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Computational Tools for Analysing Air Pollutants Dispersion: A Comparative Review †

E. Antuña Yudego [1,*], JL. Carús Candás [1], E. Álvarez Álvarez [2], MJ. Suárez López [2], L. García [2] and VM. Fernández-Pacheco [2]

1 TSK Company, Ada Byron, 220 Gijón, Asturias, Spain; juanluis.carus@grupotsk.com
2 Energy Department, University of Oviedo, 220 Mieres, Asturias, Spain; edualvarez@uniovi.es (E.Á.Á.); suarezlmaria@uniovi.es (M.J.S.L.); garciaexpositolaura@gmail.com (L.G.); victorpacheco.ing@gmail.com (V.M.F.-P.)
* Correspondence: elena.antuna@grupotsk.com; Tel.: +34984495491
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Abstract: Atmospheric pollution is one of the biggest problems and concerns in modern society, especially in industrial and highly populated areas. Poor air quality can have adverse impact on human health and ecosystems. For this reason, air quality forecasting becomes increasingly important, especially for governments and administrations, which use these predictions to enhance the design of mitigation actions in order to reduce air pollution in urban areas. In this framework, process of pollutant dispersion simulation is the best way to predict the most affected areas by industrial and other kinds of emissions. To carry out these simulations, there is a great number of computational tools currently available. However, not all of them have the same functionalities, nor can they be applied to the same case studies, so it is necessary to establish the advantages and disadvantages of each one of them in order to choose the most suitable tool in each case. Therefore, the objective of this paper is to identify the main available simulation tools and to make a comparative review between them in order to define advantages and disadvantages.

Keywords: modelling; pollutant dispersion; air quality

1. Introduction

Atmospheric dispersion modelling consists of the mathematical simulation of pollutant dispersion process in the ambient atmosphere, which is achieved by the use of computers and algorithms to solve the mathematical equations that govern the pollutant dispersion. Nowadays there are many air pollutant dispersion models available [1], as well as tools in which these models are combined with other meteorological and chemical ones. When selecting a model, attention should be paid to the particularities of each case study, as long as they will determine the tool that best meets the requirements. In order to classify and select a model or a tool to predict air pollutant dispersion, some important parameters should be considered:

- Spatial resolution. It consists of the detail level visible in the results, and it is related to the cell size of the grid of the model.
- Type of emission. A distinction can be made between point and diffuse emissions. The first ones come from a point source like a chimney in an industry, while the second ones are produce by non-point sources, like the exhaust pipes of cars.
- Domain extension. This feature is related to the spatial resolution and it represents the land surface that can be tackled in the air pollutant dispersion study. Usually, the higher the

resolution of a model, the smaller the extension of the terrain, because of the need of a high computational capacity.

- Results visualisation. In general, current tools to predict air pollutant dispersion show the results in the form of maps using a colour scale to pose different levels of pollutant concentrations or lines that represent spaces with an equal level of concentration. However, some tools designed for more specific applications show the results adapted to the shape of some urban elements like roads.
- Data input. Meteorological data or forecasts (wind direction and velocity, radiation, temperature, pressure…), as well as initial pollutant data are basic data input for the models. Nevertheless, some models can work not only with these data but also with terrain topography as an input, which allows for obtaining better results as it considers the local effects of the landform on the dispersion of pollutants.
- Ownership. These tools can be based on an Open-Source software, and so accessible to anyone, or proprietary, which implies acquiring a commercial license.

In this paper, a review of the main models and tools to predict air pollutant dispersion is made, as well as a classification according to the aforementioned criteria. This work is part of a research project on the dispersion of air pollutants in an industrial region for which it was necessary to select the most appropriate tool during the first stage. The aforementioned project is called EventRisk (Metodología de predicción de eventos de riesgo en ambientes industriales), and it was developed in collaboration between the company TSK and University of Oviedo.

2. Methodology

Six different tools have been selected for the review, some of them recommended by the EPA (Environmental Protection Agency) for the study of air pollutant dispersion as a proof of reliability. The main features of these tools are summarised below.

