H13-126

PERFORMANCE ASSESSMENT OF REGULATORY AIR QUALITY MODELS AERMOD AND CALPUFF - A NEAR FIELD CASE STUDY IN METROPOLITAN REGION OF RIO DE JANEIRO, BRAZIL

Luiz Claudio Gomes Pimentel[1,2] *, Bruno D'Aiuto da Cunha*[2] *, Maurício Soares da Silva*[1] *, Luiz Landau*[2]*, Jesus Salvador Perez Guerrero*[3]

[1]Department of Meteorology, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil
[2]Alberto Luiz Coimbra Institute Graduate School and Research in Engineering - COPPE-UFRJ, Rio de Janeiro, Brazil
[3]Brazilian Nuclear Energy Commission - CNEN

Abstract: Environmental Agencies have been recommended the use of AERMOD and CALPUFF air quality models for use in regulatory purpose. Due to their differences in physical assumptions they are indicated for applications in distinct dispersion characteristics, and the scientific community is still evaluating the uncertainties of these models. The present study aims to assess the uncertainties on the use of both models in near-field dispersion in Rio de Janeiro Metropolitan Region that presents an increasing in the petrochemical industry and an atmospheric pollutant emission growth. The complex topography, the presence of a bay and the proximity to Atlantic Ocean provide an inhomogeneous condition for atmospheric pollutant dispersion making it a challenge to manage the local air quality. The statistical indexes applied for the evaluation between simulation results and observed concentrations indicates better results for CALPUFF simulations.

Key words: *Near-Field, AERMOD, CALPUFF***.**

INTRODUCTION

The AERMOD and CALPUFF air quality models have been recommended by environmental agencies for use in regulatory purpose (EPA, 2005). The AERMOD is a Gaussian model that deals with surface and upper air meteorological data from only one station processed by AERMOD meteorological preprocessor AERMET (EPA, 2004). CALPUFF is a Lagrangian puff model that assimilates meteorological data for one or more stations by CALMET diagnostic meteorological model (Scire *et al.*, 2000). The AERMOD is recommended for near-field regulatory applications (EPA, 2009) (less than 50 kilometers) and CALPUFF is recommended for environmental impact assessment in long range transport (LRT) (beyond 50km), it been considered as an alternative model on a case-by-case basis for near field applications involving complex winds (EPA, 2005). The CALPUFF application in near field situations is under discussion on scientific community as presented at ***9th Conference on Air Quality Modelling***, USA in 2008.

The Rio de Janeiro Metropolitan Region (RJMR), RJ, Brazil, present the second largest vehicles and industry concentration of Brazil with a high pollutant emissions density. According to atmospheric pollutant emissions sources inventory reported by Rio de Janeiro Environmental State Institute (INEA, 2004) the mobile sources represent 77% of total pollutant emission, while stationary sources contribute with 22%. However, 88% of SO_2 emission comes from stationary and just 12% from mobile sources. Among the stationary sources, the petrochemical industry has a major contribution on RJMR pollutant emissions with 51% of SO_2, 38% of NO_x and 90% volatile organic compounds (VOC). The most part of the oil and gas national production of Brazil occur on Rio de Janeiro continental shelf (80%) and the recent discovery of oil in the subsalt layer represents the possibility to increase the oil production in a few years (MME, 2010). It will be expected that demand of petrochemical industries activities will increase and the local air quality management will require the best and most realistic tools.

The RJMR is inserted on a complex topography area influenced by the Atlantic Ocean and Guanabara Bay (fig.1) providing an inhomogeneous condition for atmospheric dispersion**.** The features of this region, involving different time and space scales phenomena, cause changes in the local atmospheric circulation, such as: South Atlantic Subtropical Anticyclone, Cold Front, South Atlantic Convergence Zone, Convective Activity, valley/mountain and land/sea breeze.

The main goal of this study concerns assessing the uncertainty of air quality models, by using statistical index, in order to simulate the pollutant transport in inhomogeneous dispersion conditions into RJMR to near-field scenarios.

