EVALUATION OF AIR QUALITY: SIMUATION OF AIR POLLUTANTS DISPERSION IN PAULINIA (BRAZIL) USING ISCST3

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Abstract. *The purpose of this paper is to study main pollutants (NO_x, SO_2, CO and PM_{10}) dispersion in Paulinia (SP – Brazil) atmosphere from January 1st to December 31st. It was considered both vehicular and industrial emissions. ISCST3 was the dispersion model used. To validate the methodology, the simulated NO_x and SO_2 concentrations were compared to data from air quality monitoring stations held by CETESB (Companhia Ambiental do Estado de São Paulo). The relative difference between simulated and monitored period mean NO_x concentrations for Paulinia-Center station was about 30% and for Paulinia-South station was about 55%. It was expected because the emission factor considered for NO_x was the mean emission factor established in PROCONVE (Programa de Controle da Poluição do Ar por Veículos Automotores), due to lack of measured data for this pollutant. The relative difference between simulated and monitored period mean SO_2 concentrations for Paulinia-B.Cascata station was about 162%. It is expected due to the non consideration of chemical reactions in the dispersion model which may transform SO_2 into another substance. In spite of the observed differences between simulated and monitored concentrations of NO_x and SO_2, it evidences the ISCST3 model performance as a tool in simulation of air pollution dispersion. The air quality evaluation showed that NO_x concentrations were above air quality standards for hourly mean concentration but below air quality standards for annual mean concentration. SO_2 concentration was below the primary air quality standards and above secondary one. CO and PM_{10} concentrations were below air quality standards. It means the air quality of Paulinia was good for year 2009. It also can be seen that the concentration of CO was the only one which followed more directly mobile sources location, the other pollutants followed the plume from industrial emissions of Replan point sources. We can conclude that the major sources of CO pollution are vehicles and the other pollutants are emitted mainly from industrial sources.*

Keywords: *air pollution dispersion, ISCST3, air quality.*

1. INTRODUCTION

Due to the concern about population's life quality improvement and the increasing air pollution emissions, more studies about air pollutants transport is needed. So, there was a significant increasing in air pollution dispersion researches in urban areas (Clemente, 2000; Levy *et al*., 2002; Amorim, 2003; Moraes, 2004; Lyra, 2008) because of the computational technology improvement. Despite this, quantify air pollution dispersion is still a complex task, as the lower atmosphere flow, called Planetary Boundary Layer (PBL), is controlled by turbulence whose physics is still far from completely understood (Moraes, 2004). However, nowadays simulate air pollution dispersion is feasible due to the technological progress that made the results closer to real data and describes the inherent complexity, including the atmospheric physicochemical processes.

The dispersion modeling is the main tool to simulate air pollutants transport and became important not only for air quality evaluation in big cities but to identify the proper regions for the installation of new industries. Beforetime, topographical characteristics and meteorological data haven't been considered in determining the appropriate region to install an industry. For example, in Cubatão (SP – Brazil) due to adverse atmospheric conditions (meteorology - wind direction; topography – mountains) to air pollutants dispersion, the air pollution concentration was too high that new technologies air pollution control has been developed. Currently, situation in Cubatão was controlled and before installing a new industry in Brazil an Environmental Impact Study is required by the law (Alonso and Godinho, 1992).

The newest air pollution dispersion models are those with meteorological models attached, which are California Photochemical Grid Model (CALGRID), California Puff Model (CALPUFF), Urban Airshed Model (UAM) and American Meteorology Society – Environmental Protection Agency – Regulatory Model (AERMOD). These models are used in developed countries by environmental agencies and researchers (Moraes, 2004).

In spite of these new technologies, in developing countries like Brazil, the unattached models are still being used due to the lack of reference in CONAMA (*Conselho Nacional do Meio Ambiente*) legislation and mainly to lack of meteorological data in some cities. That's why there are a lot of difficulties in air pollution dispersion studies held in Brazil.

So, this study aims to simulate the transport of the main air pollutants like nitrogen oxides (NO_x), sulphur dioxide (SO_2); carbon monoxide (CO) and inhalable particulate matter (PM_{10}) from stationary and mobile sources in Paulinia (SP – Brazil) from January 1st to December 31st, 2009. The simulated results were compared against monitoring stations cared by São Paulo State environmental agency - CETESB aiming the model validation. Then, air quality was evaluated by comparing the simulated results with air quality standards. To do so, we choose the ISCST3 dispersion model (Industrial Source Complex, Short Term, 3rd generation) due to its smaller meteorological data requirements, even though recently the US-EPA (United States Environmental Protection Agency) has recommended the use of AERMOD, also developed by EPA (1995).

