# AIR QUALITY AND POLLUTANT DISPERSION ON PARAÍBA RIVER VALLEY

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#### 1. INTRODUCTION

Air pollution is the introduction of chemicals, Particulate Matter, or biological materials that cause harm or discomfort to humans or other living organisms, or damages the natural environment, into the atmosphere. The atmosphere is a complex, dynamic natural gaseous system that is essential to support life on planet Earth. Stratospheric ozone depletion due to air pollution has long been recognized as a threat to human health as well as to the Earth's ecosystems.



Figure 1: Before flue gas desulfurization was installed, the emissions from this power plant in New Mexico contained excessive amounts of Sulfur Dioxide. (Font: http://en.wikipedia.org/wiki/Air pollution).

An air pollutant is known as a substance in the air that can cause harm to humans and the environment. Pollutants can be in the form of solid particles, liquid droplets, or gases. In addition, they may be natural or man-made.<sup>[1]</sup> Pollutants can be classified as either primary or secondary. Usually, primary pollutants are substances directly emitted from a process, such as ash from a volcanic eruption, the Carbon Monoxide gas from a motor vehicle exhaust or Sulfur Dioxide released from factories. Secondary pollutants are not emitted directly. Rather, they form in the air when primary pollutants react or interact. An important example of a secondary pollutant is ground level ozone - one of the many secondary pollutants that make up photochemical smog. Note that some pollutants may be both primary and secondary: that is, they are both emitted directly and formed from other primary pollutants. Particulate Matter particulates, alternatively referred to as Particulate Matter (PM) or fine particles, are tiny particles of solid or liquid

suspended in a gas. In contrast, aerosol refers to particles and the gas together. Sources of Particulate Matter can be man made or natural. Some particulates occur naturally, originating from volcanoes, dust storms, forest and grassland fires, living vegetation, and sea spray. Human activities, such as the burning of fossil fuels in vehicles, power plants and various industrial processes also generate significant amounts of aerosols. Averaged over the globe, anthropogenic aerosols—those made by human activities—currently account for about 10 percent of the total amount of aerosols in our atmosphere. Increased levels of fine particles in the air are linked to health hazards such as heart disease, altered lung function and lung cancer. (http://en.wikipedia.org/wiki/Air pollution#cite note-0).

According to Akula Venkatram and John C. Wyngaard, 1988 most industrial pollution sources are stacks with discharges of momentum and heat as well as pollutants. The resulting plume rise can be considerable - hundreds of meters - and can substantially aid the dilution of plume constituents before they reach ground level. Thus, plume rise is an important factor to consider in diffusion modeling. For power plants and other moderate-to-large industrial sources, the major contribution to the rise is from the heat flux. For example, a modern power plant typically discharges ~ 100 MW of heat from its stack. Source momentum can be important for smaller sources, such as those typically found in light manufacturing. Although we will address the plume rise due to source momentum, we will give most attention to the effects of source buoyancy. Plume rise varies not only with source conditions, but also with the local meteorological conditions the wind speed, ambient stratification (i.e., potential temperature gradient), and ambient turbulence and is a strong function of distance form the source. The distance dependence was ignored in much of the early empirical work (e.g., HOLLAND, 1953), in which the rise was taken simply as the most distant observation as determined visually or by remote sensing. The diverse behavior of plumes dictates that one have a sound theoretical model along with good observations to assess the effects of the controlling variables. Furthermore, a simple model is generally more useful than a complex one, not only for diffusion applications but also in the interpretation of experimental data. This chapter focuses on an integral model, in which one writes down the differential equations governing the total fluxes of mass, momentum, and energy through a plume cross section (e.g., MORTON et al., 1956;

