DESIGN AND DEVELOPMENT OF DATA ANALYSIS MODULES FOR THE AERMOD AND CALPUFF SIMULATION MODELS

Wellens A.[(a)], García G.[(b)]

[(a)(b)]Facultad de Ingeniería, UNAM-MÉXICO

[(a)]wann@unam.mx, [(b)]gamarzaid@gmail.com

ABSTRACT

Mathematical models for atmospheric dispersion are being used in a wide variety of industrial applications. Even simplified models have improved their formulation incorporating up-to-date knowledge regarding micrometeorology and dispersion, and can be used to estimate air pollution concentrations around, for example, industrial facilities. Two dispersion models based on Gaussian modeling of the dispersion plume, are of special interest in the simulation of small and medium scale dispersion: AERMOD and CALPUFF are recommended by the US EPA to determine air pollution dispersion.

Both models are freely distributed by EPA, although independent developers offer graphical interfaces (for example ISC-AERMOD, View, Breeze, CALPUFF View) to be able to integrate in a friendly way the topographic, land use and meteorological data, and to represent the results graphically. Although these graphical interfaces are quite complete, specific research projects may need some data manipulation not provided by these interfaces.

This paper proposes some external modules to AERMOD and CALPUFF that extract and prepare in a specific way the output data for certain research needs, such as comparison of the model data with DOAS measurements, etc.

Keywords: consequence analysis, dispersion modeling, CALPUFF, AERMOD.

1. INTRODUCCIÓN

Mathematical models are used extensively in a variety of applications related to the study of air pollution. Examples are, among others, emission modeling, pollutant dispersion modeling, determination of the minimum chimney height, safety audit studies or the modeling of accident consequences. There exists a big variety of models that differ in application type, generated model output, spatial scale, temporary resolution, complexity, method of solution, reference system and required resources.

Pollutants enter the environment in diverse ways. The dispersion of industrial chimney pollutants depend on many correlated factors, as for example:

- The physical and chemical nature of the effluent.
- The meteorological characteristics in the environment.
- The location of the chimney with respect to possible obstructions for the free movement of air.
- The nature of the area located downwind the chimney.

With very few exceptions, the basic approach of the current regulative platform of the EPA for air pollutant modeling in the surroundings of an industrial source has been maintained fundamentally without changes from the beginning of the air programs, approximately 30 years ago. Most used models have been Gaussian ones; they give quick results, but their development is based on quite severe assumptions. Nevertheless, in the last years significant scientific advances have been reached: these have been incorporated in the ISCST3 model (Industrialist Source Complex – Short Term Model) to design advanced Gaussian models able to evaluate pollutant transport at long distances and in complex topographical and meteorological conditions. Two of these advanced models are CALPUFF and AERMOD.

1.1 The Gaussian model

The Gaussian model is a particular solution of the general equation for pollutant concentration transport.

Figure 1 illustrates the problem to be studied, including the used coordinate system where the origin is located at the base of the chimney.

In a simple Gaussian model the concentration *c* of a compound located at the coordinate point (*x*, *y*, *z*) can be described by:

$$c(x,y,z) = \frac{Q}{u\, 2\pi\, \sigma_y\, \sigma_z}\; exp\left[-\frac{1}{2}\frac{y^2}{\sigma_y{}^2} + \frac{(z-H_e)^2}{\sigma_z{}^2} \right]$$

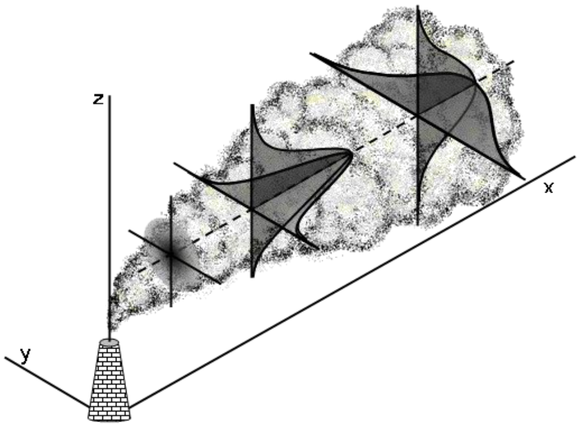


Figure 1. The Gaussian dispersion model.

