $H=20$ cm height was placed with its centre 4 m downwind the test section entrance, and at the test section horizontal centre ($y/H=0$). Mean wind direction was normal to the building. The emitted compound consisted of a mixture of air and ethylene, released from a stack at $x/H=0$, at $H_s=H$ height, 30 cm upwind from the centre of the building. Averaging time was 40 s and length scale ratio was 1:250. The simulated atmosphere stability was neutral. The Reynolds number, based on the boundary layer height and on the wind speed measured at the top of the boundary layer was 4.00×10^4 . Kato and Hanafusa (1996) found out the critical Reynolds number for a wind tunnel scaled representation of the atmospheric flow over a flat terrain was 3.7×10^4 , thus Reynolds number independence was established for the experiment.

LES simulation was performed on a domain measuring 2.5 m, 1.0 m and 1.0 m (x, y and z). The obstacle ($H = 20$ cm) was located 1.45 m downwind of the domain entrance. The domain was divided in a mesh of 100, 65 and 53 elements (x, y and z). Inflow velocity turbulent fluctuation was generated using random numbers.

Wind velocity, horizontal and vertical turbulence intensities, average concentration and concentration fluctuation intensity profiles were generated for several positions downwind the source ($x/H = 0$; $x/H = 1.5$; $x/H = 2.5$; $x/H = 3.5$ and $x/H = 5.0$, at $y/H = 0$). The experimental schematic configuration is shown in Figure 5-1.

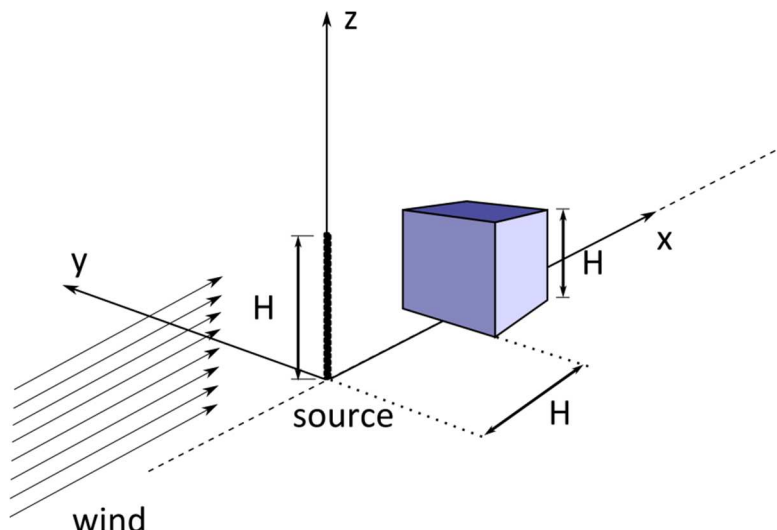


Figure 5-1: Schematic configuration of Sada and Sato (2002) experiments, showing relative positions of the source and the building, as well as wind direction.

5.1.2 Wind tunnel experiment on wind flow and dispersion around a complex shaped obstacle (Aubrun and Leidl, 2004): Experiment B

The second experiment used for validation in the present work consisted on a wind tunnel simulation of dispersion of an odorant gas emitted from a stack on top of a 1:400 model of a pig barn (Aubrun and Leidl, 2004). A detailed dataset of the wind tunnel experiments is available online at the University of Hamburg website, at http://www.mi.uni-hamburg.de/CEDVAL_Validation_Data.427.0.html. A close-up view of the building model is shown in **Erro! Fonte de referência não encontrada.b** and its detailed dimensions are shown in Figure 5-3 and Figure 5-4.

The wind tunnel test section (**Erro! Fonte de referência não encontrada.a**) measured 1.5 m wide, 1 m high and 4 m long. The modelled boundary layer reproduced a real neutral atmospheric boundary layer up to 100 m high. The tracer gas was a mixture of air and ethane and the concentration time series was measured with a 1.25 Hz (full scale).

The approaching flow mean wind speed and velocity fluctuations are shown in Figure 6-23 presented in chapter 6.

The available experiment dataset contains the result for average concentration for a 2000 min (full scale) averaging time, as well as the intermittency factor, defined as

the percentage of time during which the instant concentration was higher than a defined threshold of $0.0025C_s$, where C_s is the concentration measured at the source.

Different wind directions were tested, however, the present work only uses the results corresponding to the wind direction of 220° . The origin of the coordinate system is located at the source and the x-direction is considered parallel to the mean wind direction (Figure 5-5).



Figure 5-2: (a) Wind tunnel test section with the building model and (b) close view of the pig barn model used in the wind tunnel.

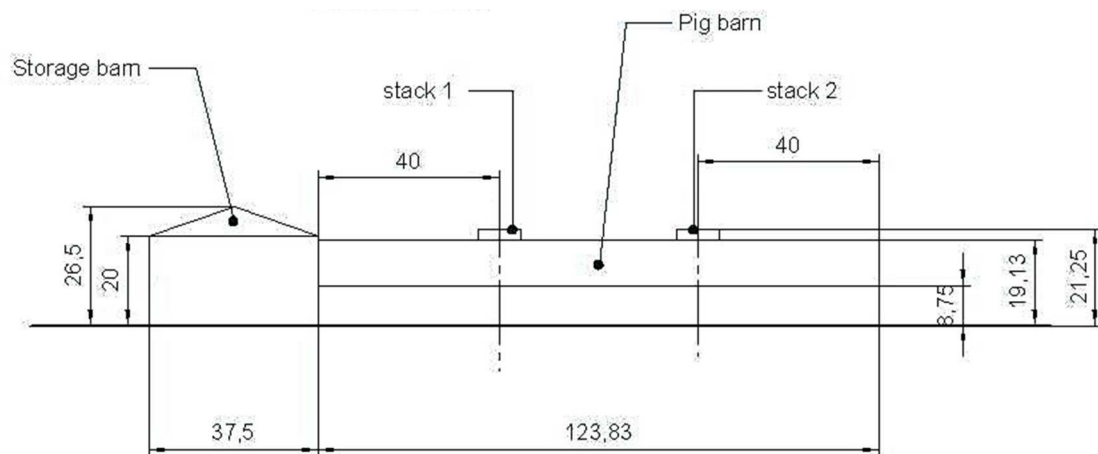


Figure 5-3: Lateral view of the building model used in the wind tunnel (dimensions in mm).

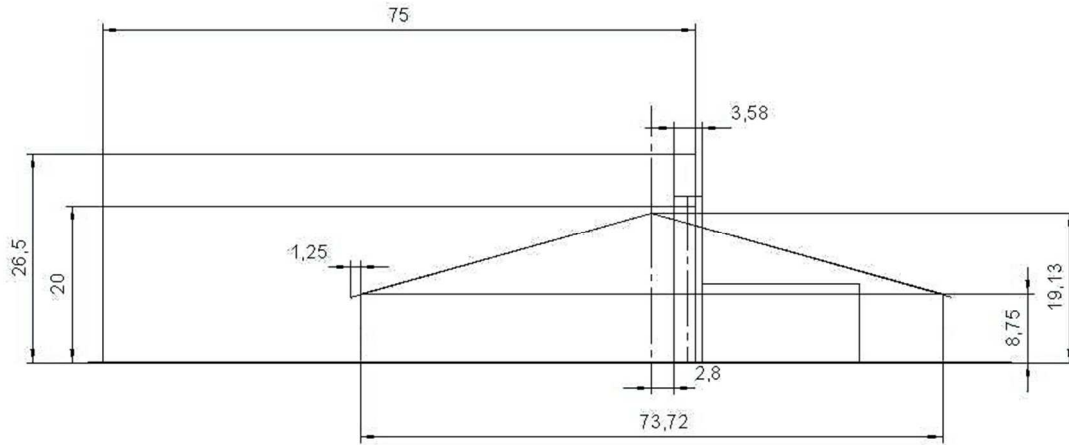


Figure 5-4: Frontal view of the building model used in the wind tunnel (dimensions in mm).

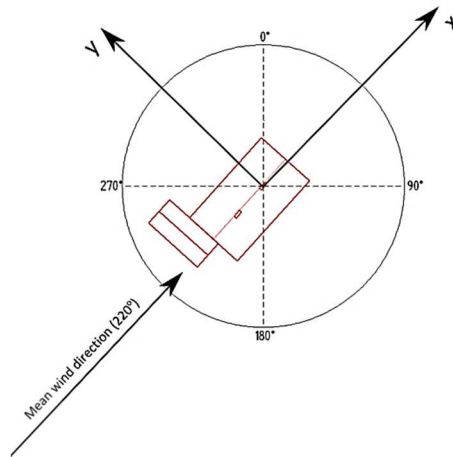


Figure 5-5: Top view of the obstacle, showing the mean wind direction (220 degrees relative to the obstacle north) and the system of coordinates used to express the results (adapted from CEDVAL, 2006).

5.1.3 Field experiment on dispersion around a cubical obstacle (Mavroidis et al., 2003): Experiment C

This experiment was conducted at the Altcar Field Site, northwest coast of England, a site with fairly flat terrain. Different obstacle geometries and source positions were tested, but in the present work only the data concerning the cube obstacle with a source aligned with the centre of the cube is used. The cube side measured $H = 1.15$ m, and was positioned normal to the mean wind direction. The source (located at $x/H = y/H = 0$) was positioned $2.0H$ upwind of the centre of the frontal face of the building, at a $0.5H$ height (Figure 5-6). Atmospheric conditions varied from slightly neutral to neutral. The cube model represented a full scale building of 10 m height.

Concentration results were measured at different downwind distances from the leeward face of the building: $0.5H$, $2.0H$, $3.0H$, $4.0H$ and $5.0H$. The averaging time was 3 minutes. For each receptor position, the intermittency factor (defined as the percentage of time during which the concentration was zero) has been measured. The dataset of the experiment was provided by Dr. Ilias Mavroidis via personal communication.

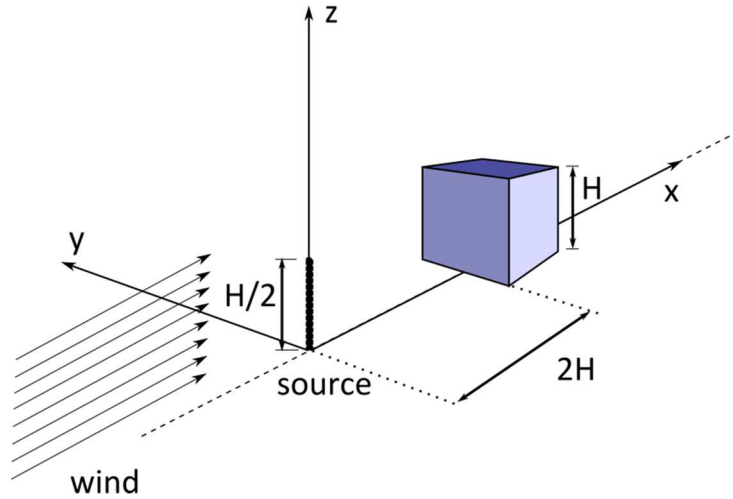


Figure 5-6: Schematic configuration of Mavroidis et al (2003) experiment, showing relative positions of the source and the building, as well as wind direction.

5.2 Numerical simulations of wind flow and dispersion in the presence of obstacles

5.2.1 Transport phenomena equations and numerical methods

The set of transport filtered equations for a Newtonian and incompressible fluid (Equations 5-1, 5-2, and 5-3) are solved through the use of numerical methods. Atmospheric stability condition is neutral. The overbar indicates a filtered variable.

Mass conservation:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (5-1)$$

Momentum:

$$\frac{\partial(\rho \bar{u})}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mu \left(\frac{\partial \bar{u}_i}{\partial x_i} + \frac{\partial \bar{u}_j}{\partial x_j} \right) \right) - \frac{\partial P}{\partial x_i} + \rho g_i - \frac{\partial}{\partial x_j} (\tau_{ij}^s) \quad (5-2)$$

where τ_{ij}^s is the sub grid stress tensor.

Conservation of chemical species:

$$\frac{\partial C}{\partial t} + \frac{\partial \bar{u}_i C}{\partial x_i} = \frac{\partial \varphi_i}{\partial x_i} + S \quad (5-3)$$

where C is the volume-averaged concentration of the chemical species, S is the source term and φ_i is the sub grid flux of concentration, modelled as:

$$\varphi_i = k_{SG} \frac{\partial C}{\partial x_i} \quad (5-4)$$

where k_{SG} , the eddy diffusivity being

$$k_{SG} = \frac{\nu_t}{Sc} \quad (5-5)$$

where ν_t is the kinematic eddy viscosity and the turbulent Schmidt number is $Sc=0.9$.

The fluid is considered a continuous medium but the numerical methods present a discrete solution (in space and time) thus the transport equations need to be discretized. Versteeg and Malalasekera (2007) points three traditional methods for solving the differential equations: finite difference, finite elements and spectral methods. Commercial computational fluid dynamics codes such as ANSYS-CFX and FLUENT employs the finite volume method, which is a special formulation of the finite difference method (FDM). First of all the domain is divided in a number of points (or nodes) which corresponds to the discrete locations where the problem variables are calculated – the numerical grid. Each grid point is surrounded by a control volume. In the FDM, transport equations are then integrated over all the control volumes. The resulting integral equa-

tions are then converted in a system of algebraic equations which in turn are solved by an iterative method. Figure 5-7 illustrate the process of domain discretization for a 1-D mesh. The grey area shows the control volume surrounding node P.

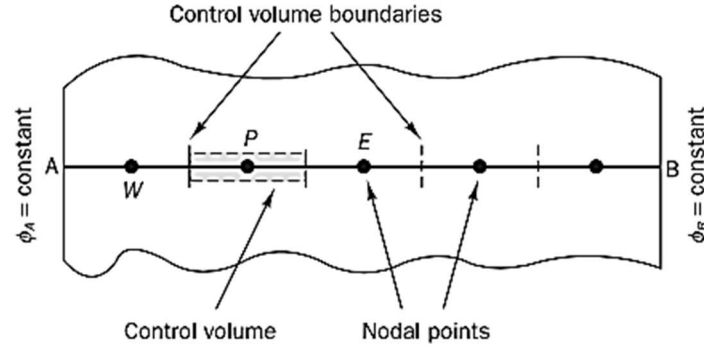


Figure 5-7 : control volume definition on a 1-D mesh (source: Malalasekera, 2007).

The numerical simulations for the present work were performed using commercial software ANSYS CFX 13 (ANSYS Inc., 2010). This software solves the transport equations numerically using the finite volume method for structured and non-structured meshes.

The turbulence effects were taken into account by employing the Large Eddy Simulation Technique (Section 3.3.1.1). ANSYS CFX includes three LES techniques, the Smagorinsky LES (Section 3.3.1.1.1), the Dynamic Smagorinsky LES (Section 3.3.1.1.2) and the Wall Adaptive Local Eddy-viscosity (WALE) model (Section 3.3.1.1.3). In the present work, the simulation of Experiment A is performed in order to compare the use of Dynamic Smagorinsky and the WALE models, the simulations of Experiment B and C are carried out using the best performing model.

The software was run in a computer cluster with 8 Intel X3210 quad-core (2.13 GHz) processors, with 4GB of RAM each.

Mesh were generated using ANSYS ICEM CFD (ANSYS, 2010), for uniform mesh generation, and ANSYS CFX-MESH (ANSYS, 2010), for non-uniform unstructured mesh generation.

5.2.2 Inflow turbulence generation

One of the major challenges for atmospheric flow simulations is the adequate representation of the approaching flow, including the representation of the atmospheric

turbulence, which requires fluctuating velocity inlet conditions. Tabor and Baba-Ahmadi (2009) revised the techniques currently employed for the generation of inflow turbulent fluctuations in LES simulations and listed the desired characteristics of such fluctuations:

- The generated fluctuations should present stochastically variation;
- The variation should be present on all scales, down to the filter scale (spatially and temporally);
- Variations should be compatible with the Navier-Stokes equations;
- The generated fluctuations should ‘look’ like turbulence, with coherent eddies across the range of spatial down to the Kolmogorov scales;
- Variations should allow the easy specification of turbulent properties;
- The generated inflow fluctuations should be easy to implement and adjust to new inlet conditions.

According to Baba-Ahmadi and Tabor (2009), two techniques are generally employed, (i) artificial generation of inflow turbulent profiles based on fluctuations around average values (e.g., Sada and Sato, 2002), with the use of random numbers generators, Fourier analysis or white noise, where the generated fluctuations correspond to the desired turbulence spectrum; or (ii) turbulent fluctuations generated through auxiliary simulations (e.g. Tamura et al., 2007), a technique called “precursor domain”. Fluctuations generated through the precursor domain technique are stored in a database of inlet conditions which can be further used in other simulations.

The artificial generation technique has the advantage of being easily adapted to different simulations while the precursor domain technique is more accurate as real turbulence is generated; but the scaling or adaptation of the turbulence database to simulations with different inlet dimensions might be troublesome.

In the present work inflow turbulence is generated by using a technique based on the precursor domain, adapted from Nozawa and Tamura (2002), where a boundary layer is developed over a flat surface covered with roughness elements and then over a flat surface until reaching the main obstacle, with the difference that this precursor domain is part of the main simulation. A disadvantage of this method is number of elements of the resulting mesh, but this choice was justified as ANSYS-CFX does not pre-

sent an obvious way of inserting external data as boundary conditions at each time step of the simulation.

The layout of the roughness elements used in each simulation as well as the description of the mesh employed are shown in sections 5.2.3, 5.2.4 and 5.2.5.

5.2.3 Numerical simulation details of Experiment A

For the CFD simulation of experiment number one (Sada and Sato, 2002) a calculation domain measuring 7.0 m, 1.0 m and 1.0 m ($35H$, $5H$ and $5H$) for the downwind, horizontal and vertical directions (x, y and z) was used (Figure 5-8). The cubical obstacle (height $H = 0.2$ m) has its center located 4.9 m from the domain entrance. A set of roughness elements was placed just after at the domain entrance in order to generate inflow turbulence (Figure 5-8). The mesh employed is structured, consisting of all hexahedral elements (Figure 5-9) and more than 9.76 million nodes. The length scale of the mesh elements is $H/22$. The mesh was generated with ANSYS ICEM CFD 13.0, software.

Boundary conditions at the lateral faces of the domain were set as periodic (conservative interface flux). At the upper face a free slip condition was employed. No slip conditions (smooth wall) were set at the bottom face and also at the building walls. At the domain entrance a mean velocity profile based on experimental data from Sada and Sato (2002) was used. The boundary condition at the domain exit was set as zero average static pressure. Time step size was 0.005 s. The simulations were run for at least 2,400 time steps after stabilizing. Advection scheme was set as Central Difference and Transient scheme was Second Order Backward Euler.

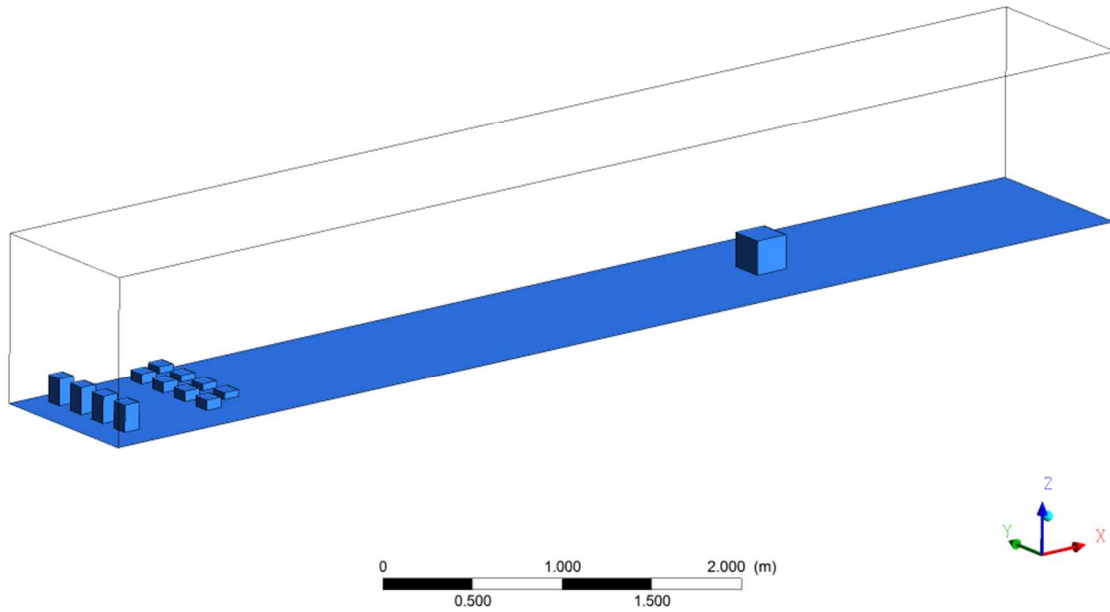


Figure 5-8: computational domain used for experiment number one, showing the cubical obstacle and the roughness elements used for generating velocity fluctuations.

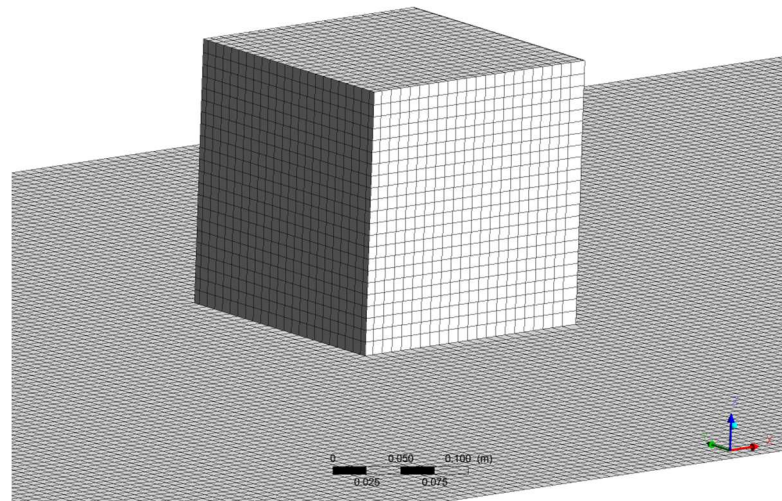


Figure 5-9: detailed view of the mesh close to the obstacle (Experiment A).

5.2.4 Numerical simulation details of Experiment B

The CFD simulation of experiment number two employed a domain measuring 396 m long, 114.4 m wide and 52.8 m high, corresponding to $45H$, $13H$ and $6H$, respec-

tively, where H is the average obstacle height (8.8 m), shown in Figure 5-10. The obstacle is the representation of a pig barn consisting of two attached buildings (dimensions shown in Figure 5-14). The simulation corresponds to the wind tunnel experiment with wind direction 220° , where the wind blows normal to the smaller building lateral wall.

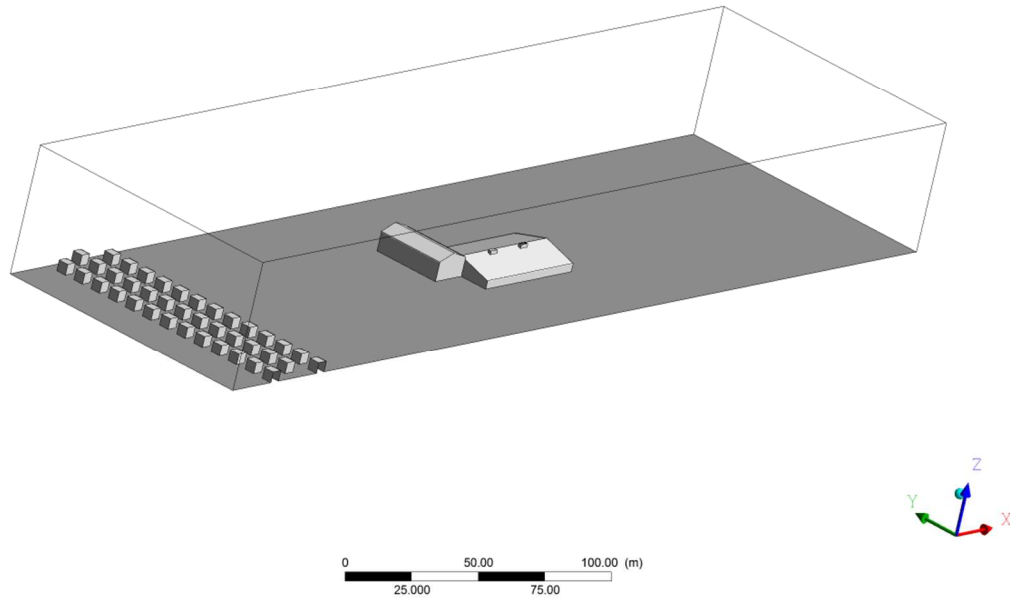


Figure 5-10: Computational domain used for experiment number two, showing the model of the pig barn and the roughness elements used for generating velocity fluctuations next to the domain .

The origin of the Cartesian coordinate system was at the ground and corresponded to longitudinal and lateral position of the source, situated 220 m ($25H$) from the domain entrance. X-direction corresponded to the main wind direction. Inflow turbulence was generated through the use of roughness elements placed after the domain entrance (Figure 5-10). The pollutant was released at $z = 8.5$ m. Due to the complex geometry of the pig barn model, a non-uniform tetrahedral mesh, generated with ANSYS CFX MESHING was employed. The mesh had a resolution of about $H/32$ near the obstacle, and comprised a total of more than 5.23 million nodes. The rate of growth of the elements size was kept under 10%. A detailed view of the mesh around the obstacle is shown in Figure 5-11.

Similarly to experiment number one, boundary conditions at the lateral faces of the domain were set as periodic (conservative interface flux); free slip wall at the top face; no slip wall at the bottom face and at the roughness elements and building walls. At the domain entrance a mean velocity profile based on experimental data from the wind tunnel dataset was used. The boundary condition at the domain exit was set as zero average static pressure.

The simulation time step was 0.02741 s and runtime was 16,450 time steps and the advection scheme was set as Central Difference and Transient scheme was Second Order Backward Euler.

