

# Physical and Numerical Models of Atmospheric Urban Dispersion of Pollutants

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**Abstract.** In this paper the application of numerical and physical models for the simulation of airborne pollutants in urban areas are presented. The assessment of the impact of cruise ships during the hoteling phase in the port of Naples is considered as case study. A physical model of the urban area of Naples has been realized (scale 1:500) and tested in the wind tunnel facility of the Ecole Central de Lyon. Results of wind tunnel tests are compared with CALPUFF and CFD simulations with the aim to validate the performances of the models. The results obtained give useful information for an optimized use of dispersion models.

**Keywords:** Air pollution · Physical models · Numerical models

## 1 Introduction

Urban air pollution is still a challenging task for the scientific community even though it is studied since several decades. Moreover, it is ever more a topic of current interest mainly due to the implications with human health but also with the preservation of historical heritage and natural systems. Some relevant political and sanitary events but also break-through in the human life-style have also direct implications with air pollution in urban areas. Examples are the terrorist threat, in the last years, and the SARS-CoV-2 pandemic in these days. They are new challenges to scholars of air pollution broadening the issues to be faced. Other feature of air pollution in urban areas is often the immediate contact with policy-makers, media and public opinion who have typically different ways of thinking and scale of time of answer with respect to researchers.

The first task in modelling air pollution was represent the urban canopies are a network of interconnected cavities. The main phenomena occurring are: pollutant emission from local sources present in the cavity, turbulent dispersion inside the cavity with chemical and physical phenomena like chemical reactions, deposition, coagulation and evaporation and, finally, mass exchange with the surrounding atmosphere at roof top level and cross-roads.

© Springer Nature Switzerland AG 2020
O. Gervasi et al. (Eds.): ICCSA 2020, LNCS 12253, pp. 692–699, 2020.
https://doi.org/10.1007/978-3-030-58814-4_56

The first attempt to model urban canopies was the definition of the "ideal street canyon": a cavity between buildings shaped like two parallelepipeds of same and constant height and infinite length with perpendicular wind [1]. It enables to highlight a fundamental geometrical parameter, the aspect ratio (AR) H/W, where H is the building height and W the road width. Street canyon are classified as: low-rise street canyon when AR $< 0.7$; regular street canyon when AR is in the range 0.7–1.5; and deep (or narrow) street canyon if AR $> 1.5$.

The first fluid dynamics studies showed as, in function of the aspect ratio, different flow regimes occur in the ideal canyon: isolated roughness flow, wake interference flow and skimming flow [2]. The skimming flow regime takes place in deep street canyons.

The bulk of the above-roof flow does not penetrate the canyon and a single vortex forms when $0.7 <$ H/W $< 1.6 - 2$ while if H/W $> 1.6$, the street canyon is classified as deep [3] and two or more counter-rotating vortices may form [4], with the bottom vortex weaker than the upper one.

For real canyons a second aspect ratio was defined H/L where L is the length of the road between two consecutives crossroads. Real street canyons are then subdivided into: short L/H $= 3$; medium L/H $= 5$; and long canyons L/H $= 7$. If the buildings that line the road have approximately the same height, the urban streets are defined symmetrical canyons, otherwise asymmetrical [3].

More sophisticated representations of street canyon require the use of parameters like building frontal area density and planar area density or packing density [5].

In recent years, with the increased of computing power and of the development and availability of GIS technologies the urban areas are represented as they are without any idealization, apart from a schematization of the real shape of buildings. However, this approach is still not feasible for large areas and several emitting or meteorological scenarios.