HOULT et al., 1969; BRIGGS, 1975). The equations are closed using the entrainment assumption (MORTON et al., 1956), which specifies that the rate of ingestion of ambient air into a plume is proportional to an "inflow" or "entrainment" velocity at the plume edge; this velocity is generally assumed to be equal to the local rise velocity times a dimensionless entrainmet parameter. For practical purposes, the entrainment parameter can be considered a constant for a particular flow geometry, e.g., a bent-over plume ina cross wind. This approach has been successful in predicting the rise and growth of plumes close to the source and the "leveled off" plume height in stable air. The success stems largely from the dominance of buoyancy effects over those of the ambient atmospheric turbulence in these problems: i.e., buoyancy-generated turbulence due to the plume's upward motion is the principal cause of mixing with ambient air. There are two other important diffusion applications in which plume behavior is not totally resolved. One is the penetration of an elevated inversion by a buoyant plume. The second is predicting the effect of ambient turbulence on plumes in a near neutral or a Convective Boundary Layer (CBL), when the turbulence is sufficiently strong to bring the plume, or parts of it, to the surface. This problem has benefitted. Our discussion of plume rise addresses fundamental aspects and major problems, but it isn't exhaustive in that some problems such as rise from multiple stacks, plume downwash, moisture effects, etc., aren't covered. For these and other details the reader is referred to the review by BRIGGS (1984).

Modeling of air pollution is a difficult issue, since the turbulence is a phenomenon always present, where the atmosphere experienced different types of conditions of stability (stable, unstable and neutral), changing its thermodynamic condition constantly. However, in recent years the monitoring of air quality has become very important activity in order to industrial society in which we live.

According to Oliveira Júnior (2008), in the 80s, the Meteorology of air pollution in complex terrain emerged as a major breakthrough at the time. Part of it gave to the new plants and buildings industries near the coastal and mountainous regions, mainly in the U.S. Besides Moreover, many industries of their environment are located near the west hills or ridges. With that there was a need to establish procedures for modeling the dispersion of pollutants on land complex (HANNA et al., 1982). Initially, these models were relatively simple and basically believed in modeling a shift of the center line of the plume of pollutants on irregularities of the land. Currently, the models show a mesoscale more realistic treatment for this effect on the flow, and consequently, the dispersion of pollutants.

Atmospheric dispersion modeling is the mathematical simulation of how air pollutants disperse in the ambient atmosphere. It is performed with computer in the ambient atmosphere. It is performed with computer programs that solve the mathematical equations and algorithms which simulate the pollutant dispersion. The dispersion models are used to estimate

or to predict the downwind concentration of air pollutants emitted from sources such as industrial plants and vehicular traffic. Such models are important to governmental agencies tasked with protecting and managing the ambient air quality. The models are typically employed to determine whether existing or proposed new industrial facilities are or will be in compliance with the National Ambient Air Quality Standards (NAAQS) in the United States and other nations. The models also serve to assist in the design of effective control strategies to reduce emissions of harmful air pollutants.

The dispersion models require the input of data which includes:

- Meteorological conditions such as wind speed and direction, the amount of atmospheric turbulence (as characterized by what is called the "stability class"), the ambient air temperature and the height to the bottom of any inversion aloft than may be present.
- Emissions parameters such as source location and height, source vent stack diameter and exit velocit, exit temperature and mass flow rate.
- Terrain elevations at the source location and at the receptor location.
- The location, height and width of any obstructions (such as buildings or other structures) in the path of the emitted gaseous plume.

Many of the modern, advanced dispersion modeling programs include a pre-processor module for the input of meteorological and other data, and many also include a post-processor module for graphing the output data and/or plotting the area impacted by the air pollutants on maps.

The atmospheric dispersion models are also know as atmospheric diffusion models, air dispersion models, air quality models, and air pollution dispersion models (http://en.wikipedia.org/wiki/Atmospheric dispersion modeling).

The importance of the issue has become evident with the increase of emissions of pollutants caused by the growth of urban and industrial areas. A tool that has been used for the monitoring of pollution are the numerical models of dispersion of pollutants. The CALPUFF (CALinfornian PUFF Model) is a model of Gaussian Lagrangian puff dispersion of nonstationary, which allows validation of a concentration camp, simulating the transport, processing and removal of pollutants into the atmosphere from weather variables in space and time. Mathematically, the concentration of pollutants in each puff is represented by a Gaussian distribution evolves in time and space. The movement of each puff is calculated at each interval of time, moving its center of mass of this agreement with the wind at that point and at that moment. The concentration camp at each step of time is calculated by adding the contribution of each puff (SCIREA et al., 2005). The CALPUFF model is completely public, including its manuals and can be obtained at website www.src.com.

