Transactions on Ecology and the Environment vol 21, © 1998 WIT Press, www.witpress.com, ISSN 1743-3541

Calibration of the dispersion code SAFE_AIR against measurements in a complex coastal area

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Abstract

The SAFE_AIR code (Canepa and Ratto [1]; Canepa et al. [2]; Canepa et al. [3]) simulates the transport and diffusion of airborne pollutants. This dispersion code is based on the advection of Gaussian segments and puffs driven by a 3D diagnostic wind model, able to deal with both non-stationary and non-homogeneous conditions. SAFE_AIR is an evolution of the AVACTA II code (Zannetti [4]), a code «recommended» by the U.S. EPA. In this work, we applied SAFE_AIR to the region of Ilo, Peru, where large SO2 emissions from a copper smelter plant affect the local air quality. The smelter is located in a complex coastal area. The field project (Wilkerson [5]) is based on a large set of meteorological and tracer (SF6) field data collected in the area of interest. Among the eighteen tracer experiments performed, under a variety of meteorological conditions and at different times of the day, we selected the most representative one and simulated it. The preliminary results presented here are encouraging.

1 Introduction

In this work, we applied the latest version of the SAFE_AIR (Simulation of Air pollution From Emissions _ Above Inhomogeneous Regions)

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code (a commercial version of SAFE_AIR is distributed by FiatLux Publications, Fremont, California, USA, http://www.envirocomp.org/html/news/safe-air.htm) in the region of Ilo, Peru (the same as Jackson and Zannetti [6]), where large SO2 emissions from a copper smelter plant affect the local air quality. The tracer project is based on a large set of meteorological, SO2, and tracer (SF6) field data collected in the area of interest. It was designed to collect transport and dispersion data to simulate stack and fugitive SO2 emissions from the Ilo smelter under a variety of meteorological conditions and at different times of the day. The aim of this calibration exercise was directed to investigate possible future operational use of the code. The strong non-stationary and non-homogeneity of the experimental conditions created a challenge to the code. Among the eighteen tracer experiments performed (eleven stack and seven fugitive tracer releases) we selected the most representative one for our purposes and simulated it. The preliminary results presented here are encouraging.

2 Model Description

The SAFE_AIR code is an evolution of the AVACTA II (AeroVironment Air pollution model for Complex Terrain Applications) code, a code «recommended» by the U.S. EPA and by the Italian Ministry of Health (Bassanino et al. [7]). SAFE_AIR consists mainly of two parts: a meteorological pre-processor (Wind-field Interpolation by Non-Divergent Schemes, WINDS) and a pollutant diffusion simulator (Program Plotting Paths of Pollutant Puffs and Plumes, P6). SAFE_AIR is extremely versatile in the sense that the user may select the level of complexity and detail. Hence, the computational effort may be easily adapted to this type of application.

The meteorological pre-processor WINDS (Ratto et al. [8]; Ruaro et al. [9]; Ratto [10]) computes the wind field necessary for the subsequent description of the transport of the pollutant plume above complex orography. WINDS is a mass-consistent model (Ratto et al. [11]) developed at the Department of Physics of the University of Genoa, Italy; it builds a three-dimensional (3D) wind field by the following two steps. First, an initial wind field is constructed, through an interpolation procedure, starting from available wind data at given points. Second, an adjustment is performed based on the variational method proposed by Sasaki [12], to achieve a non-divergent flow field. WINDS can use different initialisation possibilities: ground station data and/or geostrophic wind, observed vertical profiles (sodar, etc.), profiles

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coming from larger scale meteorological models (e.g., Limited Area Models, Mazzino et al. [13]), etc. WINDS is written in conformal co-ordinates that have several advantages with respect to Cartesian co-ordinates: the terrain surface is better represented, consequently, more accurate boundary conditions can be used and this allows higher resolution near the terrain surface. In neutral and stable atmosphere, the model uses the formulae of the vertical wind profile proposed by Zilitinkevich [14]. In conditions of unstable atmosphere, the model uses some extensions of the cited formulae. WINDS considers the following phenomena: roughness effect, roughness change (Internal Boundary Layer, see for instance Castino and Tombrou [15]), variations of the wind direction due to the Coriolis' force, effects due to the atmospheric stability, etc.

