Evaluation of atmospheric pollutants dispersion using CFD numerical models

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Abstract This paper describes the approach of studying air pollution by using Computational Fluid Dynamics (CFD) models. It also includes a report of a series of investigations performed in order to illustrate the potential of such models with the aim to give a solution to the dispersion to resolve the question of the dispersion of solid and gases pollutants into the atmosphere by using different validation techniques.
Keywords: Air Quality, CFD, Pollution, Pollutant dispersion.

1. Introduction

One of the main consequences of industrial development is air pollution, which is increasing due to growing populations in cities, high consumption of fossil fuels and widespread of car use. Air pollution causes many environmental and health problems. Specifically, it has been estimated that there are about 500,000 premature deaths per year in Europe due to air pollution (European Environment Agency 2019).

Air quality is a major concern of regional, national and European governments. Authorities are developing strict regulations and controls to reduce emissions of atmospheric pollutants. According to the European Union, these measures should ensure a clean atmosphere, free of anthropogenic pollutants by 2030 (Council of the European Union 2017).

Most of the tools used to analyze air pollution (AERMOD, CALPUFF, etc.) has a closed architecture and is focused on the analysis of specific pollutants, such as SO_2, NO_2, PM_{10}, $PM_{2.5}$, Pb, VOC, NH_3 (US EPA 2020). Within this framework, Computational Fluid Dynamics (CFD) models allow these analyses with higher accuracy and without restrictions. It is possible to evaluate the dispersion of any kind of pollutant in different environments, and it is especially useful on a small or medium scale taking into account orography or buildings, including complex three-dimensional geometries.

The main phases of a CFD methodology are the development of the geometric model, definition of the models and boundary conditions, the simulation and the validation of the results. In this work the development of the numerical model is presented, analyzing Navier-Stokes equations, turbulence models, multispecies model, boundary conditions and resolution parameters. In addition, results obtained with this type of CFD model are shown. Finally, a methodology to test at real or laboratory scale will be presented.

2. Geometric model

The first thing to do in the CFD methodology is the development of the geometric model. For this, it will be necessary to know the study area, so that the limits of the computational domain can be defined. The domain dimensions will be set taking into account the requirements, the computational resources or the time needed to simulate.

One advantage of CFD models is the allowance for the use of very complex geometries. Thus, the orography of the terrain, which is not considered by the rest of the tools, can be incorporated into the model and, even, a detailed modeling of the city considering the streets and buildings (Fig.1).

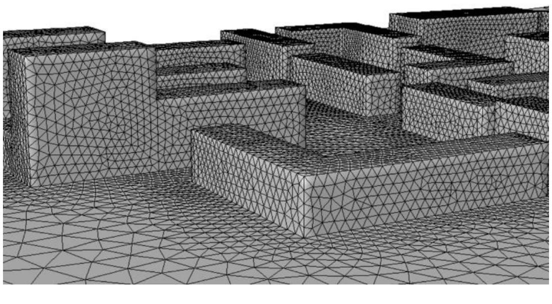

Figure 1. Detail of a mesh for pollutant dispersion study considering the geometry of buildings (Suárez-López et al. 2018).

After the geometry definition, it is necessary a discretization of the domain generating an appropriate meshing, since it is a key point in the accuracy of the results. There are different tools and techniques to optimize this process. Therefore, meshing is the basis of the finite element methods, since it is in each cell where the software applies the proposed models and equations, solving them through iterative calculation by means of numerical methods up to a limit value known as residual.

3. Numerical model

The CFD techniques are used to study fluid flows, solving the mathematical equations expressing the governing laws. Thus, using numerical techniques, the distribution of pollutants in the domain studied can be revealed. With these simulations, a lot of variables can be obtained results, such as air flow and pressure, temperature variations, forces exerted on adjacent solids, energy exchanges, etc.

