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Comparação entre o modelo CALPUFF e o modelo lagrangiano LAMBDA com fonte linha

Comparison between the models CALPUFF and lagrangian LAMBDA with line source

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Resumo

O objetivo deste estudo é comparar os modelos CALPUFF e LAMBDA e avaliar acurácia do modelo regulatório CALPUFF em situações de emissões de fontes em linha instantâneas. As fontes em linha são muitas vezes utilizadas em simulações de dispersão de poluentes para representar as emissões atmosféricas de vias não pavimentadas e pavimentadas (suspensão de material particulado pela passagem de veículo sobre a via). No setor de mineração estes dois tipos de fontes de emissão constituem uma influência antropogênica importante no ambiente. O experimento OLAD é apropriado para avaliar estes modelos e estabelecer a acurácia de ambos nestas situações descritas. Os resultados do modelo CALPUFF mostrou nas simulações de curtas e longas distâncias uma sistemática tendência de sub previsão das concentrações. O modelo LAMBDA apresentou melhor precisão mesmo desconsiderando a variabilidade espacial do campo meteorológico e da topografia. Quando o modelo LAMBDA é utilizado, o fluxo de poluentes para distâncias maiores é menos pronunciado, especialmente pelo passo de tempo de um segundo adotado na simulação.

Palavras-chave: *CALPUFF, modelo de regulação, LAMBDA, Camada Limite Neutra, fonte em linha de emissão instantânea.*

Abstract

The aim of this study is to compare the CALPUFF and LAMBDA models and evaluate the regulatory model CALPUFF accuracy in situations of line instant source emissions. Line source emissions exist in a variety of situations in the environmental field. Paved and unpaved roads are the most common examples of line sources. For instance, in the mining sector these two types of sources play an important role of anthropogenic influences in the environment. The OLAD experiment is appropriate to evaluate these models and check the accuracy of both. The CALPUFF results show in the simulations for short and long distances a systematic tendency of sub-prediction for the concentration. The LAMBDA model presented better accuracy in the prediction of natural pollutant dispersion even disregarding the spatial variability of meteorological field and topography. When the LAMBDA model is used the flow of pollutants to greater distances is less pronounced, especially because of the time step of one second adopted in the simulation.

Keywords: *CALPUFF, Regulatory Model, LAMBDA, Neutral Boundary Layer, line source instantaneous emission.*

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1 Introduction

Dispersion and transport models of contaminants are useful tools to evaluate anthropogenic influences in the environment. Actually, there are different kinds of dispersion models and in general, Gaussian models are used worldwide by environmental agencies in regulatory application. The CALPUFF model is one of them. This model is a non-stationary puff with Lagrangian algorithm. As part of a study to design and develop a generalized non-steady-state air quality modeling system for regulatory use, Sigma Research Corporation developed the CALPUFF dispersion model and related models and programs, including the CALMET meteorological model. The original development of CALPUFF and CALMET was sponsored by the California Air Resources Board (CARB) (Scire et al., 2000).

Another model used to study and predict the environmental impact is the stochastic Lagrangian dispersion model LAMBDA (Ferrero and Anfossi, 1998). Particle models are efficient and fundamental tools in the investigation and study of turbulent diffusion phenomenom in the planetary boundary layer. In the stochastic Lagrangian model the turbulent dispersion was established by the particle movement of the fluid that follows turbulent flow. In this kind of model and to represent the eddies motions the particles velocities are subject to a random forcing (Rodean, 1996). There, these dispersion models are based on a stochastic Langevin equation. This equation is derived assuming that the particle speed can be written as the sum of a deterministic and a stochastic term. In this case, for each time step, the fluid particle moves due to the action of mean wind and turbulent diffusion. The latter is caused by the action of wind velocity fluctuations. This flow is characterized by certain initial conditions and physical constrains. As a result, the movement of any particle is independent of the remainder. Thus, the concentration field, the estimated spatial distribution of particles, should be interpreted as an average performed over the total number of simulated particles (Degrazia et al., 2007). Further, the model LAMBDA was employed in this study to simulate the contaminant concentration field.

Therefore, the aim of this study is to compare these two models and evaluate the regulatory model CALPUFF accuracy in situations of line source emissions. Line source emissions exist in a variety of situations in the environmental field. Paved and unpaved roads are the most common examples of line sources. For instance, in the mining sector these two types of sources play an important role of anthropogenic influences in the environment. The Over-Land Alongwind Dispersion experiment (OLAD) is quite appropriate to evaluate these tools and check the accuracy of both models.