Paraíba River Valley is an industrial region, and cut through a highway of traffic called President Dutra Highway. Therefore, this road is a source of line where the vehicle moving it emit pollutants. There are also point sources that represent the plants and other points of pollution. The cities are surrounded in a valley between the Sea Ridge (Serra do Mar) and Mantiqueira Ridge (Serra da Mantigueira). This topography will cause interesting situations from the weather, such as passageways catabatic and anabatic (schemes wind forced by the presence of the topography) and the effects of the wind pipe (MORAES, 1995). Given the proximity of the coast, effects of sea breeze is superimpose the effect sinotico (+ breeze fronts), creating a microclimate of the region. All this complexity of atmospheric flow can in principle be modeled from meteorological models of limited area as the model BRAMS (Brazilian Regional Atmospheric Modeling System), and the CPTEC/INPE is responsible for their development (Barros, 1998, Mendes and Panetta, 1999).

For assessment of urban planning and decision-making, such as the demarcation of industrial areas, it is vital to establish criteria that minimize the impact of pollution on the population. Models of dispersion of pollutants are important tools in this analysis. However, strategy for urban and regional planning based on minimizing the effects of air pollution, it is essential to carrying out a study of the climatology of the region.

The objective is to evaluate a scenario of dispersion of air pollutant in the region of Paraíba River Valley primarily through an approach using the numerical model CALPUFF. The aim is to model the dispersion of pollutants through the estimation of two-polluting sources, Carbon Monoxide (CO) and Particulate Matter (MP<sub>10</sub>) that are emitted by motor vehicles that travel by the President Dutra Highway axis in São Paulo and Rio de Janeiro in 200 km, passing through the cities of the Valley is estimated in the cities of Jacareí, São José dos Campos, Taubaté and Pindamonhangaba. Section 2 of this paper presents the methodology used in this analysis, and the settings of the models. Section 3 presents the results and finally, in section 4 are presented the findings.

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## 2. DATA AND METHODOLOGY

The numerical modeling used in this work is to monitor the dispersal of pollutants in the Paraíba River Valley through the estimate of the concentration of pollutants in this field. For both, it was necessary to define a period of study is determined from a systematic observation on a case, the output of the model reanalyses ETA of 40 km, where it was a typical air flow perpendicular to the topography of the area chosen.

This flow characteristic was found during the days 01/01/2004 - 00Z until 06/01/2004 - 00Z, called the period of summer and the days 11/07/2004 - 16/07/2004 until 00Z - 00Z, called period of winter. After the choice of periods for the simulation of the dispersion of pollutants was used with initial condition of the model CALPUFF the BRAMS regional analysis of the model which was started by the model's Global CPTEC.

The sources of pollution to boot CALPUFF considered are: (a) 200 km from the President Dutra Highway that bisects the Paraíba River Valley axis in São Paulo - Rio de Janeiro and (b) the cities of Jacareí, São José dos Campos, Taubaté Pindamonhangaba. Air quality is assessed through two tracers, and the concentration of CO and particulate matter (MP<sub>10</sub>). The emissions from road vehicles, were estimated through the study of the Health Effects Institute, while the issue for the city of São José dos Campos was established from the annual report of CETESB 2005 and estimated for the other cities.

Figure 1 is a diagram of the steps used to achieve the desired results. In the first stage of the numerical modeling was used in the analysis BRAMS with a resolution of 5 km, as well as geophysical data of the study region. The model is responsible for meteorological Calmet interpolation of grade between the BRAMS and CALPUFF, yielding an output with a resolution of 1 km. The initial information is used to feed the CALPUFF in the second stage, which along with the values of tracer concentrations of CO and MP<sub>10</sub> will result in the amount of desired concentration during the study period. The simulation of CALPUFF was held in a period of 36h two distinct periods, one representing the season of summer 03/01/2004 - 00Z and the other the season of winter 12/07/2004 - 00Z. In the third stage, there was the post-processing the output generated by the software for displaying graphics SURFER.

The CALPUFF model was developed in Windows platform. This version of the package, was developed in the LAC / INPE and adapted to the Linux environment (DEGRAZIA et al., 2007) and Calmet code has been adapted to read data output of BRAMS.