2. METHODOLOGY

ISCST3 is a Gaussian plume model which can be applied to describe air pollutants transport from a variety of sources such as: industrial complexes; vehicles; wet and dry deposition, building downwash effect, chemical transformations, etc (U.S.EPA, 1995). The ISCST3 simulations can vary according to information complexity considered and the results one wants to achieve. In this paper were considered:

- Source characteristics: Each industrial source was characterized as a point source and its emissions was estimated based on the regional emission inventory (CETESB, 2009) or stack sampling data for some sources when these data were available (location, height, diameter; emission rate; temperature and velocity gas exit). The mobile sources (vehicles) were considered as line sources, so it was need to know the city main streets and develop a vehicular emission inventory.

- Meteorological data: The required meteorological data are ambient temperature, wind speed and direction, stability category and mixing height. Below it will be shown these data for this study.

- Topography: A 90 meter digital topography data resolution was obtained from U.S.GS (2009) (U.S. Geological Survey).

Paulinia was chosen as our case study. Its characteristics are shown below, with the details of industrial and vehicular emission inventory.

3. CASE STUDY

Paulinia is one of the most industrialized areas of São Paulo state. Currently, Paulinia has 84,577 inhabitants and an area of 139 km^2 from which 60% is urban area (IBGE, 2010; Clemente, 2000). It's part of the Metropolitan Region of Campinas and is 25 km northwest distant from Campinas. Its surface is almost flat and its height goes from 510 to 660 meters, as shown in Fig. 1 (A).

The meteorological data used in this research (hourly data from January 1st to December 31st, 2009 of ambient temperature, wind speed and direction, solar radiation and cloud cover) were obtained from the automatic meteorological station of Paulinia's refinery (Replan). About wind speed and direction, Fig. 1(B) shows the 2009 wind rose. It can be seen that the prevailing wind direction is from southeast (from Campinas to Paulinia) and northeast (from industrial zone to urban area of greater population density). The stability category was calculated according to the Pasquill stability category (Seinfeld and Pandis, 2006), which relates the wind speed standard deviation with the wind scalar mean speed, by the sigma A method (U.S.EPA, 2000). The mixing height was calculated according to Randerson (1984) method published in U.S.EPA (1995). With Paulinia's whole characteristics defined, it will be shown the methodology used in the emission inventory.

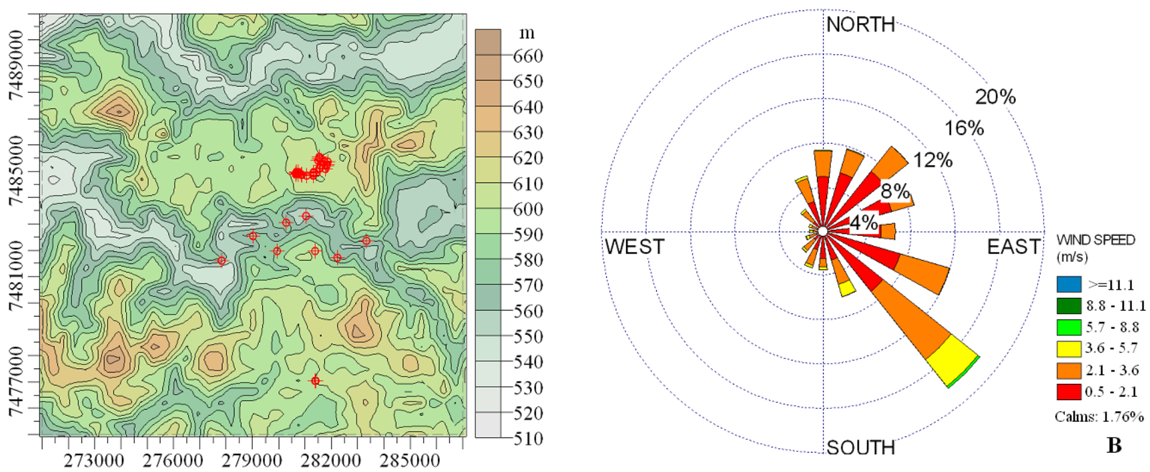


Figure 1. Topography of Paulinia (A); Paulinia's wind rose for 2009 (B)

3.1. Industrial emission inventory

In this research we considered industrial emission from the main industries of Paulinia as in CETESB (2009). The industries names and emission rates by pollutant are in Tab. 1, where the major contribution to all pollutants is from Replan. Rhodia is a great emitter of NO_x as well as of CO and Evonik Degussa is a great emitter of SO_2. Due to the lack of data for all stacks, it was considered that each industry emission came from only one point source like showed in Tab. 1. The Petróleo Brasileiro S/A – Replan was exception with 27 stacks considered according to Petrobras (2006). It was considered a total of 38 point sources in this paper and its location is shown in Fig. 2. It can be seen that most industries are at northeast area and, according to the wind direction (Fig. 1(B)) the pollutants shall go in central area direction. Data such as gas exit temperature (K) and velocity (m/s); stack height (m) and diameter (m) from each point source is needed, but there is no information about this, so we considered typical values as in Tab. 2, except for *Replan* which was considered the data from Petrobras (2006).

