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PrOlor: a Modelling Approach for Environmental Odor Forecast

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Odor episodes control due to low threshold perception odorants, as H_2S, is extremely difficult, as they are detected in very low concentrations. Even low odorants emissions without any health effects can derive in odor episodes, highly dependent on the changeable meteorology.
PrOlor system is an environmental odor forecast system based in WRF/CALMET/CALPUFF models. WRF model settings includes four one-way nested grids, with 1x1 km^2 horizontal resolution for the innermost grid, and initial and boundary conditions from GFS model forecast. CALMET horizontal resolution is 250x250 m^2 to provide meteorological input to CALPUFF dispersion model.
CALPUFF odorants dispersion modelling includes not only mixing, but also first order chemical decay. In addition, in order to estimate short odor events (minutes) from hourly CALPUFF concentrations peak-to-mean approach was adopted. Finally, chemical odorant peak concentrations were converted to odor intensity and odor concentration applying the Steven's law.
Traditionally, pulp paper mills using Kraft process produce TRS (Total Reduced Sulphur) odorants emissions, so their environment can be affected by odors. ENCE-Pontevedra pulp paper mill, located at the NW of the Iberian Peninsula, developed significant improvements to avoid any odor impact. Particularly, PrOlor system was developed and applied in order to prevent any odor event. Around the paper mill environment, both wind and temperature WRF and CALMET models results were compared and validated against four surface meteorological sites, using Openair software. About CALPUFF results, after several months under operation, PrOlor forecasted most of the sporadic short odor events registered as qualitative observations around the paper pulp mill.

1. Introduction

Usually, paper pulp mills using Kraft process produce odorants emissions included in the TRS group (total reduced sulphur); although those emissions are harmless both for health and environment (according to standard thresholds, as EU and WHO limits), their very low odor thresholds (Leonardos et al., 1969) can produce troublesome events. Considering potentially odor activities, the use of atmospheric models can help to prevent those events (Carrera-Chapela et al., 2014).
ENCE-Pontevedra paper pulp mill developed along the last six years several investments in order to reduce systematically its TRS emissions, to avoid persistent odor around it. However, due to the changeable conditions of its environment, the possibility of short and sporadic odor events (minutes) remains. In order to prevent those short events, PrOlor Pontevedra system is presented in this work, as a model-based software tool to forecast any odor event produced by the TRS emissions sources previously characterized.

2. PrOlor system

PrOlor is an operational odor forecast system. It can work considering the operational conditions of the odorants source, with 72 hours in advance. Also, it can work in real-time, that is, using real-time emissions measurements and running every hour to nowcast the environmental odor in the following hours. Finally, PrOlor includes a Web-based interface for data analysis and also an app for android/IOS smartphones is available, in order to check the estimated environmental odor levels and, specially, the zones where the odor thresholds will be superseded.

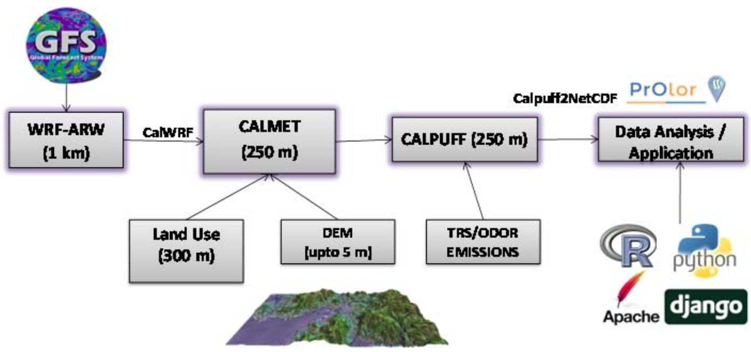


Figure 1: General scheme of PrOlor system, showing the models, input dataset, and data analysis and application modules

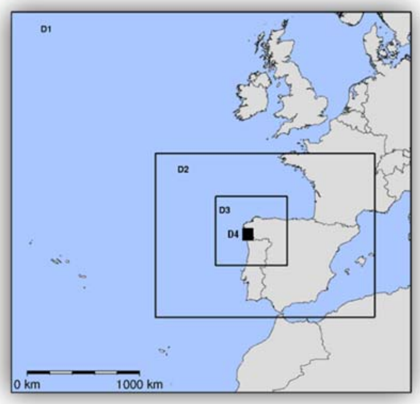


Figure 2: WRF model nested domains at four different horizontal resolutions, in order to achieve up to 1.3x1.3 km^2 resolution over the innest D4 domain.