1.2 The AERMOD model

Of all available models, few are widely accepted. The US Environmental Protection Agency (EPA) proposes and recommends AERMOD to model the dispersion of pollutants of fixed sources.

AERMOD, developed by the US-EPA and the American Meteorological Society, was designed to support the EPA's regulatory modeling programs (EPA 2010). AERMOD is a regulatory steady-state plume modeling system and includes a wide range of options for modeling air quality impacts of pollution sources, making it a popular choice among the modeling community for a variety of applications (Lakes AERMOD VIEW USER GUIDE). Together with the AERMOD code, the US-EPA provides three complementary components: AERMAP (AERMOD Terrain Preprocessor) AERMET (AERMOD Meteorological Preprocessor) and AERSURFACE, a tool that produces surface characteristics data.

As AERMOD includes recent scientific knowledge with respect to the understanding of the planetary boundary layer, it has a more realistic approach in treating plume interaction with the earth's surface than older Gaussian air dispersion models like ISCST3. Since December 2006, AERMOD replaced ISCST3 as the standard regulatory model.

AERMOD, as any other mathematical dispersion model, provides only an estimate of the atmospheric concentration of environmental pollutants, and its results depend on the quality of the corresponding input data, and the methodology used for its determination.

1.3 The CALPUFF model

CALPUFF is an advanced non-steady-state meteorological and air quality modeling system, adopted by the U.S. Environmental Protection Agency in its Guideline on Air Quality Models as the preferred model for assessing long range transport of pollutants and their impacts on Federal Class I areas and on a case-by-case basis for certain near-field applications involving complex meteorological conditions. The modeling system consists of three main components and a set of preprocessing and postprocessing programs. The main components of the modeling system are CALMET (a diagnostic 3-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a postprocessing package). Each of these programs has a graphical user interface (GUI). In addition to these components, there are numerous other processors that may be used to prepare geophysical (land use and terrain) data in many standard formats, meteorological data (surface, upper air, precipitation, and buoy data), and interfaces to other models such as the Penn State/NCAR Mesoscale Model (MM5), the National Centers for Environmental Prediction (NCEP) Eta/NAM and RUC models, the Weather Research and Forecasting (WRF) model and the RAMS model.

This model has been evaluated and improved by institutions and/or groups like the Interagency Workgroup on Air Quality Modeling (IWAQM-US), the EPA and other north-American and foreign organizations, and at present it is one of the most used models due to the EPA support.

Both AERMOD and CALPUFF are models recommended by the United States Environmental Protection Agency and have been used in a variety of applications and countries. In México, they have been used for example by the Universidad Nacional Autónoma de México in air pollution studies around petroleum refineries or electricity generation facilities (Ruiz Suárez *et al*., 2010; Jazcilevich *et al*. 2009; Grutter *et al*. 2008). However, the nature of these research projects requires transformation of model results provided by AERMOD or CALPUFF to be able to compare them with real-time measurements.

2. PROPOSED METHODOLOGY

Both AERMOD and CALLPUFF are written in Fortran, which is a not a very flexible programming language. For the proposed external modules, new programming technologies will be used, independently of the original Fortran code of the specific model. In this stage, the development platform .NET is proposed, as it is a powerful system, which provides quick and reliable results.

The methodology used in the.NET platform will help to improve significantly the tasks and the interaction of the modules to be developed with the original AERMOD and CALPUFF code. In .NET a three layer architecture is used, in which every part of the programming is organized in the most efficient way in order to access the information rapidly and efficiently. The programming time is short due to the large number of tools provided in .NET and the versatility of its use.

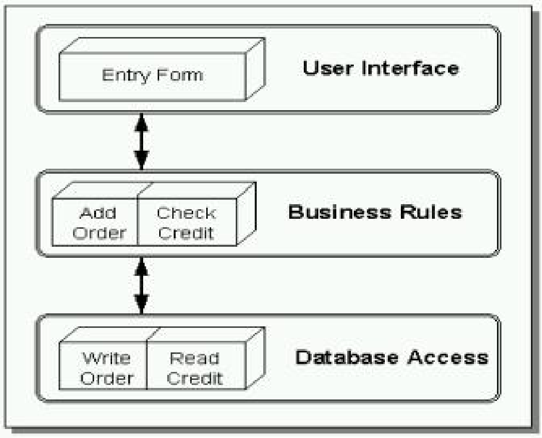


Figure 4. Architecture of the three .NET layers.