Table 1. Atmospheric emissions estimate for point sources of Paulinia (Adapted from CETESB, 2009)

Industry[(1)]	Pollutants emission (t/year)			
	NO_x	SO_2	PM_{10}	CO
Bann Química Ltda (BAN)	18.20	0.07	1.78	4.55
Cargil Nutrição Animal Ltda (CAR)	8.54	24.02	1.93	0.79
Evonik Degussa Ltda (EVO)	101.56	751.93	28.13	30.84
Galvani Ind. Com. e Serviços Ltda (GAL)	27.05	196.50	46.43	-
Hércules do Brasil Produtos Químicos Ltda (HER)	4.8	13.49	1.08	0.44
Invista Brasil Ind. e Com. de Fibras Ltda (INV)	6.65	0.68	0.68	1.63
Kraton Polymers do Brasil S/A (KRA)	6.76	8.94	1.65	4.71
Nutriara Alimentos Ltda (NUT)	7.74	0.03	0.76	1.94
Orsa Celulose, Papel e Embalagens S/A (ORS)	43.96	1.28	4.35	10.93
Petróleo Brasileiro S/A – Replan (REP) [(2)]	7,584.00	12,074.00	1,201.00	2,267.00
Rhodia Poliamida e Especialidades Ltda (RHO)	1,292.28	85.18	13.68	95.44
Syngenta Proteção de Cultivos Ltda (SYN)	2.31	6.50	0.55	0.21

[(1)]*: Abbreviations in parentheses are those used in Fig. 2.*
[(2)]*: Total emission of the 27 stacks considered.*

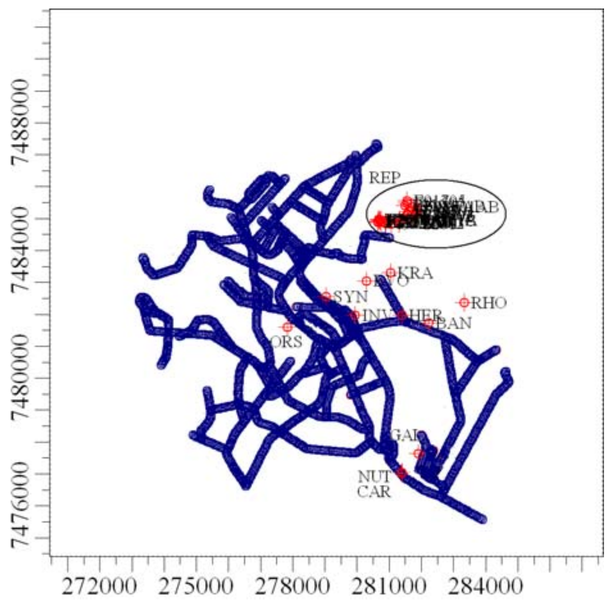


Figure 2. Point and line sources location

Table 2. Stacks data

Variable	Value
Height (m)	20
Diameter (m)	1
Exit Temperature (K)	600
Exit Velocity (m/s)	20

3.2 Vehicular emission inventory

To include vehicular emissions in dispersion model, it was needed to create the Vehicular Emission Inventory (VEI). Details of the methodology used are in Tadano *et al.* (2010). Here it's shown the main information. The fuel inventory for vehicules is presented in Tab. 3. It can be observed that the gasoline is used by the majority of the cars. Gasoline C (gasoline with 22% of ethanol) is used by 50 and 35% of passenger and commercial car, respectively. Ethanol is used by 34 and 22% of passenger and commercial car, respectively. Diesel is used by 85% of the trucks and 100% of the bus uses this fuel. The fleet age is presented in Fig. 3, where vehicles older than 1989 wasn't included and corresponds to 33% of the fleet. It can be seen that the fleet gradually increased until 1997 when had quite a decrease and then came back increasing.