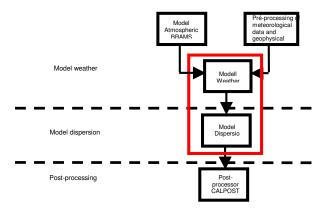


Figure 2: Outline of numerical modeling.

#### 3. RESULTS

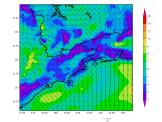


Figure 3: Winter: Output of numerical simulation of BRAMS of wind direction and intensity with spatial resolution of 5 km for the July 12, 2004 at 00Z.

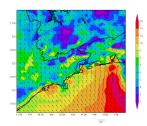
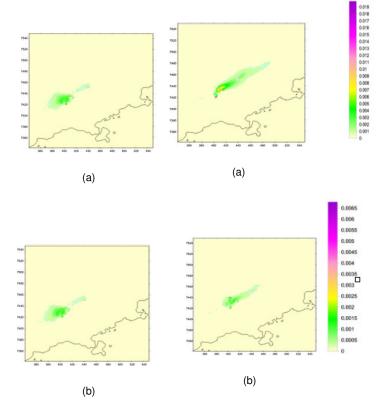


Figure 4: Summer: Output of numerical simulation of BRAMS the direction and intensity of the wind at 850 hPa, with spatial resolution of 5 km for the day 03 January 2004 at 00Z.



the model of dispersion of dispersion pollutants CALPUFF concentration spatial resolution of 1 km for and 24 h (b). the day July 12, 2004 at 12 h (a) and 24 h (b).

Figure 5: Winter: Output of Figure 6: Summer: Output of the model of of pollutants **CALPUFF** concentration of CO with spatial resolution of CO with 1 km for the day 03 January 2004 at 12 h (a)

The model was implemented BRAMS to play an interesting meteorological condition: the wind has a main direction which is approximately cross the Valley. both for the winter and for the situation in summer. Figure 3 shows the result of simulation on July 12, 2004 at 00Z (from winter) and Figure 4 shows the simulation for on 03 January 2004 at 00Z (from summer). In these pictures, the field of wind is displayed at the surface, the intensity of the wind represented by the color chart and the wind direction arrows. It is clear that the air flowing in the direction perpendicular to the valley from south to north. This condition will generate a flow within the valley towards the west-east (ie direction São Paulo -Rio de Janeiro). In the simulation performed is noted that during the summer the intensity of the wind was stronger than in the period of winter.

The fields generated by the model BRAMS are read by the code Calmet, where some parameters are calculated (height of boundary layer, scale, speed, etc.) and the fields are set for the resolution and map projection of the model CALPUFF. As mentioned, two tracers were configured for the CALPUFF: CO and PM<sub>10</sub>, is displayed here only the CO gas. Figure 5 shows an output of the model of dispersion of pollutants to the tracer CO with resolution of 1 km for the July 12. 2004 to daytime hours to 12 hours (Figure 5a) and night at 24 pm (Figure 5b), in both figures is shown the concentration to the level of surface.

Figure 6 shows an output of the model of dispersion of pollutants CALPUFF concentration of CO with spatial resolution of 1 km for the day 03 January 2004 to daytime hours to 12 hours (Figure 6a) and night at 24 h (Figure 6b), both for the level of surface.

The simulations with the model CALPUFF show the influence of the intensity of the wind in the dispersal of pollutants in the Valley. In the simulation for a day of winter, there is a shift in direction in the flow direction in São Paulo - Rio de Janeiro, but it is clear that the effect of diffusion (mass transport) of the effect of pollutant concentration gradient is clearly noted ( Figure 5a and 5b). For a system of wind more intense. as shown in Figure 6a and 6b, the pollutant is carried by wind and pollution produced in the Valley nearest the city of São Paulo is dragged to the region more in the bottom of the Valley (the nearest Rio de Janeiro).