Initially, two modules will be developed: the first integrates concentration values at different vertical levels to a sole integrated concentration (in ppm m) to be compared with DOAS integrated concentration data. The other one integrates monthly or seasonal data in an annual concentration, as – due to the size of the meteorological input data – the yearly average cannot be defined in a sole simulation run. In the future, a third module is planned, determining the region were predefined ambient standards are violated when AERMOD or CALPUFF surface concentrations are known.

Once the requirements of each module are defined, the graphical interfaces are developed; the trial version will be evaluated to correct programming errors or to obtain information for future implementations.

3. CASE STUDY

3.1 Study area

The infrastructure of the Mexican Federal Commission of Electricity (CFE) includes 154 energy generation facilities. The number of thermoelectric generation plants distributed in Mexico is 79, of which the Petacalco thermoelectric facility is one of the most important. The Plutarco Elías Calles facility in Petacalco has a capacity of 2100 MW, in six production units. The electric power produced is transported through fifteen transmission lines between 115 and 400 kV.

The plant uses coal as a primary fuel to produce high pressure steam (between 120 and 170 kg/cm^2) and high temperature (of the order of 520°C), to move the electrical generator connected to the rotor of the steam turbine.

The electricity generation plant is an important pollution source, emitting among other SO_2, NOx, particulate matter and CO.

Figura 3. Petacalco thermoelectricity facility.

3.2 Objectives

The general target is to compare the Gaussian model of dispersion of atmospheric pollutants AERMOD and CALPUFF with the spectroscopic skill DOAS in the industrial Petacalco complex, the Warrior's State by means of the creation of external modules to these models that realize the above mentioned comparison and help to work in a practical way the information.

The specific targets of the same sound the following ones:

1. To use the skill DOAS to estimate by implication and wind below the entire emission of SO2 as well as its spatial distribution about the industrial Petacalco complex.
2. To shape the dispersion of this pollutant gas with AERMOD and CALPUFF using the topography and available meteorological information.
3. To evaluate the exits of the models AERMOD and CALPUFF using the sets of meteorological data, with the results of the measurements of the DOAS.
4. To use the modules designed to work with the information of exit of both measurements.

3.3 DOAS

The Optical Spectroscopy of Distinguishing Absorption (DOAS, for its initials in English) is a method to determine the gas concentrations in the ambience by means of the analysis of the light, principally in the spectral status of the ultraviolet and visible one. The light that travels across the ambience is partially absorbed by the gases along the covered trajectory.

Analysis in the vertical one

For this project, the radiation dispersed by the blue sky is collected by means of a telescope and it analyzed espectroscópicamente to obtain column concentrations in units of ppm*m. The concentration in column of a gas represents the concentration integrated along an indefinite trajectory.

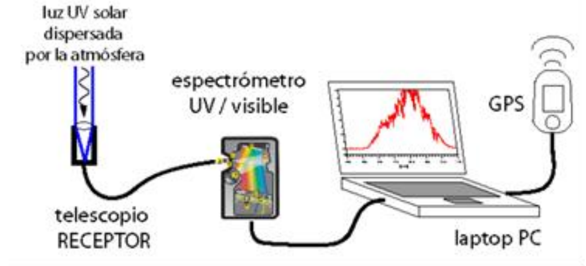


Figure 7. DOAS function

The remarks with the DOAS, on having been measured from a vehicle realizing passages below the pen, give the possibility of estimating the gas flows making use of the speeds of spread of the pen.

The column concentration measures itself to this skill while it passes below a pen or cloud of pollutant gases. The target of this strategy is to obtain the measurement of a "slice" of the pen that disperses perpendicularly over the measurement trajectory.

