Analysis of the Middle Range Transport of the Aerosol from Cubatão by means of a Modelling System for Complex Terrain

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1 Introduction

The modelling system RMS, consisting of the mesoscale model RAMS, the Lagrangian dispersion model SPRAY and the interface code MIRS, was used to investigate the middle range dispersion of inhalable particulate matter emitted at Cubatão, Brazil (23.53S, 46.25W). This industrial city is located on the flat terrain between the escarpment of Serra do Mar mountain range (700 to 1000 m high) and the sea. The modelling of pollutant dispersion over such a complex terrain requires a model system able to give reliable simulations of the atmospheric transport and diffusion processes. Only the particulate matter emitted by 5 Fertiliser Plants placed in Vila Parisi, a town of Cubatão, at the entrance of the Moji Valley, was studied. They give the heaviest contribution to the PM10 local levels (Kerr and Orsini, 1996) that also are the worst levels in all the São Paulo State (annual average between 80 and 200 µg/m³ - CETESB, 1988 to 2000).

The industrial complex at Cubatão is the main factor for the local bad air quality and for the damage brought about to the tropical forest in the neighbour Biological Reserve. We simulated concentration fields related to typical regional circulation. The city itself has 100.000 inhabitants, and the nearby area is densely populated: Santos and São Vicente, 12 km far, have 700.000 inhabitants and the São Paulo metropolis, whose centre is 40 km far, has nearly 17.2 million inhabitants.

2 3D-wind field and dispersion models

The good performances of RAMS (Pielke et al., 1992) in real applications are described in several works (e.g. Pielke and Pearce, 1994). RAMS' two way nesting technique allows the user to start from large computation domains and to downscale to smaller regions. It is non-hydrostatic, so that all meteorologically relevant spatial scales can be represented, and the vertical coordinate is a terrain-influenced coordinate. RAMS outputs relevant to this model system are: 3-D wind, temperature and diffusion coefficient fields, and the 2-D topography and surface layer fluxes.

SPRAY (Tinarelli et al., 1994 and 1999; Ferrero and Anfossi, 1998 a,b) is a LSM (Lagrangian Stochastic Model) for the simulation of the dispersion of inert gases in complex terrain, based on the Langevin equation (Thomson, 1987). A Gaussian PDF is used in the horizontal directions and a Gram-Charlier PDF, truncated to the third order, in the vertical. MIRS reads the RAMS outputs, prescribes the turbulence information not given by RAMS and prepares the SPRAY inputs (Trini Castelli and Anfossi, 1997).

3 Models' parameterisation

RAMS - Our simulations focused on an area of roughly 100 km² with an inland-displaced centre, allowing a detailed analysis of the pollutant penetration toward the big urban centres placed in the plateau. Besides that, we used a larger grid, accounting for the general circulation characteristics, and a fine resolution grid, to evaluate the model performance around the critical topography near the sources of pollutants (Table 1). The meteorological information for the model initialisation was available every six hours at the standard pressure levels, with a resolution of 2.5 degrees (NCAR-USA). The topography file distributed by the EROS data Center (30” resolution) was supplemented for the local area by a file (resolution of nealy 3”) obtained by the digitalisation of a map with 1/50.000 scale (IGGSP, 1972). The vertical grid had a depth of 100 m in the first level, while the next 29 levels increased by a rate of 1.2, until reaching a maximum value of 500 m. The land/water percentage and sea temperature came from RAMS inner files (resolution of 10´ and 1 degree, respectively). Vegetation type (evergreen-broadleaf tree), soil type (clay loam) and roughness length (0.1 m) were kept constant.

MIRS - From RAMS tke and diffusion coefficients gridded values, MIRS calculated the 3-D wind standard deviations and the Lagrangian decorrelation time scales. PBL heights were defined using the criterion of the critical value for the Richardson number. Third order moment of the vertical velocity was prescribed according to Chiba (Trini Castelli and Anfossi, 1997).

SPRAY - Dispersion simulations were relative to the RAMS second grid. Source attributes are the same as described by Kerr et al.(2000b).

Table 1 Horizontal grids defined in the RAMS’ simulations.