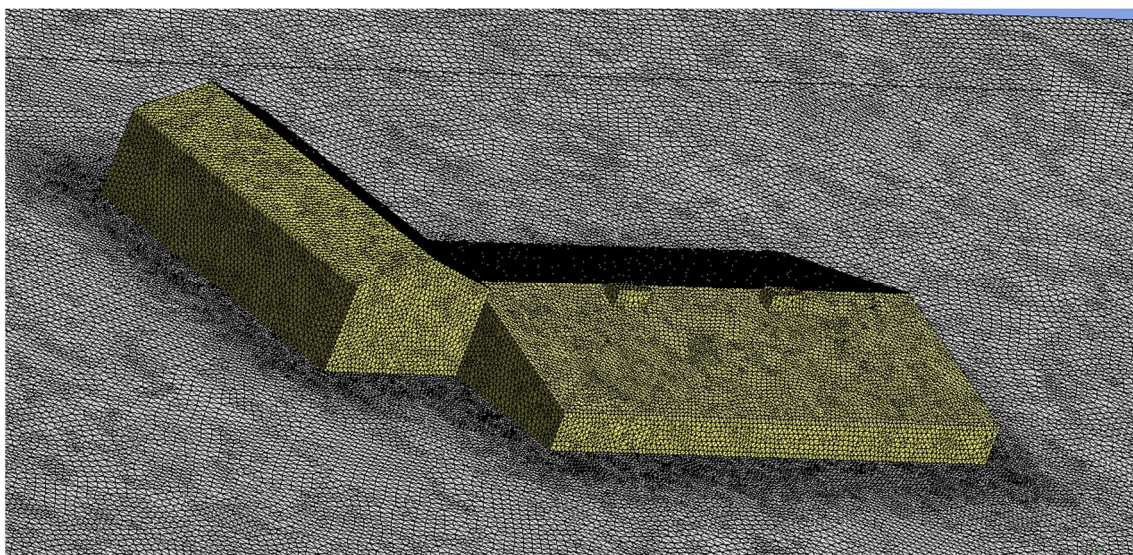


Figure 5-11: close up view of the mesh around the obstacle in experiment B.

5.2.5 Numerical simulation details of Experiment C

Experiment number three has a similar geometry to experiment number one (the obstacle is a cubical building) but the employed domain has different proportions and a finer mesh near the obstacle. The domain measured 39.1 m long ($34H$), 12.65 m wide ($11H$) and 6.9 m high ($6H$) and consisted of more than 11.3 million nodes. The mesh consisted of hexahedral elements, with $H/32$ resolution near the obstacle. A close up view of the mesh around the obstacle is shown in Figure 5-12. The rate of growth of the elements size was kept under 10%. The origin of the Cartesian system of coordinates was at the ground and corresponded to the source position. The main wind direction

corresponded to the x -direction. The source was located $2H$ upwind of the building and the pollutant was released at $z/H = 0.5$.

Boundary conditions were similar to experiments number one and two, with periodic conditions at the lateral faces of the domain, free slip condition at the upper face, no slip conditions were set at the floor and at the roughness elements and building walls. At the domain entrance a mean velocity profile based on the experimental data was used. The boundary condition at the domain exit was set as zero average static pressure. Time step size was 0.0025s and run time was 6,669 time steps.

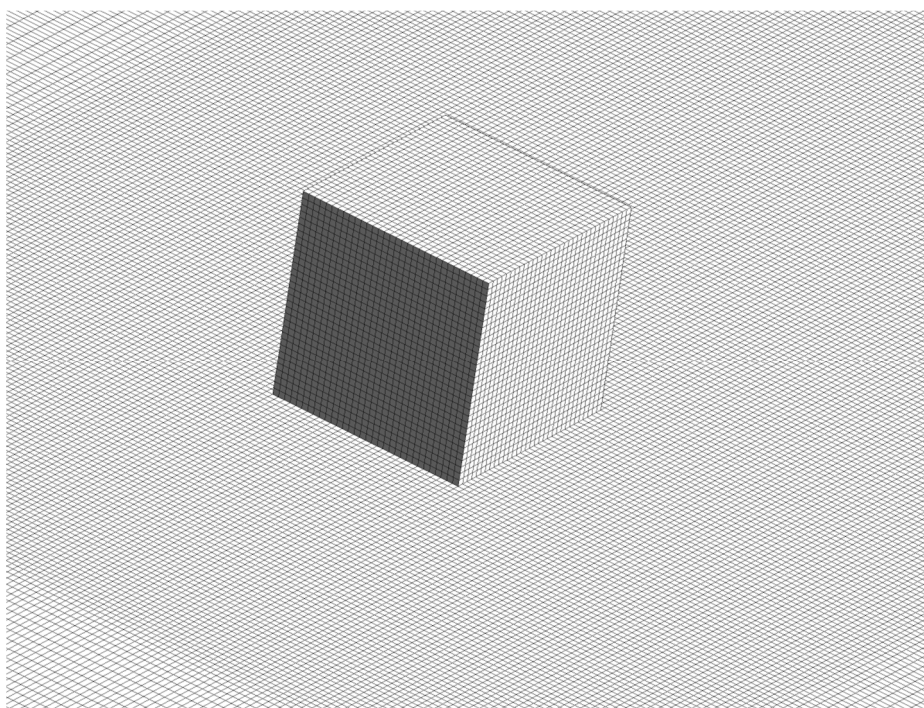


Figure 5-12: close up view of the mesh around the obstacle in experiment C.

5.3 PRIME

As mentioned in section 3.6.7, PRIME was developed to include the effects of plume elevation and downwash due to buoyancy and the presence of obstacles. PRIME calculates the concentration field in the building wake region based on the plume trajectory influenced by velocity and turbulence fields (Figure 5-13). A detailed description of the model is available in Schulman et al., 2000 and its main points are shown in the following sections.

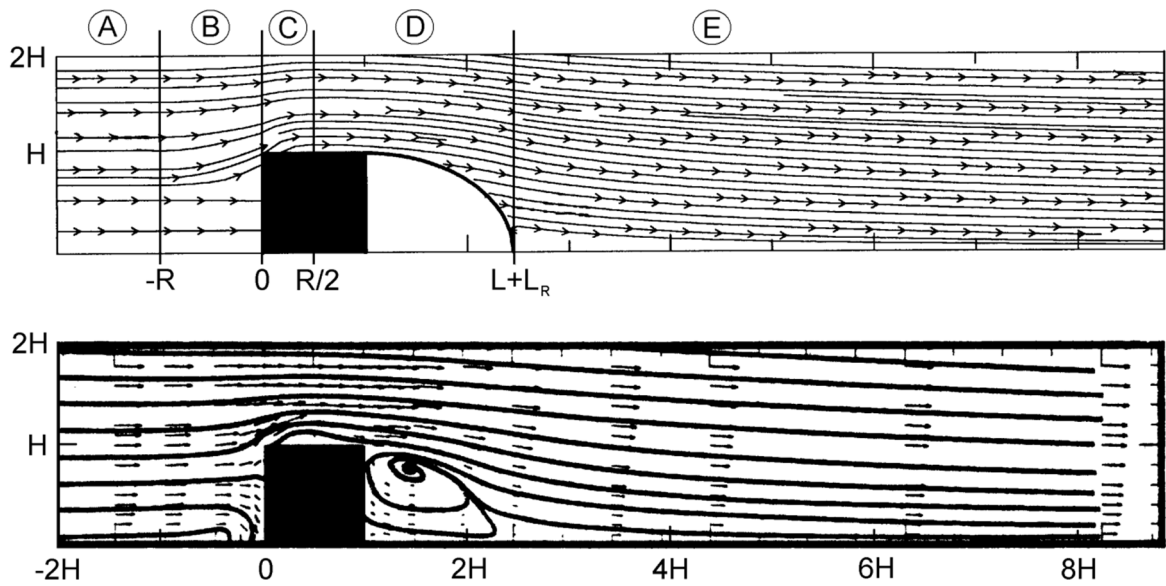


Figure 5-13: streamlines predicted by PRIME compared to wind tunnel observations, showing the five distinct regions. Distances are scaled by building height. (Source: Schulman et al., 2000)

5.3.1 Cavity and wake dimensions

In order to determine the building effects, cavity and wake dimensions are determined using equations 5-6 to 5-19 (shown in the next page). Calculated parameters are cavity (H_C and W_C) and wake (H_W and W_W) height and half-width, cavity maximum height (H_R), cavity length (L_C) and also the building length scale (R), with x measured along wind from the obstacle upwind face. H is the building height, W is the along flow projected building width and L is the along flow building length. B_L is the maximum between building height and width and B_S is the minimum between building height and width.

$$R = B_S^{2/3} B_L^{1/3} \quad (5-6)$$

$$H_R = H \quad [\text{if } L < 0.9R \text{ - roof top cavity reattaches to the building}] \quad (5-7)$$

$$H_R = H + 0.22R \quad [\text{at } x = 0.5R, \text{ if } L < 0.9R, \text{ no reattachment}] \quad (5-8)$$

$$L_R = \frac{1.8W}{\left[(0.3)^{0.3} (1.0 + 0.24W/H) \right]} \quad [\text{for } L/H \leq 0.3] \quad (5-9)$$

$$L_R = \frac{1.8W}{\left[(L/H)^{0.3} (1.0 + 0.24W/H) \right]} \quad [\text{for } 0.3 \leq L/H \leq 3.0] \quad (5-10)$$

$$L_R = \frac{1.8W}{\left[(3.0)^{0.3} (1.0 + 0.24W/H) \right]} \quad [\text{for } L/H \geq 3.0] \quad (5-11)$$

$$H_C = H \quad [\text{for } 0 < x \leq L, \text{ when the flow reattaches}] \quad (5-12)$$

$$H_C = H \left[1 - \left(\frac{x-L}{L_R} \right)^2 \right] \quad [\text{for } L \leq x \leq L + L_R, \text{ when the flow reattaches}] \quad (5-13)$$

$$H_C = H_R + \frac{4 \left(x - \frac{R}{2} \right)^2 (H - H_R)}{R^2} \quad [\text{for } 0 \leq x \leq R/2, \text{ no flow reattachment}] \quad (5-14)$$

$$H_C = H_R \left[1 - \frac{\left(x - \frac{R}{2} \right)^2}{(L + L_R - R)^2} \right]^{1/2} \quad [\text{for } R/2 \leq x \leq L_R, \text{ no flow reattachment}] \quad (5-15)$$

$$W_C = \frac{W}{2} + \frac{R}{3} - \frac{(x-R)^2}{3R} \quad [\text{for } 0 < x \leq R] \quad (5-16)$$

$$W_C = \left(\frac{W}{2} + \frac{R}{3} \right) \sqrt{1 - \left(\frac{x-R}{L + L_R - R} \right)^2} \quad [\text{for } R < x \leq L + L_R] \quad (5-17)$$

$$H_W = 1.2R \left[\frac{x}{R} + \left(\frac{H}{1.2R} \right)^3 \right]^{1/3} \quad (5-18)$$

$$W_W = \frac{W}{2} + \frac{R}{3} \left(\frac{x}{R} \right)^{1/3} \quad (5-19)$$

5.3.2 Mean streamline slope

Based on wind tunnel experiments, the velocity field was divided in five regions where the mean streamlines slope (dz/dx) were determined (Figure 5-13). The mean streamlines slopes are most influenced near the building, decreasing with horizontal as well as vertical distance from the obstacle. In region E, the slopes gradually decay to zero. The formulation used to calculate the mean streamline slope is shown in Table 5-1. For crosswind distances outside of the projected obstacle width the calculated slopes are linearly attenuated until zero at a lateral distance of $(W/2) + (R/3)$ measured from the building centerline.

Table 5-1: PRIME formulation for mean streamlines slope

Region	Streamline slope	Downwind distance from upwind face	Factor for $z > H$	
A	$\frac{dz}{dx} = 0$	$x < -R$	$F_z = 1$	(5-20)
B	$\frac{dz}{dx} = \frac{2(H_R - H)(x + R)}{R^2}$	$-R \leq x < 0$	$F_z = \left(\frac{z}{H}\right)^{-3}$	(5-21)
C	$\frac{dz}{dx} = \frac{-4(H_R - H)\left(\frac{2x}{R} - 1\right)}{R}$	$0 \leq x < 0.5R$	$F_z = \left(\frac{z}{H}\right)^{-3}$	(5-22)
D	$\frac{dz}{dx} = \frac{(H_R - H)(R - 2x)\left(\frac{z}{H}\right)^{0.3}}{\left(L + L_R - \frac{R}{2}\right)^2}$	$0.5R \leq x < L + L_R$	$F_z = \left(\frac{z}{H}\right)^{-1}$	(5-23)
E	$\frac{dz}{dx} = \frac{-2(H_R - H)\left(L + L_R - \frac{R}{2}\right)}{\left[x - \left(\frac{L + L_R - R}{R}\right)\right]}$	$x > L + L_R$	$F_z = \left(\frac{z}{H}\right)^{-1}$	(5-24)

(Source: Schulman et al., 2000)

5.3.3 Plume rise

Initial plume rise is calculated through a numerical solution of the mass energy and momentum equations, allowing for arbitrary ambient temperature stratification, arbitrary unidirectional wind shear and arbitrary initial plume sizes. Wind speed is mod-

ified within the building wake as a function of building downwind distances. After the plume reaches its final rise then it starts to be influenced by the ambient velocity field determined in the previous section. The governing equations as solved in PRIME are:

$$\text{Mass} \quad \frac{d}{ds}(\rho U_{sc} r^2) = 2r\alpha\rho_a |U_{sc} - U_a \cos \phi| + 2r\beta\rho_a |U_a \sin \phi| \quad (5-25)$$

where $\alpha=0.11$ and $\beta=0.6$ are entrainment parameters, $U_a(z)$ is the ambient wind speed, ρ is the plume density, ρ_a is the air density, s is the distance along the plume centerline measured from the source, r is the plume radius, ϕ is the plume centerline inclination and U_{sc} is the velocity of the plume cross section along its centerline, calculated as a function of the plume along wind (u) and vertical (w) velocity components as:

$$U_{sc} = \sqrt{u^2 + w^2} \quad (5-26)$$

$$\text{Momentum (along wind):} \quad \frac{d}{ds}(\rho U_{sc} r^2 (u - U_a)) = r^2 \rho w \frac{dU_a}{dz} \quad (5-27)$$

$$\text{Momentum (vertical):} \quad \frac{d}{ds}(\rho U_{sc} r^2 w) = gr^2 (\rho_a - \rho) \quad (5-28)$$

where g is the gravitational acceleration.

$$\text{Energy:} \quad \frac{d}{ds}(\rho U_{sc} (T - T_a)) = -\left(\frac{dT_a}{dz} + \frac{g}{c_p}\right) \rho w r^2 - R_p r (T^4 - T_a^4) \quad (5-29)$$

where T is the plume temperature, T_a is the ambient temperature, c_p is the ambient air specific heat and $R_p = 9.1 \times 10^4 \text{ kg}/(\text{m}^2 \text{K}^3 \text{s})$ is a parameter characterizing radiation properties.

Considering that plume entrainment is dominated at times by plume growth due to wake turbulence, the mass conservation equation is solved as:

$$\frac{d}{ds}(\rho U_{sc} r^2) = \text{Maximum} \left[\left(\frac{d}{ds}(\rho U_{sc} r^2) \right)_{\text{entrainment}}, 2 r \rho_a U_a \left(\frac{dr}{ds} \right)_{\text{wake}} \right] \quad (5-30)$$

Where:

$$\left(\frac{d}{ds} \right)_{\text{wake}} = \sqrt{\frac{\pi}{2}} \frac{d\sigma_z}{dx} \quad (5-31)$$

The formulation for σ_z is discussed in the next section.

The ambient wind speed profile downwind of the building is obtained from:

$$U_w(z) = F(z) U_a(z) \quad (5-32)$$

With F constant inside the wake ($F = F_c$), above the wake ($F = 1$) and varying linearly as a function of height between H_c and H_w as:

$$F = F_c + \left[\frac{1 - F_c}{H_w - H_c} \right] (z - H_c) \quad [H_c \leq z \leq H_w] \quad (5-33)$$

$$F_c = 1 - \left[\frac{0.7 H_w}{0.5 (H_w + H_c)} \right] \quad (5-34)$$

5.3.4 Dispersion coefficients

The effect of the building wake is to increase plume dispersion. This is reflected in the value of the dispersion coefficients. PRIME calculates the turbulent wake turbulence field. Turbulence values are highest at the obstacle lee wall, and decays downwind the building. At the point where the plume centerline intercepts the obstacle wake until a distance equivalent to the cavity length, a probability density function (pdf) model is used for plume dispersion. Beyond the cavity, an eddy diffusivity model is used until the turbulence values have decayed to ambient values, where the dispersion coefficients are obtained from traditional formulations, such as the P-G curves or Briggs formulas (Table 3-3).

Horizontal and vertical turbulence intensities are calculated as:

$$i_y = i_{y0} \left[1 + \frac{\left(\frac{0.136}{i_{y0}} - 1 \right) + 0.7}{\left(\frac{\xi}{R} \right)^{\frac{2}{3}} - 0.7} \right] \quad (5-35)$$

$$i_z = i_{z0} \left[1 + \frac{\left(\frac{0.102}{i_{z0}} - 1 \right) + 0.7}{\left(\frac{\xi}{R} \right)^{\frac{2}{3}} - 0.7} \right] \quad (5-36)$$

where ξ is a distance defined such as $\xi = R$ at the lee wall.

Inside the pdf region, the dispersion parameters rates of growth are:

$$\frac{d\sigma_y}{dx} = i_y(x) \quad (5-37)$$

$$\frac{d\sigma_z}{dx} = i_z(x) \quad (5-38)$$

In the eddy diffusivity region, up to a distance where the turbulence intensity has decayed to the ambient turbulence intensity value or at 15R from the lee face (whichever is smaller), the plume dispersion coefficients growth rate are:

$$\frac{d\sigma_y^2}{dx} = 2\sigma_y(x_d)i_y(x) \frac{W_w(x)}{W_w(x_d)} \quad (5-39)$$

$$\frac{d\sigma_z^2}{dx} = 2\sigma_z(x_d)i_z(x) \frac{H_w(x)}{H_w(x_d)} \quad (5-40)$$

where x_d is the point of transition from the pdf to the eddy diffusivity region.

5.3.5 Concentrations in the near and far wakes

Inside the cavity, PRIME predicts a vertically mixed concentration (C_N) as a consequence of plume capture and recirculation by the near wake:

$$C_N = \frac{3fQ \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_{ycav}}\right)^2\right]}{U_H H_C W'_B} \quad (5-41)$$

where f is the fraction of the plume captured by the near wake, Q is the emission rate, W'_B is the width scale through which the plume is mixed (normally equal to the obstacle width but limited to a minimum value of $H_B/3$ and a maximum value of $3H_B$) and U_H is the ambient wind speed at building height; σ_{ycav} is the horizontal dispersion coefficient inside the cavity, considered as constant and calculated as (assuming a top-hat distribution):

$$\sigma_{ycav} = \frac{W'_B}{\sqrt{2\pi}} \quad (5-42)$$

For plumes released upwind of the obstacle, W'_B is obtained from the plume σ_{ycav} at the lee wall.

f is calculated as the maximum product of the vertical and horizontal mass distributions calculated along the near wake length, $f_y f_z$, with H_p being the plume height and f_y and f_z calculated for the full cavity width and height:

$$f_y(x) = \operatorname{erf}\left(\frac{W_c(x)}{\sqrt{2}\sigma_y(x)}\right) \quad (5-43)$$

$$f_z(x) = \operatorname{erf}\left(\frac{H_c(x) - H_p(x)}{\sqrt{2}\sigma_z(x)}\right) \quad (5-44)$$

The maximum allowed value for f_z is capped at the fraction below H_B at the end of the near wake.

The mass fraction captured by the near wake is then reemitted to the far wake as a volume source which is modelled as a point source located at the base of the lee wall. The concentration due to this volume source is used in the far wake as:

$$C_F = \frac{fQ \exp \left[-\frac{1}{2} \left(\frac{y}{\sigma_{ycav}} \right)^2 \right]}{\pi U_S \sigma_{ycav} \sigma_{zcav}} \quad (5-45)$$

where U_S is the wind speed at source height; σ_{zcav} is the vertical dispersion parameter for the cavity source, obtained by matching $C_N = C_F$ at the lee wall. The rate of growth of σ_{ycav} and σ_{zcav} is obtained with the same methods used for the elevated plume.

Finally, the portion of the plume not captured by the near wake is represented (for a ground level receptor) as:

$$C_p = \frac{(1-f)Q \exp \left[-\frac{1}{2} \left(\frac{H_p}{\sigma_z} \right)^2 \right] \exp \left[-\frac{1}{2} \left(\frac{y}{\sigma_y} \right)^2 \right]}{\pi \sigma_y \sigma_z U_S} \quad (5-46)$$

Vertical terms for receptors above ground level and reflection from top of the mixed layer are not shown in the above equation, but are the same employed in the ISC model.

The near and far wake concentrations are then calculated as:

$$C = C_N \quad (L \leq x \leq L + 0.85L_R) \quad (5-47)$$

$$C = \lambda C_N + (1-\lambda)C_F \quad (L + 0.85L_R \leq x \leq L + L_R) \quad (5-48)$$

$$C = C_p + \lambda C_N + (1-\lambda)C_F \quad (L + L_R \leq x \leq L + 1.15L_R) \quad (5-49)$$

$$C = C_p + C_F \quad (x \geq L + 1.15L_R) \quad (5-50)$$

where $\lambda = 1$ at $x = L + 0.85L_R$, with a linear decrease to $\lambda = 0$ at $x = L + 1.15L_R$.

5.4 The proposed fluctuating plume model (FPM-PRIME)

The model proposed by the present work, FPM-PRIME is based on Gifford (1959) fluctuating plume model proposition (section 3.4.3). The present section initiates

with a description of the original Gifford model and its implementation. The inclusion of the effects of the presence of obstacles based on PRIME is then described.

5.4.1 The fluctuating plume model by Gifford (1959)

As already stated (section 3.4.3), Gifford (1959) proposed that plume spreading as described by Gaussian modelling is the combined result of meandering and dispersion of plume segments. During the model averaging time (usually 60 minutes), the resulting plume and its trajectory is obtained as the average position of the centroid of each plume element which fluctuates laterally and vertically (Figure 3-9). The pollutant is dispersed inside each plume element with concentration, as well as the lateral and vertical positions of the plume elements following a Gaussian distribution.

The usual plume dispersion parameters employed in the standard Gaussian model, σ_y and σ_z , now called the long-term dispersion parameters, are then related to the variation of the position of each puff around the mean plume centerline and the dispersion within each puff by Equation 5-51:

$$\sigma^2 = \sigma_c^2 + \sigma_p^2 \quad (5-51)$$

Where:

σ is the long term dispersion parameter;

σ_c is the standard deviation of the puff position from the plume centerline;

σ_p is the standard deviation of the concentration inside each puff.

The concentration equation is then slightly modified in relation to the original Gaussian model:

$$\bar{C}(x, y, z) = \frac{Q}{2\pi \bar{u}_H \sigma_{yp} \sigma_{zp}} \exp\left(-\frac{(y - y_c)^2}{2\sigma_{yp}^2}\right) \cdot \left[\exp\left(-\frac{(z_c - z)^2}{2\sigma_{zp}^2}\right) + \exp\left(-\frac{(z_c + z)^2}{2\sigma_{zp}^2}\right) \right] \quad (5-52)$$

where σ_{yp} and σ_{zp} are the the standard deviation of the concentration inside each puff in y and z directions, respectively. Högström (1968, 1972), developed the expressions for determining σ_{yp} and σ_{zp} through field experiments. The author took successive photo-

graphs of plumes traveling in the field under different atmospheric conditions (Equations 5-53, 5-54 and 5-55):

$$\sigma_{zp} = 0.36 \frac{w_a^*}{u_a} \frac{\sqrt{2[e^{(-0.65a_0x)} + 0.65a_0x - 1]}}{0.65a_0(1 + 2.2 \times 10^{-2} \left(\frac{h}{87}\right)^{0.62} s)} \quad (\text{stable and neutral}) \quad (5-53)$$

$$\sigma_{zp} = 0.554 \frac{i_z}{b_0} \sqrt{2 \left(e^{-0.65b_0x} + 0.65b_0x - 1 \right)} \quad (\text{unstable}) \quad (5-54)$$

$$\sigma_{yp} = 50 \sqrt{2 \left[e^{-10^{-3}x} + 10^{-3}x - 1 \right]} \left(\frac{1}{1 + 10^{-2}s} \right) \quad (5-55)$$

where, h is the mean height of the plume centerline; x is the downwind receptor position; s is a stability parameter (Equation 5-57); a_0 and b_0 are empirical parameters (Equations 5-58 and 5-59); i_z is the vertical turbulent intensity (Equation); $w_a^*/\overline{u_a}$ is equivalent to the logarithmic wind profile and is obtained by Equation 5-56:

$$\frac{w_a^*}{u_a} = \left(4.31 \log \frac{h}{z_0} \right)^{-1} \quad (5-56)$$

where z_0 is the roughness length, usually taken as one tenth of the average height of roughness elements present in the terrain (Hanna, Briggs and Hosker Jr, 1982).

The stability parameter (s) is calculated with Equation 5-57:

$$s = \left(\frac{\partial \theta}{\partial z} / u_m^2 \right) \cdot 10^5 \quad (5-57)$$

where $\partial \theta / \partial z$ is the vertical potential temperature gradient at plume center height and u_m is the wind speed at the top of the mixing layer. For Neutral and stable atmospheric conditions, $s = 0$.

Empirical parameters a_0 and b_0 are obtained by Equations 5-58 and 5-59:

$$a_0 = \frac{w_a^*}{u_a} \left(\frac{1}{0.4hN_{pa}} \right) \quad (5-58)$$

$$b_0 = a_0 \left(\frac{\bar{u}_a}{16} \right)^{0.8} \quad (5-59)$$

where N_{pa} is a non-dimensional parameter, function of the roughness length (z_0): for flat terrain, $N_{pa} = 1.0$ ($z_0 \approx 0.1$ m) and $N_{pa} = 0.5$ ($z_0 \geq 0.1$ m).