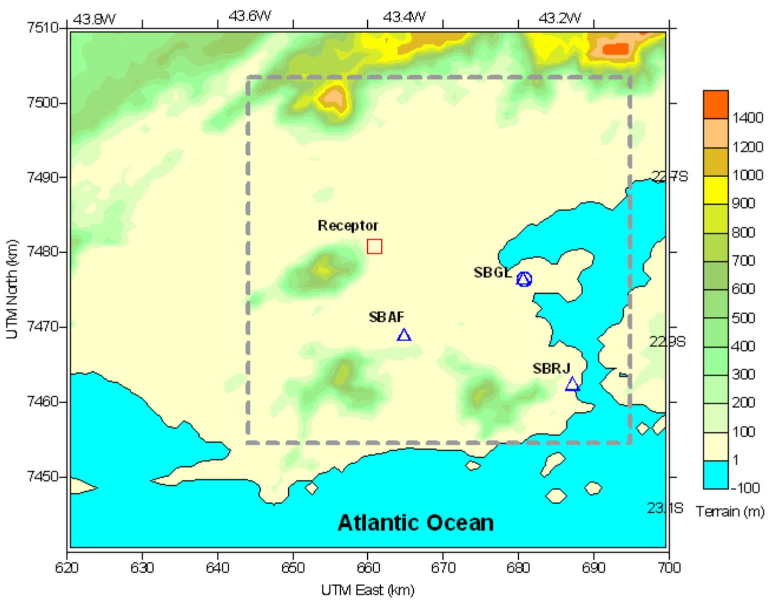

Figure 1. Rio de Janeiro Metropolitan Region. In dashed lines the domain of AERMOD and CALPUFF simulations. The red square indicates the SO_2 receptor, the blue triangles the surface meteorological stations and the blue circle the upper air station.

METHODOLOGY

The SO_2 concentrations were simulated by AERMOD and CALPUFF for RJMR from 20th August to 20th September 2008 for evaluation against observed data available in a near-field condition. Emission data from both mobile and stationary sources were used as line and area source respectively in AERMOD and just as area sources in CALPUFF. The twenty two mobile sources used (Loureiro, 2005) cover the major traffic routes of the region. For stationary sources, the facilities and industries emission from the region were distributed in 29 area sources as the methodology proposed by Pires (2005).

The AERMOD model was set up with surface and upper air data from International Airport of Rio de Janeiro (SBGL) located around twenty kilometers from the air quality station and ten kilometers of the major stationary emission sources. The CALPUFF model simulations were defined with two different configurations: The first one is the same as AERMOD simulations and named in this work CALPUFF1. The second one named CALPUFF3 was configured by using the upper air data from International Airport of Rio de Janeiro (SBGL) and surface meteorological data provide from Santos Dummont Airport (SBRJ), Afonsos Airport (SBAF) and International Airport of Rio de Janeiro (SBGL), as shown in table 1. In all configurations the pollutants removal mechanisms were neglected.

Table 1. Descriptions of Simulations performances

SIMULATIONS	SURFACE STATION	UPPER AIR STATION	METEOROLOGICAL PROCESSOR	DISPERSION MODEL
AERMOD	SBGL	SBGL	AERMET	AERMOD
CALPUFF 1	SBGL	SBGL	CALMET	CALPUFF
CALPUFF 3	SBGL, SBRJ and SBAF	SBGL	CALMET	CALPUFF

The models results were statistically compared against observed data from INEA air quality station located at Nova Iguaçu (NI), twenty kilometers away from major stationary emission sources. The scatter plot, fractional variance (FS), correlation coefficient (R), fractional bias (FB), factor of two (FAC2) and normalized mean squared error (NMSE) were applied in order to measure models uncertainties.

