Validation of CALMET/CALPUFF models simulations around a large power plant stack

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Abstract
CALMET/CALPUFF modeling system is frequently used in the study of atmospheric processes and pollution, and several validation tests were performed until now; nevertheless, most of them were based on experiments with a large compilation of surface and aloft meteorological measurements, rarely available. At the same time, the use of a large operational smokestack as tracer/pollutant source is not usual.

In this work, first CALMET meteorological diagnostic model is nested to WRF meteorological prognostic model simulations (3x3 km^2 horizontal resolution) over a complex terrain and coastal domain at NW Spain, covering 100x100 km^2, with a coal-fired power plant emitting SO_2. Simulations were performed during three different periods when SO_2 hourly glc peaks were observed. NCEP reanalysis were applied as initial and boundary conditions. Yong Sei University-Pleim-Chang (YSU) PBL scheme was selected in the WRF model to provide the best input to three different CALMET horizontal resolutions, 1x1 km^2, 0.5x0.5 km^2, and 0.2x0.2 km^2. The best results, very similar between them, were achieved using the last two resolutions; therefore, the 0.5x0.5 km^2 resolution was selected to test different CALMET meteorological inputs, using several combinations of WRF outputs and/or surface and upper-air measurements available in the simulation domain.

With respect to meteorological aloft models output, CALMET PBL depth estimations are very similar to PBL depth estimations using upper-air measurements (rawinsondes), and significantly better than WRF PBL depth results. Regarding surface models surface output, the available meteorological sites were divided in two groups, one to provide meteorological input to CALMET (when applied), and another to models validation. Comparing WRF and CALMET outputs against surface measurements (from sites for models validation) the lowest RMSE was achieved using as CALMET input dataset WRF output combined with surface measurements (from sites for CALMET model input).

Following, CALPUFF model was applied to simulate the local atmospheric diffusion of SO_2 (as an inert tracer) from a large power plant smokestack (with four parallel independent liners), considering two different stack configurations (one single point source as a summa of four liners vs. one point source per liner) and two different CALMET meteorological simulations (using as input dataset only the WRF model output vs. only surface and upper-air meteorological measurements).

Comparison of those CALPUFF simulations results against the hourly average ground level concentration (glc) measurements shows that the best model performance was obtained by using only WRF model output as CALMET input; also, better glc results are obtained considering one point source per liner in CALPUFF simulations.

Key words: CALMET, CALPUFF, WRF, model validation and intercomparison, surface and rawinsonde data, PBL depth, plume dispersion, glc, stack configuration.

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Validación de simulaciones de los modelos CALMET/CALPUFF en el entorno de una gran chimenea de central térmica

Resumen
El sistema de modelización CALMET/CALPUFF es empleado habitualmente en el estudio de procesos atmosféricos y de contaminación, y múltiples tests de validación han sido desarrollados hasta ahora; sin embargo, la mayoría de ellos están basados en experimentos con una gran compilación de medidas meteorológicas en superficie y en altura, pocas veces disponibles. Al mismo tiempo, el uso de una gran chimenea en operación como fuente del trazador/contaminante empleado para la validación de modelo CALPUFF no es habitual.

En este trabajo, en primer lugar, el modelo de diagnóstico meteorológico CALMET (con diversas resoluciones horizontales) es anidado a simulaciones del modelo de predicción meteorológica WRF (resolución horizontal de 3x3 km^2) sobre un dominio costero con terreno complejo en el Noroeste de España, abarcando 100x100 km^2, con una central térmica de carbón que emitía SO_2. Las simulaciones se han realizado durante tres períodos diferentes en los que picos horarios de inmisión de SO_2 fueron detectados. Como condiciones iniciales y de contorno del modelo WRF se aplicaron los reanálisis del NCEP. En particular, el esquema de capa límite Yong Sei University-Pleim-Chang (YSU) fue seleccionado en el modelo WRF para proporcionar los mejores datos de entrada a tres resoluciones horizontales diferentes con CALMET: 1x1 km^2, 0.5x0.5 km^2, and 0.2x0.2 km^2. Con las dos últimas resoluciones se obtuvieron los mejores resultados, muy similares entre sí; en consecuencia, la resolución 0.5x0.5 km^2 se eligió para ensayar distintos datos meteorológicos de entrada al modelo CALMET, empleando varias combinaciones de los resultados obtenidos con el modelo WRF y/o medidas meteorológicas en superficie y en altura disponibles en el entorno de simulación.

Sobre los resultados de los modelos WRF y CALMET en altura, las estimaciones de altura de capa de mezcla derivadas de medidas en altura (radiosondeos) son bastante similares a los resultados de las simulaciones CALMET, y mejores que los resultados del modelo WRF. Sobre los resultados de los modelos WRF y CALMET en superficie, se dividieron las estaciones disponibles en dos conjuntos, uno para proporcionar datos de entrada al modelo CALMET (cuando se usaron), y otro compuesto por estaciones para validación. Comparados los resultados de los modelos WRF y CALMET con medidas en superficie de las estaciones para validación el RMSE más bajo se alcanzó empleando como datos de entrada al modelo CALMET los resultados del modelo WRF combinados con medidas en superficie (de las estaciones seleccionadas para proporcionar datos de entrada al modelo CALMET).

En segundo lugar, el modelo CALPUFF fue aplicado para simular la dispersión local de SO_2 (como trazador) de una gran chimenea de central térmica (con cuatro conductos independientes), considerando tanto dos diferentes configuraciones de chimenea (un solo foco puntual suma de los cuatro conductos vs. un foco puntual por conducto) como dos resultados distintos del modelo CALMET (usando como datos de entrada: solo los resultados del modelo WRF vs. solo medidas meteorológicas en superficie y en altura). La comparación de dichas simulaciones CALPUFF frente a las medidas de inmisión disponibles (promedios horarios) mostró que el mejor rendimiento del modelo se obtuvo empleando los resultados del modelo WRF como datos de entrada para CALMET; también, mejores resultados de inmisión se obtuvieron considerando un foco puntual por conducto en las simulaciones con CALPUFF.