The vertical turbulence intensity (i_z) is calculated as:

$$i_z = \frac{w_a^*}{u_a} + 0.33 \left(1 - \frac{\bar{u}}{16} \right)^3 \quad (5-60)$$

5.4.2 The use of PRIME to include building effects in FPM

FPM-PRIME is based on Gifford fluctuating plume theory (Equation 5-51), with plume segments dispersion coefficients based on the expressions proposed by Högström (Equations 5-53, 5-54 and 5-55).

Long-term dispersion coefficients are obtained from Briggs equations (Table 3-3) and inclusion of the effects of obstacles is based on the PRIME model. PRIME was chosen because it models building effects not only in the far field, but also in the near field, which includes the building recirculation zone or near wake, where Gaussian models might not perform well (US-EPA, 1995; Schauburger and Piringer, 2004). For each receptor point, FPM-PRIME generates a series of instant concentration values corresponding to the different positions of the plume segment centroid during the averaging time.

The streamlines deflection caused by the obstacle are modelled by equations 5-20 to 5-21 (Table 5-1), and the near wake and far wake dimensions, as well as the building length scale are calculated by equations 5-6 to 5-19.

Initial plume rise is modelled using the procedure described in section 5.3.3, and the dispersion parameters growth rate inside the building influence region are obtained through the procedures described in section 5.3.4.

As shown in section 5.3.5, concentrations predicted by PRIME in the obstacle near wake and wake regions (Equations 5-47, 5-48, 5-49 and 5-50) are the result of the elevated plume – not captured by the near wake (Equation 5-46), the mass fraction recirculating inside the cavity (Equation 5-41) and the mass fraction captured by the near wake reemitted as a volume source (Equation 5-45). FPM-PRIME retains this idea, adding the plume fluctuation concept to each modelled plume. The instant concentrations are then calculated in a similar way as in PRIME, as the combined effect of different plumes, as follows.

- Inside the cavity:

$$C_N = \frac{3fQ \exp\left[-\frac{1}{2}\left(\frac{y-y_{pcav}}{\sigma_{ypcav}}\right)^2\right]}{U_H H_C W'_B} \quad (5-61)$$

where σ_{ypcav} is the plume segment horizontal dispersion parameter, calculated with Equation 5-55, at the lee wall and y_{pcav} is the plume segment centroid position. Following PRIME assumption of a constant dispersion parameter within the cavity, σ_{ypcav} also does not vary for calculations of C_N . The other terms are the same as in Equation 5-41.

- For the plume emitted by the cavity:

$$C_F = \frac{fQ}{2\pi U_S \sigma_{ypvol} \sigma_{zpvol}} \exp\left[-\frac{1}{2}\left(\frac{y-y_{pvol}}{\sigma_{ypvol}}\right)^2\right] \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-z_{pvol}}{\sigma_{zpvol}}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+z_{pvol}}{\sigma_{zpvol}}\right)^2\right] \right\} \quad (5-62)$$

where σ_{ypvol} and σ_{zpvol} are the plume segment lateral and vertical dispersion parameters, obtained from equations 5-55 and 5-54; y_{pvol} and z_{pvol} are the plume segment centroid positions. The other terms are the same as in Equation 5-45. Considering that the original Höglström formulation did not take into account the presence of obstacles and that

the obstacle effect is to increase turbulence downwind of the building, Equation 5-54 was chosen for the calculation of all plume segments vertical dispersion parameters.

- For the elevated plume – mass fraction not captured by near wake:

$$C_p = \frac{(1-f)Q}{2\pi U_s \sigma_{yp} \sigma_{zp}} \exp\left[-\frac{1}{2}\left(\frac{y-y_p}{\sigma_{yp}}\right)^2\right] \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-z_p}{\sigma_{zp}}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+z_p}{\sigma_{zp}}\right)^2\right] \right\} \quad (5-63)$$

where σ_{ypvol} and σ_{zpvol} are the plume segment lateral and vertical dispersion parameters, obtained from equations 5-55 and 5-54; y_p and z_p are the plume segment centroid positions. The other terms are the same as in Equation 5-45.

The plume segment centroid instant positions (y_{pvol} and z_{pvol} in Equation 5-62, and y_p and z_p in Equation 5-63) are obtained by a random number generator. For each run of the model, the user can choose the number of generated positions. The generated series of plume centroid vertical and lateral positions exhibit a Gaussian distribution centered in the plume centreline mean vertical and lateral positions, with a standard deviation equal to the correspondent dispersion parameter: σ_{ycav} for the cavity; σ_{zcvol} and σ_{ycvol} for the plume emitted by the cavity volume source; and σ_{zc} and σ_{yc} for the elevated plume.

The near and far wake instant concentrations are then calculated using Equations 5-47, 5-48, 5-49, 5-50. For each receptor point, the mean concentration is then the average of the instant concentration generated series.

FPM-PRIME can express concentration values in units of mass per volume or in odour units (OU), depending on the input data used. If values of rate of emission expressed in mass of emitted pollutant per unit of time are given by the user, than the output concentration results will be expressed in units of mass per volume. For concentration result in OU, then the user must insert the odour strength at the source (N_o), expressed in odour units, and the volumetric flow rate of the source (V). The concentra-

tion equation is then slightly modified, with the rate of emission replaced the product $N_0 V$. For example, the concentration due to the elevated plume will be expressed as:

$$C_p = \frac{(1-f)N_0 V}{2\pi U_s \sigma_{yp} \sigma_{zp}} \exp\left[-\frac{1}{2}\left(\frac{y-y_p}{\sigma_{yp}}\right)^2\right] \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-z_p}{\sigma_{zp}}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+z_p}{\sigma_{zp}}\right)^2\right] \right\} \quad (5-64)$$

where the concentration is given in odour units and all other parameters are the same as in Equation 5-63.

5.4.3 Intermittency factor and peak-to-mean ratio

As FPM-PRIME models concentration fluctuation and generates a series of instantaneous concentration values for each receptor point, it is then possible to calculate the intermittency factor, as well as the peak-to-mean concentration ratio, important parameters for odour impact analysis.

For each receptor point the model algorithm analyses the generated series and computes the number of concentration values exceeding the user-chosen concentration threshold; this quantity is then divided by the number of concentration values in the generated series.

$$I_{r(x,y,z)} = \frac{\sum_{i=0}^{i=n} (C_i > C_{thresh})}{n} \times 100 \quad (5-65)$$

where $I_{r(x,y,z)}$ is the percentage of time during which the instant concentration (C_i) is higher than the user-defined threshold concentration (C_{thresh}) at a receptor located in position (x, y, z) ; n is the number of generated concentration values.

The obtained result corresponds to the intermittency factor *Int*, if one defines it as the percentage of time during which the concentration is above the defined threshold (as in Aubrun, 2004, for instance).

$$Int_{r(x,y,z)} = I_{r(x,y,z)} \quad (5-66)$$

If the other definition is used, where intermittency is the percentage of time during which the concentration stays below a defined threshold (Higson et al., 1994; Mavroidis and Griffiths, 2001; Santos et al., 2009), then:

$$Int_{r(x,y,z)} = 100 - I_{r(x,y,z)} \quad (5-67)$$

The P/M concentration ratio for each receptor ($P/M_{r(x,y,z)}$) is then obtained by dividing the highest concentration in the respective concentration series ($\max(C_i)$) to its average value (C_{ave}):

$$P/M_{r(x,y,z)} = \frac{\max(C_i)}{C_{ave}} \quad (5-68)$$

It is important to point out that, as a direct result of the Gaussian distribution of the plume segment positions, the observed peak concentration value ($\max(C_i)$) might be the result of instant plume positions laying out of the $\pm 3\sigma$ interval, so the 98th percentile of the concentration series might be a much more representative indicator of the expected peak concentration and P/M concentration ratio.

5.4.4 Frequency of occurrence

The frequency of occurrence of each class of odour intensity (as expressed by Murray et al., 1978 and De Melo Lisboa et al., 2006) can be easily obtained through statistical analysis of the generated concentration series for a specific receptor, provided that FPM-PRIME is run with the results in OU option. FPM-PRIME algorithm outputs the concentration series of user-defined receptor positions. These series can easily be imported into any analysis software that support text files as input format, allowing the generation of histograms of odour concentrations.

5.4.5 Input data for modelling experiments A, B and C with FPM-PRIME

Input data for FPM-PRIME basically consists of (i) obstacle dimensions, (ii) roughness length and (iii) friction velocity, (iv) emission rate of the source, (v) internal diameter of the stack (vi) release velocity of emitted gases and (vii) the domain size (length, width and height). Additional data consists of receptor positions in which the generated concentration series are stored for further processing.

5.4.5.1 Experiment A

Whenever wind tunnel experiments are employed some kind of scaling needs to be done as the use of full scale models is impracticable. Sada and Sato (2002) wind tunnel experiment consisted of a 1:250 scaled model of a cubic building. In order to set up the FPM, AERMOD, and CALPUFF simulation the geometry had to be up scaled, resulting in a cubic building with $H=50$ m. The source was then placed 50 m upwind of the obstacle.

As already mentioned, Reynolds number independence was achieved as the wind tunnel experiment Reynolds number was sufficiently high. Then, in order to generate the incoming wind speed profile for the simulation, the same non-dimensional incoming wind speed profile of Sada and Sato (2002) wind tunnel experiment was employed. The non-dimensional wind speed profile equation (Equation 5-70) is obtained by taking the well-known mean wind speed ($\bar{u}$) profile equation for neutral atmospheric stability (Stull, 1988), shown in Equation 5-69, and dividing the mean along wind speed ($\bar{u}$) and the friction velocity (u_*) by a reference speed (U_{ref}), and the height (z) and roughness length (z_0) by a reference height (z_{ref}). For the full scale geometry a reference speed of $U_{ref}=2$ m/s was adopted, corresponding to the mean wind speed at the top of the boundary layer, at $z_{ref} = 75$ m. The Von Karman constant remains the same at all scales ($k = 0.4$).

$$\bar{u} = \frac{u_*}{k} \ln \left(\frac{z}{z_0} \right) \quad (5-69)$$

$$\bar{u}/U_{ref} = \frac{u_*/U_{ref}}{k} \ln \left(\frac{z/z_{ref}}{z_0/z_{ref}} \right) \quad (5-70)$$

Friction velocity and roughness length of the experimental data was obtained from the mean incoming wind speed profile and were then up scaled using the above equations.

An emission rate of 5g/s was adopted, along with a release speed of 1.82 m/s. The domain measured 250m (length), 80 m (width) and 150 m (height).

5.4.5.2 Experiment B

Although Experiment B was performed with a scale model, the database presented full scale values for velocities and distances, so the same data was used in FPM-PRIME. Full scale building dimensions are presented in Figure 5-14. An average building height of 8.8m was used (Aubrun and Leidl, 2004).

As the concentration results presented in the experiment database are normalized by the concentration measured at the source, in order to determine the emission rate a value of 1PPM was adopted, with 1atm ambient pressure; then, based on the given area of the source and exhaust velocity, an emission rate value of 0.007g/s was obtained.

5.4.5.3 Experiment C

Based on the database of Experiment C and on details given in Mavroidis et al. (2003), and adopting a value of 1m for the stack diameter, Table 5-2 presents the input data for FPM-PRIME:

Table 5-2: Input data for FPM-PRIME

Building height	10m
Roughness length	0.01m
Friction velocity	0.24m/s
Emission rate	0. 182 μ g/s
Stack diameter	1m
Exhaust velocity	0.03m/s
Domain size	300m (length), 80m (width) and 75m (height)

5.5 AERMOD

Experiments A and B were also simulated with AERMOD. PRIME was used to include the building effects on dispersion. More detailed information on the AERMOD simulations is available in Melo (2011) and Melo et al. (2012).

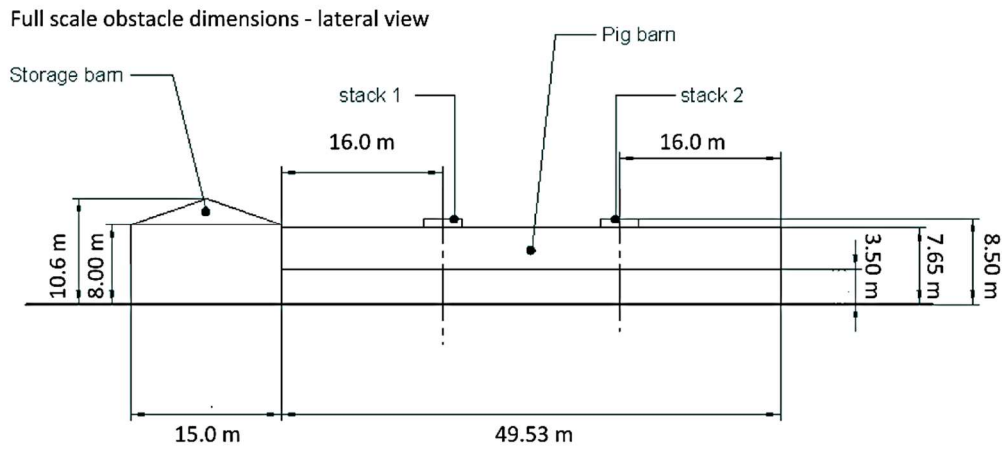
5.5.1 Experiment A

The incoming wind speed profile was generated using the same procedure described in section 5.4.5.1. A similar procedure was employed in order to generate the incoming turbulence intensity profile. Reynolds number for the AERMOD simulation was 10^7 .

AERMOD uses meteorological data generated by AERMET preprocessor. This generated data covers a period of 24 hours. As the wind tunnel experiments were performed under constant simulated atmosphere conditions, input data for AERMET consisted of profiles of wind speed, wind direction, temperature, standard deviation of wind speed direction and standard deviation of wind speed with values that remained constant for a 24-hour period. The values used in the standard deviation of wind speed direction and standard deviation of wind speed profiles were obtained from the incoming flow wind speed and turbulence intensities profiles from Sada and Sato (2002). The standard deviation of the lateral wind speed direction were calculated using Equation 5-71 (Slade, 1968):

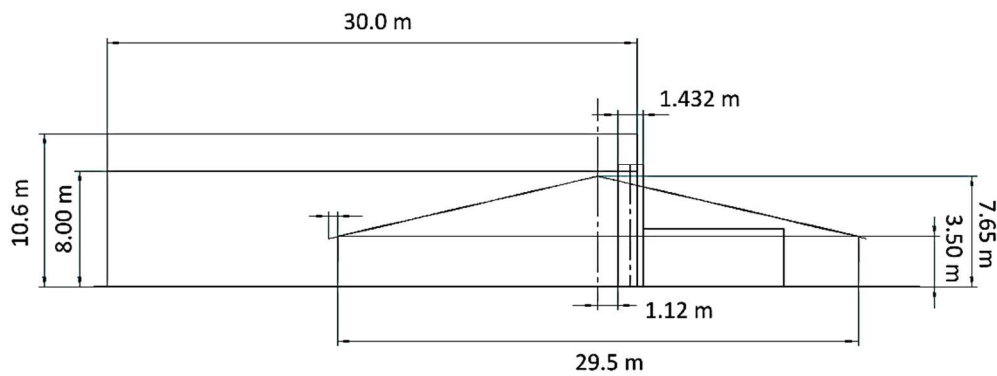
$$\sigma_\theta = \frac{\sigma_v}{\bar{u}} \quad (5-71)$$

where σ_v is the standard deviation of the lateral wind speed and $\bar{u}$ is the along flow mean wind velocity.



(a)

Full scale obstacle dimensions - front view



(b)

Figure 5-14: full scale obstacle dimensions - lateral view (a) and front view (b) (adapted from CEDVAL, 2006).

Values for the Monin-Obukhov length, as well as for the surface sensible heat flux and convective scale velocity were estimated in order to correspond to typical neutral atmospheric stability conditions.

The BPPRIME software, part of the AERMOD system and available at http://www.epa.gov/ttn/scram/dispersion_related.htm#bpipprm, calculates values of the projected building width and length for different wind directions. Mean wind direction was normal to the building wall, with the source placed 50 m upwind of the centre of the building wall. It was considered that the simulated wind direction was 270° .

Detailed input data used in the AERMOD simulation is given in APENDIX A.

5.5.2 Experiment B

The available dataset covering Experiment B included wind speed and turbulence intensities profiles corresponding to the full scale representation of the flow around the complex geometry building, so these values were used as input data for the AERMOD simulation. Similarly to Experiment A, the same values were used for a 24-h period, with standard deviation of the lateral wind direction obtained from Equation 5-71 using the available data.

Using the full scale building dimensions (Figure 5-14) and the software BPPRIME, values for the projected building width and length for different wind directions were generated.

Similarly to Experiment A, values for the Monin-Obukhov length, as well as for the surface sensible heat flux and convective scale velocity were estimated in order to correspond to typical neutral atmospheric stability conditions. Detailed input data used in the AERMOD simulation is given in APENDIX B.

The simulated situation corresponded to a wind direction of 220° and the results will be given relative to a Cartesian reference situated at the source, with the x-direction parallel to the mean wind direction (Figure 5-5).

5.6 CALPUFF-PRIME

Experiments A and B were also simulated with CALPUFF, using PRIME to include the effect of the obstacles. The meteorological conditions used were similar to the AERMOD simulations, with specific assumptions in order to generate input data for the model. More detailed information on the CALPUFF simulations is available in Melo (2011) and Melo et al. (2012).

A similar computational domain was used for experiments A and B. It consisted of a 300 m x 400 m mesh, comprising 30 cells in the lateral direction and 40 cells in the longitudinal direction. Figure 5-16 and Figure 5-17 show the respective meshes used for experiment A and experiment B.

The vertical grid consisted of 12 layers of cells, showed in Figure 5-15, with indication of the height of each cell face, as well as the height of each cell center. The wind speed, direction, pressure and temperature profiles were similar to those on the AERMOD simulations. Detailed input data used in the CALPUFF simulations for experiments A and B are given in APENDIX C and APENDIX D.

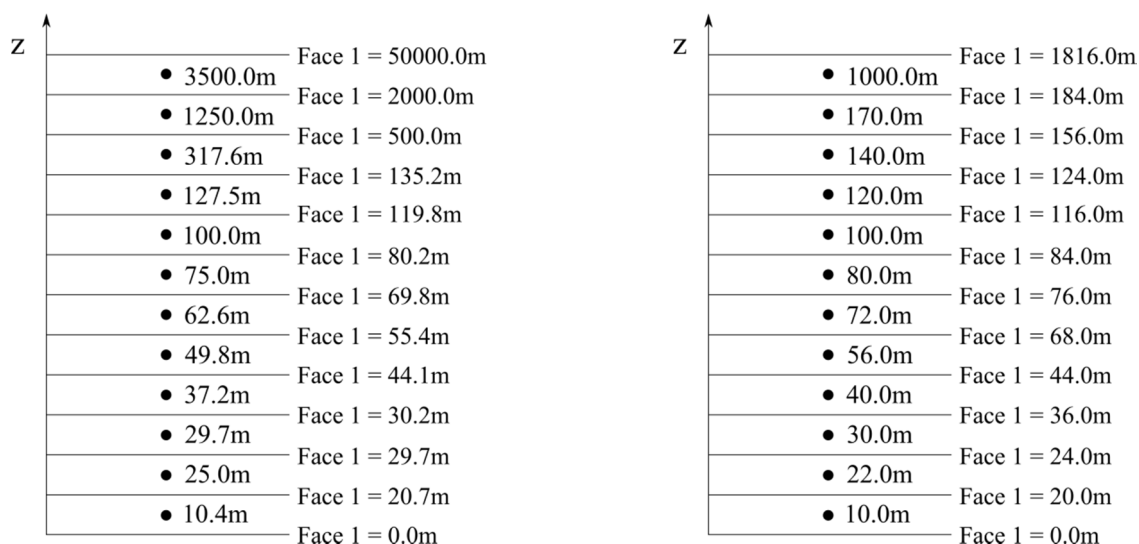


Figure 5-15: vertical levels used in CALPUFF for (a) Experiment A and (b) Experiment B.

The turbulence intensity profiles used on the CALPUFF simulations were the same used in AERMOD, which were obtained from each wind tunnel experiment data. Dispersion coefficients were calculated using the Pasquill-Gifford curves and were valid for a 1-hour period. CALPUFF processor output, containing the rough hourly concentration data was then exported to CALPOST post processor.

CALPOST generates output concentration data from the CALPUFF results. In addition to the hourly mean concentration values, short period (3 minutes) concentration values were also generated. As already mentioned, CALPUFF generates short-time concentrations with Equation 3-50.

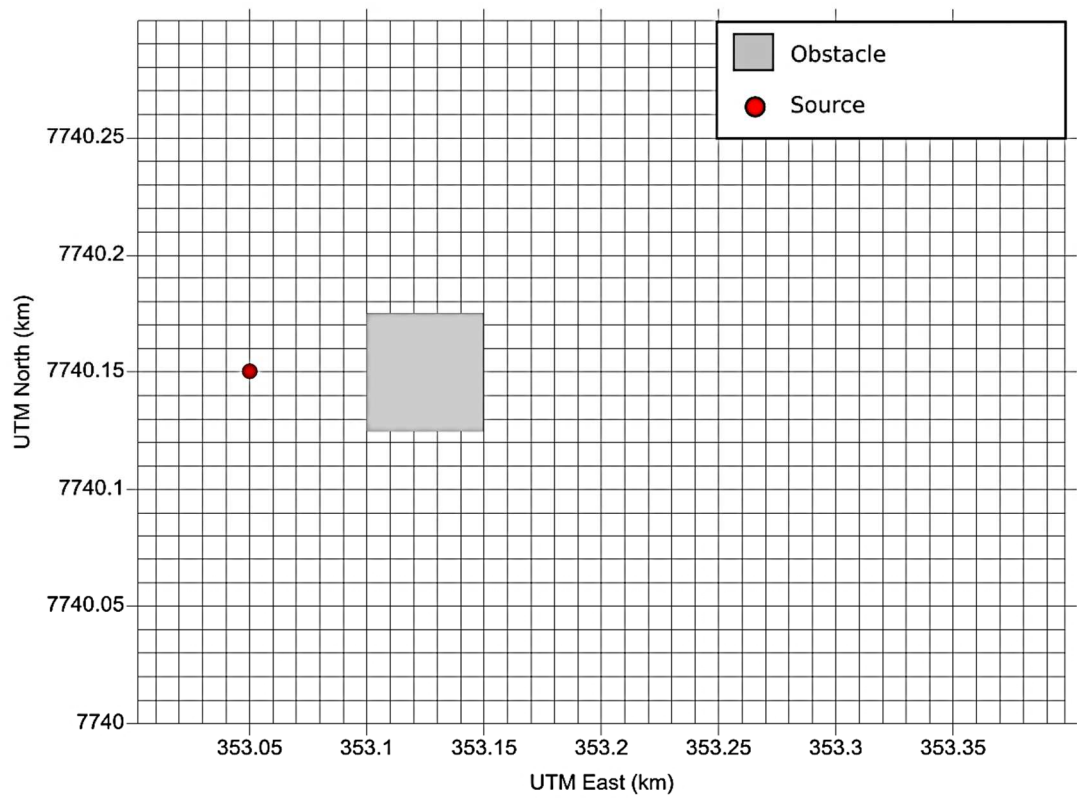


Figure 5-16: Computational mesh used for CALPUFF simulation of experiment A.

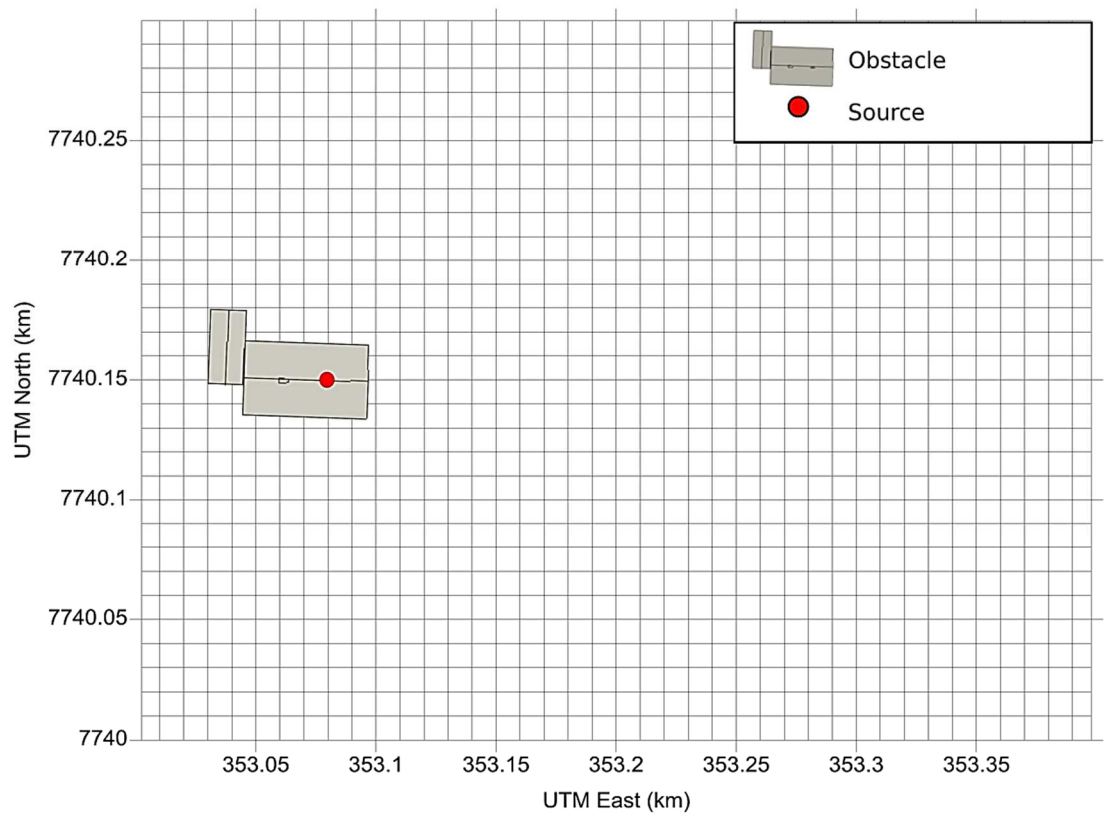


Figure 5-17: Computational mesh used for CALPUFF simulation of experiment B.