Table 3. Vehicle percentage by type of vehicle and kind of fuel used

Type of Vehicle	Gasoline	Gasoline C	Ethanol	Diesel	Total
Passenger Car	16.58%	49.58%	33.84%	-	28,016
Commercial Car	20.10%	35.36%	21.80%	22.74%	4,079
Truck	13.68%	0.07%	0.37%	85.88%	2,968
Bus	-	-	-	100%	2,413
Motorcycle(1)	-	-	-	-	7,742
Total	5,871	15,336	10,379	5,889	45,218

(1): Motorcycle data wasn't divided by kind of fuel used.

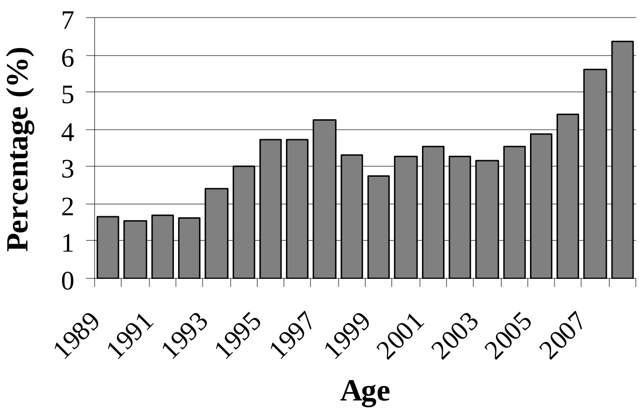


Figure 3. Vehicles of Paulinia by age

- Fleet emission calculation

It was possible to determine fleet emission according to the methodology proposed by CETESB (1994) after obtaining data about vehicular fleet and emission factors by type of vehicle, kind of fuel used and age as described in Tadano *et al.* (2010). The vehicles mileage was set by type as showed in Tab. 4 for new cars. For older vehicles was considered 2% decrease in annual mileage (Lents et al., 2004).

Table 4. New vehicles annual mileage

Type of Vehicle	Annual km(1)
Passenger Car(2)	20,000
Commercial Car(2)	20,000
Truck(3)	51,500
Bus(3)	73,500
Motorcycle(4)	5,200

(1): To new vehicles;
(2): Lents et al. (2004);
(3): Ferreira et al. (2008);
(4): CETESB (1994).

Finally, the fleet total emission was calculated according to CETESB (1994) as shown in Eq. (1). The fleet emission values for each pollutant are presented in Tab. 5. It can be seen that trucks and buses are the major emitters of NO_x and SO_2 because they are moved by diesel. Passenger vehicles are the major emitters of CO due to the great amount moved by gasoline C. The data of the vehicular emission are included in the ISCST3 model as line sources then it has to be distributed on the main streets of Paulinia as shown in Fig. 2.

$$E_F = FE_F \cdot \overline{KM} \cdot N \cdot 10^{-6}, \qquad (1)$$

where:
E_F : Fleet emission of the considered pollutant (t/year);
FE_F : Fleet emission factor for the considered pollutant (g/km);
$\overline{KM}$: Annual mean mileage (km);
N : Fleet vehicles number.

Table 5. Paulinia's vehicular fleet emission for each pollutant

Type of vehicle	Fleet emission (t/year)			
	NO_x	SO_2	PM_{10}	CO
Passenger Car	935.935	177.823	360.722	28,310.677
Commercial Car	268.950	24.897	53.693	3,771.056
Truck	8,624.777	1,926.042	658.807	11,903.636
Bus	1,495.971	333.813	114.135	2,052.962
Motorcycle	35.970	43.625	46.026	6,870.229
Total	**11,361.540**	**2,506.200**	**1,233.383**	**52,908.561**

3.3 Receptors

We considered a uniform cartesian grid of 256 km^2 covering Paulinia city. The grid central point was UTM X 279000 and UTM Y 7483000. The space between each receptor was of 200m giving 6561 points. Moreover, it was added three discrete receptors where the air quality monitoring stations of Paulinia are located, as shown in Tab. 6.

Table 6. Air quality monitoring stations held by CETESB and its elevation and UTM coordinates

Monitoring Stations	Elevation (m)	UTM Coordinates	
		X	Y
Paulinia-Center	595.89	278829	7480128
Paulinia-South	592.59	280680	7478503
Paulinia-B. Cascata	595.4	278996	7486352

4. RESULTS

After obtaining all data needed to simulate the pollutants (NO_x, SO_2, CO and PM_{10}) dispersion in Paulinia's atmosphere from January 1st to December 31st, 2009 using ISCST3, it is necessary to validate the methodology before evaluating the air quality. To validate the model, the results for NO_x and SO_2 where compared with monitoring data from CETESB (2009).