Palabras clave: CALMET, CALPUFF, WRF, validación e intercomparación de modelos, datos de superficie y radiosondeos, altura de capa de mezcla**,** dispersión de penachos atmosféricos, inmisión, configuración de chimenea.

Contents:

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1. Introduction

The knowledge of atmospheric processes and pollution is essential for the handling of air quality. In this respect, the interpretation of the spatial and temporal evolution of air pollution requires extensive and detailed weather information, as both are strongly related. Even though the measurements obtained by weather sites, surface and upper air, provide a significant basis for driving meteorological studies, their biggest limitations are the lack of site in every location and time (including upper air data) and the need to know in detail the evolution of atmospheric phenomena. Accurate meteorological models allow covering those faults. Any user of an atmospheric model usually can choose among a large number of possible model setups to obtain its best output, suited to the characteristics of the region and the phenomena being studied. Then, there is no universal model setup that can be applied to every region and every phenomena, as the model must be validated against measurements to determine the degree of accuracy of the simulation results and to obtain a suitable model setup (Hernández-Ceballos et al., 2010). Particularly, Ames et al. (2002) emphasized the significance of meteorological model validation related to CALMET model configuration, as it can strongly influence the results of the CALPUFF dispersion model.

The use of different statistics and methods for the validation of meteorological models was previously studied: The advantages of using RMSE to evaluate meteorological models was pointed out for Willmott (1981), as other statistics drive to either large errors overestimation or small errors masking. More recently, Snyder et al. (2007) applied a bayesian statistical method to validate the RegCM3 model, and artificial neural networks were applied by Cao et al. (2012). Nevertheless, many meteorological models evaluations are still based in statistical parameters as RMSE, BIAS, etc (Souto et al., 2001; Emery et al., 2001; Chang and Hanna, 2004).

The estimation of the local dispersion of an air pollutants' plume emitted from a smokestack is a problem conditioned by both the emission source and the meteorological conditions. In the first case, the smokestack is often seen as a point source that emits gaseous and particulate pollutants. In the second one, an accurate estimation of the meteorological conditions around the source is required, also with high temporal and spatial resolutions.

The application of CALMET/CALPUFF is well-known, as a well-established Lagrangian modelling system, and several validation tests were published (Cohen et al., 2005; Dresser and Huizer, 2011; Fishwick and Scogie, 2011; Ghannam and El-Fadel, 2013; Levy et al., 2003; Protonotariou et al., 2005; Yau et al., 2004). In order to achieve the best model performance evaluation, most of them were based in specific experiments with passive tracers and a large compilation of surface and aloft meteorological measurements during the experiments. Nevertheless, with limited available meteorological and pollution datasets, as in an operational scenario, uncertainties arise (both in measurements and models results) and worse performance of the models is expected.

In this work, a CALMET diagnostic model nested to WRF model simulation is evaluated by comparison to both surface and upper air measurements, along specific periods. PBL depth and surface data are considered. Also, the CALPUFF model is applied to simulate the local dispersion of SO_2 (as a tracer) from a large smokestack, in an operational scenario, considering both different stack configurations and meteorological inputs. Because of the limited availability of air quality data around the smokestack, a new approach for CALPUFF validation is applied.

2. Case study: As Pontes Power Plant

Galicia occupies the extreme northwestern corner of the Iberian Peninsula, between 42° and 44° N and 7° and 9°30’ W. In Galicia, the study area is located around As Pontes Power Plant (Figure 1), a 1,400 MWe coal-fired power plant with large smokestack that is selected as tracer source. A simulation domain of 100x100 km^2 was selected in order to cover any pollutants source local impact. This domain is a coastal and complex terrain environment, with a mixing of several granitic mountains achieving up to 1000 asl-m (above sea level meters), valleys and a narrow coastal line.

About the tracer source, SO_2 was selected because As Pontes Power Plant is the largest SO_2 source in the domain, so usually any other sources contribution to SO_2 ground level concentration (glc) can be neglected. About its SO_2 emissions, until year 2006 this facility burnt a mix of local lignite (2% in S) and foreign subbituminous coal (0.1% in S) (Dios et al., 2013) in four boilers, with a 70:30 (lignite:subbituminous) weight ratio; during each validation periods selected this ratio kept constant, so SO_2 emissions were also quite constant along each period. However, the facility could change this ratio to achieve a SO_2 emission reduction if high SO_2 ground level concentration (glc) levels were expected along the next day in its surrounding area (Souto et al., 2009). Nowadays, 100% of subbituminous coal is burnt, so current SO_2 emissions are 20 times lower and no SO_2 pollution episodes were observed.

This power plant includes a smokestack (356.5 agl-m height, above ground level meters height) with four independent liners (one per boiler) in the same concrete shaft (Figure 2). Therefore, it should be considered as four different point sources practically located in the same point; alternatively, it can be considered as a single point source, with an emission and stack section as the sum of the four liners. SO_2 emissions are very much higher than other local contributions, so this pollutant could be considered as a tracer of this power plant emission in a radio of 30 km. In fact, an air quality network in this area (Figure 1) allowed the control of these power plant emissions, with 17 glc monitoring sites located over sectors with more frequent SO_2 hotspots.