Grid	side size (km)	Resolution (km)	Centre (Lat, Lon)	SW Corner (Lat, Lon)
Grid-1	560	14.4	23.740S; 46.330W	26.240S; 49.146W
Grid-2	104.4	3.60	23.805S; 46.400W	24.274S; 46.916W
Grid-3	36.9	0.90	23.870S; 46.330W	24.036S; 46.512W

3.1 Results and Discussion

3.1.1 RAMS simulations

Two periods of 96 hours were selected, beginning on 14 October 1991 and 21 October 1991, both at 6 UTC. The simplest option for humidity was chosen to avoid unnecessary complexities. Nevertheless, cloud development was enabled, since Kerr et al. (2000a) showed that its role in the thermal and radiative exchanges are important in the highly thermal coupled local circulation. These authors also enlarged the size of the finest grid toward the ocean to solve numerical problems related to the steep slopes of the mountains (simulation of unrealistic negative temperatures during the night) In the present work, the topographic definition was enhanced. The slopes became steeper, giving, again, unrealistic negative temperatures nearby the base of the mountains. This new numerical instability was solved by increasing the depth of first vertical grid cell from 50 m to 100 m. In particular, this more resolved topography allowed the dispersion process simulation to improve. Figure 1, for instance, is a NNW cross section showing the re-circulation simulated, near the ground, between the base of the mountain range and a small hill that was possible to identify only with the present topographic detail.

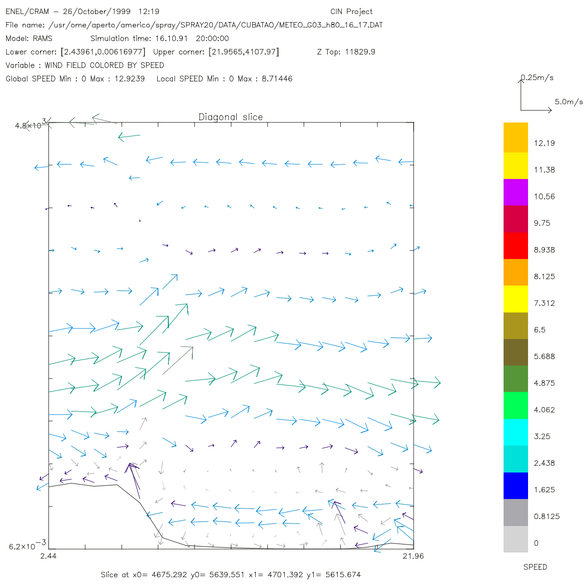

Figure 1

RAMS evaluation was performed for two ground stations: VPS (4 m a.s.l., 23.8498S; 46.3893W) with hourly horizontal wind measurements (Table 2); and IAG (799 m, 23.6491S; 46.6251W) also including temperature and humidity observations (Table 2 and 3). Comparisons were also done for one daily sounding station CNG at Congonhas airport (802 m, 23.625S; 46.650W, see Table 4). The following statistical indexes were used: MD (mean difference), RMSVE (root mean square vector error), RMSE (root mean square error) and FB (fractional bias).

For wind speed and direction, our MD values at IAG, and for the first period at VPS, are less than the best value obtained by Pielke and Pearce (1994). For the second period at VPS, only the wind intensity MD was slightly higher than their values, but the MD for the direction still was better than the minimum value they obtained. At the IAG station, *t* and *us* fit shows good statistical indexes. Our MD value for *t* are less than the Pielke and Pearces' best value (1.2ºC).

The predominant regional circulation is a sea breeze coupled with mountain breeze during the daytime, and a land breeze coupled with katabatic winds from the mountain range during night-time. This agrees with previous works (e.g. Dias et al., 1995; Bischoff-Gauβ et al., 1998).

Table 2 Statistical evaluation of the simulated horizontal wind velocity at 10m.

	14-17/October/1991		21-24/October/1991	
Station	VPS	IAG	VPS	IAG
RMSVE (u,v) - m/s	2.61	1.69	1.90	1.56
MD (speed) - m/s	-0.17	-0.06	-1.05	-0.03
MD (direction) - Degree	1	-23	-1	-13
number of cases	30	49	33	49

Table 3 Statistical evaluation of temperature and specific humidity at IAG.