4.1 Model validation

The simulated results for NO_x and SO_2 dispersion were compared with monitored concentrations from CETESB (2009). These pollutants are the most difficult ones to simulate; therefore it is enough to validate the model (Clemente, 2000; Kumar *et al*., 2006). Other reasons for not using CO and PM_{10} to validate de model is that CO isn't monitored in Paulinia and the dispersion model can't consider all the sources of PM_{10} like resuspension (the main source of PM_{10} dispersion) and emissions from burning forests, an important source in seasons with low relative humidity.

- Nitrogen Oxides (NO_x)

Table 7 presents period mean concentrations of NO_x simulated with ISCST3 and monitored by CETESB (2009) in Paulinia-Center and Paulinia-South stations. The predicted period mean concentrations using ISCT3 are lower than the monitored ones. The relative difference in Paulinia-Center station was about 30% and for Paulinia-South was about 55%. It is expected because the emission factor considered for NO_x was the mean emission factor established in PROCONVE (*Programa de Controle da Poluição do Ar por Veículos Automotores*), due to lack of measured data for this pollutant. The relative difference between predicted and monitored concentrations of Paulinia-South station is greater than those of Paulinia-Center. It may be due to stations location, so Paulinia-South receives more influence of the pollutants dispersion coming from neighbor cities.

Table 7. Comparison between predicted and monitored concentrations of NO_x in Paulinia-Center and Paulinia-South stations

Nitrogen Oxides	Annual mean (μg/m^3)	
	Paulinia-Center	Paulinia-South
Predicted results by ISCST3	16.88	10.42
Measured results by CETESB[(1)]	24	23
Deviation	30%	55%

[(1)]: Measured results by CETESB were from NO_2 (Nitrogen dioxide).

- Sulfur dioxide (SO_2)

Table 8 presents period mean concentrations of SO_2 simulated with ISCST3 and monitored by CETESB (2009) in Paulinia-B.Cascata station. The predicted period mean concentration using ISCST3 is greater than the monitored one. The relative difference was about 162%. It is expected due to the non consideration of chemical reactions in the dispersion model which would transform SO_2 into another substance.

In spite of the observed differences between simulated and monitored concentrations of NO_x and SO_2, it evidences the ISCST3 model performance as a tool in simulation of air pollution dispersion.

Table 8. Comparison between predicted and monitored concentrations of SO_2 in Paulinia-B.Cascata station

Sulfur Dioxide	Annual mean (μg/m^3)
Predicted results by ISCST3	36.62
Measured results by CETESB	14
Deviation	162%

4.1 Air quality evaluation

To evaluate Paulinia's air quality, the data simulated using ISCST3 model was compared against the national air quality standards showed in Tab. 9. It can be seen that the air quality is measured by two standards: primary and secondary. The primary standard is defined as the maximum tolerable level of air pollutants concentration and is considered as a short and medium time strategy and the secondary standard is the pollutants concentration below which is estimated a minimum adverse effect to human being as well as to animals, plants and materials. It is considered as a long time strategy (CETESB, 2009).

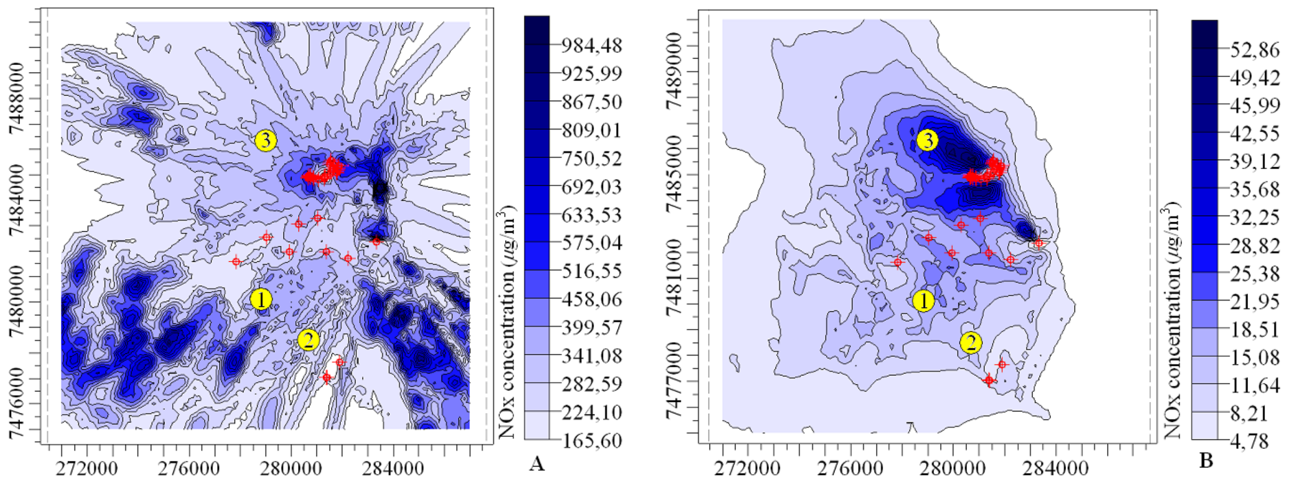
Table 9. National air quality standards (Adapted from CETESB, 2009)