2 Experiment

The OLAD experiment was conducted from 8 to 25 September 1997 in the town of Dugway (US Army Dugway Proving Ground), in the West Desert Test Center, which is located in the central-western state of Utah, about 1300 m above sea level. The OLAD was developed by the National Oceanic and Atmospheric Administration. The test was performed with the release of known amounts of tracer gas sulfur hexafluoride (SF_6) along a line perpendicular to the prevailing wind direction. The releases were made by dissemination systems mounted on a truck. Figure 1 shows the source line (red) of 10 km length. The OLAD Test 6 trials were surface releases into strong (~10 m/s) south east winds in a near-neutral boundary layer. The whole air samplers measured time-averaged (15-min) concentrations with accuracy. Tracer gas concentration sampling during OLAD was accomplished using three lines of surface-mounted samplers. Each surface sampling line, that were located 2, 5 and 10 km downstream of the dissemination line, consisted of 15 whole-air samplers spaced at 100-m intervals (Biltoft et al., 1999).

For the measurement of meteorological variables there were installed eight Portable Weather Information and Display System measuring stations (PWIDS) and eight Surface

Atmospheric Measurements Systems stations (SAMS). In addition to these stations, at certain times, meteorological balloons (radiosondes) were released to determine the atmospheric profile. The aerodynamic mean surface roughness length of 3 cm was established by the inspection method and the location has a dry, flat clay surface with sparse grass and scrub sage vegetation.

3 Metodology

The analyzed region (model domain) comprises the area of West Desert Test Center presented in figure 1. In the simulation site were included the location and amount of emissions of tracer gas, the samplers and meteorological surface and altitude stations. The topography of the region was incorporated only in the model domain area of the CALPUFF model, with satellite images. These data allowed to add a topography with spatial resolution of 90 meters in order to describe the topographic influence on the dispersion of contaminants.

The models performances was established by comparing the levels of ground-level concentrations of the tracer gas with experimental results. A test case was chosen that simulates the day September 15, 1997, with neutral planetary boundary layer, due to a significant wind speed of 10 m/s. The sampling period used in the simulation was 15 minutes for LAMBA simulations and 1 hour for CALPUFF. CALPUFF and LAMBDA models treat line sources by approximating them with volume sources along the length of the line.

For the CALPUFF simulation, the micrometeorological data were determined by the CALMET prediction tool, incorporating data of all the meteorological stations in figure 1. Therefore, in the CALPUFF dispersion simulation the spatial variability of meteorological and micrometeorological data were taken into account. In the LAMBDA simulation, a flat area was considered and the meteorological and micrometeorological variables did not vary in space. The LAMBDA model works with mean values of meteorological data. Therefore, meteorological data established by Biltoft et al. (1999) were used.

Table 1 shows the meteorological data from the CALPUFF simulation and from measurements established by Biltoft et al. (1999) that were used for the simulations of dispersion turbulence with parameterizations for the LAMBDA model.

Table 1 - Meteorological and micrometeorological parameters for the simulations

Run	h	$(u_*)_0$	U_{10m}	L	Q
	(m)	$(m \cdot s^{-1})$	$(m \cdot s^{-1})$	(m)	$(g \cdot s^{-1})$
CALPUFF	384	2,6	7	∞	0,017
LAMBDA	500	0,7	10,3	1000	0,017

Table 2 presents the observed (*Co*) and predicted (*Cp*) atmospheric ground-level concentration. Figure 2 shows the scatter diagram of atmospheric ground-level predicted concentrations plotted against observed concentrations.