6 Results

This chapter presents the modelling results of the experiments described in section 5.1.

Section 6.1 presents the numerical simulations of flow and dispersion around a cubical building in a wind tunnel described as Experiment A (section 5.1.1) performed using the Dynamic Smagorinsky LES (D-LES) and the WALE LES (W-LES) models. Details of numerical simulation can be found in section 5.2.3. These simulations allow for an evaluation of D-LES and W-LES and also Smagorinsky LES (S-LES) as Sada and Sato (2002) have performed the same simulation. Additionally, mean concentration results obtained using the FPM-PRIME (FPM), AERMOD-PRIME (AERMOD) and CALPUFF-PRIME (CALPUFF) models are compared to the previous results in order to assess the performance of Gaussian-based models. Details of input data for FPM, AERMOD and CALPUFF can be found in sections 5.4.5, 5.5.1 and 5.6, respectively. W-LES and D-LES concentration fluctuation results are explored and compared to FPM results and wind tunnel (WT) data. Peak concentrations predicted by D-LES, W-LES and FPM through determination of the 98th concentration percentile are also evaluated.

Section 6.2 shows W-LES simulation of flow and dispersion around a complex shaped obstacle in a wind tunnel described as Experiment B (section 5.1.2). This simulation was carried out in order to analyze the influence of building shape on dispersion. Details of this simulation can be found in section 5.2.4. Mean concentration results obtained using W-LES were compared with FPM, AERMOD and CALPUFF and validated by WT data. Details of input data for FPM, AERMOD and CALPUFF can be found in sections 5.4.5, 5.5.2 and 5.6, respectively. Furthermore, concentration fluctuation fields obtained using W-LES and FPM were assessed through the intermittency factor and compared with WT data. Peak concentrations predicted by W-LES and FPM are evaluated through determination of the 98th concentration percentile.

Finally, W-LES simulation of a full-scale flow and dispersion around a cubical building described as Experiment C (section 5.1.3) is presented in section 6.3. Mean concentration predicted by W-LES and FPM are compared to field experimental data. Intermittency and peak concentrations predicted by W-LES and FPM are also compared to field experimental data. Details of this numerical simulation and input data for FPM can be found in sections 5.2.5 and 5.4.5, respectively.

6.1 Flow and dispersion of odorant gases around a cubical building: a comparison between different LES sub-grid models, Gaussian based models and wind tunnel data

6.1.1 Flow field

The flow pattern around the cube obtained by the wind tunnel experiments and LES are similar (Figure 6-1); both results show two recirculating/reverse flow regions, downwind and on the top of the obstacle. The reattachment distance downwind of the obstacle ranges from 0.24 m (WT) to 0.246 m (D-LES) and 0.26 m (W-LES and S-LES), corresponding to $1.2H$, $1.23H$ and $1.3H$, respectively.

Results for the mean along-wind velocity profiles (scaled by U_∞ , the along-wind velocity at the top of the boundary layer) around the obstacle are shown in Figure 6-2. Results from both W-LES and D-LES agree well with the wind tunnel data, as well as with S-LES results. Figure 6-2 b and c clearly show the recirculation zones on top and downwind of the obstacle, which are characterized by negative along-flow velocities. Tominaga and Stathopoulos (2010) found a similar behaviour for LES simulation of flow around an isolated obstacle for the locations $x/H=1.5$ and $x/H=2.5$; Lim et al. (2009), however, observed a different behavior, with LES overestimating the Wind Tunnel results at $x/H=1.5$. They suggested that the grid resolution was not adequate to accurately resolve the region. The resolution used by Lim et al. (2009) ($H/32$) was finer than the one used in D-LES and W-LES simulations, while Tominaga and Stathopoulos (2010) employed an even finer resolution ($H/222$) using, however, a non-uniform grid. These differences with the present case could be attributed to the wall treatment used in the different LES simulations: Tominaga and Stathopoulos (2010) employed a Van Driest damping function while Lim et al (2009) followed Mason (1994). Both works used the Smagorinsky sub grid model.

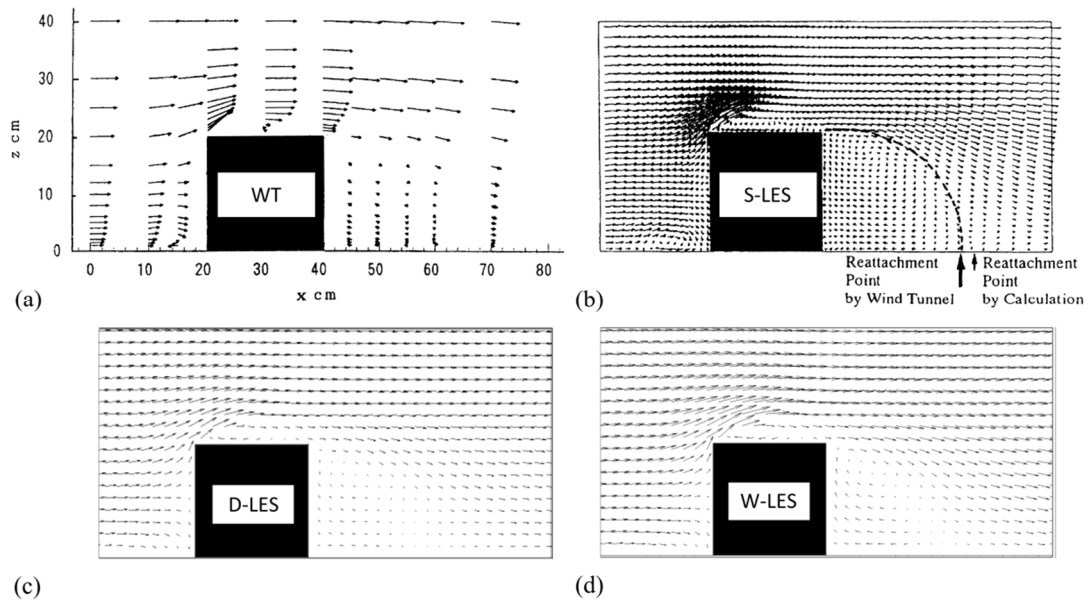


Figure 6-1: Velocity vectors around the obstacle: results of (a) wind tunnel experiment, (b) Smagorinsky LES, (c) Dynamic Smagorinsky LES and (d) WALE LES. Cavity region estimated for the wind tunnel is indicated by the dashed line in (b). ([a] and [b]: adapted from Sada & Sato, 2002)

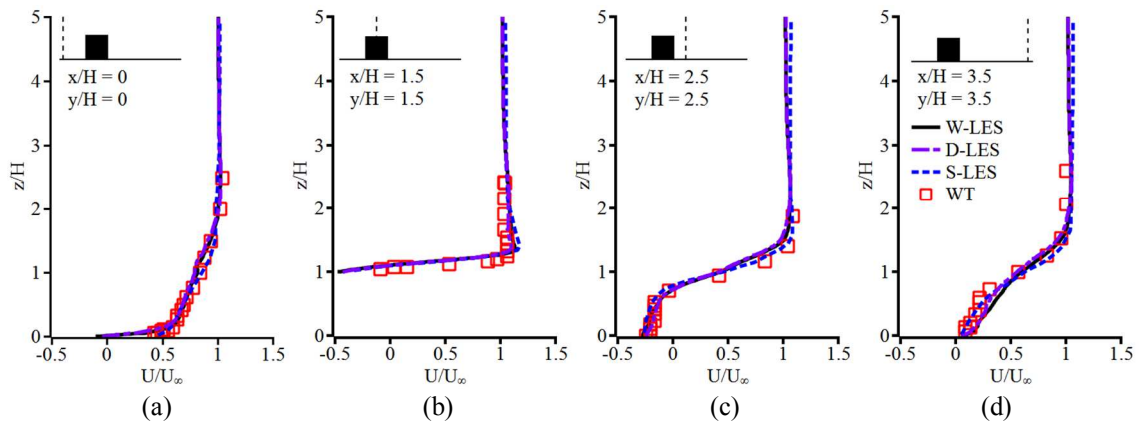


Figure 6-2: Profiles of along flow mean velocity around the obstacle.

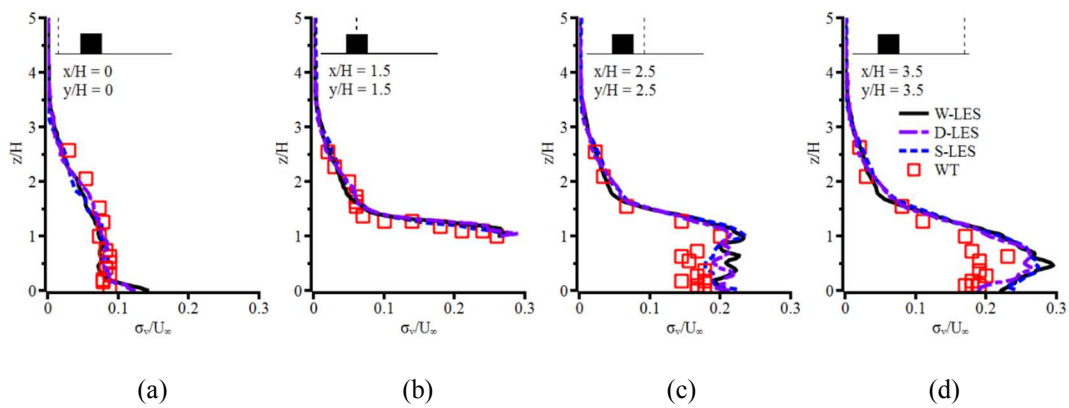


Figure 6-3: Horizontal velocity fluctuation profiles around the obstacle

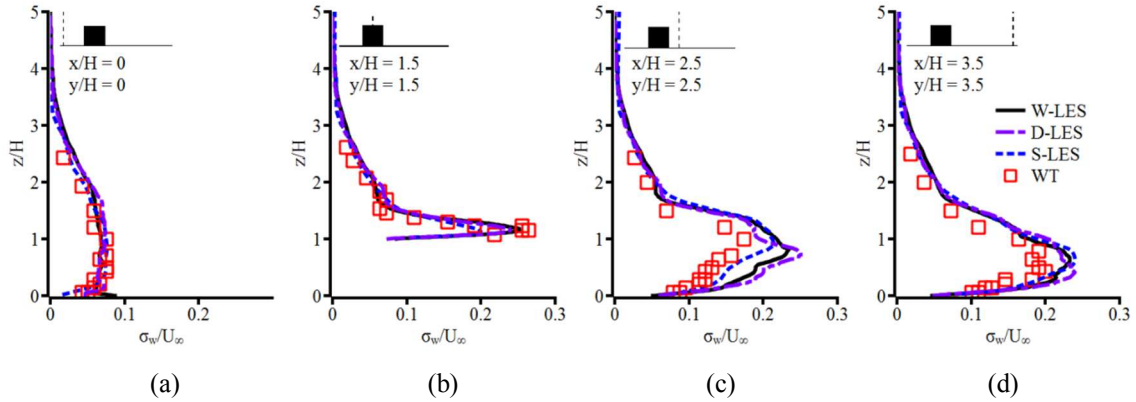


Figure 6-4: Vertical velocity fluctuation profiles around the obstacle.

Horizontal and vertical velocity fluctuation profiles (scaled by U_∞ , the along-wind velocity at the top of the boundary layer) are shown in Figure 6-3 and Figure 6-4, respectively. W-LES and D-LES results show the same general behavior as S-LES and WT data. Both mean velocity and turbulence intensity results indicate that the turbulence generated by the precursor obstacles exhibits a similar behavior to the wind tunnel turbulence. At $x/H=0$ and $x/H=1.5$, all models reproduce very well the wind tunnel results. At $x/H=1.5$ (on top of the obstacle), W-LES and D-LES reproduce the WT results for the vertical turbulence intensity better than the S-LES. At $x/H=2.5$ and $x/H=3.5$, though, all LES models overestimate WT results for both the horizontal and vertical turbulent profiles at $z/H < 1.0$. Thus, the effect of the obstacle on the flow is being overestimated by LES at the middle of the recirculation cavity and at the beginning of the obstacle wake. This overestimation is more evident for vertical turbulence intensity than for horizontal turbulence intensity. The overestimation of the vertical turbulence intensity by S-LES appears smaller at $x/H=2.5$. W-LES results are similar to D-LES results, showing good agreement with WT data; also D-LES required double the run time for the same amount of time steps when compared to W-LES, justifying the use of this subgrid model for simulations of Experiment B and C.

6.1.2 Concentration field

Mean concentration results of the emitted tracer gas are shown in Figure 6-5. Concentration was scaled by $U_{ref} \cdot H^2 / Q$, where U_{ref} is the ambient wind speed at building height (H) and Q is the source emission rate. The overall results of the differ-

ent LES models agrees with WT data. All LES models underestimate to some extent the mean concentration at $z/H < 1.0$, while results for $z/H > 1.0$ show a better agreement. These results are a consequence of LES slightly overestimating turbulence intensity at $z/H < 1.0$, causing higher plume spread. An interesting observation is that mean concentration results show a better agreement at the locations where turbulence intensity results were overestimated.

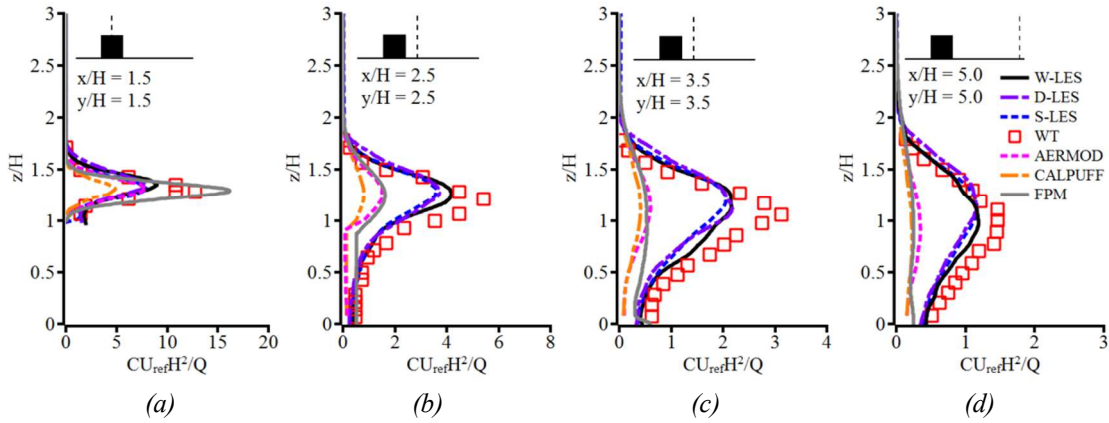


Figure 6-5: Mean concentration profiles around the obstacle

FPM, AERMOD and CALPUFF clearly underestimate the concentration in all locations examined ($x/H=1.5$, $x/H=2.5$, $x/H=3.5$ and $x/H=5.0$). FPM, AERMOD and CALPUFF results were closer to WT results at $x/H=1.5$ (top of the obstacle) than at the other locations, with FPM results agreeing better to WT than AERMOD and CALPUFF. As these three models employ PRIME to estimate the dispersion in the obstacle vicinity, this difference is possibly attributed to the way the PRIME code is implemented in each model. It is interesting to note that FPM presented the best agreement with WT results at the top of the obstacle.

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, FPM, AERMOD and CALPUFF results are closer to WT and LES. Figure 6-6 through Figure 6-10 scatter plots compare each model mean concentration with the experimental data for $x/H=1.5$, $x/H=2.5$, $x/H=3.5$ and $x/H=5.0$.

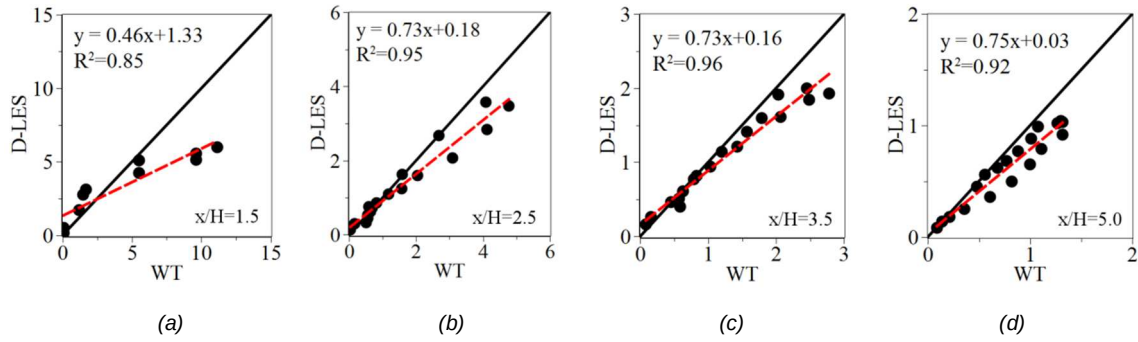


Figure 6-6: mean concentration observed in the wind tunnel and estimated by D-LES at (a) $x/H=1.5$, (b) $x/H=2.5$, (c) $x/H=3.5$ and (d) $x/H=5.0$ ($y/H=0$).

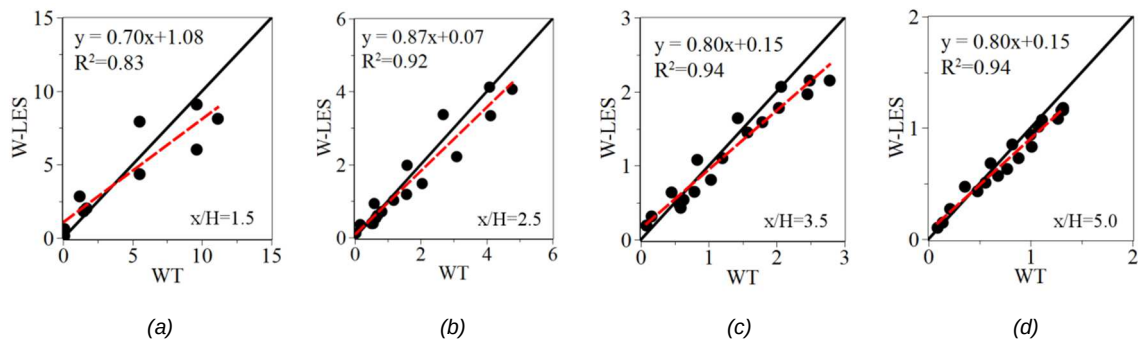


Figure 6-7: mean concentration observed in the wind tunnel and estimated by W-LES at (a) $x/H=1.5$, (b) $x/H=2.5$, (c) $x/H=3.5$ and (d) $x/H=5.0$ ($y/H=0$).

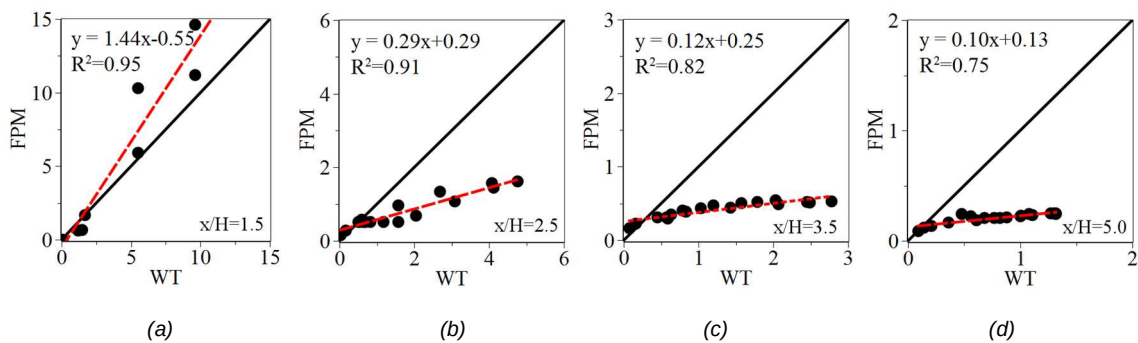


Figure 6-8: mean concentration observed in the wind tunnel and estimated by FPM at (a) $x/H=1.5$, (b) $x/H=2.5$, (c) $x/H=3.5$ and (d) $x/H=5.0$ ($y/H=0$).

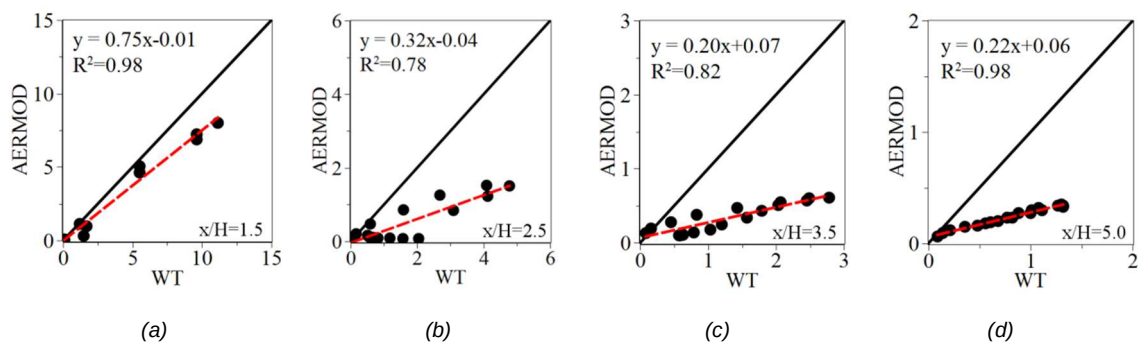


Figure 6-9: mean concentration observed in the wind tunnel and estimated by AERMOD at (a) $x/H=1.5$, (b) $x/H=2.5$, (c) $x/H=3.5$ and (d) $x/H=5.0$ ($y/H=0$).

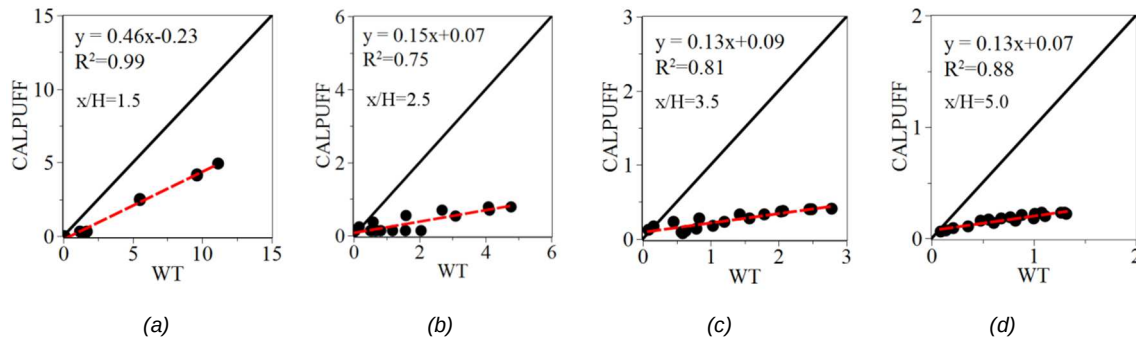


Figure 6-10: mean concentration observed in the wind tunnel and estimated by CALPUFF at (a) $x/H=1.5$, (b) $x/H=2.5$, (c) $x/H=3.5$ and (d) $x/H=5.0$ ($y/H=0$).

6.1.2.1 Concentration fluctuation

Concentration fluctuation intensity (Figure 6-11) is of great importance in odour impact assessment. Results are scaled by U_∞ , the along-wind velocity at the top of the boundary layer, and by Q , rate of emission of the contaminant. Again, results from the LES simulations show the same general trend as the WT results. With the exception of $x/H=1.5$ (where S-LES overestimates WT results), S-LES underestimates concentration fluctuations at all positions, with W-LES and D-LES showing an opposite behavior. Again, the concentration fluctuation intensity is overestimated where the turbulence intensity was also overestimated ($z/H < 1.0$), with model results agreeing with the WT data at the same locations where turbulence intensity showed good agreement. Overall, W-LES and D-LES results for the concentration fluctuation intensity show a slightly better agreement with WT than S-LES results.

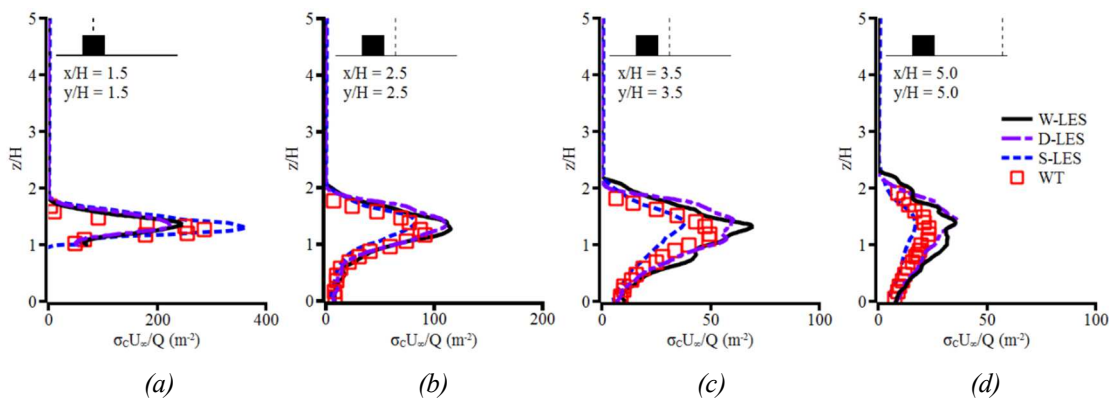


Figure 6-11: Concentration fluctuation intensity around the obstacle

As discussed previously, an important advantage of using LES simulations for odour dispersion is the possibility of using the concentration time series data to obtain

information on intermittency levels, which provides a good estimate of the impact of emitted compounds. Figure 6-12 shows the time series of the concentration value normalized by the mean concentration inside recirculation region after the building, which represents the time series of “instantaneous” peak-to-mean ratio (P/M) for D-LES and W-LES. It is interesting to note that although the time series predicted by each model are not completely similar, the size and frequency of the concentration peaks are relatively similar. This tendency can be observed in Figure 6-13, which shows the variation of the intermittency factor for D-LES and W-LES in relation to the observed concentrations scaled by the average concentration (or the P/M ratio). Here, intermittency is defined as the percentage of time during which the concentration equals or exceeds a certain threshold, which here is assumed as the mean concentration. Each intermittency curve corresponds to a different point along flow direction: top of the obstacle ($x/H=1.5$), recirculation cavity ($x/H=2.5$) and at the beginning of the far wake ($x/H=3.5$), for $y/H=0.0$ and $z/H=1.0$. It is possible to note that in spite the differences between the models, the intermittency levels are fairly similar, but the W-LES model systematically predicts higher levels of intermittency levels than D-LES. In fact, the results obtained by both LES models exhibit the same general trend for peak-to-mean ratios up to 4, but for larger values of peak-to-mean ratios the differences are more significant.