- **Aermod [2].** It is a steady-state plume model that simulates air pollutant dispersion and deposition. It was developed by AERMIC (AMS/EPA Regulatory Model Improvement Committee) and finally adopted by EPA as a preferred or recommended model in 2005. Two input data processor can be distinguished in this tool: AERMET, a meteorological data preprocessor that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, and AERMAP, a terrain data preprocessor that incorporates complex terrain using USGS Digital Elevation Data. As regards its technical capabilities, this tool allows for the simulation of different types of pollutant sources (point, areas, volumes) for different heights in a range of up to 50 km. In addition, it can work with both particulate matter and gases.
- **Caliope [3].** This tool offers hourly forecasts of the air quality levels in a time frame of 48 h and a variable spatial resolution depending on the geographic area considered. It was developed by the Earth Sciences Department of the Barcelona Supercomputing Centre. As in the previous case, it is made up of some modules: HERMES, an emissions inventory model; WRF-ARW, a meteorological model; CMAQ, a photo-chemical transport model and BSC-DREAM, a model for Saharan dust transport. The combination of these models provides its own meteorological forecasting, as well as an estimation of the levels of both pollutant gases and particulate matter.
- **Calpuff [4].** It is a non-steady-state puff dispersion model based on a Lagrangian model. It was developed by SRC (Sigma Research Corporation) and selected by the EPA as the preferred to evaluate the transport of air pollutants and the impact of complex meteorological conditions. that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation and removal. It is composed of three modules: CALMET, a meteorological model; Calpuff, an air pollutant dispersion model and CALPOST, a post-processing package. As regards its technical capabilities, it allows for modelling different types of pollutants, as it is a multi-species and multi-layer model. It simulates the effects of time and

space varying meteorological conditions on pollution transport, transformation and removal. Calpuff can be applied on scales of tens to hundreds of kilometres.

- **Copert [5].** This tool is focus on the calculation of pollutant emissions and greenhouse gases from the road traffic sector, which implies diffuse emissions. It was developed by Emisia company and funded by The European Environmental Agency. COPERT allows for the simulation of gases and particles emitted by vehicles of different categories with spatial resolution of up to 1x1 km and time steps of up to 1 h. To perform the simulations, the input data needed are maximum and minimum monthly temperatures and some information about the vehicles and fuels.
- **Smoke [6].** This tool provides hourly calculations of many types of pollutants emissions both point and diffuse ones. It was developed by CMAS (Community Modelling and Analysis System) and it is recommended by the EPA. It has to be emphasised that this tool can calculate air pollutant dispersion not only from road traffic but also from aerial traffic.
- **Ansys Fluent [7].** It is a solver for CFD (Computational Fluid Dynamics) that allows for the study of the flow performance of fluids, as well as the transport of gases and particles implied. This tool is currently used in multiple fields and applications implying fluid dynamics processes. Fluent can solve fluid dynamics problems through the discretisation of Navier-Stokes equations, using a finite-volume based approach for this purpose (FVM). In the air quality context, the usage of Ansys Fluent allows for the simulation of atmospheric circulations and the pollutants dispersion at the micro-scale, while the dimensions of the study area are limited by the computing capacity available. This process can be done by using an Eulerian model, suitable for the study of the dispersion of gases, or Lagrangian models, more appropriate for particles.

3. Results

The tools analysed were classified according to the criteria described in the first section, resulting in Table 1.

Table 1. Comparison between the different tools for air pollutant dispersion analysed.

Tool	Spatial Resolution	Domain Extension	Results	Type of Pollutants	Data Input	Ownership
Aermod	High	Medium	Pollutants concentration maps	Particulate matter and gases	Meteorology, emissions data and topography	Open-source
Caliope	Medium-low	Large	Pollutants concentration maps	Particulate matter and gases	Meteorology and emissions data	Open-source
Calpuff	High	Medium	Pollutants concentration maps	Particulate matter and gases	Meteorology, emissions data and topography	Open-source
Copert	Medium - high	Large	Pollutant concentration over roads	Particulate matter and gases	Monthly temperatures, vehicle types and fuels	Proprietary software
Smoke	Low	Large	Pollutants concentration maps	Particulate matter and gases	Meteorology and emissions data	Open-source
ANSYS Fluent	Very high	Small	Pollutants concentration maps	Particulate matter and gases	Meteorology, emissions data and topography	Proprietary software

4. Conclusions

Results show that the highest levels of resolution are provided majorly by proprietary tools, while the open-source ones have advantages when working with large geometric domains, which means medium and large scales. On the other hand, inputs are essentially the same for all of the tools analysed but those that presents high levels of resolution require information about terrain topography as an additional input. Finally, the ways in which the outputs are shown are similar in most of cases, in the form of pollutants isoconcentration maps. Other tools show results in a way that is related to pollution around infrastructures like roads or population regions, as they pursue a specific informative objective. However, these ways of showing results are closely linked to the addressed application of each tool, which can have a general character or a specific one like monitoring pollution of specific regions or roads. Finally, the most of the tools available today for predicting air pollutant dispersion can simulate both particulate matter and pollutant gases.

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