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Calibration of the dispersion code SAFE_AIR using a release in nocturnal low wind conditions

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Abstract

The SAFE_AIR code 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 inhomogeneous conditions. SAFE_AIR is an evolution of the AVACTA II code, a code "recommended" by the U.S. EPA. In this work, we applied SAFE_AIR to a tracer project designed to collect diffusion 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 field project is based on a large set of meteorological and tracer (SF6) field data collected in the area of interest under a variety of meteorological conditions and during different times of the day. Among the tracer experiments performed we simulated a nocturnal low wind conditions stack release. This release provided the best example of plume movement in the area and also contained the highest SF6 concentration measured during the entire field project. The strong time variability and inhomogeneity of the experimental conditions presented a challenge to the code. The issues we considered in this exercise concern the ability of the model to predict the temporal evolution of the tracer gas dispersion pattern. To do this, special attention was directed towards a detailed description of the nocturnal light wind field during the tracer release and the selection of the code wind speed value to discriminate between transport and calm conditions.

1 Introduction

In this work, we applied the SAFE_AIR code (Simulation of Air pollution From Emissions _ Above Inhomogeneous Regions) (Canepa and Ratto [1]; Canepa et al. [2, 3]; Canepa [4]) in the region of Ilo, Peru (the same as Jackson and Zannetti [5] and Canepa et al. [6]), where large SO2 emissions from a copper smelter plant affect the local air quality.

SAFE_AIR is included in the Model Database of the European Topic Centre on Air Quality (http://aix.meng.auth.gr/lhtee/database.html). A commercial version of SAFE_AIR is distributed by FiatLux Publications, Fremont, California, USA, http://www.envirocomp.org/ html/news/safe-air.htm). The SAFE_AIR code is an evolution of the AVACTA II code (AeroVironment Air pollution model for Complex Terrain Applications, Zannetti [7]), "recommended" by the U.S. EPA and the Italian Ministry of Health (Bassanino et al. [8]).

The tracer project (Wilkerson et al. [9]) 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 copper smelter under a variety of meteorological conditions and at different times of the day. Among the tracer experiments performed we simulated a nocturnal low wind conditions stack release. This release provided the best example of plume movement in the area and contained the highest SF6 concentration measured during the entire field project.

The strong time variability and inhomogeneity of the experimental conditions presented a challenge to the code. The issues we considered in this exercise concerned the ability of the model to predict the temporal evolution of the tracer gas dispersion pattern. To do this, special attention was directed towards a detailed description of the nocturnal light wind field during the tracer release and the selection of the code wind speed value to discriminate between transport and calm conditions.

2 The SAFE_AIR code

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. SAFE_AIR consists mainly of two parts: a meteorological pre-processor (WINDS, Wind-field Interpolation by Non-Divergent Schemes) and a pollutant diffusion simulator (P6, Program Plotting Paths of Pollutant Puffs and Plumes).

The meteorological pre-processor WINDS (Ratto et al. [10]; Ruaro et al. [11]; Ratto [12]) 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. [13]) developed at the Department of Physics of the University of Genoa, Italy, in collaboration with Prof. D.P. Lalas [14]. WINDS can use different initialization possibilities:

ground station data and/or geostrophic wind, observed vertical profiles (sodar, etc.), profiles coming from larger scale meteorological models (e.g., Limited Area Models, Mazzino et al. [15]), etc.

P6 is a model derived (Canepa and Ratto [1]; Canepa et al. [2, 3]; Canepa [4]) from part of the AVACTA II code simulating 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). Pollutant dynamics are described by the evolution of plume elements according to local meteorological conditions. This method offers the advantage of maintaining the simplicity of a Gaussian formula, while allowing a more accurate numerical simulation of both non-stationary and inhomogeneous conditions. 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. If the local horizontal transport term is less than a critical value, u_{min} (the code default is u_{min} = 1 m/s), this term is forced to zero, since it is assumed that such a small term represents more local intermittent effects than actual transport. In this case, however, a large horizontal diffusion may be produced by the large wind direction fluctuations typically encountered during these low-wind speed situations.

3 The simulated tracer release

The source is located approximately 16 km north of Ilo (Peru): this region is a desert complex coastal area (Figure 1) in which a persistent marine layer dominates the climate. There is elevated terrain within 1 km to the east of the source with elevations reaching 1,300 m within 6 km of the source and the coastal plain widens several kilometers south of the source toward the town of Ilo.

The issues we considered 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 (110 m in height) and seven ground-level 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 of this tracer release in nocturnal low-wind conditions provided the best example of 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 hours and concluded at 1900 hours 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.