P6 is a model derived from the part of the AVACTA II code simulating the pollutant dispersion. P6 is a dynamic multisource model based on the Gaussian formula in which the plume is broken into independent elements (either segments or puffs). Segments provide a numerically fast simulation of dispersion of air pollutants near their source during transport conditions. Puffs allow a proper simulation of diffusion, both far from the source and during calm or low-wind situations. Pollutant dynamics are described by the evolution of plume elements according to local meteorological conditions. The dynamics of each element consist of the following:

- generation at the source;
- plume rise (Turner method or Briggs formulae or Moore model or a value provided by the user);
- transport performed using the spatial average of the wind velocities in the volume occupied by each plume element;
- diffusion by atmospheric turbulence performed using the σ-functions (Pasquill-Gifford-Turner, Brookhaven, Briggs open country or urban, and interpolation from user's values) as a function of Pasquill-Gifford classes;
- possible chemical transformation (two species first-order chemical reaction scheme), creating secondary pollutant from a fraction of the primary pollutant;
- possible ground deposition, dry and wet, by an exponential reduction of the pollutant mass using the factor of reduction; and,
- possible gravitational settling of coarse particles.

This method offers the advantage of maintaining the simplicity of Gaussian formula, while allowing a more accurate numerical simulation of both non-stationary and non-homogeneous conditions. P6 is mainly designed for simulating air quality impact from elevated point sources. However this code can also be correctly used for line, area, and volume sources.

Recently, SAFE_AIR has been improved by adding the following algorithms: 1) the Pierce method [16] has been inserted to make the code able to decide automatically the use of either the buoyant plume or the jet formulae to describe the plume rise; 2) the simulation of the stack tip downwash phenomenon has been improved introducing the possibility for the user to choose between the Bjorklund and Bowers [17] and the Briggs methods [18]; and 3) a simple method for the simulation of building downwash has been implemented (Briggs [18]; Hanna et al. [19]; Hosker [20]).

3 Model Calibration

In this work, we applied the SAFE_AIR code to a tracer project designed to collect transport and dispersion data to simulate stack and fugitive SO2 emissions from a copper smelter under a variety of meteorological conditions and at different times of the day. The smelter is located approximately 16 kilometres north of Ilo (Peru): this region is a desert complex coastal area (Figure 1) in which the climate is dominated by a persistent marine layer. There is elevated terrain within a kilometre to the east of the smelter with elevations reaching 1,300 meters within six kilometres of the smelter and the coastal plain widens several kilometres south of the smelter toward the town of Ilo. There are four stacks at the smelter that are all approximately 110 meters in height, but also fugitive emissions are not negligible. The field project is based on a large set of meteorological and tracer (SF6) field data collected in the area of interest.

The issues we consider in this exercise concerned the ability of the model to predict the temporal evolution of the tracer gas dispersion pattern. Among the eighteen tracer experiments performed (eleven stack and seven fugitive tracer releases) we selected the most representative one for our purposes (stack release #5) and simulated it. We chose a stack release because P6 is mainly designed for simulating air quality impact from elevated point sources; we chose stack release #5 because the dispersion pattern for this experiment provided the best example of

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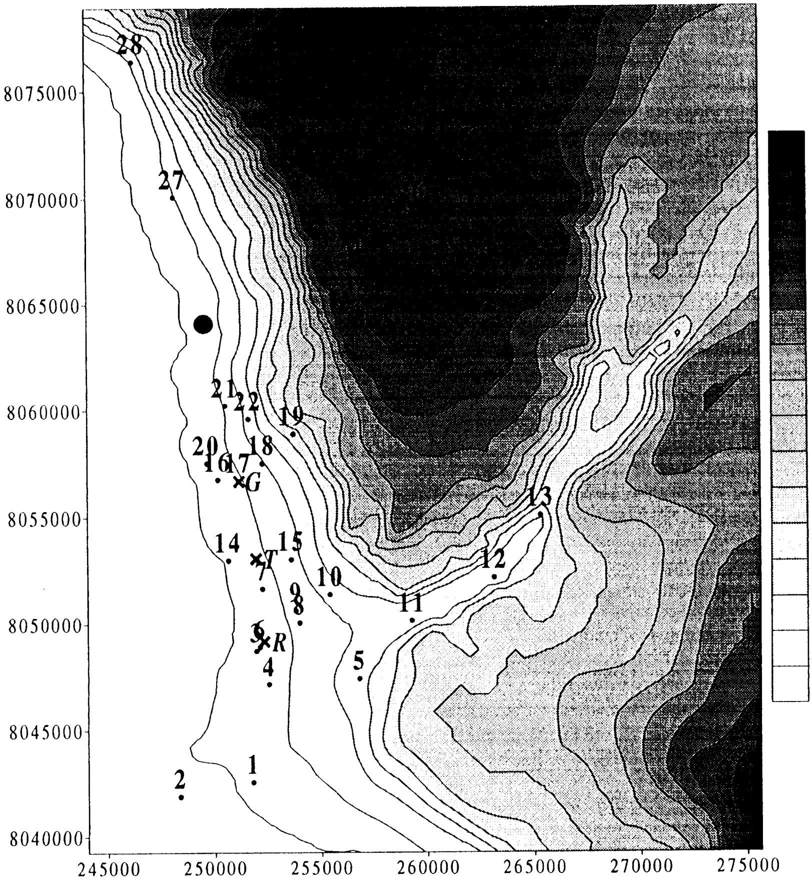