Table 2 - Observed and predicted ground-level concentrations at different distances from the source

Sampler	Sampler Distance (m)	Observed Conc. (μg/m³)	LAMBDA Predicted Conc. (μg/m³)	CALPUFF Predicted Conc. (μg/m³)
1	2000	2,87	2,28	1,37
2	2000	4,53	2,41	1,34
3	2000	2,62	2,41	1,32
4	2000	3,29	2,47	1,23
5	2000	3,78	2,38	1,40
6	2000	3,29	2,50	1,34
7	2000	4,20	2,38	1,24
8	2000	3,58	2,28	1,09
9	2000	4,26	2,32	1,00
10	2000	4,75	2,50	1,10
11	5000	1,70	1,19	0,41
12	5000	1,34	1,22	0,38
13	5000	1,35	1,04	0,35
14	5000	1,46	1,11	0,34
15	5000	1,40	0,98	0,33
16	5000	1,14	1,29	0,31
17	5000	1,41	1,20	0,28
18	5000	1,38	1,24	0,28
19	5000	1,03	1,09	0,29
20	5000	1,60	1,15	0,29
21	5000	1,56	1,05	0,29
22	5000	1,37	1,13	0,27
23	5000	1,26	1,30	0,24
24	5000	1,14	1,17	0,23
25	5000	1,19	1,07	0,23
26	10000	0,13	0,07	0,13
27	10000	0,17	0,08	0,12
28	10000	0,17	0,09	0,11
29	10000	0,21	0,08	0,11
30	10000	0,17	0,11	0,10
31	10000	0,17	0,08	0,09
32	10000	0,16	0,08	0,09
33	10000	0,23	0,08	0,09
34	10000	0,24	0,09	0,09
35	10000	0,24	0,17	0,09
36	10000	0,20	0,09	0,09
37	10000	0,31	0,07	0,09
38	10000	0,25	0,07	0,09

Table 3: Observed and predicted ground-level concentrations at different distances from the source.

Run	NMSE	FB	FS	COR
CALPUFF	3,13	1,09	1,03	0,93
LAMBDA	0,37	0,35	0,46	0,95

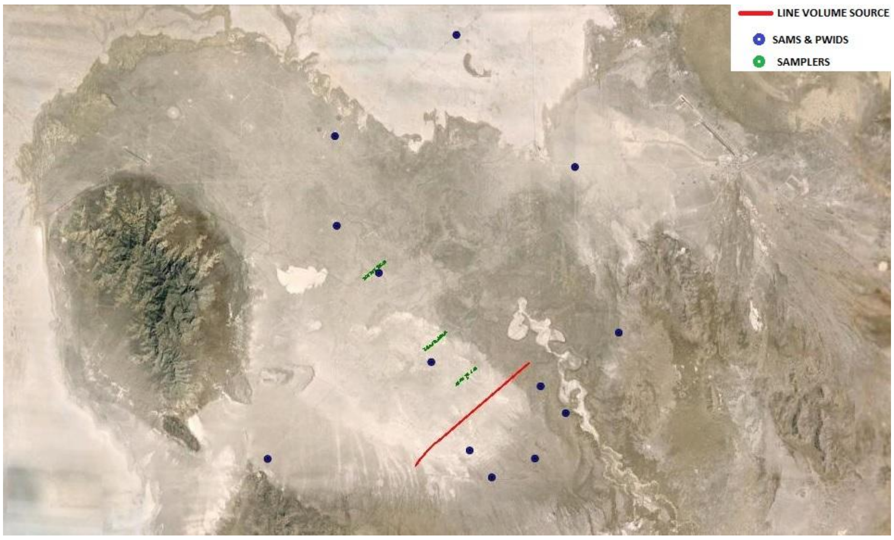

Figure 1 - OLAD test site at Dugway Proving Ground showing the locations of dissemination lines, sampling lines, and meteorological measurements sites.

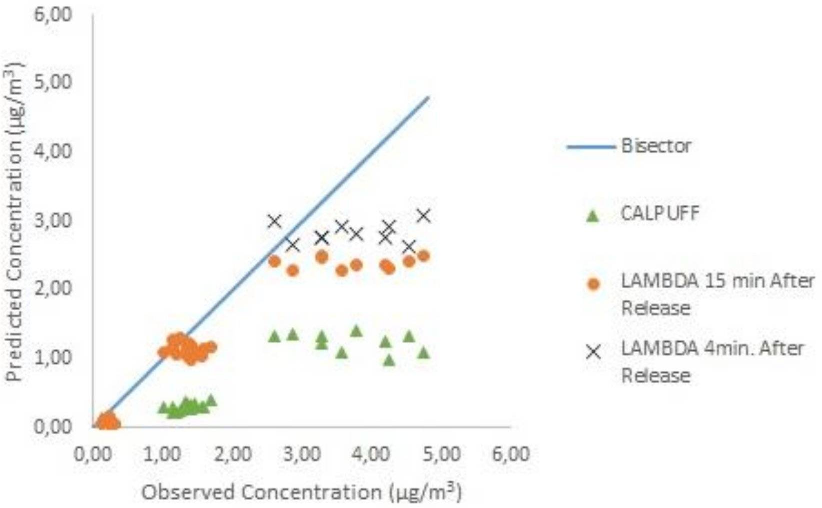

Figure 2 - Scatter diagram of modeling results in comparison with observed ground-level concentrations