### 4. CONCLUSIONS

The objective is to show that a relatively simple model (Gaussian models are comparatively simple and less demand than computational models Eulerianos and Lagrangianos, they computationally more expensive) can be applied to a complex problem of land, subject to weather interesting (sinotica coupling of conditions, with effects of sea breeze and the flow due to topography). The development for the Linux system, makes the model CALPUFF a system that can be implemented in complementing environment free software and requires no hardware equipment of high computational power. In this configuration, the system is ready to be used by any user, such as small halls and public ministry as a tool for preliminary analysis of environmental risks and urban planning.

The case simulated here is that only a preliminary result will be a set of scenarios for a performance assessment of the dispersion of pollution in the Paraíba River Valley. The simulation shows the case the "effect of tunneling", ie the flow induced within a valley caused by a condition of wind that is perpendicular to the main valley. In the case simulated, the direction of the wind in the Paraíba Valley occurred from west to east. In fact, a study climatológico advance, this behavior wind was recorded (Veiga et al., 2007).

### 5. REFERENCES

Akula Venkatram and John C. Wyngaard, 1988: Air Pollution Modeling, 1-390 pp, Boston.

Barros, S. R. M., 1998: Towards the RAMS-FINEP parallel model: load balancing aspect, Towards Teracomputing Proceedings of the 8 th ECMWF – Workshop on the Use of Parallel Processors in Meteorology, Reading (UK).

Briggs, G. A., 1975: Plume rise predictions. Lectures on Air Pollution and Environmental Impact Analyses, D. A. Haugen, Ed., Amer. Meteor. Soc., Boston, 59-111 pp.

Briggs, G. A., 1984: Plume rise and buoyancy effects. Atmospheric Science and Power Production, D. Randerson, Ed., U.S. Dept. of Energy DOE/TIC-27601, available from NTIS as DE84005177, 327-366 pp.

Calpuff site: http://www.src.com

Degrazia, F. C., Campos Velho, H. F., Cintra, R. S. C., Barbosa, J. P. S., Moraes, M. R., 2007: Sistema de Previsão da Qualidade do Ar para o Vale do Paraíba. Ciência e Natura, v. 111, 293-296 pp, Brasil.

HANNA, S.R., BRIGSS, G.A., HOSKER, R. P. Handbook on Atmospheric Diffusion. 1ª ed., New York, Department of Energy, 1982

Holland, J. Z., 1953: A meteorological survey of the Oak Ridge area: Final report covering the period 1948-1952; U.S. Weather Bureau, USAEC Report ORO99, 554-559 pp.

Hoult, D. P., J. A. Fay, and L. J. Forney, 1969: A theory of plume rise compared with field observations. J. Air Pollut. Control Assoc., 19, 585-590 pp.

Oliveira Júnior, J. F., 2008: Estudo da camada limite atmosférica na região de Angra dos Reis através do modelo de mesoescala MM5 e dados observacionais. Tese - Universidade Federal do Rio de Janeiro, COPPE, 1-272 pp.

Mendes, C. L., and Panetta, J., 1999: Selecting directions for Parallel RAMS performance optimization,

Proceedings of the 11 th Symposium on Computer Architecture and High Perfomance Computing (SBAC-PAD), Natal (RN), 85-92 pp, Brazil.

Moraes, R. M., 1995: Estudo numérico da canalização em vales em termos de parâmetros de similaridade. Tese de mestrado em sensoriamento remoto, Universidade Federal do Rio Grande do Sul, Brasil.

Morton, B. R., G. I. Taylor, and J. S. Turner, 1956: Turbulent gravitational convection from maintained and instantaneous sources. Proc. Roy. Soc. London, A234, 1-23 pp.

Scrire, J. S., Françoise, R. R., Mark, E. F., Yamartino, R. J. A., 2000: User's Guide for the CALMET Meteorological Model (Version 5), Earth Tech, Inc.

Veiga, P. M. S., Campos Velho, H. F., Freitas, S. R., 2007: Estudo Observacional da Climatologia no Vale do Paraíba: Resultados Preliminares – Workshop em Computação Aplicada – CAP/INPE, São José dos Campos, Brasil.

http://en.wikipedia.org/wiki/Air pollution#cite note-0 acessado em 30/12/2008.

http://en.wikipedia.org/wiki/Atmospheric dispersion modeling acessado em 12/01/2009.