Figure 1: The orography (as obtained using the graphical program SURFER®Golden Software): • = smelter; × = meteorological stations; 1, 2, ..., 28 = receptors.

plume movement in the area and also contained the highest SF6 concentration measured during the entire field project. The study period for stack release #5 began at 0200 hour and concluded at 1900 hour on March 15, 1996; the length of time of this experiment was 17 hours. The tracer release period began at 0200 hours and ended four hours later at 0600 hour. High pressure was over southern Peru and northern Chile. This experiment showed a two-hour period before the SF6 was measured at any of the sampling sites. By hour three, light SF6 concentrations were noted just south of the smelter south-east to inland sampling sites to the east of Pueblo Nuevo. By hours four and five, a discrete pulse of SF6 was evident just south of the smelter. Hours six to eight show continued movement of a concentrated area of SF6 south from the smelter. Concentrations are highest inland as the SF6 slides along the foothills to the south-south-east. By sunrise, the SF6 had made it well up the Ilo Valley and concentrations are just beginning to diminish. Hours nine through eleven show the influence of the southerly winds as the plume quickly dilutes and moves northward. By hours twelve to seventeen, the SF6 gas exits the area under the influence of the southerly daytime flow.

Keeping in mind, a future operational use of the code, we initialised the code in the simplest possible way. The assumptions concerning input data for the SAFE_AIR code were as follows. We reconstructed the wind field above that orographically complex area using the WINDS code, then the concentrations at the ground were simulated using the P6 code. We selected an area of $32 \times 40 \times 3$ km^3 around the smelter using, along the horizontal directions, 80×100 grid points and, along the vertical direction, 19 conformal levels (WINDS code) or 100 Cartesian levels (P6 code). For each of the 17 hours necessary to simulate the entire experiment, the WINDS code calculated the wind field making use only of data measured at the ground stations of Golf Club, Town Site, and Ross Siding situated at 10 m a.g.l. (Figure 1). At Golf Club, northerly winds persisted through the release period until 1100 hours, and speeds were less than 3 ms^{-1} at the time of release then gradually increased to 1100 hours. After 1100 hours, the winds turned southerly with speeds increasing to over 6 ms^{-1}. At Town Site wind directions were variable throughout the study period. During the release, winds were southerly and less than 3 ms^{-1}. After the release and until 0900 hour, the wind turned northerly with speeds continuing under 6 ms^{-1}. After 0900 hour until the end of the study, winds turned southerly again with speeds increasing to over 4 ms^{-1}. Ross Siding had southerly winds throughout the entire study period. Speeds averaged between 3 and 7 ms^{-1}. We have treated data measured in stable, unstable, and neutral atmosphere, both in night-time and daytime hours, as the PBL diurnal evolution is concerned. The stability class, assumed one and the same for the whole domain, was calculated using the Pasquill method [21] based on both the intensity of wind speed at 10 m a.g.l. and insolation. Stability turned out to be F by 0200 to 0700 hours (nocturnal light wind conditions); it moved from B to D by 0700 to 1700 hours (diurnal conditions with increasing wind speed); it was D by 1700 to 1900 hours (nocturnal strong wind conditions). We used a roughness length of 0.0002 m for the see and 0.005 m for the land (except close to the Refinery, Town Site, Miraflores, and Ross Siding stations where we used 0.05 m). The tracer emission rate was 17.64 gs^{-1}. The P6 code simulated the hourly tracer measured concentrations at the 28 receptors used in the experiment (Figure 1). The P6 code used as input the mixing height calculated by the WINDS code: its value ranging from 50 m (nocturnal conditions) to 2900 m (diurnal conditions, well developed mixed layer).

In order to calibrate the P6 code, we performed 20 simulations using different assumptions about: length of the elements, σ-functions, wind speed value to discriminate between transport and calm dispersion conditions, reflection terms, kind of spatial average of the wind velocities in the volume occupied by each plume element for the calculation of the advective wind speed, limitations to the vertical shifting of elements, plume rise, and stack tip downwash.