RESULTS

The wind rose representative of airport surface stations are presented in figure 2. It can be noted that for SBAF south and southwest directions predominantly occur, with maximum intensity of the 8.8 m/s and 11.5% of calm winds. At SBGL the southeast pattern is more evident with maximum intensity similar to that observed at SBAF and calm regime slightly lower at just 6.7% of calm winds. At SBRJ the calm regime is around 4.3% with main direction from the south sector and maximum intensity of the 11 m/s. The wind regime analysis shows a slight variability of the atmospheric circulation pattern surrounding the analyzed emissions area strengthening the inhomogeneous features of the region as discussed previously.

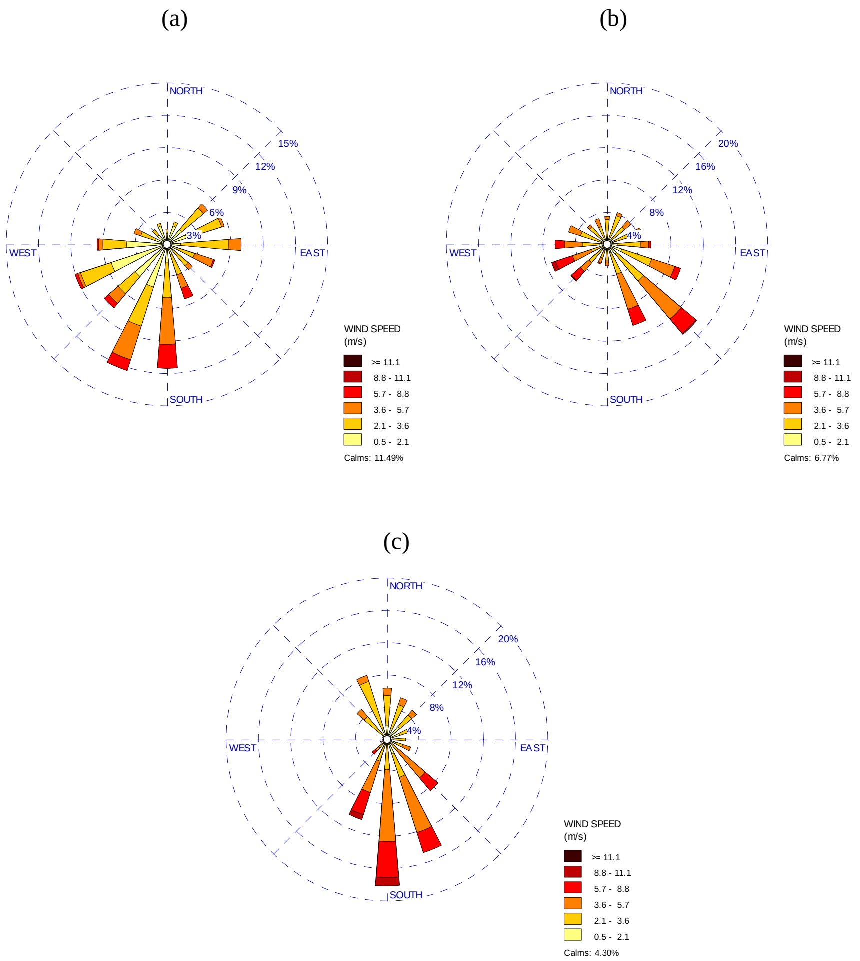

Figure 2. Wind rose for SBAF (a), SBGL (b) and SBRJ (c) during simulation period.