PrOlor is a software system based in three different atmospheric models running on Linux,

1. WRF (Weather Research & Forecast) model (Skamarock and Klemp, 2008), that provides high resolution (1.3x1.3 km^2) weather forecasts over the study domain (D4). Model input is daily provided by the US NCEP (US National Centre for Environmental Prediction) from its GFS (Geophysical Forecast System).
2. CALMET meteorological diagnostic model (Scire et al., 2000a) that produces very high resolution (250x250 m^2) meteorological fields over the study domain (D4). Also, 12 vertical layers up to 4000 m are considering, following a telescopic distribution (with thinner layers close to the surface) (Gonzalez et al., 2015).
3. CALPUFF Lagrangian dispersion model (Scire et al., 2000b), using the same 3-dimensional grid as CALMET to provide odorants concentrations and odor levels results.

This model-based system produces their numerical results in netCDF standard format, in order to facilitate the data analysis: graphical time series, statistical analysis and maps. In addition, “cloud” storage is available for web and smartphone data access.

Flow diagram of PrOlor system is shown in Figure 1. Although CALMET/CALPUFF models are included in US EPA regulatory CALPUFF system, PrOlor was developed using improved versions of both models: CALMET v. 6.334 and CALPUFF v. 6.42. Currently, CALMET meteorological input over D4 domain is provided by WRF model daily simulations over the nested domains shown in Figure 2, at four different horizontal resolutions: D1

(36x36 km^2), D2 (12x12 km^2), D3 (4x4 km^2), and D4 (1.3x1.3 km^2). Nesting technique is required in order to reduce the computational time, due to the CFL (Courant-Friedrich-Levy) convergence condition (Inness and Dorling, 2013) that relates the time step applied in the WRF model solver to its grid resolution.
CALMET also requires a detailed terrain module over D4 domain (Figure 2), including land use data and a Digital Elevation Model (DEM) as follows: Spanish Geographic Centre (CNIG) LIDAR elevation data with 5x5 m^2 resolution, and Global Land Cover Characterization (GLCC) with 300x300 m^2 resolution, considering 22 different land use as Land Cover Classification System (LCCS).
PrOlor system runs every day to get an odor forecast 72 h in advance; their hourly results include WRF numerical weather forecast, CALMET high resolution meteorological fields (specially, wind, temperature and mixed layer depth), and CALPUFF odorants concentrations and odor intensity (in OU/m^3).
Although CALPUFF model allows directly applying odor emissions measurements as input, in PrOlor chemical odorants emissions are considered. Therefore, not only odorants atmospheric diffusion, but also first order chemical decay of each odorant is calculated during the CALPUFF simulation, and odorants ambient concentrations are obtained. From these hourly results, odor intensity and odor concentration were obtained by using the Stevens' Law and a modified Steven's law relationship for H_2S, Eq. (1) (Koe, 1985, Gostelow et al., 2001),

$$C_{(ou)} = 2000 \times [H_2S] \quad (1)$$

where $C_{(ou)}$ is the odor concentration ($ou \cdot m^{-3}$) and $[H_2S]$ is the hydrogen sulfide concentration (ppm).
PrOlor system can obtain hourly odorant results, as it is designed to apply hourly meteorological inputs. However, short odor events (less than 1 hour) are also estimated by using the peak-to-mean ratio, Eq. (2) (Smith, 1973; Piringer et al., 2012),

$$\frac{C_p}{C_m} = \left(\frac{T_m}{T_p}\right)^U \quad (2)$$

where Cp is the mean odorant concentration over the Tm integration time (typically, 1 hour), Cm is the peak (short) concentration, Tp is the integration time for Cp (typically, 1 minute), and U depends on the atmospheric stability following Pasquill classes (Piringer et al., 2012).

3. Results

This section shows the validation of PrOlor results around the ENCE-Pontevedra plant environment (study domain, D4). Both WRF and CALMET meteorological validations were done against four surface meteorological sites measurements (only one for wind measurements); also, CALPUFF H_2S concentrations and odor levels were validated against short odor events observed around this plant. Validations dataset corresponds to the period April, 1st 2014 to August, 31st 2014, as it was the initial operational period of PrOlor system.
Hourly average wind speed and direction, temperature and relative humidity surface measurements were compared to both forecast results from WRF innest domain (D4) and from CALMET using only WRF-D4 results as meteorological input. From the four meteorological sites installed inside the D4 domain, only Castrove site provided valid wind measurements during this period.