3.1. Air flow characterization

Considering the air in which both solid and gases pollutants move as an incompressible fluid, the continuity equation is:

$$div\,(\vec{v}) = 0 \quad (1)$$

Where $\vec{v} = (u, v, w)$ is the velocity vector.

For the case of incompressible flow, density of the fluid remains constant with the pressure and the Navier Stokes equations in the three directions are (White 1981):

$$\rho\frac{\partial u}{\partial t} + \rho div(\vec{v}u) + \frac{\partial P}{\partial x} - div(\mu gr\vec{a}d(u)) - S_{Mx} = 0 \qquad (2)$$

$$\rho\frac{\partial v}{\partial t} + \rho div(\vec{v}v) + \frac{\partial P}{\partial y} - div(\mu gr\vec{a}d(v)) - S_{My} = 0 \qquad (3)$$

$$\rho\frac{\partial w}{\partial t} + \rho div(\vec{v}w) - \rho g + \frac{\partial P}{\partial z} - div(\mu gr\vec{a}d(w)) - S_{Mz} = 0 \qquad (4)$$

Where ρ is the density of the fluid, P its pressure, μ its viscosity, g is the gravity and S_{Mx},S_{My},S_{Mz} are the source terms, including the contributions due to mass forces (gravitational, centrifugal, Coriolis and electromagnetic).

Turbulence is defined as a phenomenon of intrinsic instability of the flow caused by apparent volatile behaviour. This turbulent agitation produces additional stresses in the flow (Reynolds stresses) giving rise to the RANS equations (Reynolds-average Navier-Stokes). The resulting system has more unknown variables than equations, which raises the problem of closure Reynolds stresses must be related to flow conditions and geometry.

3.2. Turbulence models

A turbulence model is a numerical procedure that allows closing the Reynolds system of equations so that it can be solved. As the velocity fluctuations can be small-scale and high-frequency, the direct simulations are almost impossible, since the numerical simulation would require a lot of computational effort. The Reynolds equations can be averaged out over time, collectively by using other techniques to eliminate small-scale fluctuations. With this procedure, an easily-solve set of equations is obtained.

3.3. Multispecies model

A particularization of the conservation equations used the pollutant dispersion analysis is the multispecies model. This model gives us the opportunity to study the mix and transport of chemical species by solving the conservation equation describing the sources of convection, diffusion and reaction for each component. The CFD software predicts the local mass fraction of each species Y_i, by solving a convection-diffusion equation for each "i" specie. The general form of this conservation equation is:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho\vec{v}Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (5)$$

Where R_i is the net rate of production of "i" specie by chemical reaction, S_i is the rate of creation by addition of the dispersed phase from any source defined by the user, and $\vec{J}_i$ is its diffusion flux.

3.4. Boundary conditions and simulation parameters

In order to complete the numerical model and perform the simulation, it is necessary to specify the boundary conditions setting values for the static pressure, the total pressure, the velocity, or the gradient of these variables at the limits of the domain. These conditions must also be imposed for the variables of the turbulence model used.

For non-stationary problems, it is also needed to define the initial values of the variables for all points in the domain from the initial calculation of the solutions in the successive temporal steps. In the case of a stationary problem, only some initial values of the variables must be introduced in the program to start the iterative process.

In addition, some properties of the fluid, such as viscosity and density, must be specified, considering the possible variations with temperature, pressure, etc. In this case, these variations should be introduced to the program. Finally, the parameters affecting the numerical resolution of the problem (relaxation factors, setting criteria for completion of iterations, etc.) have to be controlled.

4. Validation

Validation is the final step in the development of a CFD model. In the case of the pollutants dispersion, two types of studies can be performed depending on its scale: real scale or laboratory scale. The real-scale data collection is usually used in many projects which incorporate CFD techniques. However, air quality study requires a large number of measurements. This is conducted by placing a large number of sensors for monitoring purposes. The laboratory scale makes it possible to solve these problems, thereby providing the opportunity to the conditions by means of reduced-scale physical models. In addition, this methodology allows us to incorporate corrective measures such as plant barriers, for the study of their possible implementation on a real scale.