Pollutant	Sampling time	Primary Standard ($\mu g/m^3$)	Secondary Standard ($\mu g/m^3$)
Particulate Matter (PM_{10})	24hours(1)	150	150
	AGM(2)	50	50
Sulfur Dioxide (SO_2)	24 hours(1)	365	100
	AAM(3)	80	40
Nitrogen Oxides (NO_x)	1hour	320	190
	AAM(3)	100	100
Carbon monoxide (CO)	1hour(1)	40,000	40,000
	8hours(1)	10,000	10,000

(1): Can't be exceeded more than once a year;
(2): Annual Geometric Mean;
(3): Annual Arithmetic Mean.

- Nitrogen Oxides (NO_x)

As shown in Tab. 9, NO_x primary and secondary air quality standards for hourly mean concentration are 320 and 190 $\mu g/m^3$. Figure 4 (A) presents maximum hourly mean NO_x simulated concentrations for 2009. It can be seen that maximum concentrations go up to 985 $\mu g/m^3$ and are greater than the primary and secondary standards. It can also be seen that the highest concentrations are near the major point and mobile sources. Figure 4 (B) presents annual mean NO_x simulated concentrations. It shows that maximum concentrations go up to 53 $\mu g/m^3$ and are below air quality standards for annual mean concentration (100 $\mu g/m^3$).

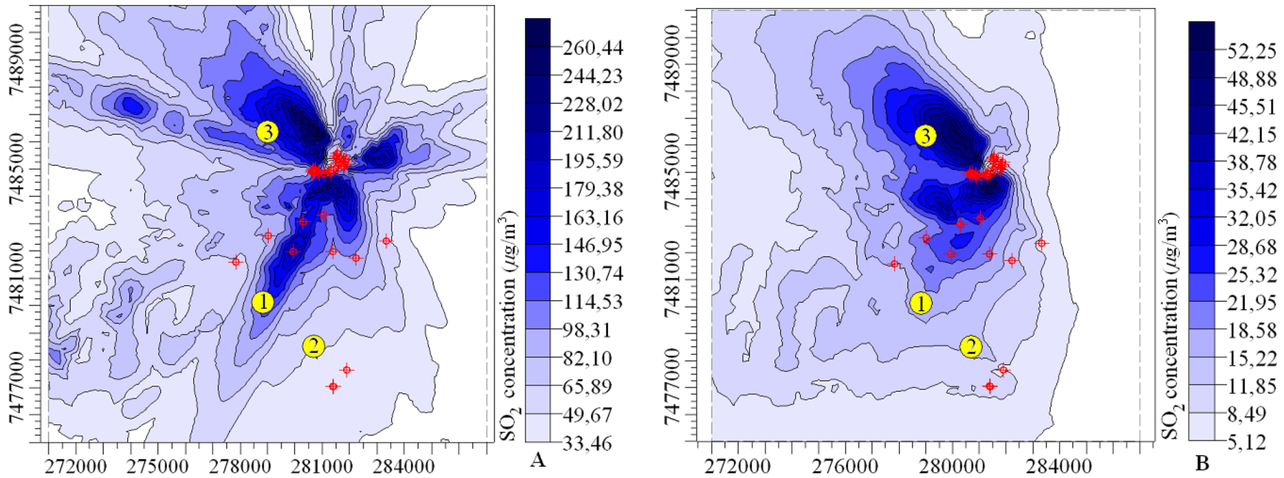


1: Paulinia-Center station; 2: Paulinia-South station; 3: Paulinia-B.Cascata station

Figure 4. Maximum hourly mean NO_x concentration (A) and annual mean NO_x concentration (B) for 2009

- Sulfur Dioxide (SO_2)

According to Tab. 9, SO_2 primary and secondary air quality standards for daily mean concentration are 365 and 100 $\mu g/m^3$. Figure 5 (A) presents maximum daily mean SO_2 simulated concentrations. It can be seen that maximum concentrations go up to 260 $\mu g/m^3$ and are below primary but above secondary air quality standard. It can also be seen that maximum concentrations are near point sources of Replan. Figure 5 (B) presents annual mean SO_2 simulated concentrations. The maximum values go up to 52 $\mu g/m^3$ and are below the primary air quality standard of 80 $\mu g/m^3$ and above secondary standard of 40 $\mu g/m^3$ for annual mean concentration.