First models developed to simulate dispersion of pollutants in urban areas were at street scale level and were box models or operational models: STREET [6], CPBM0 [7] and OSPM [8]. The key parameter of these models was the mass transfer rate between the street canyon and the above atmosphere. Many papers as Salizzoni et al. [9], Murena et al. [10], Chung and Liu [11], Yaghoobian et al. [12], have been dedicated to evaluate it as a function of external forcing like wind speed, wind angle with street axis and incoming turbulence In many cases mass transfer rate has been evaluated using a reference velocity. In the OSPM model [13], when H/W $> 1$, the concentration of pollutant in the street canyon is evaluated as:

$$c = \frac{Q}{W\sigma_{wt}}$$

where $\sigma_{wt}$ is the canyon ventilation velocity equal to $0.1u_w$ where $u_w$ is wind speed at the top of the canyon. In the model developed by Soulhac et al. [14] the mass transfer velocity is proportional to friction velocity u*. Soulhac et al. [14] observed that better results are obtained when an urban canopy, more similar to real conditions, is considered if the box model equation is modified as

$$c = \frac{Q + Q_{up}}{u_w WH + u_d WL}$$

where $Q_{up}$ is the mass flux entering in the canyon from the upwind intersection and L is the street length.

Gaussian models, developed to simulate dispersion of point sources (chimney) in industrial areas (ISC, AERMOD, CALPUFF), find application also in urban areas. In this case, the urban canopy is described assuming a surface roughness depending on the building height and density. These models have the advantage of a simple use and low computing time. They are especially adopted to simulate dispersion from point source and to assess their impact inside the urban areas. Typical example are emissions from industrial activities, waste incinerators and more recently ship emissions in ports [15, 16].

To specifically deal with dispersion phenomena associated to the dispersion within urban areas other models have been developed. An example is ADMS [17] that is essentially a Gaussian like models as AERMOD, but integrating a module to take into account the 'street-canyon effect' [18], i.e. pollutant retention within a narrow street, induced by is reduced ventilation (the module is activated when the street aspect ratio H/W is larger than 0.5). Another example is SIRANE [19], which instead includes a specific dispersion model simulating the pollutant transport within the urban canopy.

Other than the 'street-canyon effect' SIRANE simulates the horizontal advective transfer along the street axes and the pollutant dispersion at street intersections.

In the development and verification of these urban operational pollutant dispersion models, wind tunnel experiments are an essential tool. On one side they allow for an investigation of the phenomena that are responsible of the pollutant transfer, depending on the geometrical characteristics of the domain [9, 20–22]. On the other, they provide data sets that can be subsequently used to evaluate the accuracy of the dispersion models in prediction time-averaged concentrations [23–25].

To simulate pollutant dispersion at local scale in both ideal and real cases, computational fluid dynamics (CFD) is extensively used. CFD results provide insight into the role played by several parameters: wind velocity; aspect ratio; different height of buildings. Murena and Mele [26] applied the incompressible formulation of the RANS–URANS equations adopting second–order central schemes in space and time and a k–ω SST turbulence model. 3D CFD simulations were performed by Murena and Mele [27] adopting the scale adaptive simulation (SAS) model that can be ascribed to the category of hybrid models. In recent years, the large eddy simulation (LES) approach has been frequently applied to this topic. Chung and Liu [11] in a LES study on a 2D idealized canyon evaluated ventilation and pollutant removal, determining the following parameters: air exchange rate (ACH) and pollutant exchange rate (PCH).

This paper presents first results of a comparison between the experiments performed in wind tunnel with the results obtained with CFD and CALPUFF simulations.

## 2 The Case Study

### 2.1 The Area

More than 4 million people live in the Metropolitan Area of Naples (Fig. 1) which has an extension of 171 $km^2$ and a density of 2,649 inhabitants/$km^2$. Often limit values

established by the European Community for the protection of human health are exceeded by $NO_2$, PM10, Ozone and Benzene as reported by the Higher Institute for Environmental Protection and Research (ISPRA) in the Annual Report on the Quality of the Urban Environment [28].

The port of Naples with an annual traffic of $5 \times 10^5$ TEU, $6 \times 10^6$ millions of passengers and 48,000 vessels is one of main sources of some primary pollutants in the urban area of Naples. The assessment of the contribution of the ship emissions in the port of Naples is object of some published papers such as Prati et al. [15] and Murena et al. [16].

