CEST 2021

17th International Conference on Environmental Science and Technology

Athens, Greece, 1 to 4 September 2021

Air pollution assessment for regulatory purposes: a CFD approach design

ANTUÑA-YUDEGO E.[1*], FERNÁNDEZ-PACHECO V.M.[2], SUÁREZ-LÓPEZ M.J.[3], ÁLVAREZ-ÁLVAREZ E.[4] and CARÚS-CANDÁS J.L.[5]

[1, 5] TSK, Ada Byron, 220, 33203 (Gijón), Asturias, Spain.

[2, 3, 4] Energy Department, University of Oviedo, Wifredo Ricart s/n, 33204 (Gijón), Asturias, Spain.

*corresponding author:
e-mail: elena.antuna@grupotsk.com

Abstract. In a context of atmospheric pollution levels on the rise, there is a growing interest in the use of pollutant dispersion tools, especially for regulatory purposes involving industrial activities. Environmental organizations from different countries legislate and encourage the use of different types of models capable to provide fast and robust results in many scenarios. However, these models are not suitable for certain complex conditions of pollutant dispersion, where CFD tools offer a powerful alternative to consider, despite their higher demands in terms of time and resources. In order to run accurate and reliable CFD simulations, some important steps must be carefully considered, such as the definition of an appropriate computational domain. As for the concerned scenario, the pollution impact assessment of industrial facilities, building such a geometrical domain poses specific challenges that are necessary to address. The present work identifies a case study of pollutant dispersion from an industrial source for which the use of CFD models is advised. A contribution is made towards the establishment of a systematic methodology for the development of CFD computational domains in the field of pollution impact assessment of industrial facilities.

Keywords: pollutant dispersion; CFD; topography; computational domain.

1. Introduction

Atmospheric pollution has become a source of major concern in society and in the political scene, a circumstance reflected in increasingly stricter environmental regulations. As a consequence, the industrial sector is being greatly affected by this situation, as the requirements to obtain or renew the prescriptive gas emissions licenses are becoming tighter. In this scenario, there is a growing interest in the use of pollutant dispersion models as tools to perform the pollution impact assessment required by the different national environmental organizations for the license applications. Nowadays, there is a great variety of models available to carry out these studies, many of them widely recognized and validated through decades. In some cases, the national regulatory bodies recommend or even impose the use of a specific modelling tool to comply with this requirement. This is the case of the United States Environmental Protection Agency (US EPA), which accounts for resources like AERMOD or CTDMPLUS (Haq et al. 2019) in its list of preferred models, or some European countries like the United Kingdom with its ADMS model or Germany with AUSTAL 2020 (Schenk 2020; Stocker et al. 2012). The above examples, which fall within different categories (Gaussian, Eulerian, puff models, etc.), have the advantage of being relatively simple and fast in providing results and have evolved during the last years to include more powerful functionalities. Although these models yield satisfactory results in most cases, there are some conditions in which they are not expected to perform appropriately due to intrinsic constraints. Such is the case of scenarios where the dispersion is heavily influenced by turbulence, like a steep topography involving complex interactions among several terrain features (Mills et al. 1988), as well as cities and other structured built-up and industrial areas (Hajra, Stathopoulos, and Bahloul 2011; Lien et al. 2006). The dispersion in regions where sources are located in the close proximity of these obstacles constitutes also an important limitation (Holmes and Morawska 2006), especially if the heights of the chimneys and the surrounding obstacles are comparable, which greatly affects the plume behaviour (Tominaga and Stathopoulos 2016). A typical case where such conditions can be found is that of an industrial combustion facility located in a closed valley, in order to benefit from the proximity to rivers and water reservoirs for its cooling system.