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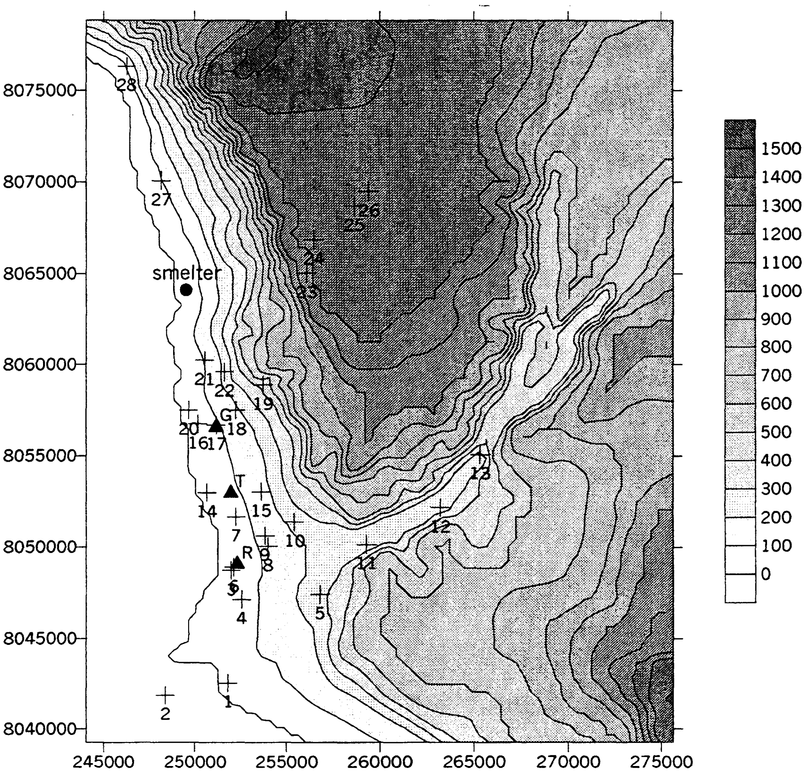

Figure 1: The orography (as obtained using the graphical program SURFER® Golden Software): • = smelter; ▲ = meteorological stations; 1, 2, ..., 28 = receptors. All the units are in m.

Wind field data were measured at the ground stations of Golf Club, Town Site, and Ross Siding situated at 10-m agl (above-ground level) (Figure 1). At Golf Club, northerly winds persisted through the release period until 1100 hours, and speeds were less than 3 m/s at the time of release, then gradually increased to 1100 hours. After 1100 hours, the winds turned southerly with speeds increasing to over 6 m/s. At Town Site, wind directions were variable throughout the study period. During the release, winds were southerly and less than 3 m/s. After the release and until 0900 hours, the wind turned northerly with speeds remaining under 6 m/s. From 0900 hours until the end of the study, winds turned southerly again with speeds increasing to over 4 m/s. Ross Siding had southerly winds throughout the entire study period. Speeds averaged between 3 and 7 m/s.

At the beginning of the experiment, there was 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 showed continued movement of a concentrated area of SF6 south from the smelter. Concentrations were highest inland as the SF6 moved along the foothills to the south-south-east. By sunrise, the SF6 had made it well into the Ilo Valley and concentrations were just beginning to diminish. Hours nine through eleven showed the influence of southerly winds as the plume quickly diluted and moved northward. By hours twelve to seventeen, the SF6 gas exited the area under the influence of the southerly daytime flow.

4 The performed simulations

We reconstructed the wind field above the orographically complex area using the WINDS code; then the concentrations at the ground were simulated using the P6 code. We selected an air space measuring $32 \times 40 \times 3$ km^3 around the source 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).

We performed two wind field simulation sets. Each set was composed of 34 half hour increments of average wind fields to simulate the entire 17-hour experiment with sufficient detail. In the first set (Set 1), we used the data measured at all the ground stations (10-m agl) of Golf Club, Town Site, and Ross Siding (Figure 1) to construct the wind field. In Set 2, we used the wind data measured at the Golf Club station - the nearest station to the smelter - to construct the wind field during the 4-hour release period, from 0200 hours until 0600 hours. We also used all the wind stations, as in Set 1, to construct the wind field during the remaining 13-hour simulation period, from 0600 hours until 1900 hours. We used this approach for Set 2 because we believe that the Golf Club station is the most representative for emissions during low wind conditions. The stability class (assumed one and the same for the whole domain) was calculated using the Pasquill method [16] based on both the intensity of wind speed at 10-m agl and insolation. Stability turned out to be F in the lower layers 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 sea 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 P6 code simulated the hourly tracer measured concentrations at the 28 receptors used in the experiment (Figure 1). The tracer emission rate was 17.64 g/s. The P6 code used as input the mixing height calculated by the WINDS code. The values ranged from about 50 m (nocturnal conditions) to about 2900 m (diurnal conditions, well-developed mixed layer). Among the different options allowed by P6, we simulated the plume rise using the Moore method [17] and the plume diffusion using the Brookhaven σ-function [18] because both furnished the best results in previous P6 model testing (e.g., Canepa [4]) with regard to emission conditions similar to the present ones. In order to calibrate

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the P6 code about the wind speed value to discriminate between transport and calm dispersion conditions, u_{min}, we performed three simulations using different values (u_{min} equal to 0.5, or 1.0, or 1.5 m/s) for each wind field set, that is to say we performed six simulations in all.