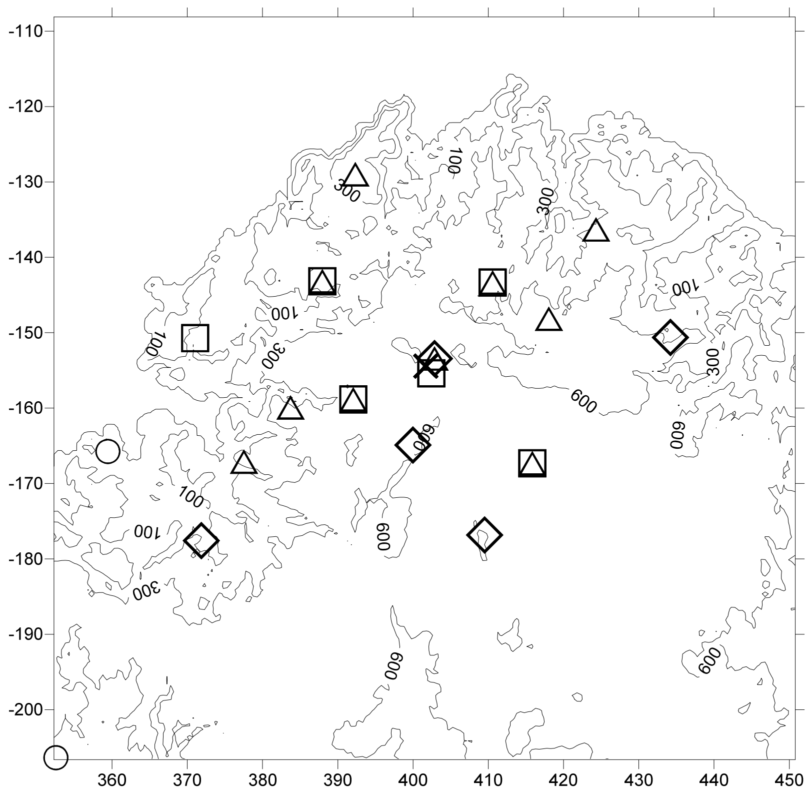

Figure 1. Surrounding area (LCC coordinates, Lambert Conic Conformal projection, WGS-84 data; in km) and physical geography (topographic lines in meters) of the simulation domain around As Pontes Power Plant stack (X), also showing 6 surface meteorological stations for model input (□), 5 surface meteorological stations for validation (◊), 2 upper-air meteorological stations (O), and 10 air quality sites (Δ).

Regarding the meteorological conditions in this region that affect the plume dispersion, the annual wind pattern in the surrounding area of this power plant is mainly NE-SW; however, significant variations are observed both at regional and local scales along every day. These complex regional conditions and the large power plant stack lead to a difficult plume dispersion simulation problem (Davakis et al., 1998). Therefore, three different periods (3-days duration) with detected SO_2 episodes in this region were selected to test CALPUFF model, following double criteria: (a) hourly maximum SO_2 ground level concentration (glc) exceeding 170 µg/m^3, and, (b) synoptic representativeness, as typical weather conditions for SO_2 episodes in the Northwestern Iberian Peninsula. These selected periods cover: P1, from 13 July 2005 to 15 July 2005; P2, from 1 June 2006 to 3 June 2006; and P3, from 9 July 2009 to 11 July 2006. All of them are anticyclonic and stable periods, typical conditions in the synoptic pattern High Pressure over Atlantic and Europe (HPAE) (Saavedra et al., 2012a).

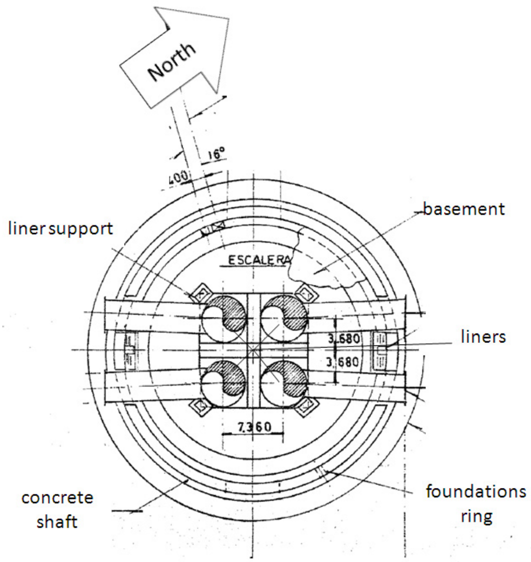

Figure 2. As Pontes Power Plant stack top view, with the four liners inside it. Measurements in mm and degrees (º).

3. Meteorological modelling

To provide meteorological input to the CALPUFF model, a CALMET diagnostic model and WRF mesoscale prognostic model are coupled. This system is run on an hour-to-hour basis, using the WRF model to obtain a mesoscale meteorological field as a first guess field and, after that, using the CALMET model to adjust the meteorological fields considering the local influence of high-resolution terrain and land use data in the study area. Then, the CALMET output is coupled with the dispersion model CALPUFF (WRF/CALMET/CALPUFF system).

In this work, a WRF v.3.2 model (Skamarock and Klemp, 2008) is configured with 30 layers in the vertical direction and 3 levels of one-way nested domains (Figure 3) to achieve a horizontal grid resolution of 3x3 km^2 over the study area. The vertical grid sizes increased gradually with height with the lowest level being at 10 m above the ground. The model top pressure was located at 100 hPa. Apart from the different planetary boundary layer (PBL) schemes tested, model settings are Kain-Fritsch scheme (Kain and Fritsch, 1993) for cumulus parameterization (for 27x27 km^2 and 9x9 km^2 domains only), the WSM3-class microphysics scheme, the RRTM longwave and Dudhia shortwave radiation, and the 5-layer soil model (Dudhia, 1996).

NCEP-GFS analysis data (1º horizontal resolution) are used as initial and boundary conditions every three hours. Neither surface nor upper-air observations are used. The United States Geological Survey (USGS, 2008) provides the elevation and land cover data. WRF model is initialized as a ‘‘cold start’’ at 0000 UTC each day and run for 72 h, updating the boundary conditions every six hours and recording data every hour. No time as model spin-up is considered. The output frequency of the WRF model is set to 1 h. In this work, Yong Sei University-Pleim-Chang (YSU) PBL scheme (Hong and Lim, 2006) is selected because of its better results (Saavedra et al., 2012b; Souto et al., 2014) after testing four different PBL schemes.