The statistical results analysis showed in table 2 presents the evaluations of models uncertainties for this analysis. The AERMOD correlation index presented the worst value in comparison with that obtained by CALPUFF simulations, with the best result to CALPUFF 3, showed more realistic temporal variability pattern of concentrations to the region. It indicate a potentiality to CALPUFF simulations, mainly by using more meteorological data (CALPUFF 3), to represent the pollutant transport on near-field in RJMR. It should be noticed that Gaussian models were not designed to attempt for temporal concentration variability due to its steady-state assumption, as non steady-state Lagrangian puff models that allow to identify the effects of time and space varying meteorological conditions on pollutant transport. The measure of mean relative scatter performed by AERMOD NMSE index presents poor value when compared with CALPUFF's values. The FS index shows the comparative values between the two CALPUFF's configurations, where an overestimative is observed of the monitored concentration dispersion field against the behavior obtained with AERMOD. From FB index analysis can be noted that the AERMOD results underestimate observed concentration levels while the CALPUFF's FB index indicates an overestimation. For regulatory purpose it is expected that simulated results should be conservative for concentration level, then it was highlighted that the AERMOD model simulation to RJMR should be done carefully.

Table 2. Statistical results of AERMOD and CALPUFF evaluations against observed data

STATISTICAL INDEXES	CALPUFF 1	CALPUFF 3	AERMOD
R	0.48	0.52	0.36
NMSE	0.71	0.68	1.67
FS	-0.60	-0.59	0.72
FB	-0.37	-0.44	0.90
FAC2	0.70	0.59	0.33

The Scatter Plots in figure 3 were designed to compare results in order to understand the best fit to observed data and the poor results to air quality regulatory practice by FAC2. It highlights that CALPUFF results were better than AERMOD, mostly overestimating observed data while the latter underestimated data. Also CALPUFF 1 performed better than CALPUFF 3 presenting a higher FAC2. It can be attributed by the weight given for the three surface meteorological data in CALPUFF 3 that are set by the parameters R1 and RMAX1 in CALMET, then this parameter must be best analyzed with sensibility studies to obtain the region appropriate value. In this work the R1 value was equal to eight kilometers and RMAX1 equal forty kilometers.