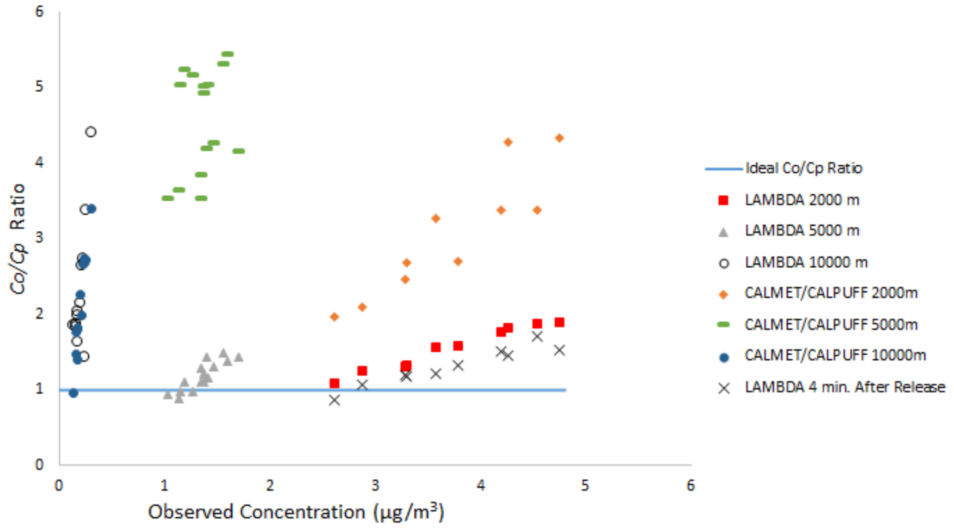

Figure 3 - Scatter diagram of the *Co*/*Cp* ratio in relation with observed ground-level concentrations

The fractional bias (FB) statistical index indicates whether the predicted quantities underestimate or overestimate the observed ones. The normalized mean square error (NMSE) statistical index represents the quadratic error of the predicted quantity in relation to the observed one. The fractional standard deviations (FS) index indicates a comparison between predicted and observed puff/particle spreading. Better results lead to values of NMSE, FB and FS that approach zero, while the correlation coefficient (COR) approaches unity.

3 Conclusion

The accuracy of CALPUFF system under neutral conditions is evaluated. Validation was performed using an instant release experiment in order to pin down the limitations of the regulatory model when line source emissions are simulated. In general, the CALPUFF simulations clearly deviate from the ideal ratio between experimental and predicted results in figure 2. The inaccuracy of the CALPUFF model increases for distant samplers as observed in figure 3. It is noteworthy that the CALPUFF model has been adopted by the U.S. Environmental Protection Agency as the preferred model for assessing long range transport of pollutants. Though, according to the results the lack of prediction is evident. To be more specific, short and long range transport simulations by CALPUFF show a systematic trend to sub-predict the concentrations from instantaneous line source emissions.

The LAMBDA model showed better accuracy in the prediction of pollutant dispersion even disregarding the spatial variability of meteorological fields and topography. This may be attributed to the stochastic character and the turbulence parameterization that play a crucial role in the model. Another difference arises from the fact that for continuous emissions close to the source, the gradients are less pronounced in comparison to instant releases. Consequently, in the instantaneous emission the flow of pollutants to longer distances is higher (Degrazia, et al., 2015). In the CALPUFF model, the minimum interval between two time steps is one hour. When the LAMBDA model is used, the flow of pollutants to greater distances is less pronounced, especially because of an adopted time step in the simulation of one second. It was also possible to observe the time evolution of the concentrations and to identify the maximum value at the location of the sampling lines for a time between 3 and 4 minutes (Biltoft et al. 1999). The LAMBDA model shows inaccuracy only at samplers over the receptor line of 10 kilometers, probably associated with the travel time uncertainty of the pollutant, the wind speed and direction variability in the domain of the study.

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