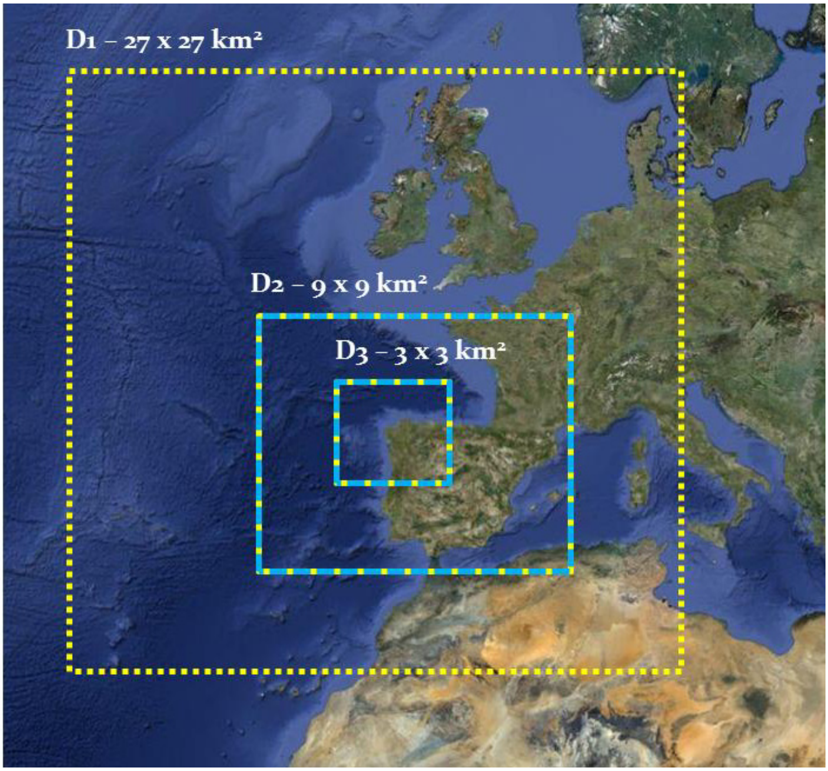

Figure 3. WRF nested domains, with D3 domain providing input data to the CALMET/CALPUFF simulation domain inside it.

Different CALMET model horizontal resolutions were tested, in order to consider complex terrain and coastal influences (Scire et al., 2000a). However, in every CALMET simulation the same vertical layers (top-faces) were applied: 20, 40, 79, 176, 290, 439, 640, 880, 1180, 1580, 2062, 2453, 3354 and 4162 agl-m.

4. CALMET modelling validation and intercomparison

For meteorological modelling validation and intercomparison, seven different CALMET simulations were done (Table 1), sorted in two groups, depending on the meteorological input applied: Group 1, using only the best WRF results as input, and different CALMET horizontal resolutions; and Group 2, using also meteorological measurements, but keeping a 0.5x0.5 km^2 CALMET horizontal resolution.

Table 1. RMSE from CALMET simulations against surface meteorological sites data: wind speed and temperature.

Simulations		**RMSE wind speed ($m \cdot s^{-1}$)**			**RMSE temperature (ºC)**		
	CALMET meteorological inputs and grids	**P1**	**P2**	**P3**	**P1**	**P2**	**P3**
Group 1 (against 11 sites)							
Best WRF	-	1.574	2.582	1.968	3.635	1.879	2.522
Cm-1/3km	WRF results only, 1 km grid resolution	1.495	2.550	1.946	3.753	2.305	3.092
Cm-0.5/3km = Cm(W)	WRF results only, 0.5 km grid resolution	1.498	2.510	1.919	3.755	2.293	3.083
Cm-0.2/3km	WRF results only, 0.2 km grid resolution	1.499	2.527	1.914	3.763	2.285	3.081
Group 2 (against 5 sites)							
Cm(S+U)	Data from 11 (all) surface and 2 upper-air sites	0.048	0.061	0.054	0.650	0.050	0.732
Cm(W+S6)	WRF results and 6 surface sites	0.493	2.018	1.982	3.480	2.005	2.736
Cm(Sw+Uw)	WRF results (as measurements), 6 surface and two upper-air sites	1.463	2.245	2.250	3.577	3.374	2.825
Cm(S6+U)	Data from 6 surface and 2 upper-air sites	1.412	2.491	2.622	1.416	2.870	2.369

Observational dataset available over the study area includes hourly average observations from eleven surface monitoring stations/sites, and upper-air data from two rawinsondes, all of them located in NW Iberian Peninsula (Figure 1). Surface sites were selected as much representative as possible of the study area meteorology, based on their local characteristics (no obstacles, uniform land use) and the typical wind and temperature in the region. For meteorological models validation, surface sites were divided in two groups, that is, when only six surface sites measurements were applied as input data, the other five surface sites measurements are applied for model testing. Upper-air observations were collected from two rawinsondes (Figure 1): EOAS-Santiago (MeteoGalicia, Regional Met Office) and A Coruña (AEMET, Spanish Met Office), alternatively launched every 6 hours.

For meteorological models validation, the following parameters were compared: PBL depth, surface temperature and wind speed.

Regarding the surface outputs assessment, Table 1 shows the root mean square error (RMSE) modelled vs. measured for the different CALMET (and also, WRF) simulations.

Group 1 simulations are described as follows,

- Best WRF is a WRF model simulation with 3x3 km^2 horizontal resolution three-dimensional grid,
- Cm-1/3km is a CALMET simulation with 1x1 km^2 horizontal resolution, using only Best WRF gridded output as meteorological input,
- Cm-0.5/3km is a CALMET simulation with 0.5x0.5 km^2 horizontal resolution, using only Best WRF gridded output as meteorological input, and,
- Cm-0.2/3km is a CALMET simulation with 0.2x0.2 km^2 horizontal resolution, using only the Best WRF simulation gridded output as meteorological input.

Group 2 simulations are described as follows,

- Cm(S+U) is a CALMET simulation with 0.5x0.5 km^2 horizontal resolution, using data from 11 (all) surface sites and 2 upper-air sites as meteorological input,
- Cm(W+S6) is a CALMET simulation with 0.5x0.5 km^2 horizontal resolution, using Best WRF gridded output and data from 6 surface sites (not used for model validation) as meteorological input,
- Cm(Ws+Us) is a CALMET simulation with 0.5x0.5 km^2 horizontal resolution, using Best WRF output over surface and upper-air locations combined to 2 upper-air sites measurements, and,
- Cm(S6+U) is a CALMET simulation with 0.5x0.5 km^2 horizontal resolution, using data from 6 surface sites (not used for model validation) and 2 upper-air sites as meteorological input.