For these more challenging cases, Computational Fluid Dynamics (CFD) models constitute a powerful alternative. They provide complete analysis of fluid flow based on conservation of mass and momentum by resolving the Navier-Stokes equation using finite volume methods. Numerical simulations with CFD are very flexible and provide results of flow features at every point in space (Moonen et al. 2012). On the contrary, the high demand of computational resources entailed by these tools, as well as the greater efforts required to set up the model and run the simulations, is well known. In this sense, one of the critical errors in CFD results arises from numerical simulation aspects such as the computational domain design and size (Frank et al. 2007), being one of the key steps in the development of the model. However, despite these shortcomings, for complex conditions and scenarios like the ones exposed, the use of CFD models is justified and necessary in order to achieve satisfactory results in the assessment of pollutant dispersion. This way, several efforts have been made during the last decades to improve the accuracy and reliability of CFD models, addressing their weaknesses and uncertainties so as to provide potential solutions. As regards of wind flow simulations over natural terrains, the use of CFD tools has substantially increased in the last years, especially for the quantification of the energy potential in new wind farm projects (Uchida and Li 2018). Other outstanding applications were the positioning of wind towers (Ha et al. 2018) or the estimation of local wind conditions for operating purposes (Blocken et al. 2015). Urban physics and their link to pollutant dispersion have also been a recurrent topic in the literature lately. According to this, guidelines and best practices have been released for the definition of the computational domain and other key parameters of the CFD models in these applications. On the contrary, few studies account for both the effect of the urban canopy and the terrain topography on the flow characteristics and pollutant dispersion simultaneously. The few examples tackling this challenge either deal with very simple topography (Zhao et al. 2019) or apply a multi-scale approach (Mochida et al. 2011). In the latter research, terrain effects are firstly simulated at a large resolution by means of a mesoscale model, and the outputs are then imposed as the input boundary conditions for a separate microscale urban simulation. However, there are almost no studies jointly integrating terrain effects and urban physics into a single modelling framework.

A possible explanation for the lack of studies undertaking this approach is the complexity behind the successful integration of these two elements (terrain and urban features) in a unique model. In addition, there are no specific guidelines for the implementation of this combined setup, and it is not clear whether the existing ones dedicated to urban scenarios can be directly applied to this approach, as it poses its own specific challenges. Therefore, it is necessary to address the definition of a computational domain which jointly accounts for terrain and urban features in order to establish a systematic methodology for this purpose.

In the present work, a case study is identified whose characteristics advice against the use of operational models for the assessment of pollutant dispersion from a chimney, and a CFD approach was chosen instead. More specifically, this research is focused on the development of the geometrical or computational domain, contributing to the establishment and application of some procedural guidelines according to the state-of-the-art. This effort aims at overcoming one of the barriers to the application of CFD models to industrial case studies, a growing need for regulatory purposes.

2. Methodology

2.1. Site location.

The case study selected for this research is a chemical industrial plant located in a mining valley in the Principality of Asturias, a province in the North of Spain. Figure 1 shows an image of the facility where the highly mountainous character of the surrounding environment and its proximity to the plant is evident. The exhaust gases of the process are released from a prominent chimney located in the geographic coordinates 43.288439, -5.674461. Information on its dimensions and other parameters required for the modelling are publicly available through the document of its integrated environmental authorization.

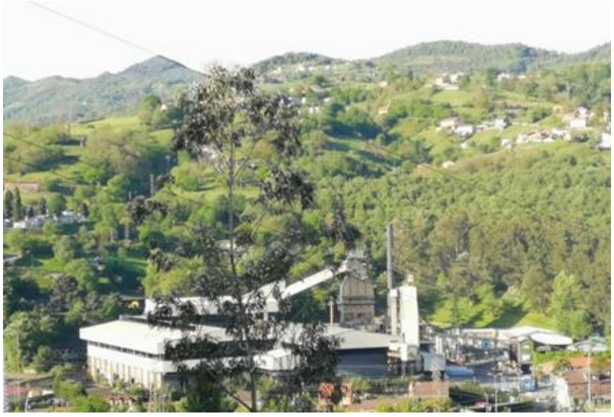

Figure 1. An image of the chemical plant of study.