The facilities chimneys emit, among other pollutants, SO_2 from 100m high chimneys. Besides this facility, four minor SO_2 pollution sources, with lower emission heights (20 to 53 m), are found in the southwest area of the modeling region (Figures 8 and 9). To be able to evaluate CALPUFF model results, Differential Optical Absorption Spectroscopy (DOAS) was used to obtain experimental information on the column concentrations of SO_2 in concentrations of ppm*m. The DOAS technique collects scattered radiation by the blue sky with a telescope and by analyzing the absorbed radiation spectroscopically, integrated SO_2 concentration in the vertical column can be obtained.

Observations were performed with the passive DOAS technique assembled on a van traveling around the industrial complex, below the emitted gas plumes. The traversals downwind were used to evaluate CALPUFF performance. Figure 8 shows a specific DOAS transversal for May 12, 2009 around the electricity generation facility, obtained between 17:03 and 17:19). However, as CALPUFF provides point concentrations, and not vertically integrated concentrations, an extern Fortran module was written to integrate CALPUFF point concentrations in different layers in a column concentration comparable with DOAS results. To assure an appropriate horizontal resolution, only 5 vertical layers of different height could be considered in a first approach, as CALPUFF's number of receptors is limited. At the moment, the programming is being extended to include more vertical layers and refine the results.

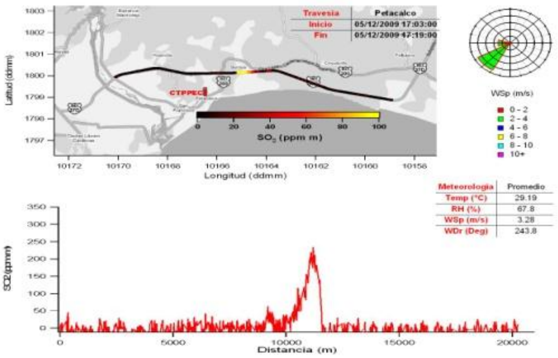
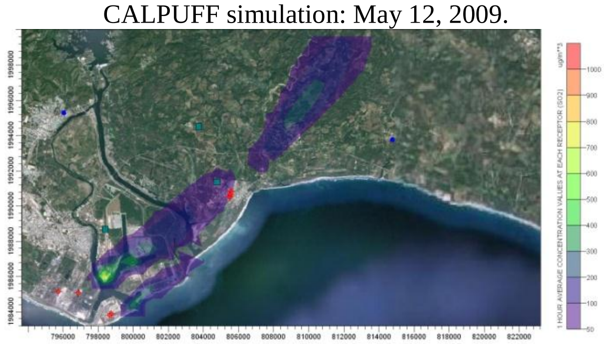
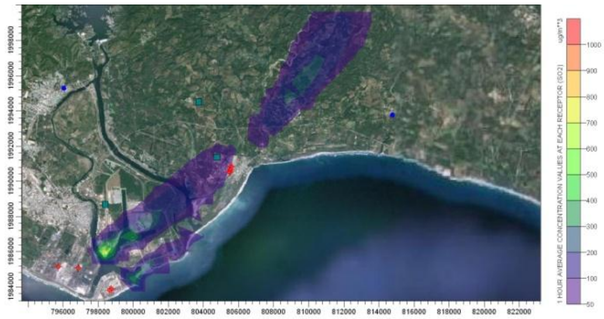


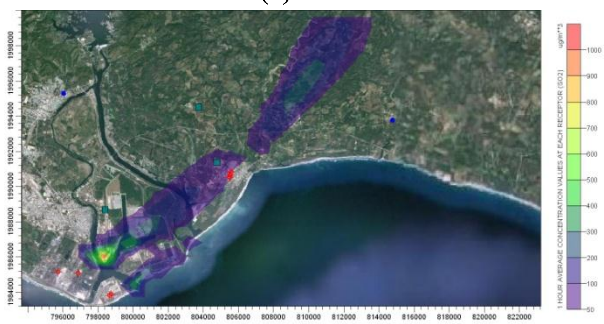
Figure 8. DOAS transversal to be compared with CALPUFF simulation: May 12, 2009.