Table 1: Statistics of hourly surface wind speed of WRF and CALMET results against measurements at Castrove site, 04/01/2014-08/31/2014. Absolute statistics in $m \cdot s^{-1}$.

Model	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
WRF	3672	0.60	-0.25	2.15	-0.07	0.57	2.96	0.32	0.03	0.52
CALMET	3672	0.77	-0.37	1.46	-0.10	0.39	2.03	0.73	0.34	0.67

Different statistics recommended by Chang and Hanna (2004) and Emery et al. (2001) for the validation of meteorological models to be applied as input to air quality models are shown in Table 1). Also, wind roses, quantile and Taylor diagrams are analysed. These validation dataset was calculated by using Openair module of R freeware software (Carslaw and Ropkins, 2012).
Table 1 shows the statistics of WRF and CALMET wind speed results against Castrove site measurements. Following Emery et al. (2001) benchmarks to check meteorological models for air quality application, CALMET wind speed statistics practically achieved them: IOA>0.6, RMSE<2.0 $m \cdot s^{-1}$ (CALMET RMSE is 2.03 $m \cdot s^{-1}$).

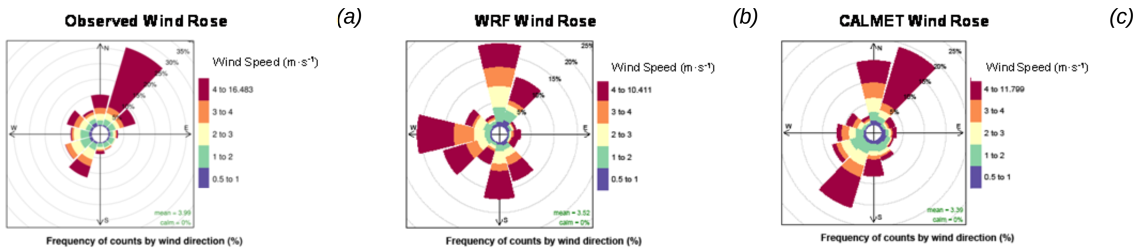


Figure3: Wind roses at Castrove site: (a) observed, (b) WRF model, and (c) CALMET model, 04/01/2014-08/31/2014.

About wind direction, Emery et al. (2001) consider a more liberal benchmark, as low wind speeds can produce unrealistic wind directions. Therefore, a qualitative wind roses comparison (Figure 3) was done at the Castrove site: it is clear that CALMET wind direction frequencies are more similar to the observed directions than WRF results, showing the necessity of applying CALMET model with higher horizontal resolution, also using a more accurate elevation model and land use distribution. However, CALMET seems to overestimate northern and southwestern wind speed at this site: these differences also produced the high RMSE value, and they can be explained by some trees around this site that cannot be considered by the model.
About temperature (Table 2), again CALMET provides better statistics than WRF at the four sites, achieving all the statistical benchmarks suggested by Emery et al. (2001): MB<±0.5 ºC, MGE<2 ºC, and IOA>0.7.

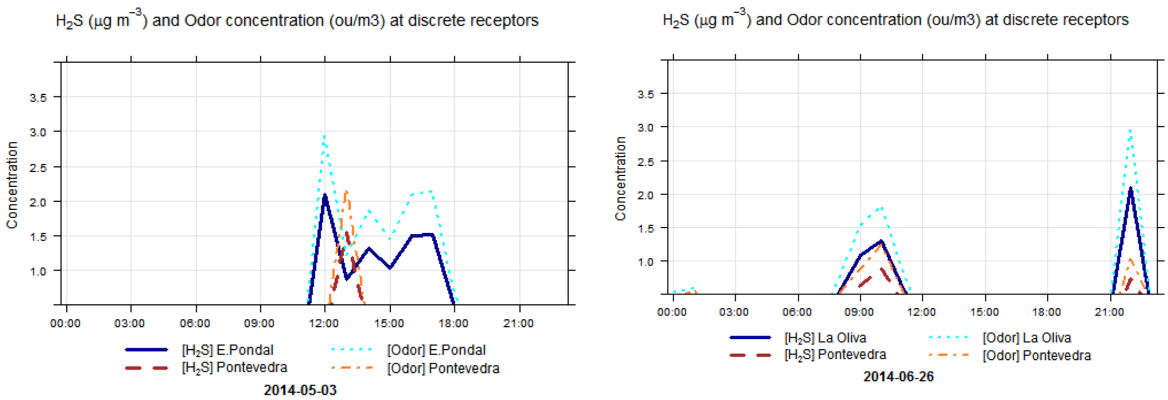
Table 2: Statistics of hourly surface temperature of WRF and CALMET results against measurements at the four sites, 04/01/2014-08/31/2014. Absolute statistics in ºC.