2.2. Data gathering.

In order to generate the terrain surface for the modelling area in the chosen location, altimetric information has been retrieved from the National Centre for Geographic Information (CNIG) in Spain. Digital terrain models (DTM) for the national territory are available in different grid spacing. However, the use of LIDAR 3D point clouds has been preferred for this work instead, given its flexibility to produce elevation models of any desired spatial resolution and to model the contour shape. This way, the terrain surface has been produced at a chosen spatial resolution of 30 m. The terrain area selected for the analysis corresponds to a circular region with a 750 m radius, the chimney of the industrial facility being located at its geometric center.

2.3. Computational domain design.

The adoption of a circular shape for the terrain domain makes it especially suitable to deal with the simulation of variable wind incoming directions. The chimney has been incorporated as a cylindrical body placed at the center of the circular region. Likewise, the buildings of interest have also been integrated as rectangular parallelepipeds in the appropriate positions. The entire process of the terrain surface generation has been developed in the commercial computer-aided design software Autocad Civil 3D. However, it is worth noting that this whole process can be alternatively undertaken by means of open-source tools. Figure 2 shows the aspect of the terrain surface, with the surface and buildings.

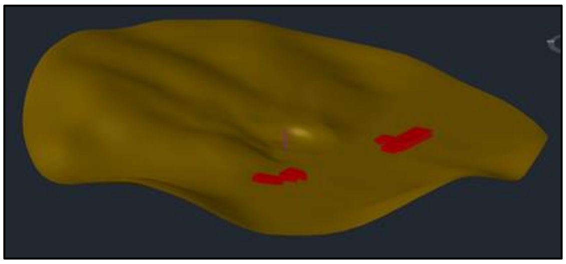

Figure 2. Terrain surface obtained.

Another key point in the design of the computational domain is the integration of empty areas surrounding the model to ensure that the inlet flow reaches a state of equilibrium before approaching the terrain and fully develops once it passes over it, out of its disturbance area. However, the coupling of these flat surfaces to the terrain portion is not straightforward given its irregular outer contour, which is highly variable in altitude. Therefore, an appropriate transition zone should be established to uniformly connect both domains. One of the studies that dealt with this issue previously was (Huang, Wenfeng; Zhang 2019), where a procedure was described to smoothly link a mountainous terrain area to a flat domain, while maintaining the circular shape throughout the new transitional surface. On the other hand, (An et al. 2020) analyzed the potential of the transitional zones to distort the vertical wind profile before it reaches the terrain if the former are improperly designed. From the analysis, it was concluded that transitional areas with inclinations beyond 30º could produce unsatisfactory results. According to this, the transitional zone has been created maintaining the circular shape and limiting the slope to a maximum value of 18º degrees at any point of the surface. This condition has been accomplished by adjusting the circular base radius of the transitional surface and the height difference between the maximum elevation point of the outer terrain contour and the elevation at which the flat domain bottom is positioned. The result is a 1400 m radius base for the transitional surface and the positioning of the flat bottom at a vertical distance of 205 m from the highest point of the terrain contour. Figure 3 shows the dimensions and composition of this transitional region. Then, the outer limits of the domain have been set and incorporated to the geometry, as shown by Figure 4.

Finally, it is important to locate the study region far enough from the model boundaries in order to avoid the flow contraction and subsequent artificial acceleration. The outer limits of the computational domain can be defined following the distance guidelines given by (Frank et al. 2007).

2.3. Domain implementation to CFD model.

After the computational domain, an appropriate mesh should be obtained prior to its integration to the solver module. Then, the boundary conditions are set and the turbulence and species transport models should be carefully selected. Once completed, the whole CFD model will be validated according to two different mechanisms. The first one relies on the use of available databases that provide airflow quantities and pollution concentrations measurements allowing for a quantitative validation. The second mechanisms will involve the development of a wind tunnel with special measurement techniques for the characterization of flow pathlines and trends, which will eventually lead to a qualitative characterization.

3. Results.

A preliminary simulation has been carried out to show the robustness of the model design proposed. The objective was to verify that the geometric domain supports the generation of a mesh, simply and without excessive efforts, capable of meeting the convergence criteria in a simulation. Figure 5 shows the results for a benzene release under neutral atmospheric conditions and north wind direction at a speed of 6 m/s.