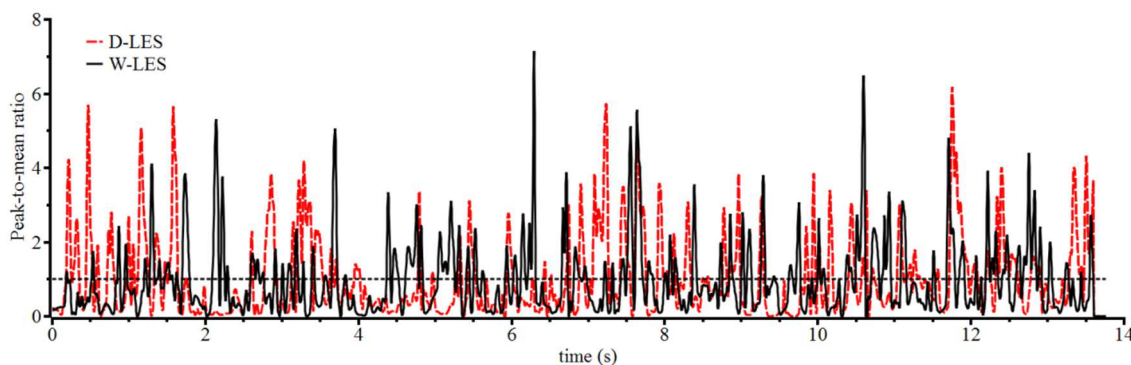


Figure 6-12: Time series of peak-to-mean ratio at $x/H = 3.5$, $y/H = 0.0$ and $z/H = 1.0$.

The FPM intermittency curves for the cavity and wake exhibit the same general trend as the LES curves up to 2. The near wake FPM curve indicate higher intermittency levels than D-LES and W-LES up to P/M 4.3 and 5, respectively, but the highest predicted value for the P/M was lower (29% lower than D-LES and 26% lower than W-

LES). The FPM wake curve indicated higher intermittency levels for all P/M thresholds when compared to the LES models (27% higher than D-LES and 17% higher than W-LES).

The FPM intermittency curve for the top of the cube showed a completely different behavior than the LES curves, with lower values for up to P/M 7.6. In fact, analysis of the FPM concentration series showed that the highest 6 observed P/M events corresponded to 4.3 (intermittency of 0.5%), 12.3 (intermittency of 0.4%), 20.9 (intermittency of 0.3%), 152 (intermittency of 0.1%) and 669 (zero intermittency). At this point the calculated average plume height is 64.76 m so the “instant” plume height fluctuates around this value following a Gaussian distribution; these high concentrations are verified when the random generated position is at the lower extreme of the Gaussian curve (closer to the receptor) and might be an indication of an under prediction of the plume segment dispersion parameter, σ_p . Considering the typical 1-hour averaging time employed in Gaussian models, an intermittency of 0.1% would correspond to 3.6 seconds, enough to generate odour perception, albeit its short duration.

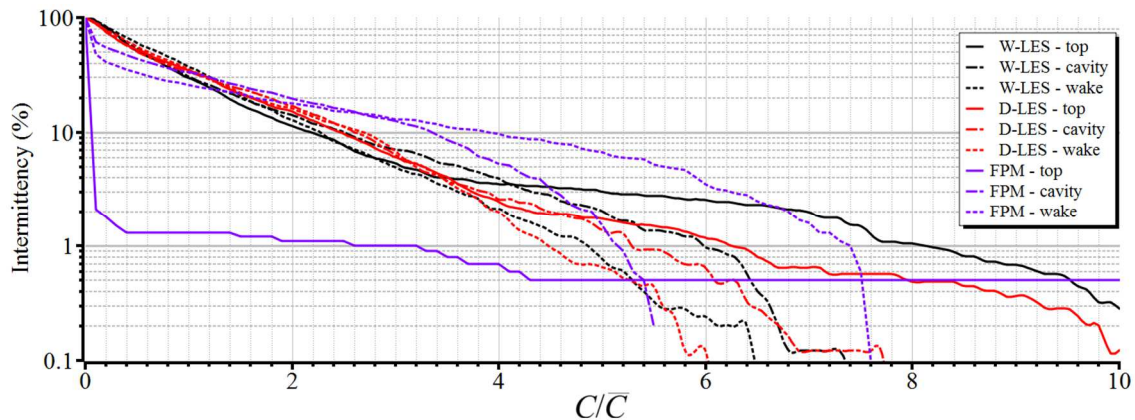


Figure 6-13: Intermittency calculated at the top of the obstacle ($x/H=1.5$), at the cavity ($x/H=2.5$) and at the far wake ($x/H=3.5$) at $y/H=0.0$ and $z/H = 1.0$

In general, the results show intermittency levels between 10 to 20% for peak-to-mean values of 2, i. e. concentration peaks twice as the average concentration are observed between 10 to 20% of the time. For the 3 locations analyzed (top of the obstacle, recirculation cavity and beginning of far wake), the LES curves are quite similar for peak-to-mean level up to 4, higher than that, the intermittency level at the top of the

building and at recirculation cavity are significantly larger than the values observed at the wake region (highest peaks were observed at the top of the cube).

This trend is probably related to the larger concentration fluctuation observed in building roof, in relation to the recirculation cavity and the wake region (Figure 6-11). In the wake region, intermittency is about 1 % between 4 and 5, in the recirculation cavity and roof of the building P/M ranges between 5 to 6 and 6 to 8, respectively. In fact, P/M results decreases as the distance from the source increases, as average concentration results become lower and turbulent eddies are of smaller scales.

The 98th percentile concentration (concentration equalled or exceeded 2% of the time) is an usual parameter in odour impact assessment (Nicell, 2008; Drew et al., 2007), and an useful indicator of peak concentration. Results for the 98th percentile concentration for D-LES, W-LES and FPM (scaled by the mean concentration) are presented in

Table 6-1. Again, W-LES results were higher than those obtained by using D-LES, both models showing lower values of the 98th percentile as the receptor distance downwind the obstacle is increased. FPM exhibited a different trend, with higher values of the 98% percentile as the receptor position was moved further downwind, indicating higher levels of concentration fluctuation, which might be a consequence of underestimation of the plume segment dispersion parameter.

Table 6-1: 98th percentile concentration $(C_{98}/\bar{C})$ at $y/H=0$ and $z/H=1$

Location (x/H)	D-LES	W-LES	FPM
1.5	4.4	7	0.13
2.5	4.5	5.1	4.9
3.5	4.0	4.1	6.8

Usually dispersion models used for regulation purposes are employed for odour impact assessment determining the P/M based on the predicted long term averaged time (usually 1-hr) concentration and Equation 3-50.

Smith (1973) recommended a value for the exponent of the power law in Equation 3-50 of $p = -0.35$ for neutral conditions and Santos et al. (2009) pointed out that values ranging from -0.12 to -0.7 are employed in the literature, depending on the type

of source. If a short averaging time tp is chosen equal to 5s, it gives $tp/tm = 0.0014$. By breaking up the concentration time series predicted by the LES simulations into smaller time intervals and calculating the respective mean concentrations it is possible calculate the value of p . These results are shown in Figure 6-14, which presents the variation of the calculated P/M ratio in terms of the ratio between averaging time and total time series duration for D-LES and W-LES, calculated at the top of the obstacle ($x/H=1.5$), at the cavity ($x/H=2.5$) and at the far wake ($x/H=3.5$) for $y/H=0.0$ and $z/H = 1.0$. Results are presented for tp/tm ranging from 0.0012 to 1.00. For each position, a linear fit of the results gives the value of the exponent p . At the top of the cube ($x/H = 1.5$) $p = -0.37$ ($R^2 = 0.88$) for D-LES and $p = -0.39$ ($R^2 = 0.89$) for W-LES. At the cavity ($x/H = 2.5$), $p = -0.31$ ($R^2 = 0.98$) for D-LES and $p = -0.32$ ($R^2 = 0.90$) for W-LES. At the beginning of the obstacle wake ($x/H = 3.5$), $p = -0.28$ ($R^2 = 0.96$) for D-LES and $p = -0.28$ ($R^2 = 0.96$) for W-LES. Santos et al. (2009) calculated the value of p close to the walls of a complex-shaped building in a field experiment, and found results ranging from -0.22 to -0.34 ($R^2 \geq 0.89$) for neutral atmospheric conditions, depending on the wind direction (tp/tm ranging from 0.0028 to 1). It is observed in Figure 6-14 that the calculated value of p decreases as the distance from the obstacle is increased, in accordance with the lower fluctuation levels observed downwind the obstacle (Figure 6-11). D-LES and W-LES results were similar although W-LES results were systematically higher, but within a maximum difference of 5.4% (observed at $x/H = 1.5$). The calculated values of p (absolute values) were higher than the value used in CALPUFF and AERMOD ($p = -0.2$) which gives a P/M concentration ratio of 3.73. LES results indicate $p = -0.2$ would probably be obtained further downwind the obstacle far wake. The results indicate that the use of a constant value for exponent p is not adequate. For instance the Smith (1973) recommended value would under predict the P/M ratio close to the obstacle and over predict the P/M ratio downwind the obstacle. Equation 3-50 was originally proposed to be used for an open terrain. The larger turbulent eddies close to the obstacle increase the dilution of the emitted pollutant resulting in lower concentration levels downwind. Schauburger et al. (2002), using a regulatory Gaussian model for odour impact assessment, suggested the use of an attenuation function where the P/M ratio obtained with the use of Equation 3-50 is lowered based on the distance from the source, wind speed and atmospheric stability for open terrain.

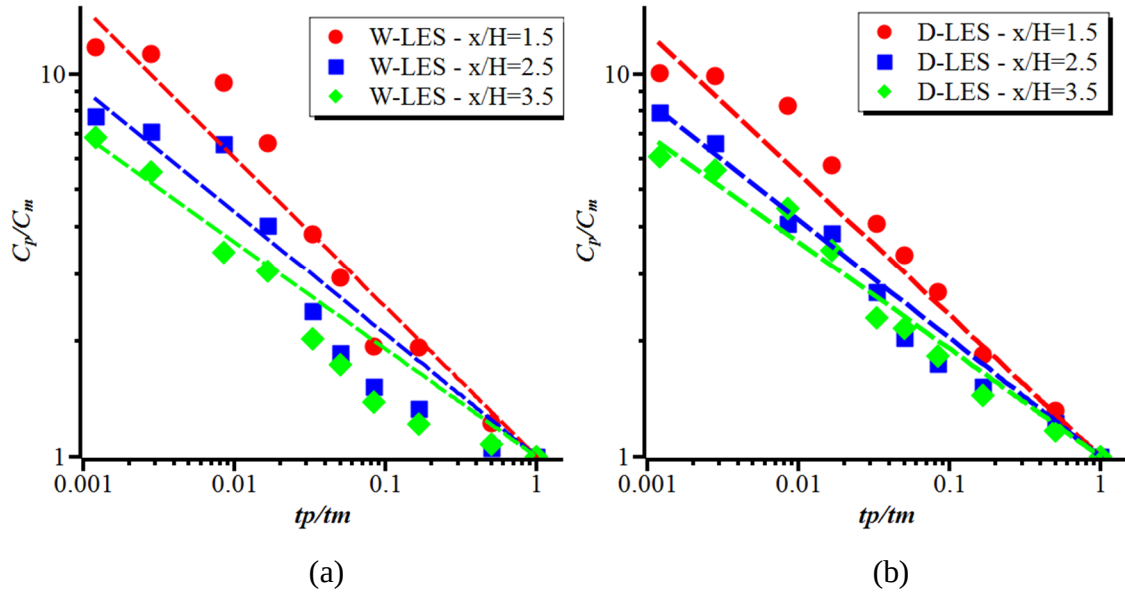


Figure 6-14: Peak-to-mean ratio in terms of the ratio between averaging time and total time series duration for W-LES (a) and D-LES (b), calculated at the top of the obstacle ($x/H=1.5$), at the cavity ($x/H=2.5$) and at the far wake ($x/H=3.5$) for $y/H=0.0$ and $z/H = 1.0$

In general, W-LES results showed better agreement with WT results than D-LES, although the results for mean wind speed, velocity fluctuation, mean concentration and concentration fluctuation profiles were similar. Due to its double filtering technique, D-LES simulations required twice the W-LES CPU time for each time step, so the use of W-LES is justified. The WALE sub grid scale model is thus employed in Experiments B and C, described in sections 6.2 and 6.3.

6.2 Flow and dispersion of odorant gases around a complex shaped building: a comparison between WALE LES model, Gaussian based models and wind tunnel data

6.2.1 Flow field

Figures 6-15, 6-16 and 6-17 present the velocity field on vertical planes: longitudinal ($y=0$ m), lateral ($x=0$ m), and horizontal ($z=1.6$ m) clearly showing the effect of the obstacle on the flow field. The colored backgrounds in these figures correspond to the mean vorticity. As the wind flows around the obstacle, regions with increased vorticity appear. It is interesting to note that the flow is highly asymmetrical in the y -direction, as a direct consequence of the building geometry. The observation of Figure

6-16 indicates that the left horseshoe vortex is higher larger and more intense than the right one. Also the complex shape of the building originates two recirculation zones which correspond to the blue zones downwind the obstacle shown in Figure 6-18, which also shows the mean velocity in a xy plane located at $z=1.6$ m (equivalent to humans nose height). This reference plane was chosen in accordance with wind tunnel data, where mean concentration and intermittency were measured (Section 6.2.2). The effect of the obstacle as a source of mechanical turbulence is also shown in Figures 6-19 to 6-22, where contours of vertical and horizontal mean velocity fluctuations are shown. Velocity fluctuation was higher for the horizontal component in the upwind face of the obstacle. This is a consequence of the aspect ratio of the building, with $W/H > 1$. Horizontal velocity fluctuation was also high in the first recirculation zone, upwind of the source. The mean wind speed in Figure 6-18, as well as the mean velocity fluctuations in Figures 6-19 to 6-22 are normalized by the reference ambient wind speed measured at 10 m height.

The reattachment point is located 12.4 m downwind the obstacle lee face according to W-LES results, and 26 m according to FPM results. FPM prediction was higher, as it models the obstacle as 42.5 m wide block. If the longest part of the building is considered, the obstacle dimensions would be 64.5 m (length) and 29.5 m (width) and 7.65 (height), which would result, according to Equation 5-9, in the reattachment point located at 14.54 m downwind the lee wall, very close to the distance predicted by W-LES.

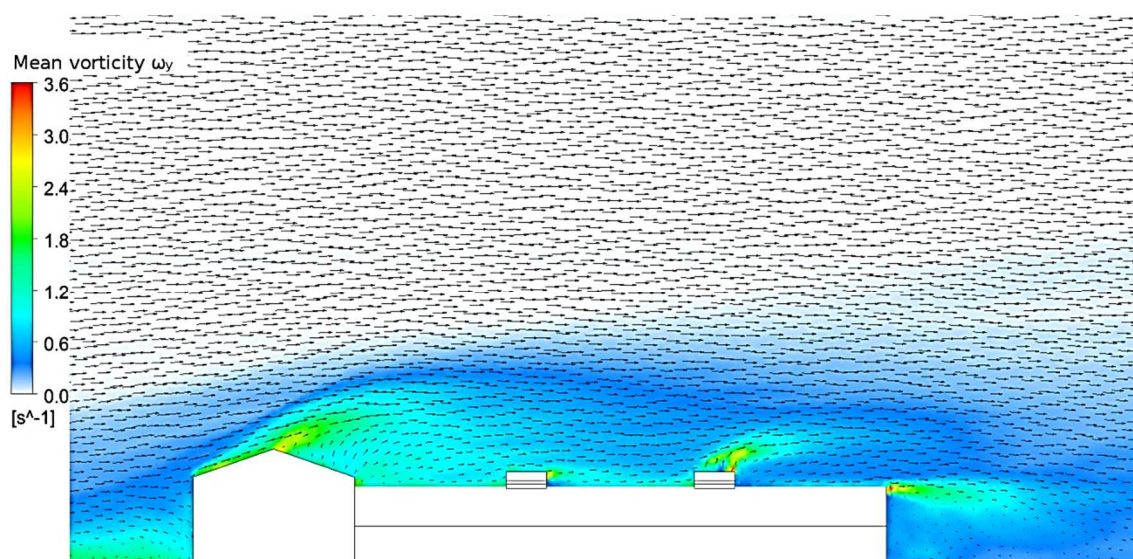


Figure 6-15: Mean velocity field around the obstacle (vectors) and mean vorticity (colours) at x - z plane ($y=0$).

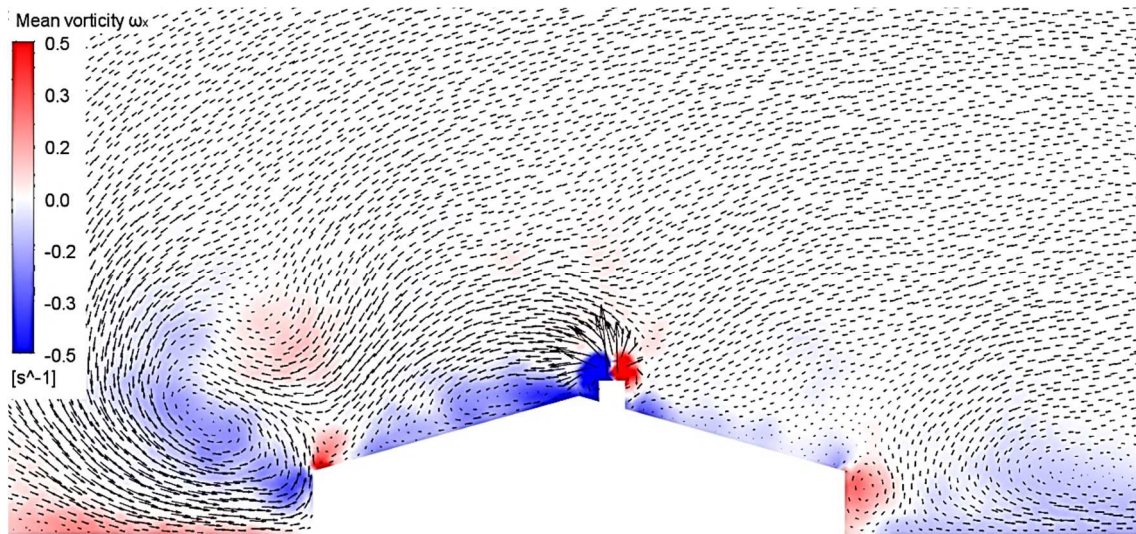


Figure 6-16: Mean velocity field around the obstacle (vectors) and mean vorticity (colours) at y-z plane ($x=0$).

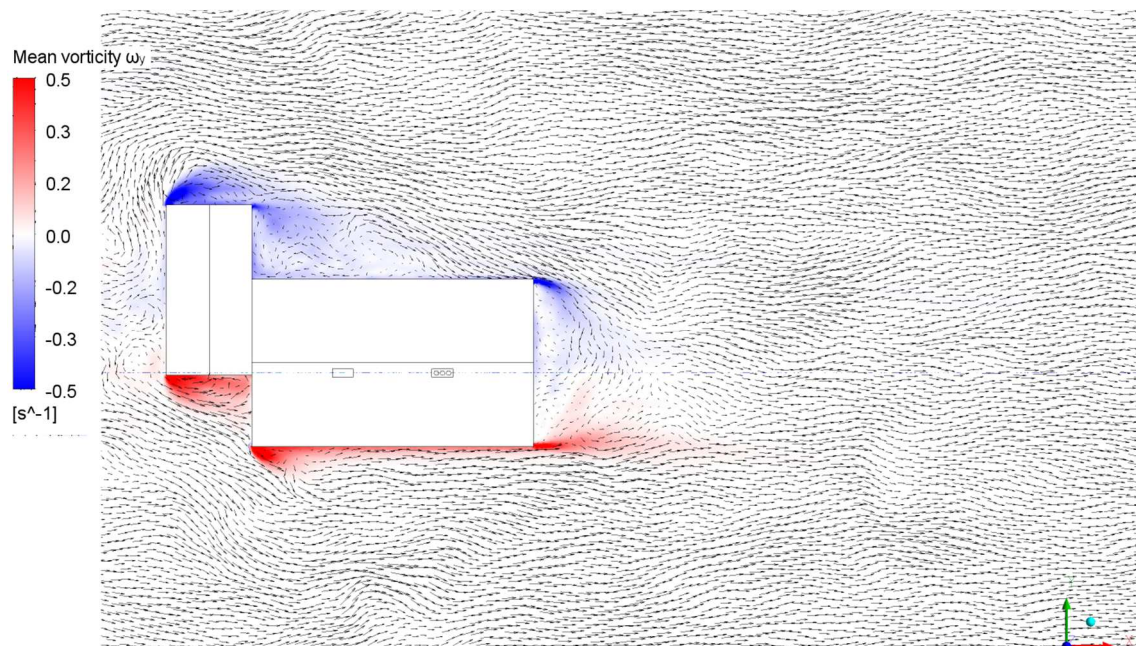


Figure 6-17: Mean velocity field around the obstacle (vectors) and mean vorticity (colours) at x-y plane ($z=1.6$ m).

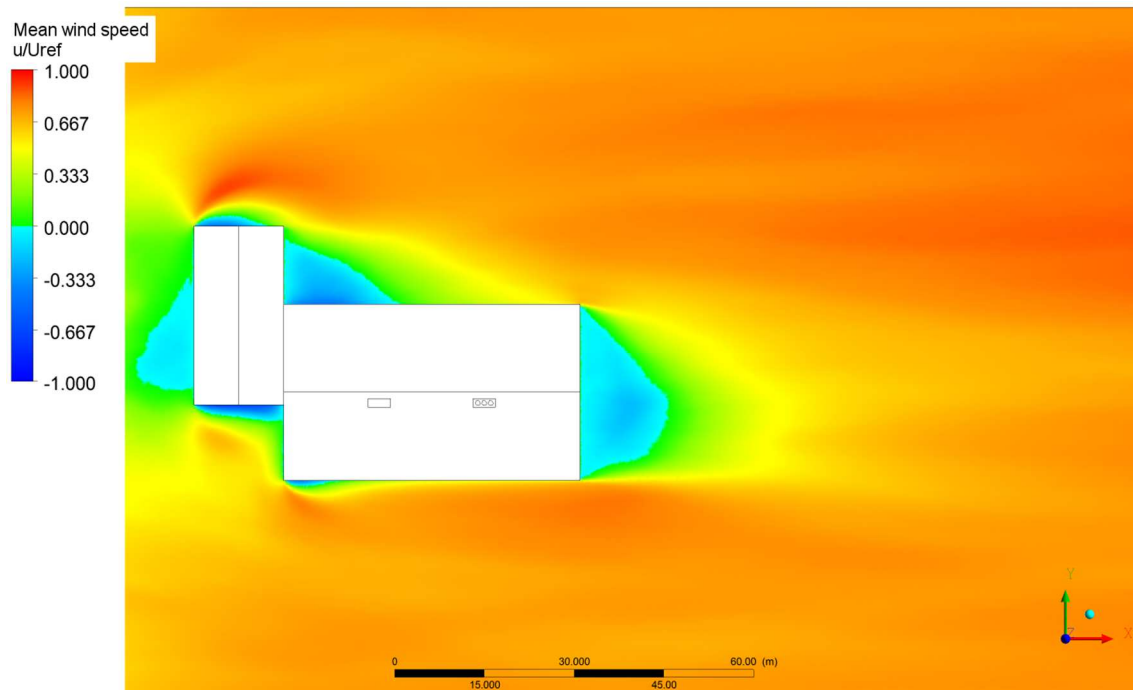


Figure 6-18: Mean normalized velocity contours around the obstacle at x-y plane ($z=1.6$ m). The blue areas correspond to negative values, indicating the recirculation zones.