	14-17/October/1991		21-24/October/1991	
	t (ºC)	us (g/kg)	t (ºC)	us (g/kg)
RMSE	2.81	1.85	2.25	2.35
FB	-0.01	-0.08	-0.03	-0.13
MD	-0.20	-	-0.63	-
number of cases	49	49	49	49

Table4 Statistical evaluation of the simulated sounding at Congonhas airport (São Paulo).

DATE	u,v (m/s)		θ (K)			us (g/kg)		
	rmsve	n	rmse	FB	n	rmse	FB	n
14-oct-1991	4.12	8	2.45	0.01	8	2.02	-0.22	8
15-oct-1991	3.65	8	2.57	0.00	10	1.59	-0.14	10
16-oct-1991	4.45	8	2.24	0.00	9	3.08	-0.39	9
17-oct-1991	4.99	8	1.62	-0.00	13	2.30	-0.26	13
21-oct-1991	2.48	13	2.57	0.01	12	2.19	-0.33	12
22-oct-1991	5.37	8	1.97	0.01	5	2.68	-0.26	5
23-oct-1991	3.94	8	2.46	-0.00	10	2.22	-0.35	10
24-oct-1991	3.66	8	1.56	0.00	8	2.93	-0.40	8

SPRAY's middle range dispersion simulations

The symbols used in Figures 2-4 are the following: 4 indicates the source location, TOP (842 m, 23.7797S; 46.3099W) and BOT (5 m, 23.8294S; 46.3697W) refer to the sampling stations; the other abbreviations refer to some municipalities of the São Paulo Metropolis. In the concentration scale, the first three concentration levels are small, providing a visualisation of the limits of the plume penetration. The other levels enable the comparison with the air quality standards for the inhalable particulate in the State of São Paulo.

Figures 2 and 3 show the concentration fields obtained for typical daytime regional circulation. In both cases the sea breeze overcame the mountain ridge and penetrated deep into the land. Concentration levels are high on the sierra slopes, at the Biological Reserve. On Figure 2, the centre axis of the inhalable particulate matter plume goes toward São Paulo. Some areas of the metropolis