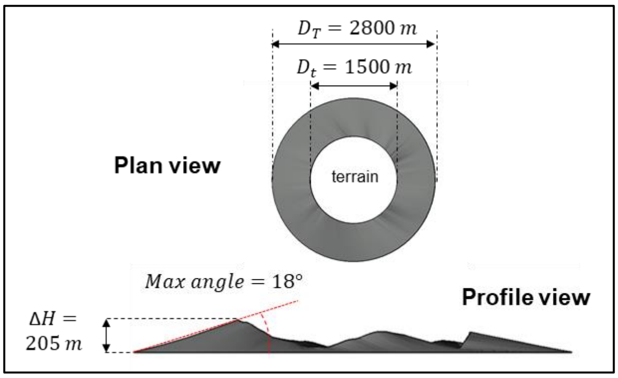

Figure 3. Transitional surface dimensions.

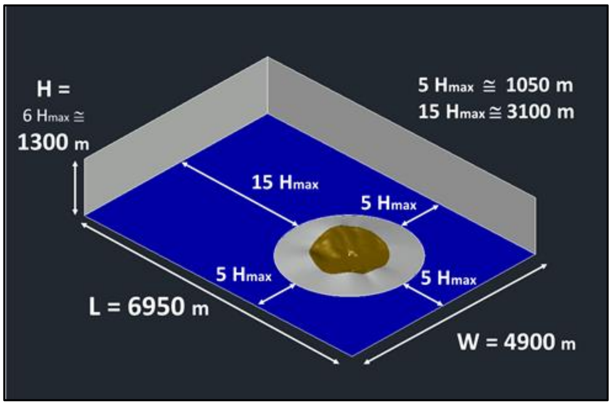

Figure 4. Computational domain dimensions.

4. Conclusions.

When it comes to the pollution evaluation impact of an industrial facility, CFD models represent a powerful alternative for those cases studies where more widespread and faster models cannot perform appropriately. However, the application of CFD tools for regulatory purposes still has to overcome some barriers related to the uncertainties and typical errors associated to this approach. One important step in the development of a CFD model which is subject to improvements is the definition of the computational model. In order to establish a systematic methodology for this purpose. A case study of pollutant dispersion from an industrial chimney has been tackled through a CFD approach in the present work. The research is focused on the development of a computational domain that jointly accounts for terrain and urban features. For that purpose, the study targeted the establishment and application of different procedural guidelines according to the state-of-the-art. The ultimate purpose of this research is the contribution to the establishment of a systematic methodology for the development of CFD computational domains for pollution regulatory purposes in the industrial field.

Acknowledgements

This research includes actions funded by the *Agencia Estatal de Investigación* (AEI) of Spain, reference DI-17-09630/AEI

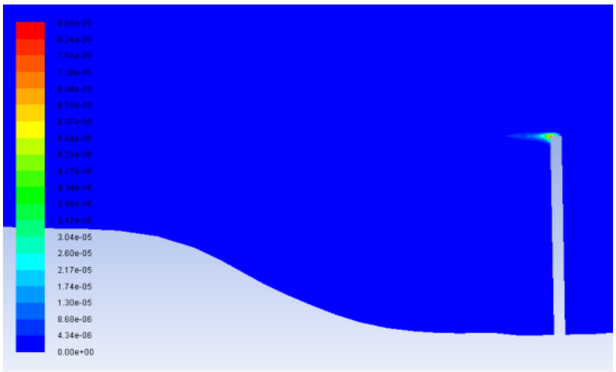

Figure 5. Contours of C_6H_6 concentration of the XZ-plane in a mid-cut of the model.

ReferencesAn, Karl, Sze Ming Wong, Jimmy Chi Hung Fung, and Edward Ng. 2020. "Revisit of Prevailing Practice Guidelines and Investigation of Topographical Treatment Techniques in CFD-Based Air Ventilation Assessments." *Building and Environment* 169:106580.