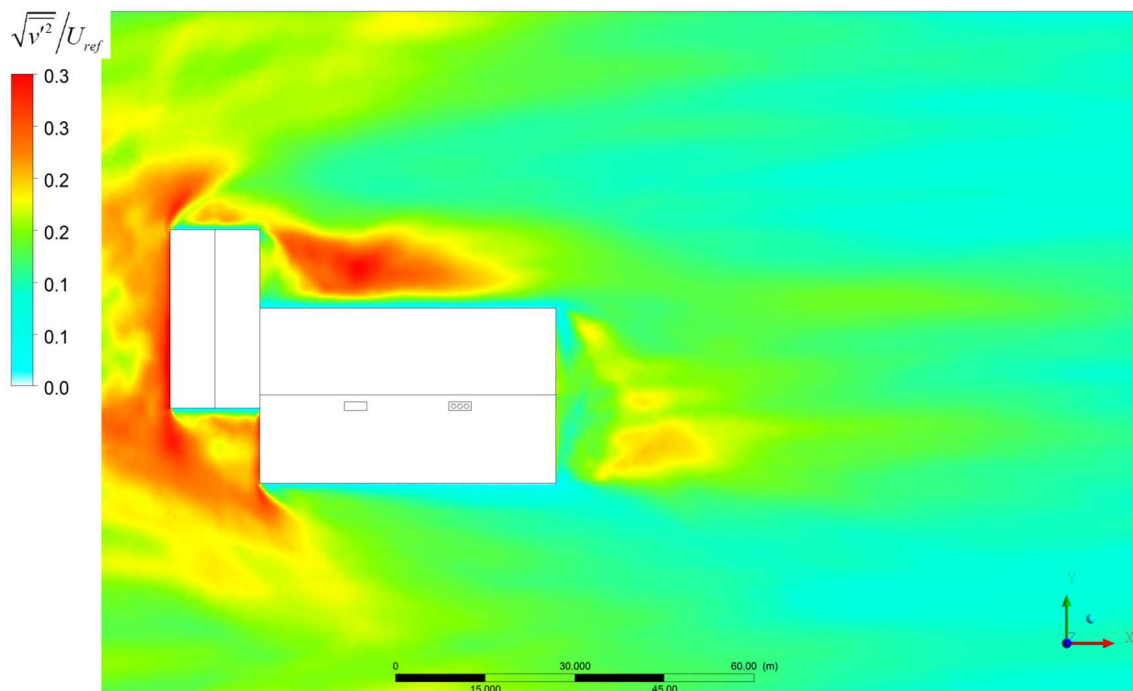


Figure 6-19: Normalized horizontal velocity fluctuation contours around the obstacle at x-y plane ($z=1.6$ m).

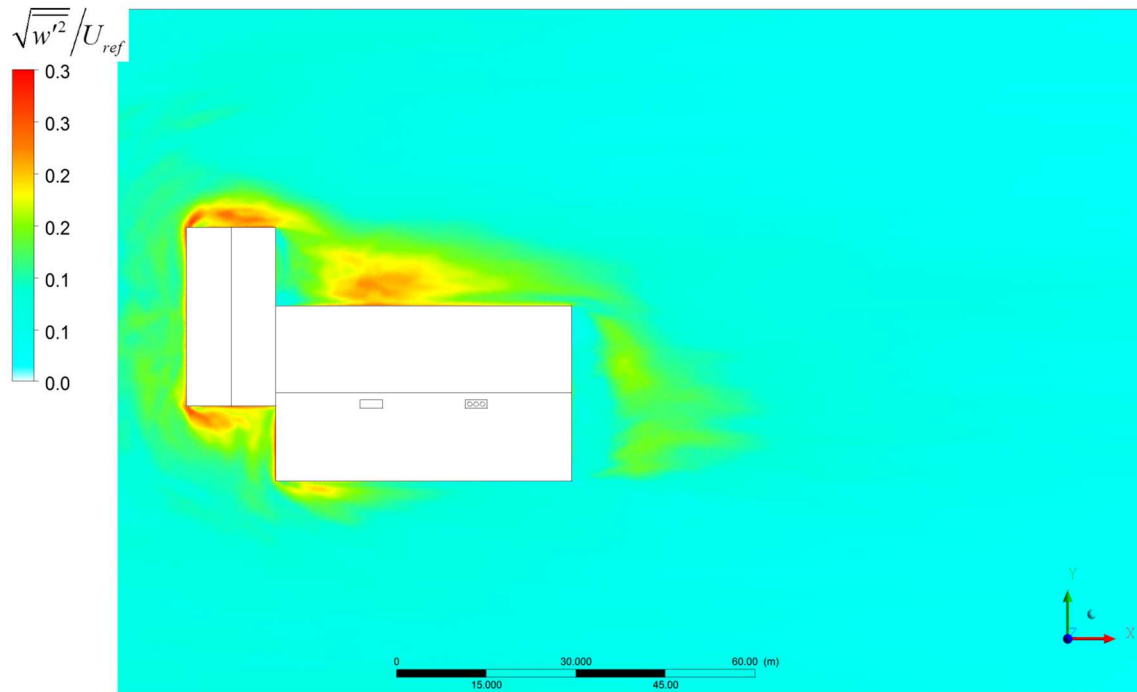


Figure 6-20: Normalized vertical velocity fluctuation contours around the obstacle at x-y plane ($z=1.6$ m).

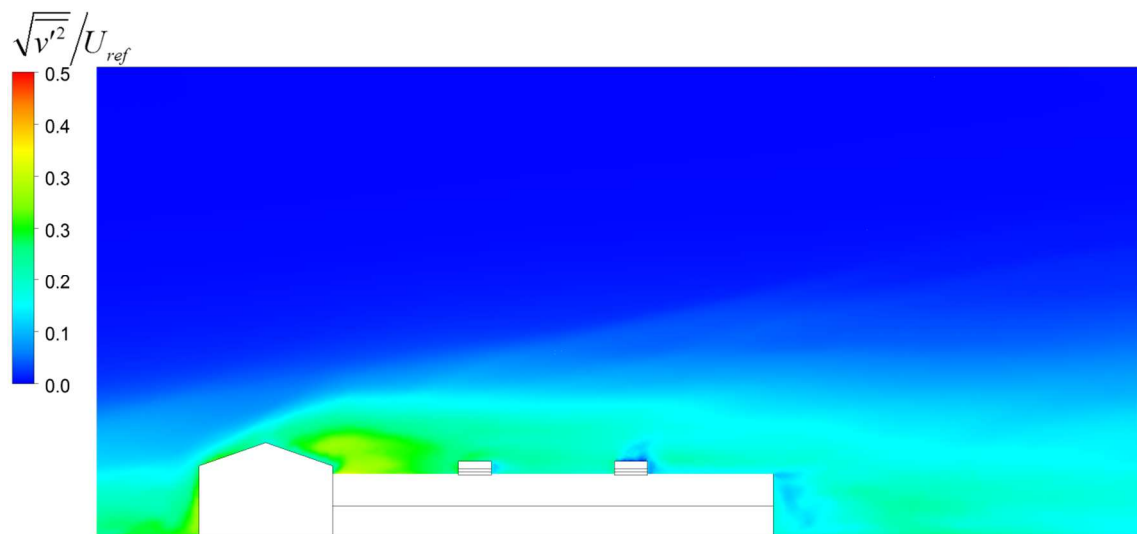


Figure 6-21: Normalized non-dimensional horizontal velocity fluctuation contours around the obstacle at y-z plane ($x=0$).

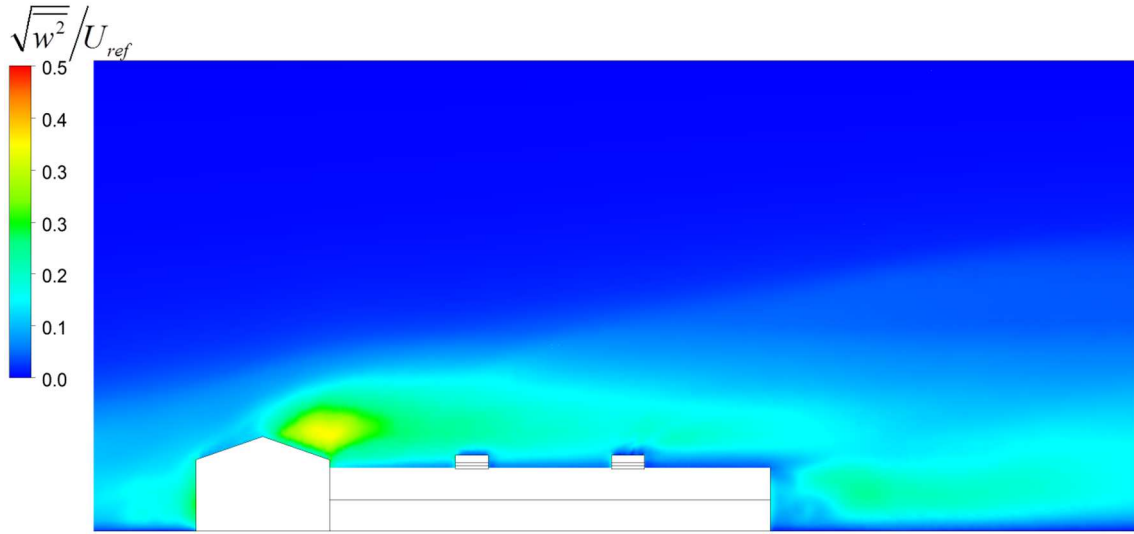


Figure 6-22: Normalized vertical velocity fluctuation contours around the obstacle at y-z plane ($x=0$).

Figure 6-23 shows the mean wind velocity, mean velocity fluctuation and shear stress profiles measured 80 m upwind the source. Values are normalized by the reference speed (mean wind speed measured at 10 m height). The W-LES wind speed profile agreed well with WT data (Figure 6-23a), although values below the reference height (10 m) were underestimated by a small amount. W-LES velocity fluctuation and shear stress results were close to WT data up to the reference height (10 m), which is higher than the obstacle height. Velocity fluctuations of the incoming flow for the numerical simulation are higher than WT data for $z < H_{ref}$, while shear stress is lower.

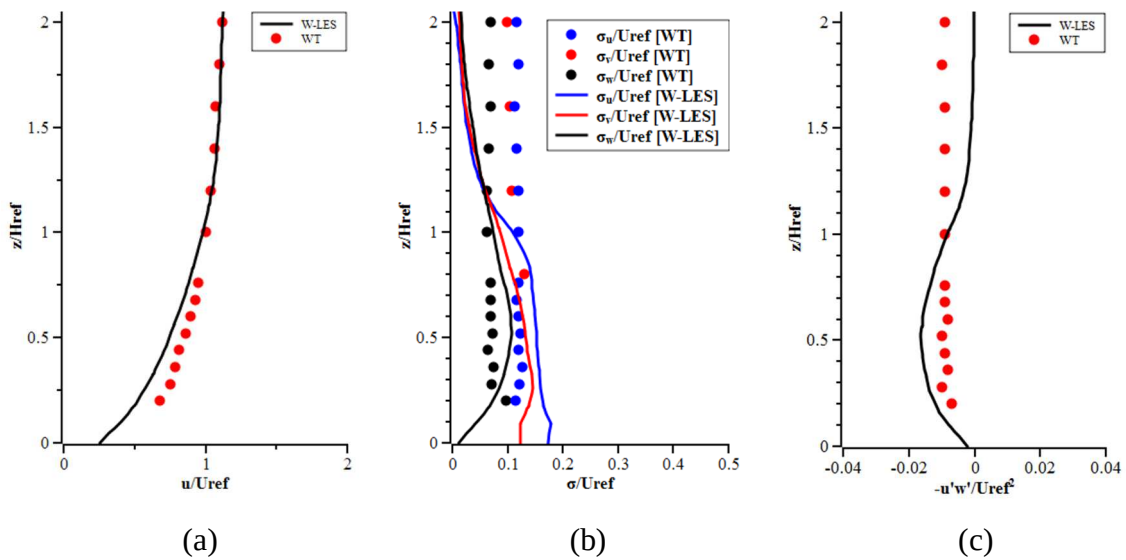


Figure 6-23: (a) incoming mean wind velocity profile, (b) mean velocity fluctuation and (c) shear stress profiles at 80 m upwind of the source. Values are normalized by the mean wind speed measured at $z=10$ m.

Figure 6-24 shows the longitudinal velocity spectral density $S_{uu}(f)$ of the axial incoming turbulent flow, measured at $z = H$, normalized by U_H and L_u (the axial integral turbulence length scale), compared to the theoretical ESDU (2001) spectrum for flat terrain under neutral stability (red dashed line). Overall, results showed lower levels for the W-LES spectrum in the inertial subrange, which presents a slightly faster decay rate than the theoretical $-5/3$ decay of the ESDU spectrum. The W-LES inertial subrange extends for about 3 decades before dropping at $fL_u/U_H = 400$ due to the grid resolution.

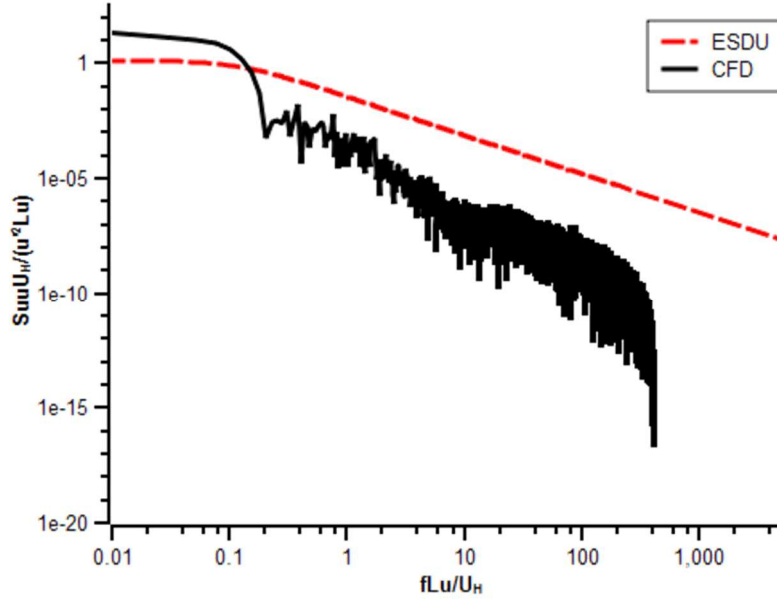


Figure 6-24: Spectral density of the incoming axial turbulence component at $z=H$, compared to the theoretical ESDU (2001) spectrum for flat terrain under neutral atmosphere condition.

In order to evaluate the averaging time choice, the autocorrelation functions of the three velocity components of the incoming flow, measured at $z=H$ are pictured in Figure 6-25, normalized by the square of the standard deviation of the respective velocity component. For instance, $R'_x(t) = R_{uu}(t) / \sigma_u^2 = \overline{u(t_0)u(t_0 + t)} / \sigma_u^2$. The correlations for all velocity components are small for a non-dimensional time interval $U_H t / H$ between 1 and 2, indicating that the employed computational averaging time of $169U_H / H$ is adequate. The area under each curve in Figure 6-25, computed between the points corresponding to $R'_x(t) = 1$ and $R'_x(t) = 0$ corresponds to the integral time scale (T), allowing

the determination of the turbulence integral length scale (Kaimal and Finnigan, 1994; Lim et al., 2009), $\Lambda = U_H T$. For the streamwise direction, $\Lambda/H = 4.4$, lower than expected for a typical neutral planetary boundary layer of a hundred meters, but sufficiently high to ensure the obstacle is fully immersed in the turbulent flow.

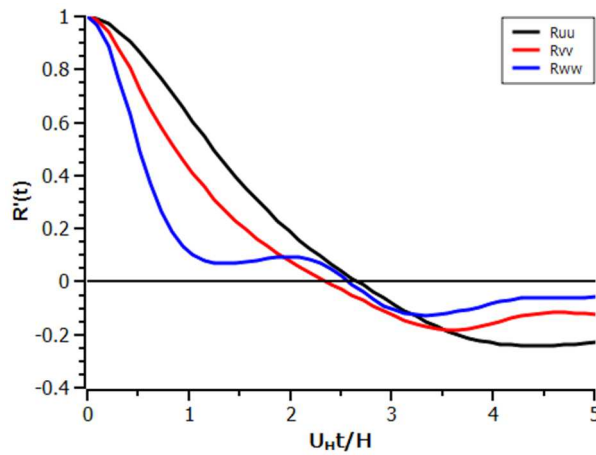


Figure 6-25: Normalized autocorrelation functions of the incoming flow, at $z=H$

6.2.2 Concentration field

Average concentration results are presented in Figures 6-26 to 6-28. Concentration results are normalized by the concentration measured at the source. Receptor height is 1.6 m above ground. AERMOD, CALPUFF, FPM and W-LES downwind concentration levels are within the same order of magnitude of the wind tunnel results (Figure 6-26a). As expected, concentration decayed with distance within the obstacle wake.

The highest average concentration predicted by the FPM model was observed just after the obstacle recirculating cavity, which seems to agree with the wind tunnel results, although the lack of other monitoring points within the cavity in the wind tunnel experiment does not give a detailed behavior of the tracer gas dispersion in that region. The same is true for the W-LES results, which show the maximum concentration occurring after the cavity. FPM predicted concentrations within the cavity did not show great variation as the model approach, based on PRIME, employs the same value for the dispersion coefficients within the cavity limits. The predicted average concentration peak near $x=50$ m is situated on the transition zone, where the cavity starts to act as a volume source emitting through the obstacle wake. Inside the cavity, AERMOD, CALPUFF

and FPM results showed much lower values for the concentration. This might indicate PRIME overestimates the plume dispersion parameter inside the cavity region.

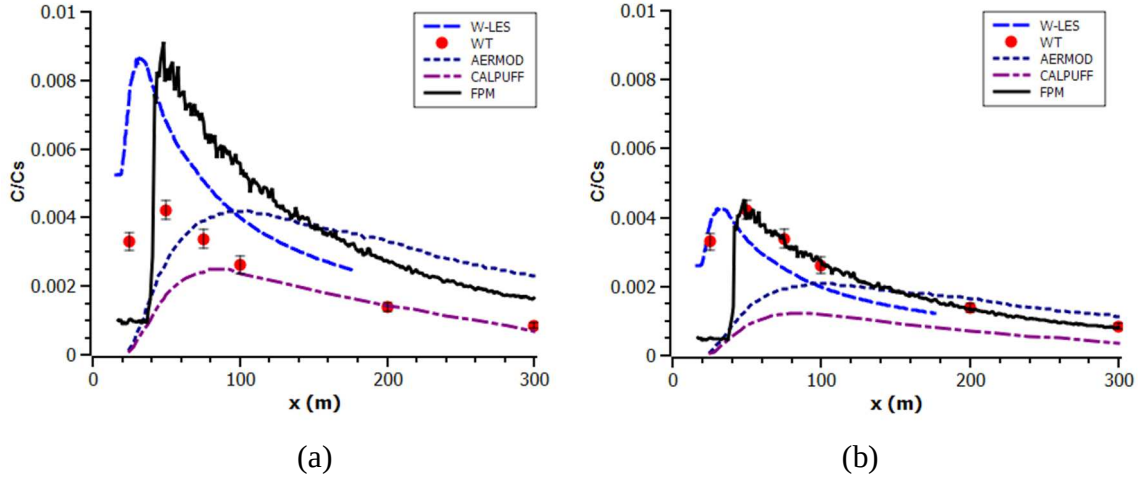


Figure 6-26: (a) non-dimensional average downwind concentration levels ($z=1.6$ m); (b) non-dimensional downwind average concentration levels ($z=1.6$ m) for an averaging time of 2000 minutes obtained by using Equation 3-50 ($t_p/t_m=0.03$ and $p=-0.2$)

The highest concentration values predicted by AERMOD and CALPUFF occurred further downwind than indicated by W-LES and FPM and also observed in the wind tunnel. Downwind $x=100$ m, CALPUFF concentrations agreed well with WT results.

It is important to note that the WT results correspond to a 2000 minutes averaging time period, while FPM, AERMOD and CALPUFF results are for a 1 hour averaging time. The numerical simulation run corresponded to 10.4 minutes. In terms of non-dimensional time ($t^* = tU_H/H$) the averaging times were $t^*_{WT} = 36000$, $t^*_{FPM} = 1080$ (same for AERMOD and CALPUFF) and $t^*_{W-LES} = 169$. As observed in section 6.2.1, t^*_{W-LES} was adequate to the simulation domain. The WT time series of measured quantities was split in shorter intervals in order to assess the influence of the averaging time (Aubrun and Leitl, 2004) and although the available database does not include the actual time series, the standard deviations of the 1-hour averaging time statistics from the 2000-minute statistics are included, and are shown on the error bars of WT results in Figures 6-26, 6-27 and 6-28. It is interesting to note that, despite the averaging time difference, the deviations from the mean are small. This is a direct consequence of the physical size of the WT domain, which limits the size of larger turbulent scales, responsible for the plume meandering (Mavroidis et al, 2003, Aubrun and Leitl, 2004, Lim et

al., 2009). Downwind $x > 100$ m, CALPUFF results are within the expected WT 60 minute range.

Mean concentrations for the longer averaging time of 2000 minutes for FPM, CALPUFF and AERMOD can be estimated using Equation 3-50, with $t_p = 60$ minutes, $t_m = 2000$ minutes, $(t_p/t_m) = 0.03$ and $p = -0.2$ (Figure 6-26b). Although the value of p might depend on the downwind distance, the value $p = -0.2$ was employed as it is the recommended value in the CALPUFF guidelines. FPM results showed excellent agreement with WT in receptor positions located after the cavity. Concentration results inside the cavity are still under estimated, following AERMOD and CALPUFF results. W-LES, and AERMOD converted results are much closer to WT, with AERMOD approaching WT downwind $x > 100$ m, while W-LES and CALPUFF values underestimate WT results.

Figure 6-27 shows the lateral concentrations observed at $x = 50$ m (Figure 6-27a) and at $x = 100$ m (Figure 6-27b). Again, all results were within the same order of magnitude. Maximum concentrations are predicted at the centreline plume location ($y \approx 0$ m) by all models, but both W-LES and FPM over predicted the wind tunnel results. Lateral concentration decay values predicted by W-LES were much closer to WT data than predicted by FPM. AERMOD and CALPUFF results showed less lateral spread of the plume. Results show W-LES predicts the effect of the obstacle on the lateral plume spreading caused by the obstacle better than the Gaussian based models. FPM results suggest the plume is much wider than what is observed in WT experiment and predicted by W-LES, possibly indicating an over prediction of the lateral dispersion coefficients and thus, higher levels of fluctuation of the plume centerline. The same trend is observed at $x = 50$ and $x = 100$ m. These results might be explained by a possible combination of over prediction of σ_y and σ_z and under estimation of σ_{yp} and σ_{zp} . It is worth mentioning that Högström original formulations for σ_{yp} and σ_{zp} did not include the effect of obstacles. At $x = 100$ m, CALPUFF results agreed very well with WT data, while AERMOD results were closer to W-LES.

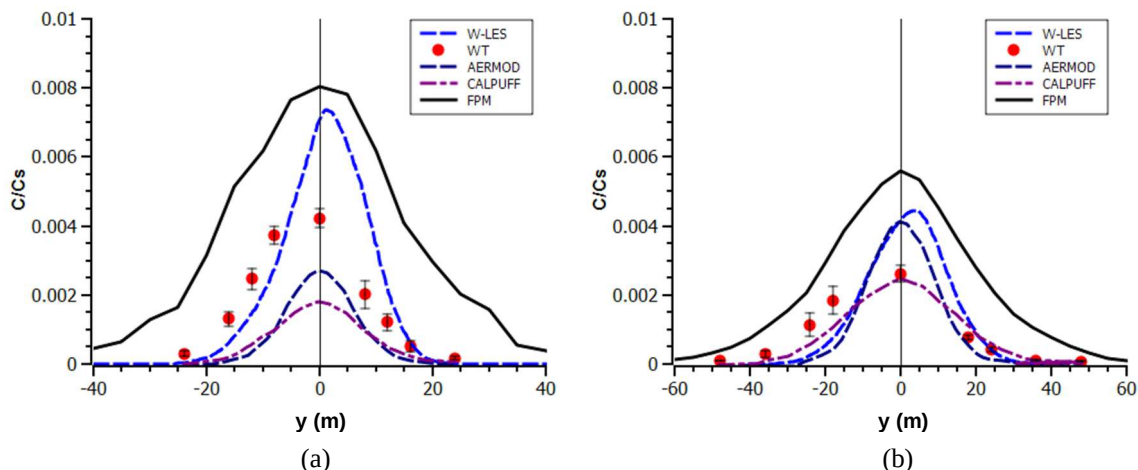


Figure 6-27: (a) non-dimensional average lateral concentration levels ($x=50$ m, $z=1.6$ m); (b) non-dimensional average lateral concentration levels ($x=100$ m, $z=1.6$ m).

If Equation 3-50 is applied (with the same parameters used for downwind concentration), FPM results agreement with WT data is improved, while all the other results start to underestimate plume spread, as shown in Figure 6-28.

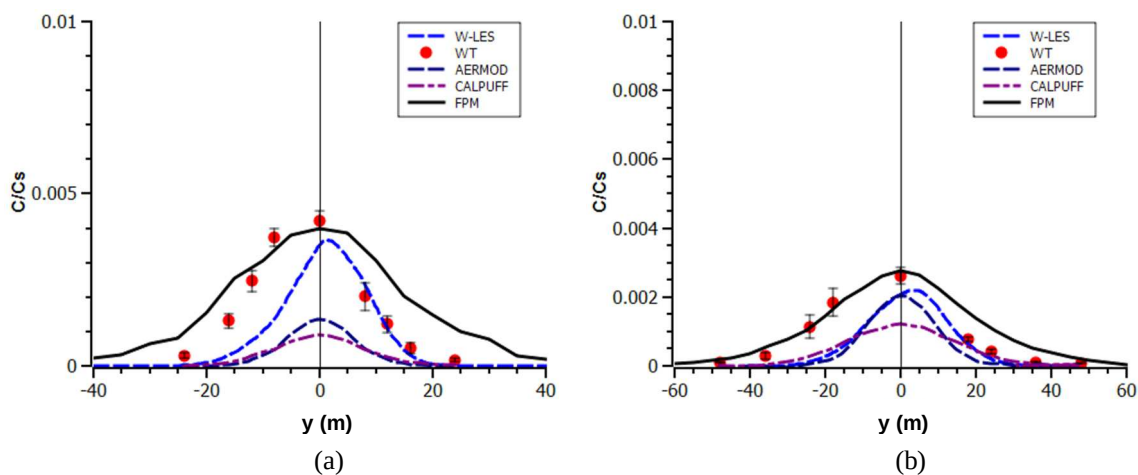


Figure 6-28: (a) non-dimensional average lateral concentration levels ($x=50$ m, $z=1.6$ m) and (b) non-dimensional average lateral concentration levels ($x=100$ m, $z=1.6$ m), for an averaging time of 2000 minutes obtained through the use of Equation 3-50 ($t_p=60$ minutes, $t_m = 2000$ minutes and $u=0.2$).