The direct comparison of the results of these simulations with the measured concentrations allowed us to select the most appropriate assumptions. Among them we report the Brookhaven [22] σ-function, the Yamartino's method [23] of multiple reflections, and the plume rise Moore method [24].

For sake of brevity, we will limit our considerations to the best performance of the code. The code described well both temporal and spatial behaviour of the pollutant pattern with respect to information provided with receptors (see, for example, Figure 2), but systematically underestimated measured concentrations. In more detail, the code: 1) correctly predicted the two-hour period before the SF6 was noted at any of the sampling sites; 2) did not point out light concentrations by hour three nor pulse of SF6 by hours four and five just south of the smelter; but 3) exactly located both time and receptor at which maximum measured concentration occurred (even though the code underestimated the measured concentration, 6.6 against 32.2 μgm^{-3}); 4) correctly predicted both the channelling of the pollutant in the Ilo valley by hours seven and eight and the influence by hours nine to eleven of the southerly winds which diluted and moved northward the plume; 5) well depicted the gas exit from the study area under the influence of the southerly daytime flow by hours twelve to seventeen.

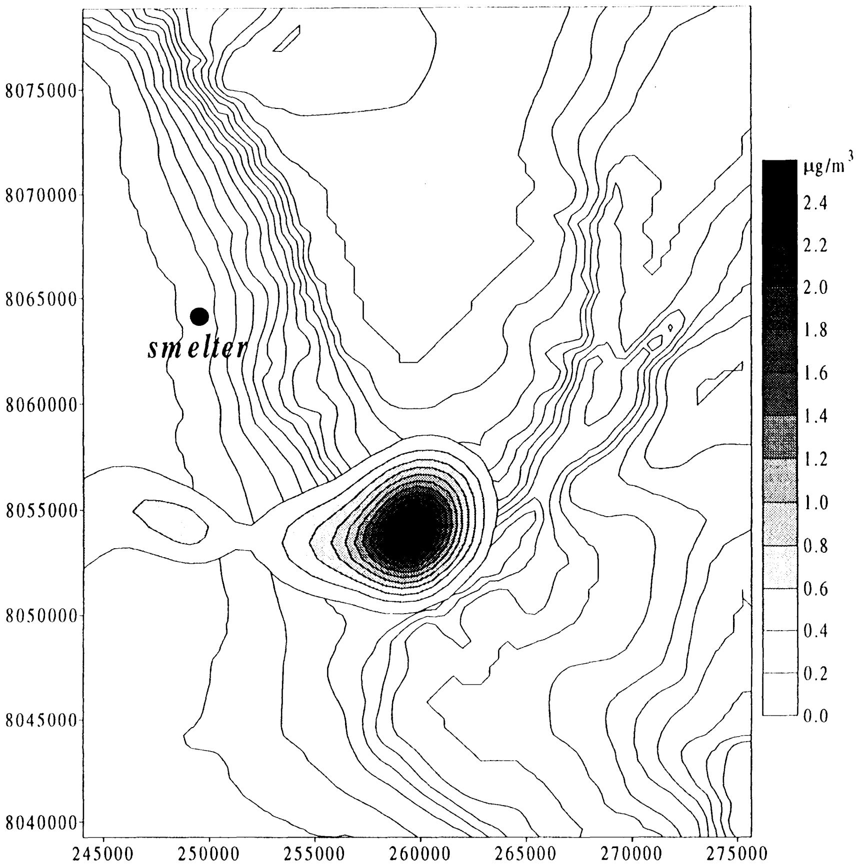

Figure 2: The pollutant channelling beginning (as obtained using the graphical program SURFER® Golden Software).

4 Conclusions

We presented a calibration of the latest version of the SAFE_AIR code against tracer (SF6) data in the region of Ilo, Peru, a complex coastal area where large SO2 emissions from a copper smelter plant affect the local air quality. The code well described both temporal and spatial behaviour of the pollutant pattern with respect to the information provided by the receptors, but systematically underestimated measured concentrations.

We will direct our future efforts towards a deeper investigation of the reasons of the underestimation. We also plan to apply the code to other tracer experiments to verify the reliability of our preliminary results.

Acknowledgements

We want to thank Prof. A. Longhetto for his constant help in this study. We also want to thank Drs. D. Anfossi and N. Arena for many fruitful discussions and helpful suggestions. Appreciation is extended to Jim Jackson and Dario Oviedo of Southern Peru Limited, who provided the data used in this study.

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