Blocken, Bert, Arne van der Hout, Johan Dekker, and Otto Weiler. 2015. "CFD Simulation of Wind Flow over Natural Complex Terrain: Case Study with Validation by Field Measurements for Ria de Ferrol, Galicia, Spain." *Journal of Wind Engineering and Industrial Aerodynamics* 147:43–57.

Frank, J., A. Hellsten, H. Schlünzen, and B. Carissimo. 2007. "Best Practice Guideline for the CFD Simulation of Flows in the Urban Environment. COST Action 732." *Quality Assurance and Improvement of Meteorological Models. University of Hamburg, Meteorological Institute, Center of Marine and Atmospheric Sciences.*

Ha, Taehwan, In bok Lee, Kyeong seok Kwon, and Seung Jae Lee. 2018. "Development of a Micro-Scale CFD Model to Predict Wind Environment on Mountainous Terrain." *Computers and Electronics in Agriculture* 149:110–20.

Hajra, B., T. Stathopoulos, and A. Bahloul. 2011. "The Effect of Upstream Buildings on Near-Field Pollutant Dispersion in the Built Environment." *Atmospheric Environment* 45(28):4930–40.

Haq, Amin ul, Qaisar Nadeem, Amjad Farooq, Naseem Irfan, Masroor Ahmad, and Muhammad Rizwan Ali. 2019. "Assessment of AERMOD Modeling System for Application in Complex Terrain in Pakistan." *Atmospheric Pollution Research* 10(5):1492–97.

Holmes, N. S. and L. Morawska. 2006. "A Review of Dispersion Modelling and Its Application to the Dispersion of Particles: An Overview of Different Dispersion Models Available." *Atmospheric Environment* 40(30):5902–28.

Huang, Wenfeng; Zhang, Xibin. 2019. "Wind Field Simulation over Complex Terrain under Different Inflow Wind Directions." *Wind and Structures* 28(4):239–53.

Lien, F. S., E. Yee, H. Ji, A. Keats, and K. J. Hsieh. 2006. "Progress and Challenges in the Development of Physically-Based Numerical Models for Prediction of Flow and Contaminant Dispersion in the Urban Environment." *International Journal of Computational Fluid Dynamics* 20(5):323–37.

Mills, M., R. Paine, E. Insley, and B. Egan. 1988. "Complex Terrain Dispersion Model(CTDM) Terrain Preprocessor System. User Guide and Program Description." *NTIS, SPRINGFIELD, VA(USA)* 177.

Mochida, Akashi, Satoru Iizuka, Yoshihide Tominaga, and Isaac Yu Fat Lun. 2011. "Up-Scaling CWE Models to Include Mesoscale Meteorological Influences." *Journal of Wind Engineering and Industrial Aerodynamics* 99(4):187–98.

Moonen, Peter, Thijs Defraeye, Viktor Dorer, Bert Blocken, and Jan Carmeliet. 2012. "Urban Physics: Effect of the Micro-Climate on Comfort, Health and Energy Demand." *Frontiers of Architectural Research* 1(3):197–228.

Schenk, Rainer. 2020. "Integral Sentences and Numerical Comparative Calculations for the Validity of the Dispersion Model for Air Pollutants AUSTAL2000." *Environmental Systems Research* 9(1):1–28.

Stocker, Jenny, Christina Hood, David Carruthers, and Christine McHugh. 2012. "ADMS-Urban: Developments in Modelling Dispersion from the City Scale to the Local Scale." *International Journal of Environment and Pollution* 50(1–4):308–16.

Tominaga, Yoshihide and Ted Stathopoulos. 2016. "Ten Questions Concerning Modeling of Near-Field Pollutant Dispersion in the Built Environment." *Building and Environment* 105:390–402.

Uchida, Takanori and Graham Li. 2018. "Comparison of RANS and LES in the Prediction of Airflow Field over Steep Complex Terrain." *Open Journal of Fluid Dynamics* 08(03):286–307.

Zhao, Yu, Peng Wang, Liangdong Ma, and Jili Zhang. 2019. "Prediction of Pollutants Dispersion Patterns around Two Adjacent Urban Road Tunnels." *Journal of Dispersion Science and Technology* 40(1):82–93.