Group 1 simulations are compared to eleven (all) sites measurements; Group 2 simulations are compared to five sites measurements not applied as meteorological input in those simulations; except in Cm(S+U) simulation, as those five sites also provide CALMET input, so this is just a reference simulation that provide the best performance any other simulation could achieve.

About the surface wind speed, Group 1 simulations provide similar surface performance, showing that CALMET model (Cm-1/3km, Cm-0.5/3km, Cm-0.2/3km) cannot improve WRF surface results (Best WRF) without adding surface measurements as CALMET input. With respect to Group 2 simulations, of course the lowest RMSE values are obtained in the Cm(S+U) simulation, as it is tested against the surface sites measurements which are also used as input data; so this is not properly a Cm(S+U) simulation validation, it is just a reference test. About the rest of Group 2 simulations, a significant improvement respect to WRF output is obtained using this WRF output and six surface sites data (Cm(WRF+S6) simulation) as CALMET input dataset, even better than using surface and upper-air measurements (Cm(S6+U) simulation). As a consequence, WRF output (Best WRF) provide better upper-air data as CALMET model upper-air input than two rawinsondes alternatively launched every 6 hours in the study area.

Regarding surface temperature, with most of RMSE values above 3 ºC, poor performance is achieved in all tests and periods, except in the reference test, Cm(S+U). As a matter of fact, the use of surface measurements from the other six sites (different than testing sites) as CALMET input does not improve model surface temperature results. As an example, Table 2 shows RMSE values for the P2 period, site by site. The worst statistics are usually achieved in Mabegondo (coastal) site, and in Fragavella and B1-Magdalena (inland) sites.

Figure 4 shows surface temperatures simulated by WRF and CALMET (several inputs) and observed at Mabegondo and Fragavella sites along P2 period. At Fragavella the simulated temperature is usually higher than observed, with some improvement when measurements from other sites are combined to WRF results as CALMET input; only WRF results provide a bit lower nocturnal temperatures than observed, which are corrected by CALMET. On the other hand, at Mabegondo all simulations provide lower daily temperature oscillations. These differences cannot be corrected by using measurements from the other six sites as CALMET input.

Table 2. MB (mean bias) and RMSE of surface temperature results (ºC) from different WRF and CALMET simulations against 5 different testing sites, along P2 period.

	Best WRF		**Cm(W)**		**Cm(W+S6)**		**Cm(S6+U)**	
Site	**MB**	**RMSE**	**MB**	**RMSE**	**MB**	**RMSE**	**MB**	**RMSE**
Fragavella	1.040	2.369	1.386	1.937	1.386	1.937	3.500	4.314
Guitiriz	0.894	1.537	0.933	1.229	0.933	1.229	0.944	2.033
Mabegondo	-0.384	1.912	0.265	2.798	0.265	2.798	-2.401	3.632
Marco da Curra	0.374	1.133	0.327	0.914	0.327	0.914	0.249	1.374
B1 Magdalena	-0.205	1.334	-0.666	2.482	-0.666	2.483	-1.384	1.830

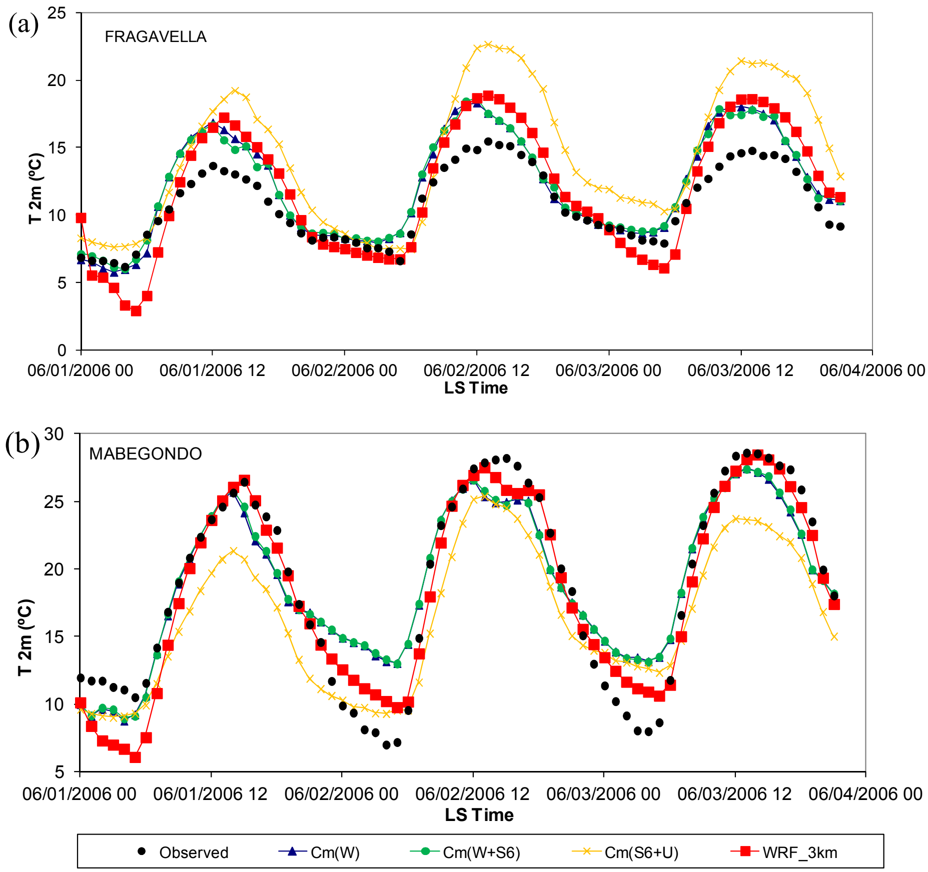

Figure 4. Surface temperature time series both simulated by WRF and CALMET (several simulations) and observed at (a) Fragavella and (b) Mabegondo sites, along P2 period

Considering the upper-air results' evaluation, PBL depths both modelled (Group 1 simulations) and estimated from rawinsonde data are compared. CALMET PBL depth is modelled as follows: in land, using Holtslag and van Ulden (1983), and overwater using a profile technique, considering air-sea temperature difference (Scire et al., 2000a). PBL depth estimation from rawinsonde measurements follows the critical bulk Richardson number method (Vogelezang and Holtslag, 1996) in dry atmosphere (as a function of potential temperature). A critical Richardson number of 0.25 is applied. As it is shown in Figures 5 and 6, CALMET PBL depth results using different horizontal resolutions are quite similar, but significantly better than WRF results. Both 0.5x0.5 km^2 and 0.2x0.2 km^2 resolutions provide a good agreement between CALMET and estimated PBL depth.