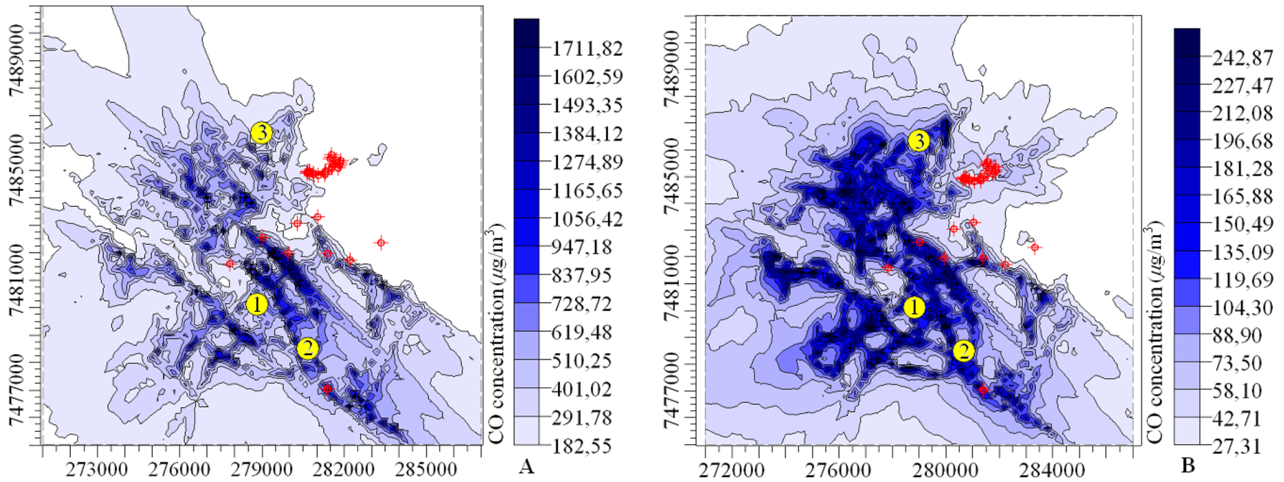


1: Paulinia-Center station; 2: Paulinia-South station; 3: Paulinia-B.Cascata station

Figure 5. Maximum daily mean SO_2 concentration (A) and annual mean SO_2 concentration (B) for 2009

- Carbon Monoxide (CO)

According to Tab. 9, CO primary and secondary air quality standards for hourly mean concentration are 40,000 $\mu g/m^3$. Figure 6 (A) presents maximum hourly mean CO simulated concentrations. It can be seen that maximum concentrations go up to 1712 $\mu g/m^3$ and are below air quality standards. It can also be seen that maximum concentrations are near mobile sources. Figure 6 (B) presents maximum 8 hours mean CO simulated concentration. The maximum values go up to 243 $\mu g/m^3$ and are below air quality standards for 8 hours mean concentration (10,000 $\mu g/m^3$).

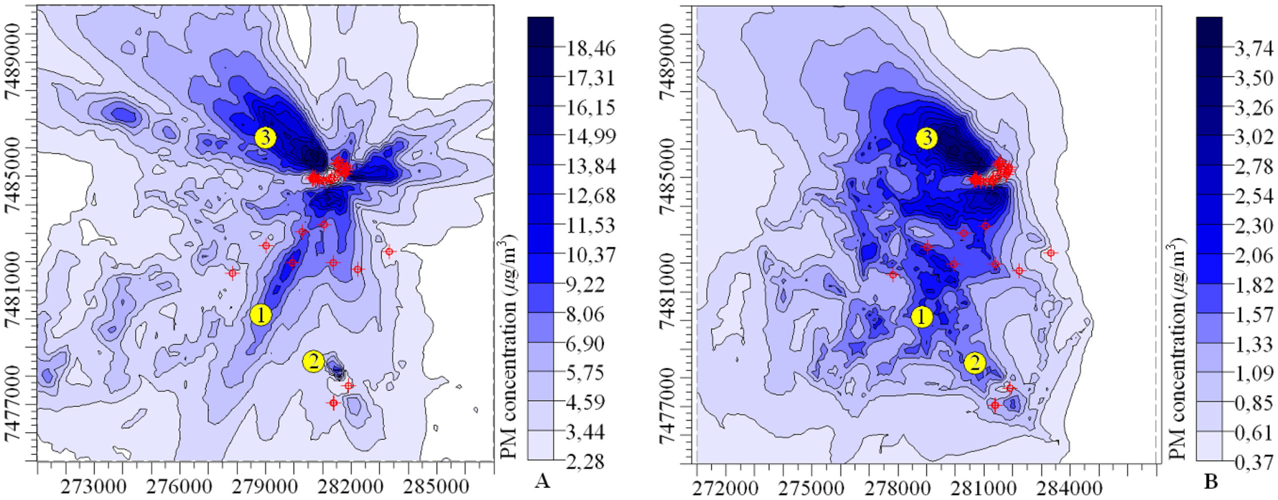


1: Paulinia-Center station; 2: Paulinia-South station; 3: Paulinia-B.Cascata station