The direct comparison of the results of these simulations with the measured concentrations allowed us to select the most appropriate assumptions with respect both the wind field initialization and the u_{min} value. To select those assumptions we took into account the SAFE_AIR accuracy with respect to the simulation of: 1) the beginning of the tracer survey by the receptors; 2) the maximum of the tracer concentrations; 3) the channeling of the tracer in the Ilo valley; and 4) the tracer going out from the simulation area. As an example, see Table 1. Taking into account all the previous items, we can assert: a) the dispersion simulations performed using the wind field Set 2 gave better results than those performed using Set 1; b) among the dispersion simulations performed using the wind field Set 2, the assumption u_{min} = 1.5 gave the best results.

For sake of brevity, we will limit our considerations to the best performance of the code. On the whole, the code described well both the temporal and spatial behavior of the pollutant pattern with respect to the information provided by the receptors (e.g., Figure 2). In more detail, the code: 1) correctly predicted the two-hour period before the SF6 was noted at any of the sampling sites, but predicted the first concentrations different from zero by hour four instead of by hour three; 2) exactly located the receptor at which the maximum concentration occurred, but underestimated the measured concentration, 18.8 against 32.2 μg/m^3, and predicted the maximum two hours early; 3) correctly predicted the channeling of the tracer in the Ilo valley by hours seven and eight, but again underestimated the tracer concentrations (e.g., 5.8 against 18.5 μg/m^3 at Receptor 11 by hour seven); 4) depicted both the influence by hours nine to eleven of the southerly winds which diluted the plume and moved it northward and the gas efflux from the study volume, even if two hours early, under the influence of the southerly daytime flow.

Table 1: The maximum of the tracer concentrations: measured versus simulated values.

	value (μg/m^3)	Receptor (num)	time (hour)
measurements	32.2	18	0800
set 1, u_{min} = 0.5	7.8	20	0800
set 1, u_{min} = 1.0	10.9	21	0800
set [illegible] u_{min} = 1.5	14.8	22	0800
set 2, $u_{m[illegible]}$ = 0.5	18.4	6	0800
set 2, u_{min} = 1.0	17.0	9	0700
set 2, u_{min} = 1.5	18.8	18	0600

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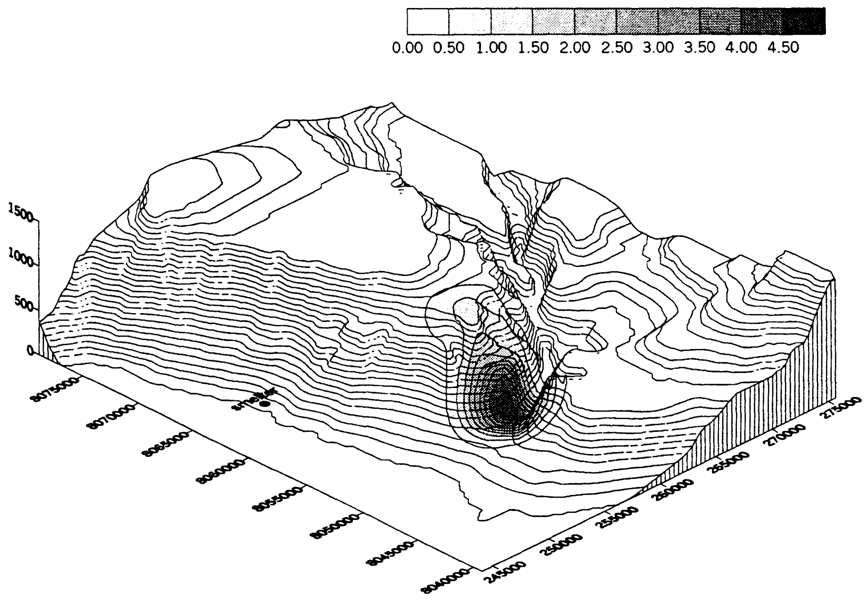

Figure 2: The pollutant channeling beginning (as obtained using the graphical program SURFER® Golden Software). The distances are expressed in m, the concentrations in $\mu g/m^3$.

5 Conclusions

We presented a calibration 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.

Among the tracer experiments performed we simulated a nocturnal low wind conditions stack release. The lack of stationary and homogeneous conditions during the experiment presented a challenge to the code.

To simulate this experiment, special attention was directed towards a detailed description of the nocturnal light wind field during the tracer release and the selection of the code wind speed value to discriminate between transport and calm conditions.

On the whole, the code described well both the temporal and the spatial behavior of the pollutant pattern with respect to the information provided by the receptors. In particular, we obtained better results than those already found by us (Canepa et al. [6]) using a less detailed wind field description (17 one-hour average wind fields obtained used the data measured at all the ground stations).

As a summary, this exercise allowed us to outline two main issues: i) the wind field construction is an essential part of the dispersion simulation process; ii) both the temporal and spatial representativeness of the wind measurements have to be carefully analyzed.

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