5. Examples of this methodology

Dispersion models can be grouped depending on the type of pollutants analyzed: solid or gases. In each group there are different studies in function of the scale and the purpose.

3.1. Gas dispersion.

Focusing on the gases, it is observed that the dispersion depends on the gas density strongly (Suárez-López et al. 2018), with highly dispersed concentration plumes appearing in light gases, while heavy gases contribute to the formation of pollution berets (Fig. 2). Another example of a gas simulation is the NO_2 simulation in the Aguirre Schools neighborhood of Madrid (Santiago and Martín 2015). In this work, the validation is carried out using air quality stations located in the field (Fig. 3).

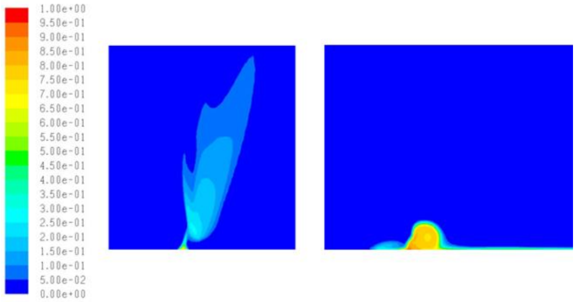

Figure 2. Differences in atmospheric dispersion between a light and heavy gas (Suárez-López et al. 2018).

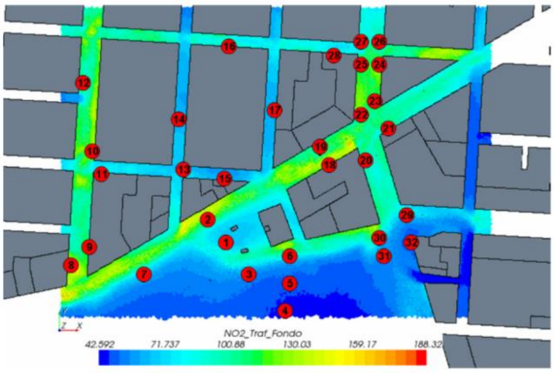

Figure 3. NO_2 obtained by CFD model and air quality measurement in the field (Santiago and Martín 2015).

3.2. Particulates dispersion.

Other studies analyze the PM_{10} particles dispersion. A first laboratory-scale example installs a particle emitter in a wind tunnel and places obstacles in its path. These obstacles attempt to simulate the behavior of pollutants when they encounter a building or other barrier (Brusca et al. 2016). In this work, the CFD model is adjusted through these tests in order to use it later in other more complex situations.

On a larger scale, there is a study of the dispersion of coke particles in the Avilés Port (Asturias 2011) offering different results depending on the wind conditions, which can explain the pollution reaching some areas of the city (Fig. 5).

Finally, sensitivity studies can be done. In this way, incorporation of vegetable barriers in order to improve air quality in an avenue can be tested (Buccolieri et al. 2011). For that purpose, this work uses physical models on a reduced scale in a wind tunnel (Fig. 6). Another factor that will affect the simulation is the turbulence model. Therefore, there are studies (Salim et al. 2011) that compare the results of several models, including LES models with high computational cost. In this way, it is possible to observe the differences that exist with eddies in PM_{10} in the vertical profile of a street (Fig. 7).

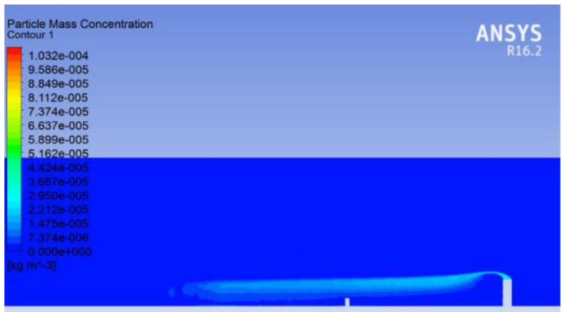

Figure 4. PM_{10} concentration fraction in simulation of pollutant dispersion in wind tunnel (Brusca et al. 2016).