6.2.3 Intermittency

Intermittency is defined as the percentage of time during which the concentration stays above a defined threshold (Aubrun, S. & Leitl, B., 2004). Following the WT experiments, the chosen concentration threshold was 0.25% of the average concentration measured at the source (C_s), simulating the detection threshold of an odorant compound. Intermittency results are presented in Figure 6-29, and Figure 6-30. Figure 6-29

shows W-LES and WT downwind intermittency levels observed at selected points along the x-direction ($z=1.6$ m). All results indicate intermittency levels decay with downwind distance after reaching its maximum value. W-LES results over predicted WT at the measured points ($x=25$ m, $x=50$ m, $x=75.2$ m and $x=100$ m, $y=0$ and $z=1.6$ m), although the location of the highest intermittency was at $x=50$ m. As for FPM results, the highest predicted intermittency level was much further downwind than the observed in WT data. The observed behavior of FPM results might be due to the formulation used for calculating concentration: in the far wake, concentration is the result of the elevated plume and the portion of the plume captured by the near wake and re-emitted by the cavity as a volume source, obtained by Equation 5-50. As downwind distance increases, the influence of the cavity emitted plume decreases. High intermittency levels, along with increased lateral plume spread (Figure 6-30a and Figure 6-30b) indicate that values of σ_{yp} and σ_{zp} are also under predicted outside the cavity, resulting in increased mean concentration and intermittency levels in the portion of the plume not captured by the near wake.

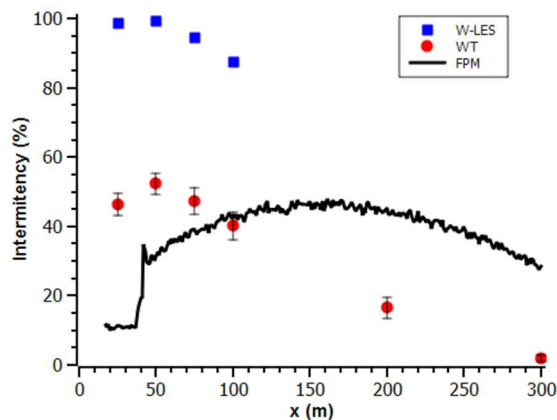


Figure 6-29: downwind intermittency levels ($z=1.6$ m).

It can be noted that although FPM average concentrations observed at downwind distances greater than about 220 m (60 min. averaging time), or about 150 m in WT, are below the chosen concentration threshold, fluctuation would still produce odour events which can cause odour perception to a nearby receptor. This fact demonstrates the importance of modelling plume fluctuation.

Figure 6-29 also indicates that intermittency levels are greatly over predicted by W-LES, even at locations where the predicted concentration is close to WT observed levels. This result indicates that the W-LES plume centreline fluctuation is much less

intense than WT and FPM. In fact, the analysis of the FPM and CFD concentration series at the four selected points located at $x=25.2$ m, 50 m, 75.2 m and 100 m ($y=0$ and $z=1.6$ m) shows concentration fluctuation intensity levels (standard deviation of the concentration time series divided by the average concentration) are between 4 and 5 times higher in FPM than W-LES (

Table 6-2), possibly due to lower turbulence intensity levels predicted by W-LES at $y=0$ and $z=1.6$ m in relation to WT data, although this fact cannot be confirmed because of the lack of turbulence measurements downwind the obstacle in the WT database. This behaviour was not observed in the lateral intermittency distribution (Figure 6-30a and Figure 6-30b), where W-LES results were close to WT levels, indicating the lateral influence of the obstacle is correctly reproduced. Both at $x=50$ m and at $x=100$ m, WT lateral intermittency levels were over predicted by FPM. Again this might be due to FPM under estimating σ_{yp} and σ_{zp} for the elevated plume portion, resulting in higher concentration levels.

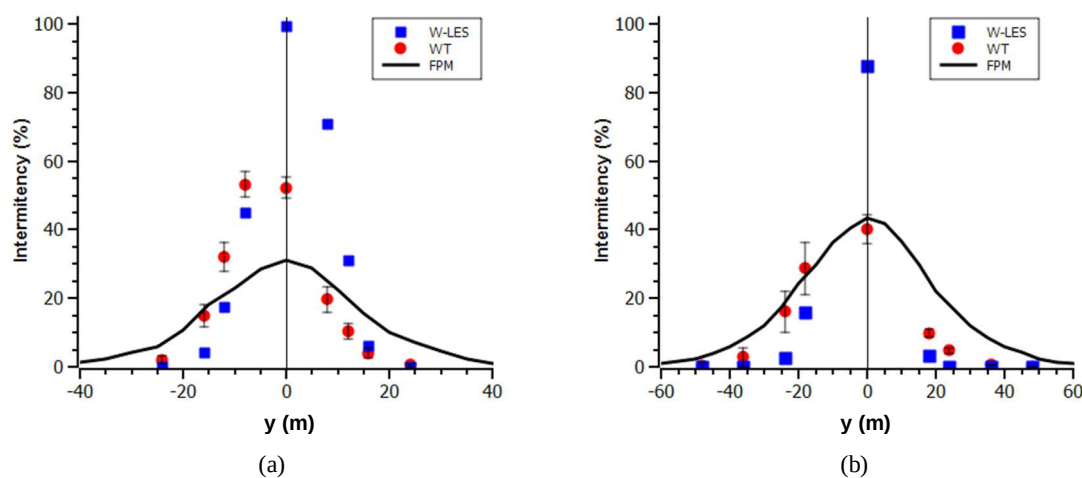


Figure 6-30: intermittency levels at (a) $x=50$ m, $z=1.6$ m; and at (b) $x=100$ m, $z=1.6$ m.

Table 6-2: FPM and W-LES concentration fluctuation intensity for different receptor positions ($y=0$ and $z=1.6$ m)

	$x = 25.2$ m	$x = 50$ m	$x = 75.2$ m	$x = 100$ m
FPM	1.59	1.12	1.24	1.25
CFD	0.28	0.28	0.34	0.32

The 98th percentiles concentrations normalized by C_s for different receptor positions are presented in Figure 6-31a at downwind distances at $x=25$ m, $x=50$ m, $x=75$ m and $x=100$ m. W-LES results showed good agreement with WT. Except at $x=25$ m, FPM overestimated WT data, with the maximum difference observed at $x=50$ m. If Equation 3-50 is used to estimate concentration for a 2000-minute averaging time ($t_p/t_m = 0.03$), FPM results present a better agreement with WT data, especially at $x=75$ m and $x=100$ m, while CFD results under estimate WT (Figure 6-31b).

Additionally, AERMOD and CALPUFF concentration results, converted using Equation 3-50 for a 5-second averaging time are also presented, with $t_p/t_m = 0.001389$ and $p = -0.2$, following the practice of estimating peak concentrations from long-term results; the converted results under estimate the WT 98th percentile concentration, showing better agreement at receptor positions further than $x=75$ m.

Lateral distribution of the 98th percentile concentration normalized by C_s are shown in Figure 6-32 ($x=50$ m) and Figure 6-33 ($x=100$ m). Similarly to the downwind variation, W-LES results agreed to WT, with FPM agreeing best with WT after conversion using Equation 3-50. AERMOD and CALPUFF concentration results, converted using Equation 3-50 for a 5-second averaging time are also presented, with predicted peak concentrations under estimating the WT 98th percentile.

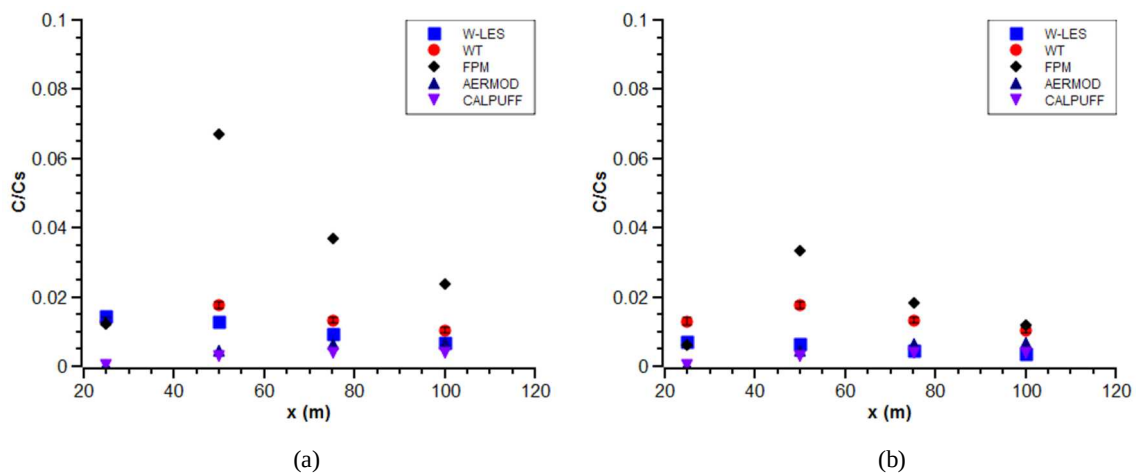


Figure 6-31: Downwind distribution of the 98th percentile concentration normalized by C_s : (a) FPM results for a 60-minute averaging time and (b) FPM and W-LES results for $t_p/t_m=0.03$ after conversion using Equation 3-50. AERMOD and CALPUFF peak concentrations for a 5-second averaging time predicted by Equation 3-50 are also shown.

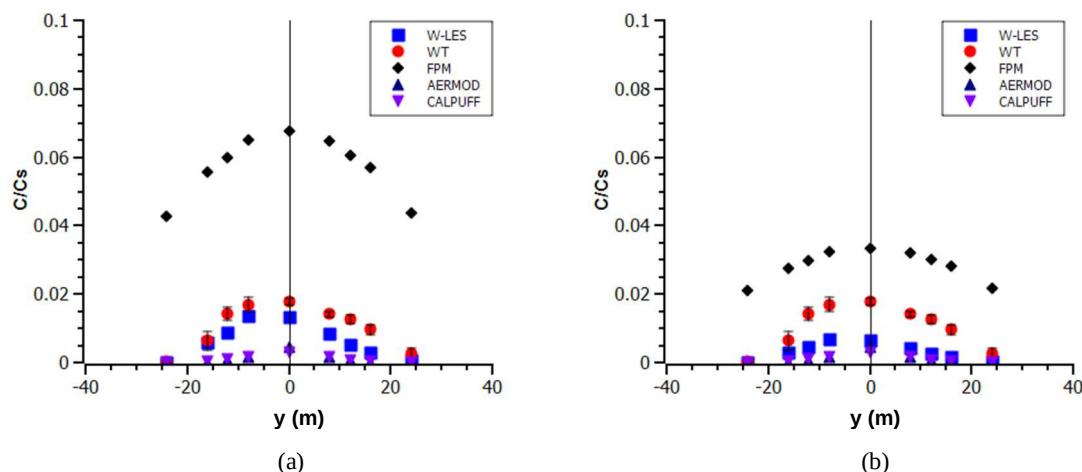


Figure 6-32: Lateral distribution of the 98th percentile concentration normalized by CS at $x=50$ m: (a) FPM results for a 60-minute averaging time and (b) FPM and W-LES results for $t_p/t_m=0.03$ after conversion using Equation 3-50. AERMOD and CALPUFF peak concentrations for a 5-second averaging time predicted by Equation 3-50 are also shown.

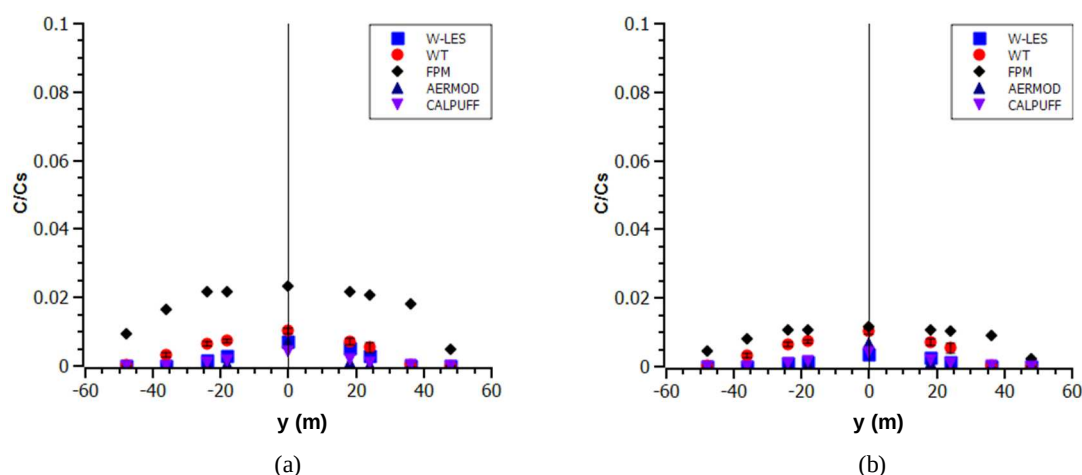


Figure 6-33: Lateral distribution of the 98th percentile concentration normalized by CS at $x=100$ m: (a) FPM results for a 60-minute averaging time and (b) FPM and W-LES results for $t_p/t_m=0.03$ after conversion using Equation 3-50. AERMOD and CALPUFF peak concentrations for a 5-second averaging time predicted by Equation 3-50 are also shown.

6.3 Flow and dispersion of odorant gases around a cubical building: a comparison between WALE LES model, Fluctuating Plume Model and field experimental data

The obstacle was a model of a cubic building with height $H=1.15$, corresponding to a full scale building of 10m. The FPM simulation used full scale dimensions.

6.3.1 Flow field

Mean velocity field are shown in Figure 6-34 (xz plane, $y=0$), Figure 6-35 (xy plane, $z=H/2$) and Figure 6-36 (yz plane, $z=2$). Recirculation zones are originated on top and downwind the building, as well as near the ground, near the upwind face of the cube, as can be seen in the red zones shown in Figure 6-37. The reattachment point was at $2.44H$ from the building lee face, a higher value than that for Experiment A ($1.3H$) and calculated by FPM using Equation 5-10 ($1.46H$). It is interesting to note that the shape of the downwind cavity (xz plane, $y=0$) follows the expected trend until the lower third of the obstacle and then it starts to extend downwind.

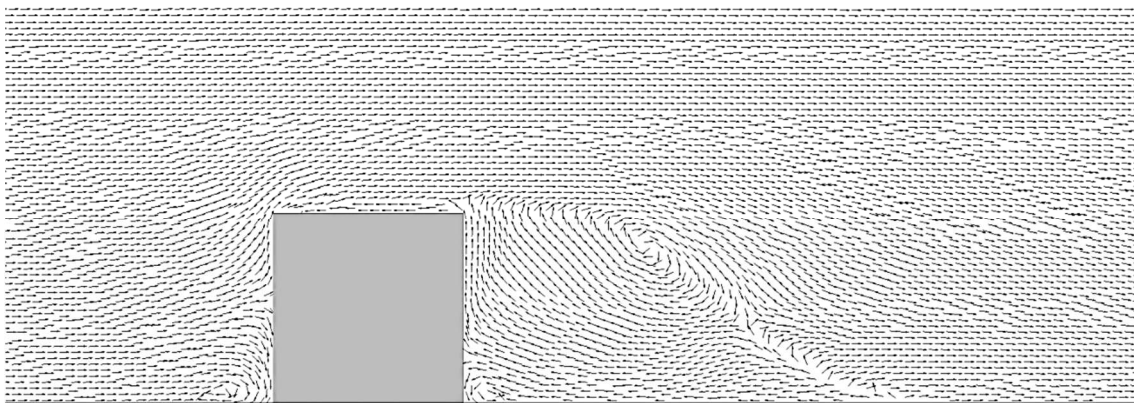


Figure 6-34: Mean velocity field around the obstacle, at plane xz ($y=0$).

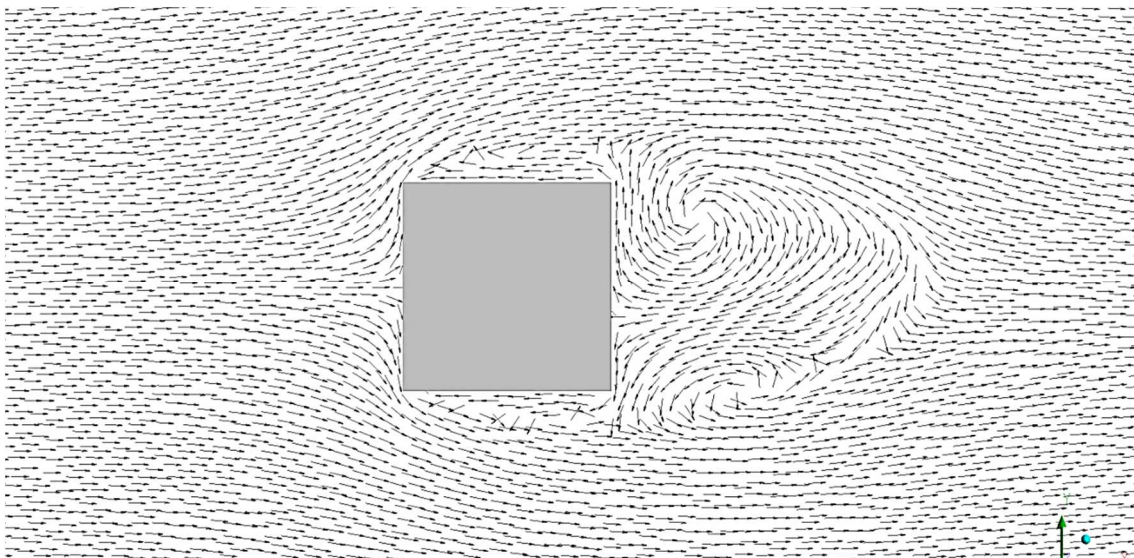


Figure 6-35: Mean velocity field around the obstacle, at plane xy ($z=H/2$).

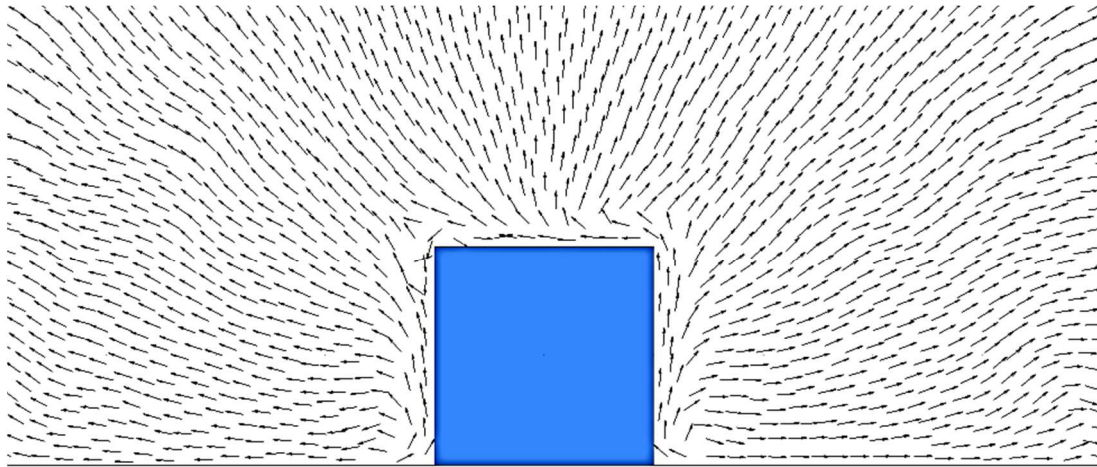


Figure 6-36: Mean velocity field around the obstacle, at plane yz ($x=2.5H$).



Figure 6-37: Recirculation zones upwind, on top and downwind the obstacle, showing the observed and the expected cavity length.

The incoming non-dimensional wind velocity profile along with the fluctuation velocities are shown in Figure 6-38a and 6-38b. Values are normalized by the wind speed measured at building height. Although there was no direct measurement of the incoming profile on the experiment database, a theoretical profile is developed based on available data on the mean wind velocity measured at building height (U_H), the roughness length (z_0) and friction velocity (u_*). W-LES wind velocity profile is presented at $x/H=0$ and $y/H=0$, corresponding to the source position. It shows a small reduction in velocity between $z/H=1$ and $z/H=0.2$ compared to the theoretical field profile, possibly due to the proximity of the obstacle.

Mean velocity fluctuation profiles normalized by U_H presented in Figure 6-38b show that longitudinal and horizontal turbulence levels are slightly under predicted when compared to the theoretical ambient levels, obtained from the field friction velocity using Arya (2001) expressions for neutral atmosphere (Equations 6-1):

$$\frac{\sigma_u}{u_*} = 2.4, \quad \frac{\sigma_v}{u_*} = 1.9 \quad \text{and} \quad \frac{\sigma_w}{u_*} = 1.3 \quad (6-1)$$

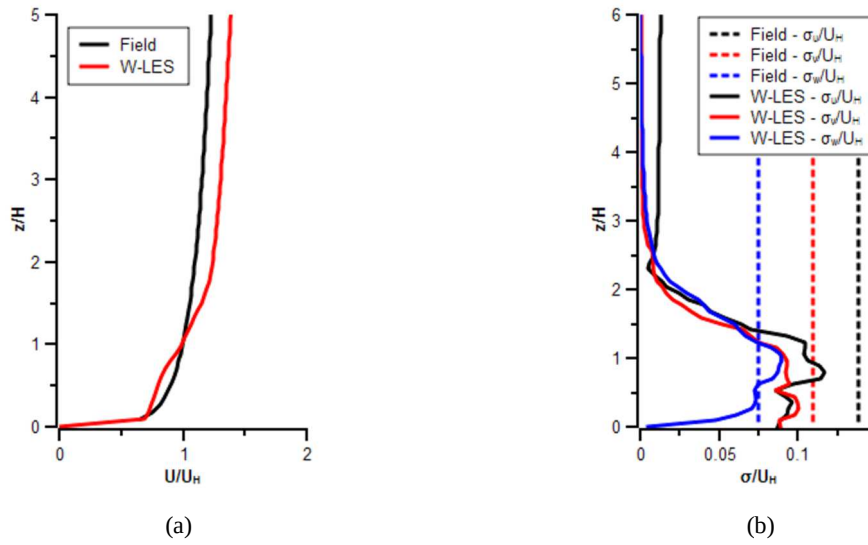


Figure 6-38: (a) incoming mean wind velocity profile and (b) incoming mean velocity fluctuation profiles. CFD profiles measured at $x/H=0$ and $y/H=0$ are compared to theoretical field profiles.

The longitudinal velocity spectral density $S_{uu}(f)$ of the axial incoming turbulent flow, measured at $z = H$, normalized by U_H and L_u (the axial integral turbulence length scale) is shown in Figure 6-39 and is compared to the theoretical ESDU (2001) spectrum for flat terrain under neutral stability (red dashed line). W-LES spectrum agreed well with ESDU for about a decade on the inertial subrange and then presented a faster decay. A similar result was found by Lim et al. (2009) in a LES simulation of flow around a cubical obstacle. W-LES inertial subrange extends for 2.5 decades before dropping at $fL_u/U_H = 320$ due to the grid resolution.

Figure 6-40 presents the autocorrelation functions of the three velocity components of the incoming flow normalized by the square of the standard deviation of the respective velocity component, measured at $z=H$. As already mentioned, the autocorrelation function is defined as $R'_x(t) = R_{uu}(t) / \sigma_u^2 = \overline{u(t_0)u(t_0+t)} / \sigma_u^2$. The correlations for

all velocity components are small for a non-dimensional time interval $U_H t/H = 1$, indicating that the employed computational averaging time of $60U_H/H$ is adequate.

The turbulence integral length scale (Kaimal and Finnigan, 1994; Lim et al., 2009), defined as $\Lambda = U_H T$ is determined based on the area under the normalized autocorrelation curve between $R_x'(t)=1$ and $R_x'(t)=0$, which corresponds to the integral time scale (T). For the streamwise direction, $\Lambda/H = 3.5$, sufficiently high to ensure the obstacle is fully immersed in the turbulent flow.

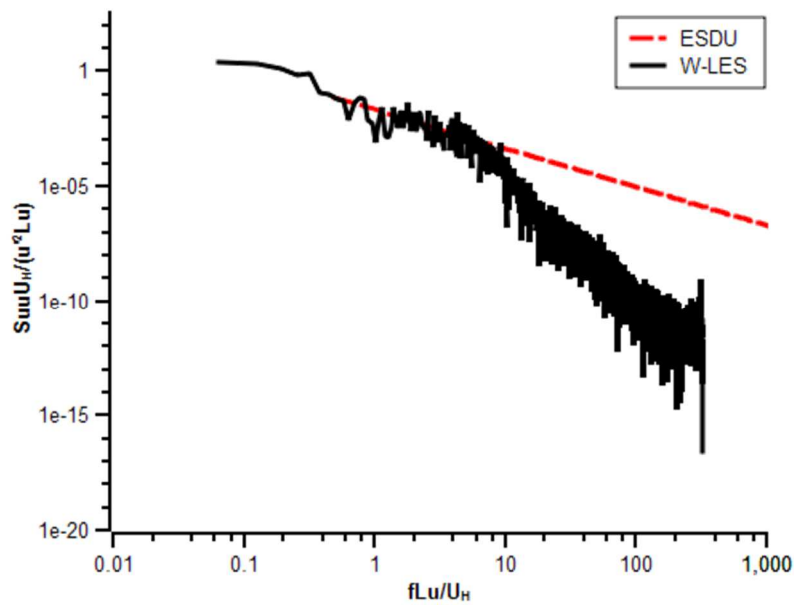


Figure 6-39: Spectral density of the incoming axial turbulence component at $z=H$, compared to the theoretical ESDU (2001) spectrum for flat terrain under neutral atmosphere condition.