	Site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
WRF	Areeiro	3672	1.00	0.68	1.48	0.04	0.09	1.99	0.91	0.59	0.80
WRF	Castrove	3672	1.00	1.68	2.04	0.11	0.13	2.37	0.94	0.47	0.73
WRF	Lourizán	3672	1.00	0.30	1.80	0.02	0.10	2.38	0.87	0.54	0.77
WRF	Mourente	3672	1.00	-0.85	1.76	-0.05	0.10	2.09	0.91	0.52	0.76
	Site	**n**	**FAC2**	**MB**	**MGE**	**NMB**	**NMGE**	**RMSE**	**r**	**COE**	**IOA**
CALMET	Areeiro	3672	1.00	-0.41	1.61	-0.02	0.09	2.07	0.89	0.55	0.78
CALMET	Castrove	3672	1.00	0.30	1.18	0.02	0.07	1.49	0.95	0.69	0.85
CALMET	Lourizán	3672	1.00	-0.47	1.89	-0.03	0.11	2.42	0.87	0.51	0.76
CALMET	Mourente	3672	1.00	0.05	1.33	0.00	0.08	1.79	0.92	0.64	0.82

Concerning the odor forecast validation, a register of short odor events based in qualitative observations was considered. As odor panelists, paper pulp mill staff members provided to a database any observed short odor event when they detected it, inside and outside the plant, using an IOS smartphone app; including date, time and odor event location. These registered events were compared to the results obtained using PrOlor system during four months (May-August 2014) at discrete receptors located either close to the paper pulp mill (less than 1 km) or far away from the factory (more than 1 km far from emission sources).
As PrOlor forecast consists in hourly average odorants concentrations, in order to compare PrOlor results to the observed short odor events, average concentrations were converted to short odor concentrations using the peak-to-mean approach (Beychock, 1994; Piringer, 2014), with 1 minute as peak integration time (C_p); and also considering different values for the power law parameter (U) depending on atmospheric stability.
Although the ambient odor should be a combination of different odorants effect, considering the odorants emitted from this paper pulp mill, H_2S is the emitted odorant with highest emission rate and very lowest odor threshold, 0.7 µg/m^3 (McGinley et al., 2008); in fact, this odorant concentration was well correlated to odor levels in the past (Gostelow et al., 2001). Therefore, odor intensity was calculated from peak H_2S concentration forecasts using the Steven's Law.

During the validation period of study, 34 short odor events were reported, and 5 of these events were detected like a strong odor, while the other 29 were rated like slight odors. Comparing to the peak odor intensity forecasts, 32 of these short odor events were correctly forecasted by PrOlor. Only 2 short odor events could not be correctly predicted: one of them was caused by an accidental increase in H_2S emissions at stripping process in the paper pulp mill; no explanation was found for the other failed event.