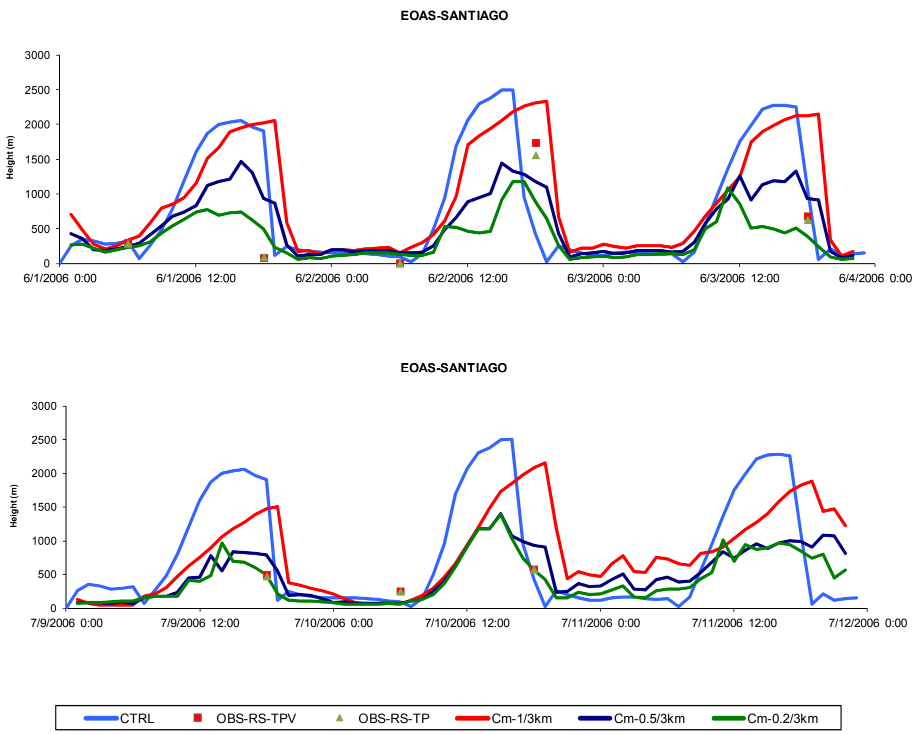

Figure 5. PBL depth time series over EOAS-Santiago (at 06 UTC and 18 UTC every date) modelled by WRF model (CTRL line) and different CALMET model resolutions (other lines) and estimated from the available EOAS-Santiago rawinsonde data (dots), only 2006 periods (P2 and P3). PBL depth estimated using observed virtual potential temperature (OBS-RS-TPV), and using observed potential temperature (OBS-RS-TP) (Vogelezang and Holstlad, 1996).

As an example of PBL profiles, Figure 7 shows temperature and wind speed profiles on June/01/2006 at 0 UTC and 12 UTC, both measured by A Coruña rawinsonde and calculated by different models simulations, as follows: WRF output, Cm(S6+U), and Cm(0.5/3km); the rest of CALMET simulations results (also using surface measurements) are very similar to Cm(0.5/3km). Modelled 0 UTC temperature profiles can reproduce observed upper air lapse rate and thermal inversion between 500-1000 m, but less strong. Of course, the best agreement is obtained by the Cm(S6+U) simulation. At 12 UTC, a light stability change is observed between 500-1500 m, which is only reproduced by the Cm(S6+U) simulation; also, WRF model produces a small change between 1000-2000 m. Observed wind speed at 0 UTC is very sparse, with values between 5-12 $m \cdot s^{-1}$ and the lowest values around 2000 m; Cm(S6+U) produces a quite flat wind speed profile, around 6 m·s^{-1}, with the highest value close to surface level. The other simulations provide a wind speed peak at 500 m, which is not observed. Better simulations results are achieved at 12 UTC, with an upper-air wind speed increment both observed and modelled, although the small number of measurements drives to a sparse profile.