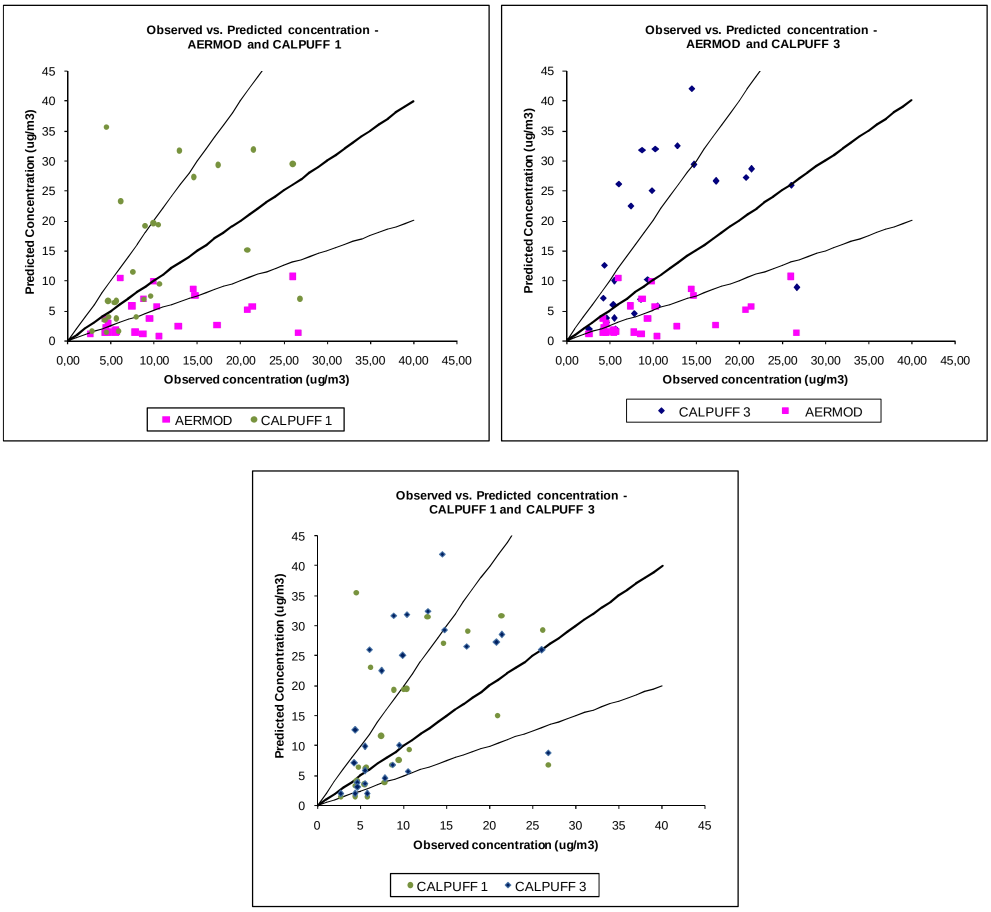

Figure 3. Observed vs. Predicted concentration by AERMOD, CALPUFF 1 and CALPUFF 3.

CONCLUSIONS

The evaluation of modeling concentrations results against observed data performed by statistical indexes indicated that the CALPUFF simulations presented better performance than AERMOD in near-field scenarios at RJMR. The CALPUFF pattern tends to overestimate the monitoring data against the behavior obtained with AERMOD. It shows that the CALPUFF model performed a conservative pattern, however it is hoped that the use of a removal process would improve results. The highest meteorological data assimilation from surface stations on CALMET played an important role on correlation and NMSE results while worsening the FAC2 and FB. Thus it is important to emphasize that extensive studies of wind station weight are required in order to play more realistic CALPUFF simulations in RJMR with several wind data. Besides AERMOD is the recommended model for regulatory purposes in near-field situations, CALPUFF indicated to be more promissory for studies in this region based on the relevant features inhomogeneous local conditions for atmospheric dispersion. Based on these results the use of air quality models require more studies for this region in longer periods and a variety of atmospheric conditions.

ACKNOWLEDGEMENTS

We would like to thank the Rio de Janeiro State Institute of Environment (INEA) and the Brazilian National Institute of Meteorology (INMET) for the pollutants and meteorology observed data, the Brazilian National Council of Research and Development (CNPq) and Fund to Support Research in the State of Rio de Janeiro (FAPERJ) for financial support.

REFERENCES

EPA. *AERMOD: Description of Model Formulation*. North Carolina, U.S. Environmental Protection Agency, 2004.

EPA. *Revision to the Guideline on Air Quality Models: Adoption of a Preferred General Purpose (Flat and Complex Terrain) Dispersion Model and Other Revisions.* North Carolina, U.S. Environmental Protection Agency, 2005. Federal Register / Vol. 70, No. 216 / Rules and Regulations. Appendix W of 40 CRF Part 51.

EPA. *Model Clearinghouse Review of CALPUFF Modeling Protocol for BART*. North Carolina, U.S. Environmental Protection Agency, 2009. Office of Air quality Planning and Standards Memorandum.

Pires, D.J. *Rio de Janeiro Metropolitan Region atmospheric emission stationary sources inventory and its contribution for Atmospheric pollution*. Tese de M.Sc., COPPE/UFRJ, Rio de Janeiro, Brasil, 2005.

INEA. *Rio de Janeiro Atmospheric Pollutant Emissions sources Inventory*, 2004. Instituto Estadual do Ambiente, http://www.inea.rj.gov.br

MME. *New Regulatory Reach: Strategic Areas and Subsalt layer*. 2009. Ministério de Minas e Energia, http://www.mme.gov.br/mme.

Loureiro, L. N. *Case study for atmospheric emission: Atmospheric emission inventory Evaluation of mobile sources on Rio de Janeiro Metropolitan Region*. Tese de M.Sc., COPPE/UFRJ, Rio de Janeiro, Brasil, 2005.

Scire, J.S., Strimaitis, D.G., Yamartino, R.J. *A User's Guide for the CALPUFF Dispersion Model (Version 5.0)***.** Concord, MA, Earth Tech, Inc., 2000. 468 p.