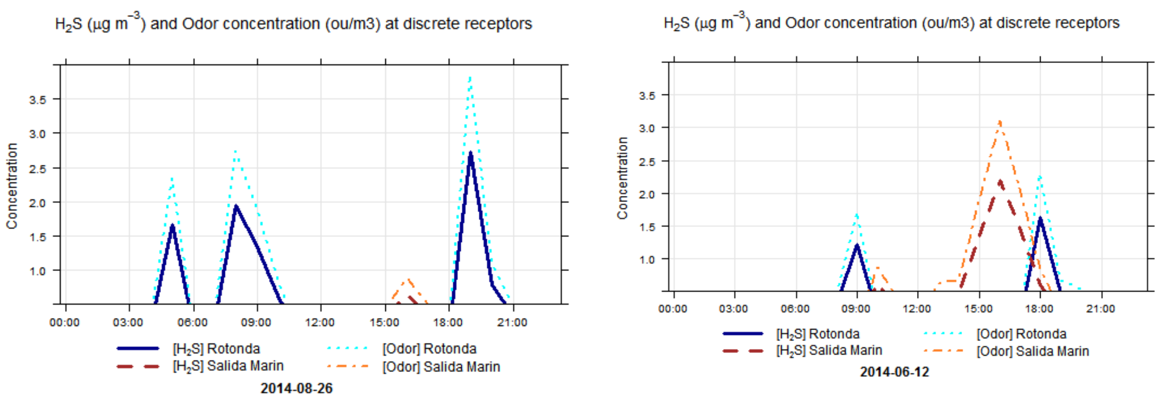
Concerning the short odor events far away from the plant, Figure 5 shows some PrOlor results of peak H_2S ground level concentration and odor intensity at three discrete receptors located in Pontevedra downtown (Pontevedra, E. Pondal and La Oliva), where short odor events with different odor intensities were detected by the panelists. During the afternoon on May 3rd, 2014 a short odor event was registered at Pontevedra downtown; as it is observed in Figure 5a, for that date PrOlor forecasted H_2S peaks up to 1.5-2 µg/m^3 (odor intensity, 3 OU/m^3) from 15:00 to 18:00 UTC at discrete points located far away (Pontevedra and E. Pondal, up to 3 km from the paper pulp mill odor sources). Also, a short odor event at Pontevedra downtown was registered on June 26th, 2014 in the morning. About PrOlor results, Figure 5b shows a H_2S peak up to 1.3 µg/m^3 (odor intensity < 2 OU/m^3) after 9:00 UTC at two downtown receptors, La Oliva and Pontevedra.



(a) (b)

Figure 5: PrOlor H_2S ground level concentration (µg/m^3) and odor intensity (OU/m^3) at three receptors during two different intensity short odor events far away from the plant: (a) May/03/2014 - strong odor event in the afternoon (b) Jun/26/2014 - slight odor event in the morning.

About short odor events close to the plant odor sources (i.e., Rotonda and Salida Marín Receptors), all the events registered by the panelists were faint odors. As it is shown in Figure 6a, along August, 26th 2014 PrOlor forecasted a peak of 2 µg/m^3 (almost 3 OU/m^3) between 8:00 and 9:00 UTC at Rotonda receptor, when a slight short odor event was registered in this receptor area by the panelist. Also, PrOlor forecasted (Figure 6b) a smaller peak (up to 1 µg/m^3) at Rotonda receptor in June, 12th 2014 at 9:00 UTC in agreement to a slight odor event registered (figure 6b).



(a) (b)

Figure 6: PrOlor H_2S ground level concentration (µg/m^3) and odor intensity (ou/m^3) at two receptors during two different morning slight odor events near the plant: (a) August/28/2014 (b) Jun/12/2014.

However near the odorants sources (< 1 km distance), the odor intensity observed by the panelists is not always in agreement to the PrOlor H_2S peak concentration, as CALPUFF usually overestimate this concentration. On the opposite, PrOlor peak concentrations are usually lower than expected at far way receptors. This can be related to the peak-to-mean decrease factor applied with travel time (Mylne, 1990), as its value should be adjusted to each specific environment.

4. Conclusions

Operational ambient odor PrOlor system for the simulation and forecast of short odor events around a pulp paper mill was developed and installed at Pontevedra city, northwest of the Iberian Peninsula, based in meteorological models and a Lagrangian dispersion model. Meteorological models WRF and CALMET were validated against the available surface measurements along five months, showing that CALMET results (with WRF results as meteorological input) passed the statistical benchmarks for wind and temperature suggested by Emery et al. (2001) to apply its results as meteorological input to CALPUFF Lagrangian dispersion model. Also, peak-to-mean ratios were applied to estimate peak short odorant concentrations, and converted to odor intensities.During four months at the study period, 34 short ambient odor events were registered by the paper pulp mill staff outside this plant; and PrOlor forecast agreed in 32 of those events in date and time period; only during one of the failed events a fugitive H_2S emission from the paper pulp mill was detected. In spite of this good qualitative agreement, PrOlor usually underestimated the odor intensities observed far away from the emission sources. On the opposite, odor intensities estimated by PrOlor close to the emission sources was usually higher than observed, showing the necessity of calibrating the peak-to-mean decrease factor applied with travel time, using chemical odorants measurements at different receptors.

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