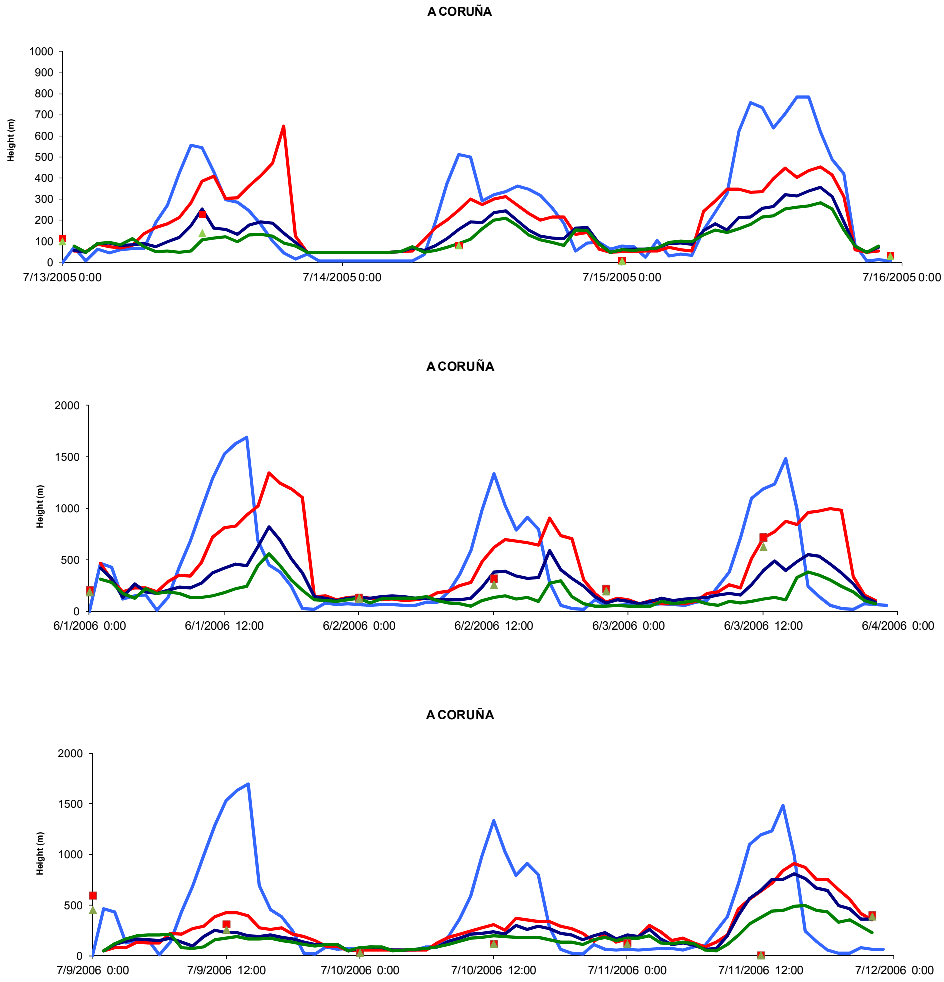

Figure 6. PBL depth time series over A Coruña (at 00 UTC and 12 UTC every date) modelled by WRF model (CTRL line) and different CALMET model resolutions (other lines) and estimated from the A Coruña rawinsonde data (dots). PBL depth estimated using observed virtual potential temperature (OBS-RS-TPV), and using observed potential temperature (OBS-RS-TP) (Vogelezang and Holstlad, 1996).

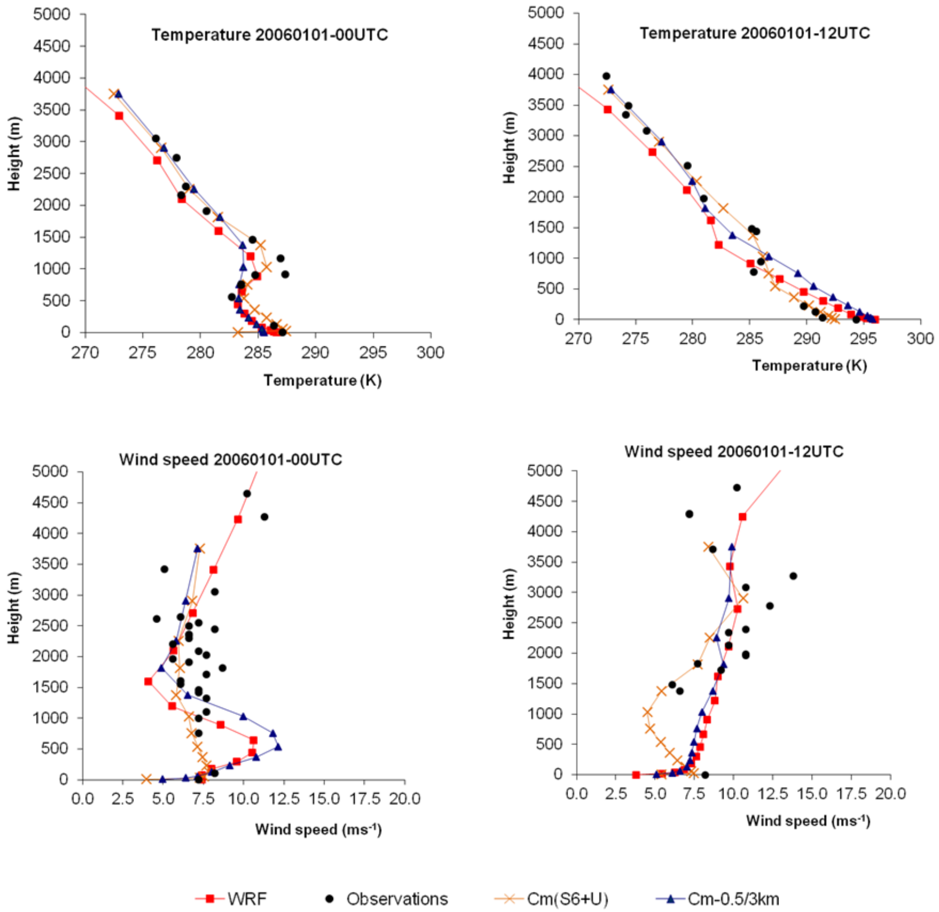

Figure 7. Temperature and wind speed profiles on June/01/2006 at 0 UTC and 12 UTC, both measured by A Coruña rawinsonde and calculated by different models simulations: WRF output, Cm(S6+U), and Cm(0.5/3km).

In summary, considering meteorological surface measurements the combination of WRF output and surface measurements provide the best input to CALMET model, as this CALMET simulation achieves the lowest RMSE. Also, PBL depth results are better using WRF output as CALMET input, no matter if surface measurements are also applied.

5. CALPUFF modelling validation and intercomparison

CALPUFF (Scire et al., 2000b) is a well-known Lagrangian puff model, with releases included in the US EPA regulatory models. CALMET diagnostic meteorological model provides the meteorological input, using either measurements or other models outputs and, even, a combination of both datasets. About the CALPUFF setup, default options recommended in the regulatory release were applied, including entrainment and complex terrain influence.

In this work, CALPUFF was tested considering, (1) one virtual or four actual (liners) point sources, and (2) CALMET output using the best WRF model output or meteorological measurements.