### 2.2 The Wind Tunnel Experiment

The experiments were performed in the atmospheric wind tunnel of the LMFA at the Ecole Centrale de Lyon. This is a recirculating wind tunnel with a working section measuring 14 m long, 3.7 m wide and about 2 m height. The air temperature in the wind tunnel is regulated so that its variations during a 1-day experiment can be maintained in the range ±0.5 °C. A neutrally-stratified boundary layer was generated by combining the effect of a grid turbulence and a row of spires, placed at the beginning of the test section, and roughness elements on the floor. The spires were of the Irwin [29] type with a height $H = 0.5$ m, spaced by a distance H/2. Hot-wire constant temperature anemometer and fast flame ionization detector were used as techniques to investigate respectively flow fields and concentration levels. Ethane was used as tracer since it has a density like air.

The modelled area extends for about 1.2 $km^2$ and scale model is 1:500. Receptor points are 37 (Fig. 1). Scenario tested is: wind direction blowing from South-East; velocity ratio $u_s/u_h = 1$ ($u_s$ is funnel gas velocity and $u_h$ is wind velocity at stack height); emissions by three cruise ships at hotelling.

The model of the urban area of Naples reproduced in the wind tunnel and a map with the position of sampling point in the wind tunnel experiments are reported in Fig. 1.

### 2.3 CALPUFF and CFD Simulations

The fluid dynamic experimental conditions realised in the wind tunnel were reproduced with CALMET. $SO_2$ emission rates were calculated as the product of the emission factors for the power applied in the hotelling phase by each ship. The S content in the fuel was assumed at 0.1% by weight following a resolution by the Port Authority of Naples.

CFD simulations have been performed adopting ANSYS fluent software. The computational domain is 7 $km^2 \times 1$ km height, ships and buildings reproduce the wind tunnel model. A multiblock mapped mesh of about 10 million hexahedral cells with refinements at the walls has been generated. The incompressible formulation of the Reynolds Averaged Navier-Stokes (RANS) equations with k-ω SST turbulence model have been employed together with species transport equations (air-$SO_2$ mixture), neglecting chemical reactions and thermal effects. These settings well reproduce the wind tunnel configuration.




**Fig. 1.** Model of the urban area of Naples reproduced in wind tunnel experiments (up) and map of Naples with the locations of sampling points in the wind tunnel experiments (bottom)

## 3 Results

The main input data of CALPUFF simulations ($Q_{SO_2}$, $H_f$, $D_f$, WD) are reported in Table 1. $H_f$ (funnel height from sea level) and $D_f$ (funnel diameter) were scaled by a factor 1/500 to design the WT test. The flow field parameters measured during WT tests ($WS_f$ wind speed at funnel height, u* and $z_0$) are also reported in Table 1. The non-dimensionalised vertical profiles of the average wind speed and the turbulence intensity measured in WT experiments are normalized with respect to the reference height δ (z/δ) and reported in Fig. 2. These profiles were used to define the input data ($WS_f$, $\sigma_v$ and $\sigma_w$) of CALMET/CALPUFF modelling chain to ensure the similarity of the flow fields.

**Table 1.** Main parameters of the wind tunnel experiments and CALPUFF simulations

| Source | $Q_{SO2}$ (g/s) | $H_f$ (m) | $D_f$ (m) | $WS_H$ (m/s) | WD (deg) | u* (m/s) | $Z_0$ (mm) |
|---|---|---|---|---|---|---|---|
| A | 0.34 | 30 | 1.1 m | 3.2 | 135 | 0.13 | 2 |
| B | 0.89 | 40 | 1.1 m | 3.4 | 135 | 0.13 | 2 |
| C | 0.92 | 40 | 1.1 m | 3.4 | 135 | 0.13 | 2 |

Vertical concentration profiles in correspondence of the sampling points (Fig. 1) are produced to compare results obtained by wind tunnel experiments with CALPUFF and