Figure 6. Maximum hourly mean CO concentration (A) and maximum 8 hours mean CO concentration (B) for 2009

- Particulate Matter (PM_{10})

As shown in Tab. 9, PM_{10} primary and secondary air quality standards for daily mean concentration are 150 $\mu g/m^3$. Figure 7 (A) presents maximum daily mean PM_{10} simulated concentrations. It can be seen that maximum concentrations go up to 18.5 $\mu g/m^3$ and are below air quality standards. It can also be seen that maximum concentrations are near point sources of Replan. Figure 7 (B) presents annual mean PM_{10} simulated concentrations. The maximum values go up to 4 $\mu g/m^3$ and are below air quality standards for annual mean PM_{10} concentrations (50 $\mu g/m^3$).



1: Paulinia-Center station; 2: Paulinia-South station; 3: Paulinia-B.Cascata station

Figure 7. Maximum daily mean PM_{10} concentration (A) and annual mean PM_{10} concentration (B) for 2009

The results showed that NO_x concentrations were above air quality standards for hourly mean concentration but below air quality standards for annual mean concentration. SO_2 concentrations were below the primary air quality standards and above secondary ones. CO and PM_{10} concentrations were below air quality standards. It means Paulinia's air quality was good in 2009. It can also be seen that the concentration of CO was the only one that followed more directly the location of mobile sources, the other pollutants followed the plume from industrial emissions of Replan point sources. We can conclude that the major sources of CO pollution are vehicles and the other pollutants are emitted mainly from industrial sources.

5. CONCLUSION

Atmospheric dispersion modeling as main tool able to simulate air pollutants transport was applied in this research aiming to evaluate Paulinia's air quality. ISCST3model was used to analyze NO_x, SO_2, CO and PM_{10} dispersion from January 1st to December 31st, 2009. The main difficulty in air pollution dispersion studies is to develop the industrial and vehicular emission inventories. To industrial emissions the main problem is to obtain sources details because of industries privacy. They are not receptive to researchers of air pollution. To vehicular emissions, there are a lot of problems due to lack of information of all parameters; fleet information separated by categories of vehicle and fuel; measured emission factors; annual vehicles mileage for each city and so on. Then it was necessary to make a lot of considerations and approximations that can sometimes under or overestimate the pollutants emissions. In spite of this, the study showed good results. The predicted NO_x and SO_2 concentrations comparison with air quality monitoring data showed great relative differences (30% for annual mean concentration of NO_x in Paulinia-Center station and 55% relative difference in Paulinia-South station; 162% for annual mean concentration of SO_2 in Paulinia-B.Cascata station), but all these differences were expected. For NO_x it happened because the emission factor considered was the mean emission factor established in PROCONVE and for SO_2 it is due to the non consideration of chemical reaction of the atmosphere which is able to transform SO_2 in another material. Although there were differences between simulated and monitored concentrations of NO_x and SO_2, it evidences the ISCST3 model performance as a tool in simulation of air pollution dispersion. The air quality evaluation showed that NO_x concentrations (maximum hourly mean up to 985 $\mu g/m^3$ and annual mean up to 53 $\mu g/m^3$) were above air quality standards for hourly mean concentration but below air quality standards for annual mean concentration. SO_2 concentrations (maximum daily mean up to 260 $\mu g/m^3$ and annual mean up to 53 $\mu g/m^3$) were below the primary air quality standards and above secondary ones. CO (maximum hourly mean up to 1712 $\mu g/m^3$ and maximum 8 hours mean up to 243 $\mu g/m^3$) and PM (maximum daily mean up to 18.5 $\mu g/m^3$ and annual mean up to 4 $\mu g/m^3$) concentrations were below air quality standards. It means the air quality of Paulinia was good for year 2009. It also can be seen that the concentration of CO was the only one that followed more directly the location of mobile sources, the other pollutants followed the plume from industrial emissions of Replan point sources. We can conclude that the major sources of CO pollution are vehicles and the other pollutants are emitted mainly from industrial sources.

6. ACKNOWLEDGEMENTS

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