Then, three different dispersion simulations were compared: Calpuff.1 (CALMET with WRF data input and four liners), Calpuff.2 (CALMET with meteorological measurements and four liners) and Calpuff.3 (CALMET with WRF data input, and one virtual source).

Because of the limited air quality monitoring sites in this domain (Figure 1) the typical statistical site-by-site comparison between model and measurements was changed by an integrated plume impact evaluation (De Castro, 2001), based in the hourly maximum SO_2 glc, Cmax, obtained over a 0.5×0.5 km^2 resolution ground level grid. Also, the mean hourly travel distances, Xmax, from the point sources to Cmax grid cell were calculated. To obtain these hourly Cmax and Xmax values, SO_2 glc over that grid were obtained by either from the three CALMET/CALPUFF configurations or by using the available glc measurements, applying a weighted average interpolation. So, four different hourly Cmax and Xmax datasets were obtained, in order to compare the three simulation outputs against one interpolated Cmax/Xmax hourly datasets.

Measurements interpolation applied a modified weight function of De Arellano et al., (1993) recommended to take into account the representativity of the observed concentration at a station for its surroundings [Equation (1)] (De Castro, 2001),

$$c(i,j) = \frac{\sum_{1}^{ns} c_n \cdot \exp\left[\frac{1}{r_n(i,j)}\right]}{\sum_{1}^{ns} \exp\left[\frac{1}{r_n(i,j)}\right]} \qquad (1)$$

where c_n is the measured glc in site n, ns is the number of glc sites, and $r_n(i, j)$ is the distance between the site n and the (i, j) grid point where $c(i,j)$ glc is calculated.

About Cmax comparisons, statistics results from ASTM (2000) for every simulation testing period and CALMET/CALPUFF setup compared to the interpolated Cmax are shown in Table 3. BOOT software (Chang and Hanna, 2005) was applied to check these results. Calpuff.1 simulation statistics are better (lower) than Calpuff.2 and Calpuff.3 statistics, showing that accurate WRF outputs are better than a limited measurements dataset as input data to CALMET model (Hernandez et al., 2014). Also, the use of a single virtual source in Calpuff.3 simulation provide worse statistics than using four sources in Calpuff.1 simulation, with the same meteorological input. However, the improvement achieved using WRF output as meteorological input (respect to using measurements) is higher than using four sources (respect to one virtual source).

Table 3. Cmax statistics (ASTM, 2000) for the three simulation periods, using Calpuff.1, Calpuff.2 and Calpuff.3 setups.

	13-15 July 2005			01-03 June 2006			09-11 July 2006		
	Calpuff.1	Calpuff.2	Calpuff.3	Calpuff.1	Calpuff.2	Calpuff.3	Calpuff.1	Calpuff.2	Calpuff.3
FB	**-0.14**	-1.08	-1.31	**-0.30**	1.58	0.76	**0.04**	-1.71	1.02
MG	**0.98**	0.50	0.24	**0.63**	29.63	1.88	**1.26**	0.16	3.86
NMSE	**3.37**	22.41	12.80	**0.93**	12.27	2.49	**1.39**	46.48	3.92
VG	**4.60**	14.94	36.64	**2.51**	241050	3.52	**13.13**	592	99.13
FAC2	**0.50**	0.33	0.25	**0.47**	0.16	0.37	**0.44**	0.32	0.28
FBFN	0.48	0.15	**0.04**	**0.43**	1.70	1.03	0.45	**0.02**	1.08
FBFP	**0.62**	1.23	1.35	0.44	**0.01**	0.13	0.41	1.73	**0.06**
MAE	**11.02**	166.55	269.71	**40.63**	99.93	62.24	**3.77**	1084	62.90
MGFN	1.60	1.29	1.07	1.32	30.18	2.36	1.89	1.13	4.20
MGFP	1.63	2.59	4.50	2.10	1.02	1.26	1.50	6.84	1.09
MOEFN	0.49	0.67	0.87	0.67	0.08	0.30	0.56	0.87	0.29
MOEFP	1.49	1.23	1.11	1.14	-0.01	7.80	2.10	1.08	-0.50

FB: fractional bias; MG: geometric mean bias; NMSE: normalized mean square error; VG: geometric variance; FAC2: factor of two of observations; FBFN and FBFP: False-negative and False-positive FB; MAE: mean absolute error; MGFN and MGFP: False negative and False-positive MG; MOEFN and MOEFP: False-negative and False-positive Measure of Effectiveness.

6. Conclusions

Meteorological simulations over complex terrain are critical to achieve accurate plume dispersion simulations; often, they require high resolution grids and, besides, a large input dataset. In this work, different CALMET/CALPUFF system setups were tested in the local simulation of a large smokestack emission, with two different emission source configurations.

Regarding the meteorological testing, seven different CALMET simulations along three different periods over a coastal and complex terrain Atlantic domain were done, using both WRF results and surface and upper-air measurements. CALMET simulations results were compared to surface wind and temperature observations (not applied as models input), to upper-air observations, and to estimated PBL depths (from upper-air data). The best surface wind results were obtained by CALMET using WRF results and surface measurements as input dataset, as the best option to obtain meteorological fields for CALPUFF modeling. However, surface temperature results are not so good, with differences in some coastal and inland testing sites; although observations from other six surface sites in the domain are included as model input. Both wind speed and temperature profiles obtained by CALMET model using WRF output as meteorological input (no matter with/without surface measurements as additional input) and PBL depths are quite similar to the rawinsonde data, and better than WRF results. As a consequence, PBL wind speed and temperature modeled by CALMET are quite in agreement with estimated from rawinsonde observations, showing the capability of CALMET model to provide a reasonable upper-air meteorological input to CALPUFF dispersion model.

About plume dispersion testing, statistical comparison of the CALPUFF model results using different configurations for the simulation of a large smokestack emission shows that CALMET meteorological output based in a regional numerical WRF meteorological simulation vs. measurements dataset (both surface and upper air data) provides better glc results; especially, because of the limited upper air measurements available. Additionally, a more realistic smokestack (which is divided in four independent liners) provides a more realistic glc than a virtual one liner-chimney.

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