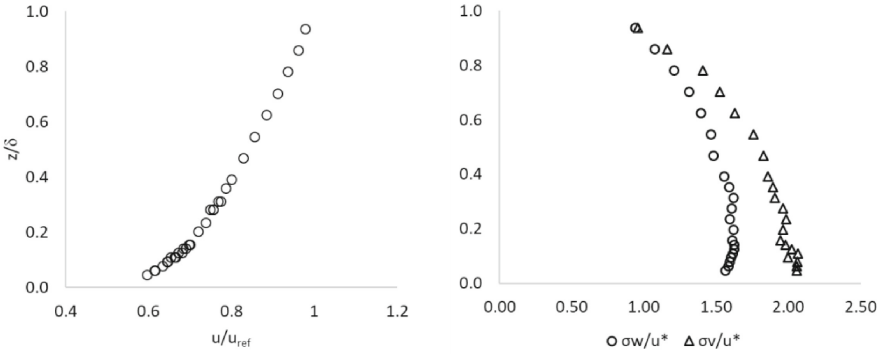



**Fig. 2.** Mean velocity and turbulence intensity profiles from WT experiments

CFD simulations. The ethane concentration measured in WT experiments were scaled to be compared with $SO_2$ concentration obtained by CALPUFF and CFD simulations. Comparison of WT experiments with CFD simulations are reported in Fig. 3 at receptor point: 1, 8, 10 and 28 sampling points (Fig. 1).

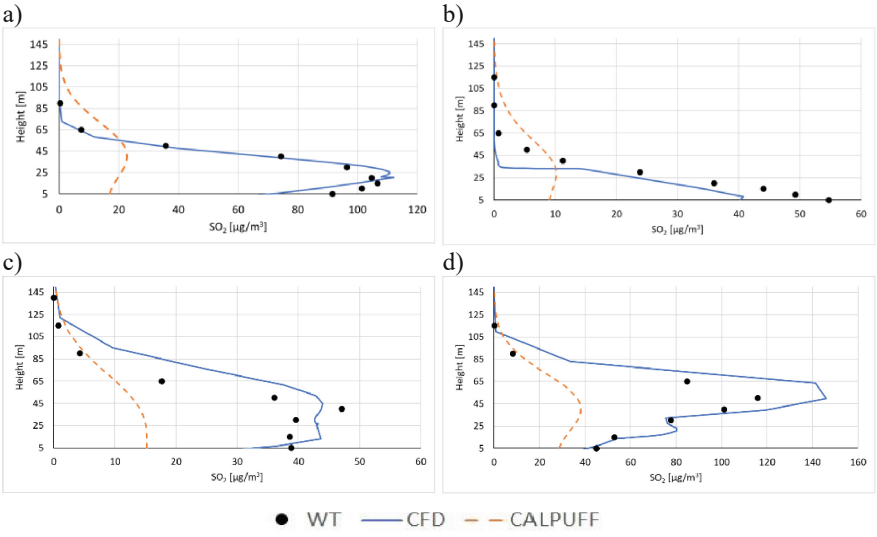



**Fig. 3.** Vertical Profiles of $SO_2$ concentration of Wind tunnel experiments, CFD and CALPUFF simulations at sampling points: a) 1; b) 8; c) 10; d) 28

As can be observed the agreement is in general quite good. The same agreement is not observed when results of wind tunnel experiments are compared with CALPUFF simulations. In fact, Fig. 3 shows how CALPUFF generally underestimates $SO_2$ concentrations (sampling points 1-8-10-28).

## 4 Conclusions

The preliminary results of our research show how the urban canopy can modify in a significant way the impact of ship emissions emitted during the hotelling phase. Our study is focused on cruise ships, but the results can be extended to other ship categories.

The effect of buildings in the urban area is not represented by the building downwash option of CALPUFF that is able to capture only the flow field modifications due to the ship itself and to some port structures near to the docks when present and if of enough height. Preliminary results indicate a good agreement between Wind Tunnel experiments with CFD simulations and a tendency of CALPUFF to underestimate ground level concentrations.

Port and port urban areas all over the world are quite different in dimensions, volume of ship traffic, meteorological conditions, orography, and relative distances. Therefore, a general rule cannot be established. However, in specific case the use of wind tunnel tests or CFD simulations can give important and quantitative information to validate dispersion models like CALPUFF increasing the precision of simulations. In this way more reliable results of studies of the assessment of the impact of ship emissions on port urban areas can be achieved.

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