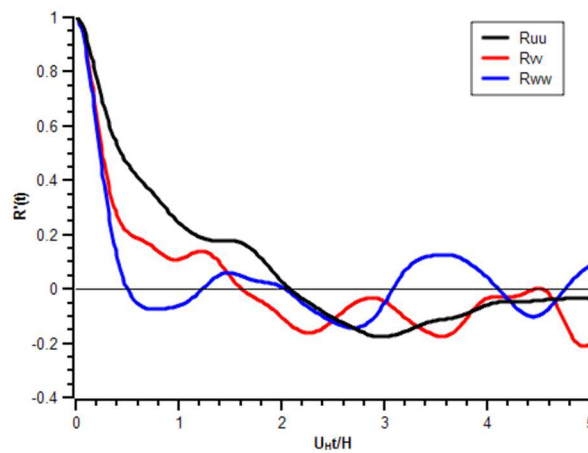


Figure 6-40: Normalized autocorrelation functions of the incoming flow, at $z=H$

6.3.2 Concentration Field

Following Mavroidis et al. (2003), concentration results are presented as non-dimensional concentration (Kc), defined as:

$$Kc = \frac{CU_H H^2}{Q} \quad (6-2)$$

where C is the measured concentration [kg/m^3], U_H [m/s] is the mean wind speed measured at $z=H$ and Q is the source flow rate [kg/s]. Concentration is presented for five different receptor positions: $x/H=0.5$, $x/H=2$, $x/H=3$, $x/H=4$ and $x/H=5$ ($y/H=0$ and $z/H=1$), with $x/H=0$ corresponding to the building lee wall. Concentration results are also presented for a wind tunnel (WT) experiment described by Mavroidis et al. (2003), which employed a cube with $H=0.15$ m. The averaging time was 3 minutes in the field experiments, corresponding to $t_{field}^* = 659$, where $t^* = U_H t / H$. For the W-LES, FPM and WT experiments, $t_{W-LES}^* = 60$ (12.55s), $t_{FPM}^* = 1516$ (60 minutes) and $t_{WT}^* = 1340$ (2 minutes), respectively. FPM results are also presented for an averaging time of 26 minutes, corresponding to $t_{FPM}^* = t_{field}^* = 659$, using Equation 3-50, with $t_p = 26$ minutes, $t_m = 60$ minutes and $p = 0.2$, $(t_m/t_p) = 1.182$.

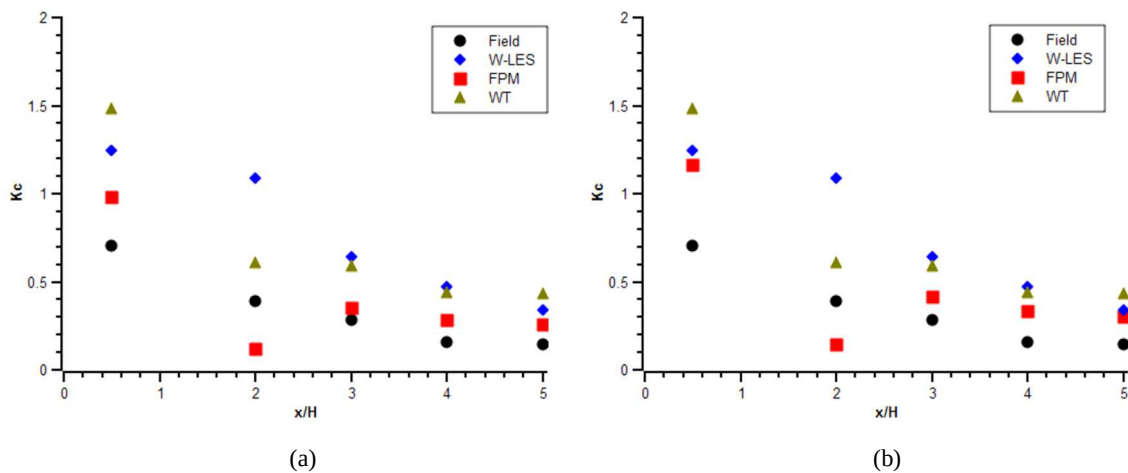


Figure 6-41: Downwind variation of the concentration coefficient (Kc) after the obstacle, with FPM results for (a) 60-minute averaging time and (b) 26-minute averaging time ($t_m/t_p = 1.182$).

Downwind concentration distribution is shown in Figure 6-41a. W-LES results agreed well with WT, especially downwind $x/H=3$ (distance measured from the obstacle lee wall). This is explained by the limited size of the W-LES and WT domains, which

limits the size of the largest turbulent scales (Mavroidis et al., 2003; Aubrun and Leiti, 2004; Lim et al., 2009). Field results were lower than WT and W-LES results due to increased dispersion.

FPM mean concentration results increased after conversion to the shorter averaging time (Figure 6-41b), but were still close to the field results, as the ratio of the longer and shorter averaging time concentration is 1.034. Another reason for the proximity of the results is that, closer to the obstacle, mechanical turbulence induced by the building plays a major role in dispersing the plume. As a consequence, as long as the averaging time is sufficiently long to capture the building induced turbulence scales it is possible that, even if the field averaging time were longer, field results would not differ, provided that the wind direction variance remains low. According to the field experiment database, the standard deviation of the mean wind direction was 7.5° , which can explain the difference between field and W-LES (and WT) results.

The largest difference between results was found at a distance $x/H=2$ from the obstacle lee wall, where W-LES has overestimated and FPM has underestimated field results. This might be explained by the fact that plume centerline height, as estimated by FPM, might be farther from the receptor position than the predicted W-LES plume, as observed in Figure 6-42, where the FPM predicted plume centerline height is superimposed over W-LES K_c contours at the $y/H=0$ XZ plane. The grey lines represent the long term dispersion parameter σ_y . As for the $x/H=0.5$, WT, W-LES and FPM over prediction of K_c in relation to field experiment data indicates that higher levels of turbulence are observed inside the cavity than these observed in the field experiment. All K_c results were in the same order of magnitude and, except for the receptor point at $x/H=2$, differed by a maximum factor of 2.

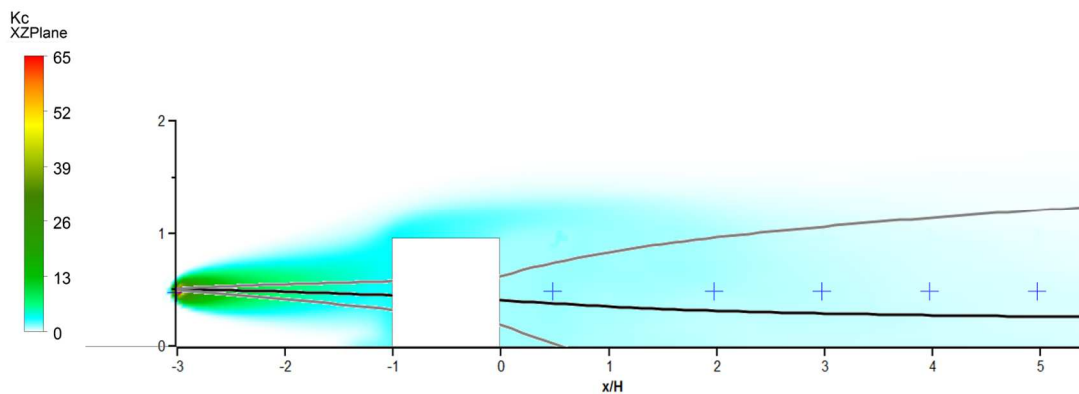


Figure 6-42: FPM predicted plume centreline height superimposed over W-LES K_c contours at the $y/H=0$ XZ plane. The grey lines represent the long term dispersion parameter σ_y .

6.3.3 Intermittency

Following Mavroidis et al. (2003) experiments, intermittency is expressed as the fraction of time during which the “instantaneous” concentration is below zero. However, due to its formulation, FPM never produces zero concentration thus a threshold of $K_c=10^{-10}$ was chosen, below which all concentrations results will be considered zero.

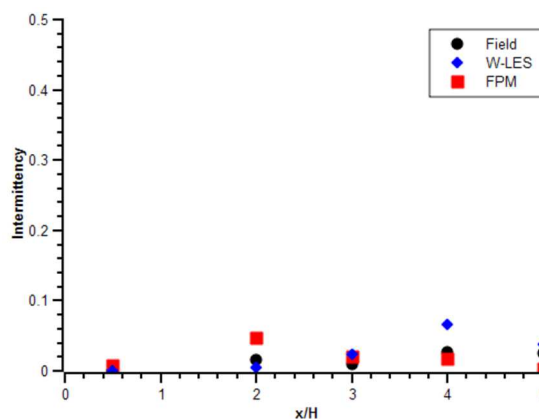


Figure 6-43: Field, W-LES and FPM distribution of intermittency.

All intermittency results show very good agreement with field results, with the exception of FPM result at $x/H=0.5$ from the building lee wall, which greatly over estimated field and W-LES results. In fact, this first monitor point is located inside the recirculation cavity, where turbulence values are small and, as a consequence, intermittency levels are also small.

7 Conclusions and recommendations for further work

The present work investigated odour dispersion modelling in the presence of obstacles (cubical and complex-shaped buildings) under neutral atmospheric conditions employing numerical modelling based on the transport equations as well as on algebraic Gaussian-based models (AERMOD, CALPUFF and FPM) and using field and wind tunnel data to validate the models results and evaluate the models performance. To include atmospheric turbulence effects on dispersion, two different subgrid scale models associated to LES were investigated (Dynamic Smagorinsk and Wale) and to include the building effects on dispersion in the Gaussian-based models, PRIME was used. The use of PRIME was also proposed for FPM as a novelty.

The experimental results comprised wind flow and dispersion around a cubical obstacle in the wind tunnel (WT) (Experiment A), wind flow and dispersion around a complex shaped obstacle in WT (Experiment B) and dispersion around a cubical obstacle in the field (Experiment C).

The two different LES techniques, Dynamic Smagorinsky (D-LES) and WALE (W-LES) results were compared with experimental results from Experiment A. D-LES and W-LES showed good agreement with WT and also with a Smagorinsky LES (S-LES) simulation (carried out by other authors), however, W-LES performed slightly better than S-LES and D-LES. As D-LES simulations employ a double filtering process, computational times are twice longer than W-LES, thus W-LES is a reasonable choice for the other simulations carried out in this study.

FPM and regulatory models AERMOD and CALPUFF (both used PRIME to include obstacle effects) concentration results were compared with of Experiment A data. FPM, AERMOD and CALPUFF results for receptors located downwind the obstacle were quite similar and underestimated WT data and also W-LES and D-LES results. This can be explained by the fact that FPM, AERMOD and CALPUFF are modelling dispersion under flow conditions in which turbulent scales are larger than those found in the WT that would increase plume spreading. Concentration results were more similar as receptor position reaches the ground. This is an important result, as ground-level concentration is usually the most sought information in atmospheric dispersion modelling. W-LES and D-LES predicted concentration fluctuation levels close to those ob-

served in WT and also those predicted by S-LES, although in the wake region, W-LES and D-LES slightly over predicted the experimental results.

Intermittency results predicted by FPM, W-LES and D-LES in the cavity and near wake regions were also similar for thresholds concentrations up to four times the local average concentration. For higher thresholds, W-LES and D-LES intermittency decreased with decreased distance and FPM results under predicting W-LES and D-LES at the cavity and over predicting at the wake. FPM intermittency results predicted at the top of the obstacle were completely off W-LES and D-LES results, which indicates that there has been an under prediction of the plume segment dispersion parameter at that location. The 98th percentile concentration at the cavity and wake predicted by W-LES, D-LES and FPM were also similar, although FPM slightly over predicted LES results in the wake.

Experiment A data and W-LES and D-LES results were also used to assess the variation of the power law exponent (p) in Equation 3-50. In accordance with other works in the literature, it was found that the absolute exponent value decreased with downwind distance, thus the use of a constant value – usual practice in regulatory models – might be inadequate, especially near the obstacle, where the usually employed value p is under predicted.

Experiment B consisted of the flow and dispersion around a complex shaped obstacle in a wind tunnel. W-LES, FPM, AERMOD and CALPUFF concentration results for receptors located near ground level were in the same order of magnitude that of observed WT results, although W-LES, FPM and AERMOD results over predicted WT concentrations. This result is due to the large averaging time used in WT (33.3 h). However, mean concentration adjusted by the power law equation to shorter averaging time agree very well with WT data, with the exception of CALPUFF results, that under estimate WT downwind concentrations. Near wake concentrations predicted by W-LES and FPM showed a much better agreement with WT results than AERMOD and CALPUFF mean concentration adjusted for a longer averaging time. FPM results predicted higher concentration levels far from the centreline of the plume mean trajectory, indicating a possible over prediction of the long term dispersion parameters and an under prediction of the short term plume segment dispersion parameters, resulting in a wider plume. Sim-

ilarly, W-LES and FPM presented a much better agreement with WT results after the adjustment for shorter averaging time.

Downwind intermittency predicted by W-LES and FPM showed a decay with distance, although at the plume centreline intermittency predicted by W-LES largely over predicted WT and FPM results. FPM intermittency far from the obstacle was higher than WT observed results, indicating that FPM predicts more strong influence of the obstacle on dispersion. On the other hand, lateral variation of intermittency showed a very good agreement between W-LES and WT results, reinforcing the ability of W-LES to adequately reproduce the influence of the complex shape of the obstacle. FPM predicted intermittency results were much higher far from the plume centreline, suggesting that the plume segment dispersion parameters are underestimated, leading to higher concentration levels. W-LES and WT results for 98th percentile concentration were similar. FPM results adjusted for shorter averaging time were similar to WT results.

Experiment C consisted in dispersion around a cubical obstacle in the field. W-LES predicted incoming flow showed good agreement with the theoretical field flow, although turbulence intensity values were slightly under predicted. Downwind variation of the average concentration results showed good agreement between field, WT, W-LES and FPM results. As expected, FPM results were closer to field experimental values while W-LES agreed best with WT results. FPM concentrations adjusted by Equation 3-50 (to match the field non dimensional averaging time) still present good agreement to field results, approaching WT and W-LES results.

Predicted W-LES and FPM intermittency results also showed good agreement to field data, except for a receptor located ~~inside the cavity~~, where FPM over estimated field data and W-LES values, indicating that FPM might be predicting lower turbulence levels and lower values of the plume segment dispersion parameters.

Overall, results indicate the use of the CFD/LES might be a useful tool for assessment of odour dispersion and impact in the presence of obstacles. The use of LES might also be a very important tool for the development of Gaussian models, as it makes possible to visualize flow patterns in the entire domain more easily than in WT and field experiments. The main drawback is still the computer power and memory requirements, not only for mesh generation but especially for solving the transport equations.

Results also indicate that the proposed FPM, which included the effects of the obstacle based on the PRIME model, is a very useful tool in odour dispersion modelling, due to its simplicity and easy set up if compared to the more complex CFD modelling and even regulatory models AERMOD and CALPUFF. The great advantage of FPM is the possibility of estimating intermittency and also the peak-to-mean (P/M) concentration ratio, which are useful parameters for odour impact assessment. Comparison to experimental and field data suggests the plume segment dispersion parameters values are under estimated, while the long-term dispersion parameters values are over estimated. This behaviour leads to higher concentration peaks and larger plumes.

Regulatory models AERMOD and CALPUFF are usually employed in odour impact assessing. These models estimate mean concentrations for averaging times of 60 minutes or more, while odour events are associated with short-duration concentration peaks of a few seconds. Common practice is to obtain estimates for concentrations valid for shorter averaging times using Equation 3-50. In fact, CALPUFF has this feature built in, where the user is able to generate the short-time averaged concentration estimates while post processing the model results. This procedure was employed in simulations of Experiment B, adopting a short averaging time of 5s. AERMOD and CALPUFF under estimated the 98th percentile concentration observed in WT. Despite the obtained results, AERMOD and CALPUFF cannot be ruled out as tools for assessing odour impact, although careful interpretation of the results might be necessary for receptors located in the obstacle near field.

Based on these discussions and conclusions, it can be realized that mathematical modelling of fluid flow is a constant evolving field and the same applies to atmospheric dispersion of odour compounds. Although the results obtained in the present work indicate that LES technique and FPM-PRIME are useful tools for assessing odour dispersion and impact, further research is still needed.

Concerning inflow turbulence generation, ANSYS-CFX would benefit of a way of inserting the results of a precursor domain simulation as an inlet boundary condition. Currently, it is possible to set up a precursor domain simulation and store the results of velocity components values at a specified plane, but there is no obvious way to insert these data back at each time step of the main simulation. It is currently possible to utilize a user created function to generate “instantaneous” values for selected variables

during run time, but ANSYS-CFX documentation does not present any way of accessing a database file. The use of roughness elements to generate inflow turbulence for large domains presents a direct impact in memory and computational time requirements.

As for the FPM-PRIME model, results obtained in the present work indicate the determination of the plume segments dispersion parameter might be improved. As currently implemented, these parameters are calculated based on field experiments where dispersing plumes was photographed at several downwind distances in order to derive the mathematical model. The advantage presented by CFD techniques in terms of detailed flow visualization could be used to refine the calculation of the plume segment dispersion parameters, especially in the presence of obstacles. Additionally, calculation of the long term dispersion parameters in the near field of the source and obstacle could also be improved based on CFD simulations.

Another important issue concerning LES and WT and/or field results comparison consists in selecting the ideal averaging time. The use of longer averaging times in LES might lead to much longer simulation run times, justifying the need for an optimized value. The present work show good agreement between WT and W-LES results obtained with a shorter averaging time; it is important to note that the autocorrelation analysis indicating the choice of the averaging time was adequate.

The present work examined flow around cubical and a complex-shaped obstacles, with the CFD simulation clearly showing the influence of the obstacle shape on the flow, however, PRIME cannot distinguish between simple and complex geometry, as it uses the projected width and length, respectively normal and parallel to the mean wind direction. The use of CFD simulations can be a useful tool in order to improve the way PRIME deals with different obstacle shapes. In addition, the effects of a group of obstacles, a representative situation in urban scenarios, on dispersion should be further developed in PRIME.

Finally, research should be extended to different atmospheric conditions, perfecting the choice of boundary conditions for the CFD simulations and comparing results with FPM-PRIME.

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APPENDIX A – Input data used for the AERMOD modeling of Experiment A

Table A-1: surface input data for AERMOD

Friction velocity (u_*) [m/s]	Sea level pressure [mBar]	Local pressure [mBar]	Cloud cover [tenths]
0.05	1013.3	1013.3	10

Table A-2: vertical profiles for AERMOD

Altitude [m]	Standard deviation of wind direction [degrees]	Standard deviation of vertical wind velocity [m/s]	Temperature [°C]	Wind direction [degrees]	Wind Speed [m/s]
3.5	0.1	0.1	25	270	1.22
5	0.1	0.11	25	270	1.3
7.7	0.1	0.12	25	270	1.38
10.4	0.1	0.13	25	270	1.43
12.6	0.1	0.13	25	270	1.45
15	0.1	0.14	25	270	1.48
20	0.1	0.14	25	270	1.53
25	0.1	0.16	25	270	1.58
29.7	0.1	0.17	25	270	1.63
37.2	0.1	0.16	25	270	1.7
49.8	0.1	0.15	25	270	1.82
62.6	0.1	0.12	25	270	1.94
75	0	0.11	25	270	2
100	0	0.07	25	270	2
127.5	0	0.04	25	270	2

Table A-3: Geophysical data for AERMOD

Roughness length [m]	Albedo	Bowen ratio
0.035	1	1

Table A-3: Source data for AERMOD

Source type	Emission rate [g/s]	Stack diameter [m]	Source height [m]	Source elevation [m]	Stack exit velocity [m/s]	Exit temperature [°C]
Point	5	1	50	0	1.82	298.1

APPENDIX B – Input data used for the AERMOD modeling of Experiment B

Table B-1: surface input data for AERMOD

Friction velocity (u_*) [m/s]	Sea level pressure [mBar]	Local pressure [mBar]	Cloud cover [tenths]
0.182	1013.3	1013.3	10

Table B-2: vertical profiles for AERMOD

Altitude [m]	Standard deviation of wind direction [degrees]	Standard deviation of vertical wind velocity [m/s]	Temperature [°C]	Wind direction [degrees]	Wind Speed [m/s]
2	0	-0.02	25	270	2.04
3.6	0	-0.01	25	270	2.36
5.2	0	-0.01	25	270	2.58
6.8	0	-0.01	25	270	2.79
10	0	-0.01	25	270	3
14	0	-0.01	25	270	3.2
18	0	-0.01	25	270	3.3
22	0	-0.01	25	270	3.4
26	0	-0.01	25	270	3.43
30	0	-0.01	25	270	3.56
40	0	-0.01	25	270	3.66
48	0	-0.01	25	270	3.68
56	0	-0.01	25	270	3.79
64	0	-0.01	25	270	3.83
72	0	-0.01	25	270	3.89
80	0	-0.01	25	270	4.02
100	0	-0.01	25	270	4.12
120	0	-0.01	25	270	4.29
140	0	-0.01	25	270	4.46
170	0	-0.01	25	270	4.71

Table B-3: Geophysical data for AERMOD

Roughness length [m]	Albedo	Bowen ratio
0.031	1	1

Table B-3: Source data for AERMOD

Source type	Emission rate [g/s]	Stack diameter [m]	Source height [m]	Source elevation [m]	Stack exit velocity [m/s]	Exit temperature [°C]
Point	0.006866	1.52	8.5	0	3	298.1

APPENDIX C – Input data used for the CALPUFF modeling of Experiment A

Table C-1: surface input data for CALMET

Wind speed [m/s]	Wind direction [degrees]	Cloud cover [tenths]	Temperature [°C]	Local pressure [mbar]	Precipitation code
1.43	270	10	298.1	1013.3	0

Table C-2: vertical profiles for CALMET

Pressure [mbar]	Altitude [m]	Temperature [°C]	Wind direction [degrees]	Wind Speed [m/s]
1013.3	0.0	298.1	270	0.0
1013.3	10.4	298.1	270	1.4
1013.3	25.0	298.1	270	1.6
1013.3	29.7	298.1	270	1.6
1013.3	37.2	298.1	270	1.7
1013.3	49.8	298.1	270	1.8
1013.3	62.6	298.1	270	1.9
1013.3	75.0	298.1	270	2.0
1013.3	100.0	298.1	270	2.0
1013.3	127.5	298.1	270	2.0
1013.3	317.6	298.1	270	2.0
1013.3	1250.0	298.1	270	2.0
1013.3	3500.0	298.1	270	2.0

Table C-3: Geophysical data for CALMET

Terrain elevation [m]	Roughness length [m]	Albedo	Bowen ratio	Surface Heat flux [w/m ²]	Anthropogenic heat flux [w/m ²]
0.0	0.035	1	1	0	0

Table C-4: Profile data for CALPUFF

Altitude [m]	Standard deviation of wind direction [degrees]	Standard deviation of vertical wind velocity [m/s]	Temperature [K]	Wind direction [degrees]	Wind Speed [m/s]
3.5	0.1	0.1	298.1	270	1.22
5	0.1	0.11	298.1	270	1.3
7.7	0.1	0.12	298.1	270	1.38
10.4	0.1	0.13	298.1	270	1.43
12.6	0.1	0.13	298.1	270	1.45
15	0.1	0.14	298.1	270	1.48
20	0.1	0.14	298.1	270	1.53
25	0.1	0.16	298.1	270	1.58
29.7	0.1	0.17	298.1	270	1.63
37.2	0.1	0.16	298.1	270	1.7
49.8	0.1	0.15	298.1	270	1.82
62.6	0.1	0.12	298.1	270	1.94
75	0	0.11	298.1	270	2
100	0	0.07	298.1	270	2
127.5	0	0.04	298.1	270	2
317.6	0	0.04	298.1	270	2
1250.0	0	0.04	298.1	270	2
3500.0	0	0.04	298.1	270	2

APPENDIX D – Input data used for the CALPUFF modeling of Experiment B

Table D-1: surface input data for CALMET

Wind speed [m/s]	Wind direction [degrees]	Cloud cover [tenths]	Temperature [°C]	Local pressure [mbar]	Precipitation code
3.00	270	10	298.1	1013.3	0

Table D-2: vertical profiles for CALMET

Pressure [mbar]	Altitude [m]	Temperature [°C]	Wind direction [degrees]	Wind Speed [m/s]
1013.3	0.0	298.1	270	0.0
1013.3	10.0	298.1	270	3.0
1013.3	22.0	298.1	270	3.4
1013.3	30.0	298.1	270	3.6
1013.3	40.0	298.1	270	3.7
1013.3	56.0	298.1	270	3.8
1013.3	72.0	298.1	270	3.9
1013.3	80.0	298.1	270	4.0
1013.3	100.0	298.1	270	4.1
1013.3	120.0	298.1	270	4.3
1013.3	140.0	298.1	270	4.5
1013.3	170.0	298.1	270	4.7
1013.3	1000.0	298.1	270	4.7

Table D-3: Geophysical data for CALMET

Terrain elevation [m]	Roughness length [m]	Albedo	Bowen ratio	Surface Heat flux [w/m ²]	Anthropogenic heat flux [w/m ²]
0.0	0.031	1	1	0	0

Table D-4: Profile data for CALPUFF

Altitude [m]	Standard deviation of wind direction [degrees]	Standard deviation of vertical wind velocity [m/s]	Temperature [K]	Wind direction [degrees]	Wind Speed [m/s]
2	0	-0.02	298.1	270	2.04
3.6	0	-0.01	298.1	270	2.36
5.2	0	-0.01	298.1	270	2.58
6.8	0	-0.01	298.1	270	2.79
10	0	-0.01	298.1	270	3
14	0	-0.01	298.1	270	3.2
18	0	-0.01	298.1	270	3.3
22	0	-0.01	298.1	270	3.4
26	0	-0.01	298.1	270	3.43
30	0	-0.01	298.1	270	3.56
40	0	-0.01	298.1	270	3.66
48	0	-0.01	298.1	270	3.68
56	0	-0.01	298.1	270	3.79
64	0	-0.01	298.1	270	3.83
72	0	-0.01	298.1	270	3.89
80	0	-0.01	298.1	270	4.02
100	0	-0.01	298.1	270	4.12
120	0	-0.01	298.1		4.29
140	0	-0.01	298.1	270	4.46
170	0	-0.01	298.1	270	4.71
1000	0	-0.01	298.1	270	4.71
2000	0	-0.01	298.1	270	4.71