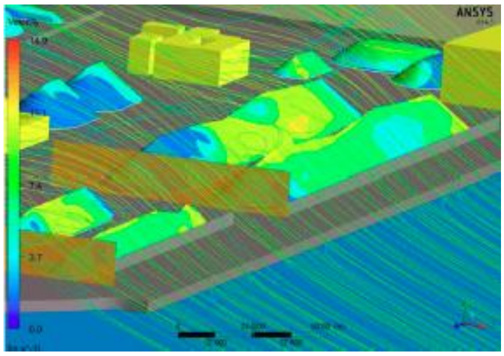

Figure 5. Path lines over coke piles in a CFD model of Avilés Port (Asturias 2011).

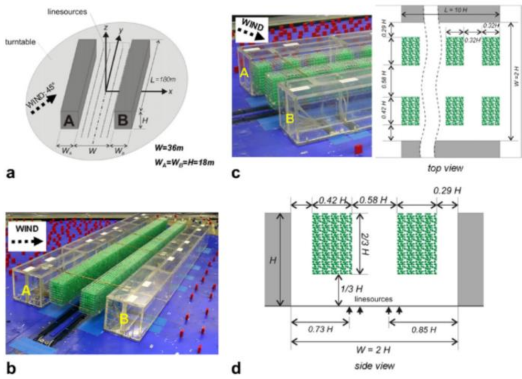

Figure 6. Physical model of a street scale (street canyon) in wind tunnel incorporating a vegetable barrier as a corrective measure (Buccolieri et al. 2011).

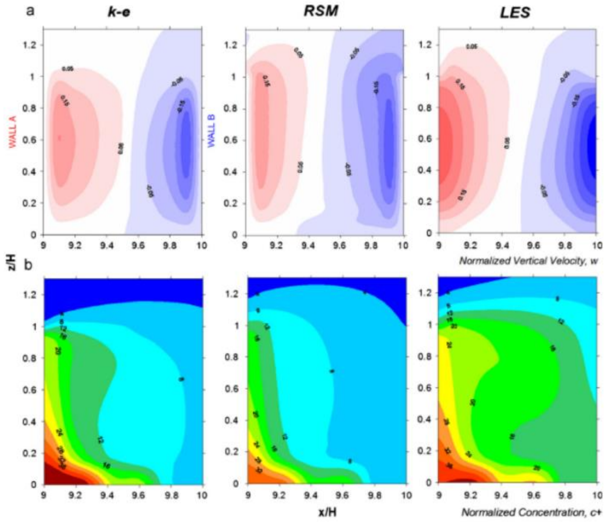

Figure 7. Velocity speed and pollutant concentration in a vertical profile of a street using different turbulence models (Salim et al. 2011).

6. Conclusions

CFD models allow for the evaluation of dispersion of all types of pollutants in complex geometries such as urban environments. These models are based on solving the Navier Stokes equations. The most common approach is to use RANS equations completed by a turbulence model ($k-\varepsilon$, $k-\omega$). Occasionally, higher computational cost models such as LES are also used to offer another interpretation of turbulence. In the case of pollution, it is common to particularize these models in a multispecies model solving the mixing and chemical transport of the species.

Validation is carried out through wind tunnel tests using physical models on a reduced scale or through measurements that require air quality stations in the field. A collection of studies employs different turbulent models and validation methodologies have been shown to illustrate the process of the development of a CFD numerical model.

Acknowledgements

This research includes actions of the EVAIR project, funded by the Government of the Principality of Asturias through the Economic Development Agency of the Principality of Asturias (IDEPA) and the Science, Technology and Innovation Plan (PCTI), as well as by the European Union through the ERDF fund.

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