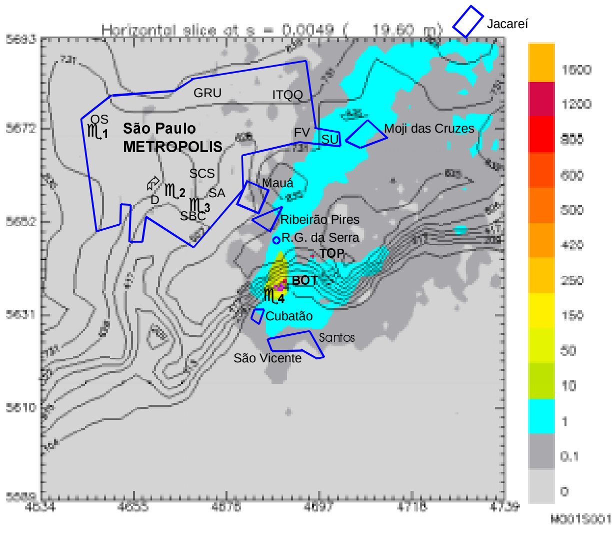

Figure 2

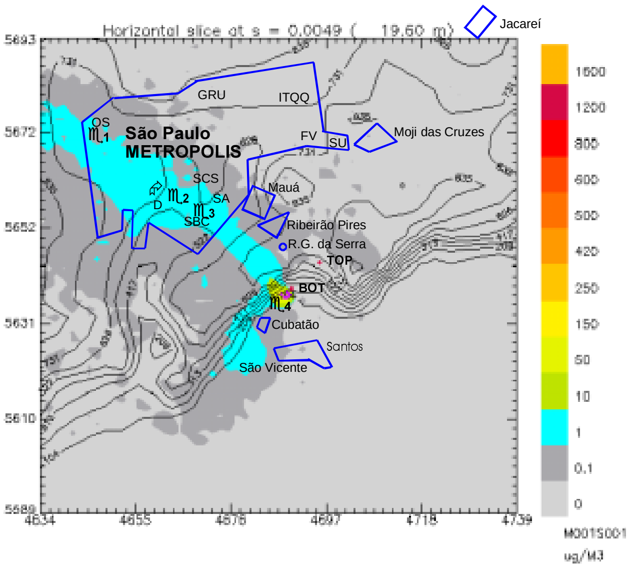

Figure 3

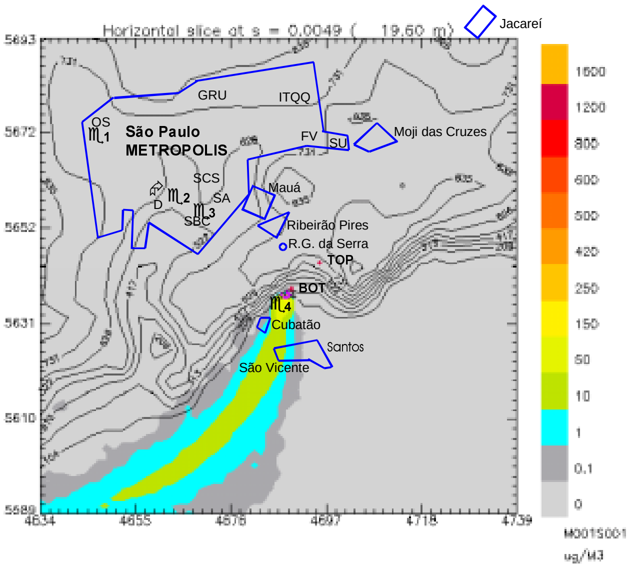

Figure 4

receive loads between 1 to 10 µg/m³.

This is not a negligible amount, although being small when compared to São Paulo's contributions itself. On Figure-3 the centre axis is directed along the Paraiba Valley. Pollutants in that direction become diluted before arriving to the out-grid most density-populated urban centres. Figure-4 is a simulation of a typical night-time regional circulation. The katabatic winds and land breeze transport the particulate matter over the shoreline plains where Cubatão, Santos, São Vicente and other small cities are settled. Concentration level remains highalong the dispersion axis, for a long distance.

Table 5 shows concentrations simulated by SPRAY and those obtained with the CMB analysis carried out on samples collected at the TOP and BOT stations (Kerr and Nascimento, 1998). D (N) in the date means that samples were collected during diurnal (nocturnal) periods. Limitations of both models should be considered. CMB is not a direct measurement of the concentrations. It is a least square fit that provides a source apportionment over the total inhalable particulate matter measured at a point. On the other side, only annual averaged source emission rates were available for SPRAY. The model inputs, such as land use, land/water surface percentage, topography resolution, should be improved. Finally there were only two points for the comparison. They were often out of the dispersion plume axis, where the modelling uncertainty increases. With these limitations, SPRAY simulations were acceptable for BOT station, when compared to the respective CMB evaluations. Moreover, the TOP station was a critical point for comparisons, because it was placed close to the level where the daytime breeze often remains trapped in the Moji Valley.

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Table 5 Comparison between concentrations values estimated by CMB and SPRAY.

	Inhalable particulate matter concentration (μg/m^3)					
	TOP station			BOT station		
Sample	CMB estimate		SPRAY	CMB estimate		SPRAY
	Fert.CMB	±Err		Fert.CMB	±Err	
14-Oct.D	79	12	0.1	63	20	34
14-Oct.N	12	5	0.0	7	4	0.0
15-Oct.D	1	4	0.0	0	-	12
15-Oct.N	9	4	0.0	-	-	0.1
16-Oct.D	11	6	3.5	12	27	288
16-Oct.N	9	4	0.0	-	-	0.4
17-Oct.D	65	16	3.6	43	14	102
21-Oct.D	6.9	2	0.0	22	5	237
21-Oct.N	19	4	0.0	21	5	14
22-Oct.D	50	9	0.0	59	15	0.0
22-Oct.N	14	4	0.0	-	-	0.0
23-Oct.D	78	11	2.4	85	20	143
23-Oct.N	10.2	2.8	0.0	-	-	0.0
24-Oct.D	30	5.8	0.2	49	16	104

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