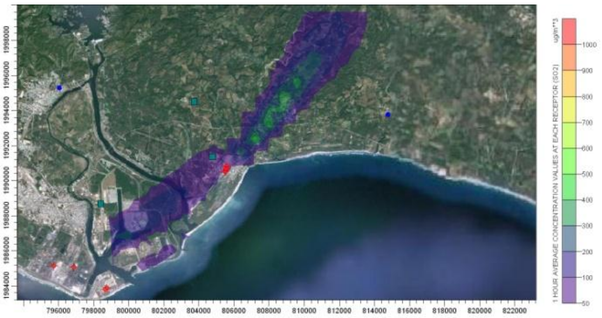
(a) 2 m



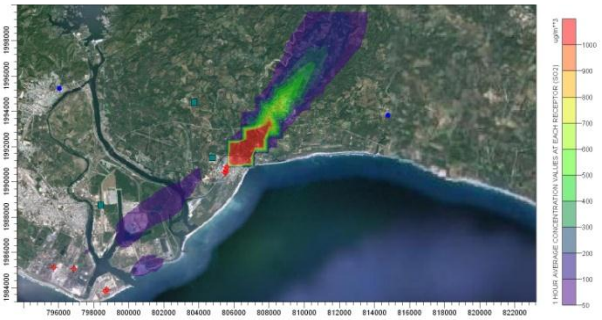
(b) 12 m



(c) 60 m



(d) 200 m



(e) 500 m

Figure 9. Point concentrations at different heights. CALPUFF, May 12, 2009 (17:00 a 18:00).

As can be seen in Figure 9, the resulting concentration is quite different in different vertical layers: at lower height (below 100 m), the smaller sources in the southwest region of the domain generate higher SO_2 concentrations, while at higher heights (see for example at 500 m), the electricity generation facility is becoming more and more important.

The resulting vertically integrated concentration of SO_2 is quite different from the default surface concentration (see Figure 9(a)) given by CALPUFF or in its case AERMOD, as concentrations in different vertical layers differ a lot. Comparison of CALPUFF/AERMOD results with DOAS was considerably better when comparing the vertically integrated concentration instead of the point concentration at the surface (Figure 10).

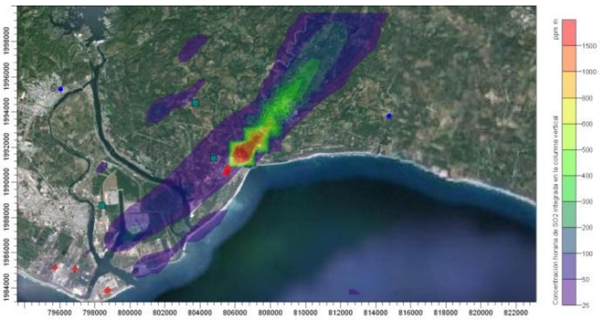


Figure 10. Integrated SO_2 concentration in the vertical column (concentrations in ppm m). CALPUFF, May 12, 2009 (17:00 a 18:00)

As could be observed after analysis of modeling results for different simulation dates and hours, the final integrated concentration, and thus the quality of the comparison between CALPUFF and the DOAS measurements, depended strongly of the number and value of the chosen heights to obtain the integrated concentration. The extern module for vertical integration of CALPUFF model results is being adapted at the moment to be able to take into account easily receptors at more than 5 heights and to change in an easy way the chosen heights to integrate, as both variables depend on the specific information of the sources in the modeling domain.

4. CONCLUSIONS

Extern modules for CALPUFF and AERMOD were developed to adapt standard output concentrations to specific research needs. Fortran models were written for vertical integration of point concentration in different layers, for integration of simulation data for different trimesters into an annual result, among others. These Fortran models were integrated to the CALPUFF and AERMOD simulation models to offer more flexibility in the results. These extern modules are being adapted at the moment to be able to make them more flexible to research needs and specific case studies.

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BIOGRAPHICAL NOTES

Gamar Castillo G. obtained his bachelor degree in Industrial Engineering (UNAM, México).

Ann Wellens is a chemical engineer with postgraduate studies in Industrial Administration (KUL, Belgium) and a master degree in Environmental Engineering (UNAM, Mexico). At the moment she is a full-time lecturer in the Systems Department of the Industrial and Mechanical Engineering Division of the National University of Mexico (UNAM). She has been working in air pollution issues for the last 15 years, dictating courses, collaborating in research projects and participating in conferences related with mathematical modeling of air pollution dispersion and statistics.