

# MAKING THE RIGHT CHOICE: TRADE-OFFS AMONG OPERATIONAL ISSUES AND MODELLING CONSTRAINTS. A CASE STUDY FOR A CEMENT PLANT LOCATED IN A COMPLEX TERRAIN DOMAIN (CALPUFF VS. ADMS)

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## Abstract:

This work is addressing the decision making process involved in the selection of the most suited air quality model to assess the impact of a cement plant located within a complex terrain domain in Northern East of Italy.

The overall objective is the description and analysis of operational issues arising from the case study which are among others: complexity of problem setting, assumptions and range of model applicability (pollutant types, spatial and temporal scales, orography description, wind calm treatment) and the input data availability. The use of a specific model and its setting up is always a trade off between consistency and accuracy of results. Two air quality models (CALPUFF vs ADMS-Urban) were used to simulate emissions from the kiln of a cement plant over a complex orography domain (6 Km x 6 Km). Both models were run under different configurations and sensitivity analysis of results was performed. On strict terms this 'field testing' was not a comparison of model performances but rather a cross-check of air quality impacts calculated by different modelling approaches. Hence a key issue was to evaluate at which point the differences between the model outputs make one model inadequate for evaluating impacts. Modelling exercise showed a discrete agreement when comparing long term averages but a strong contrast in short term outputs (high hourly percentiles).

Analysis showed that a crucial choice in determining the differences of CALPUFF outputs was the alternative use of continuous parameterisation of the turbulence properties within the atmospheric surface layer as computed by the similarity approach or by the discrete characterization through the Pasquill-Gifford dispersion coefficients; the comparison of CALPUFF vs. ADMS showed a significant contrast in modelling outputs due to the different computational treatment of the similarity approach.

Short term outputs are crucial for a regulatory point of view because they imply different compliance to air quality standards. The use of multiple models of varying complexities applied to the same case study allows useful insights into how sensitive results are to the different computational choices and how much trust should be put in the results from anyone model. This also has important implications for interpretation of model results by final users (i.e. stakeholders, policy makers).

**Key words:** cement plant, NOx emissions, ADMS, CALPUFF, sensitivity analysis, trade-offs, decision making process, model output comparison, micrometeorological input scenarios.

## INTRODUCTION: FRAMING THE ENVIRONMENTAL CONTEXT

The cement plant under study is a medium-size facility consisting of one dry-process rotary kiln with a 5-stage cyclone suspension preheater and a precalciner built into the riser duct is using scrap tires as alternative fuel. A quenching system, an electrostatic precipitator and a fabric filter system is adopted for the pollutant abatement of flue gas before the final emission into the atmosphere. The plant is located by the embankment of a major river near a residential area of a small village and close to a small mixed commercial-industrial area; also in the vicinity of the plant there are crops, a small fish farm and some natural environments of interests. The whole area is characterized by a complex terrain domain (a valley with significant altimetric variations) with diurnal thermally driven flows (mountain-valley winds, slope winds) and associated specific anemological features affecting pollutants dispersion such as stagnation (where atmospheric flows decrease or stop in speed), recirculation (polluted air initially carried away from the source is later returning back) and ventilation (stagnant air is replaced or diluted by fresh air) (Allwine and Whiteman, 1994).

## The objective

The main goal of the present study was to address the different issues involved in the selection of the 'most appropriate' air quality model to assess the *local impacts* of the cement plant in the above given computational domain. In strict terms this is not a model comparison from a theoretical point of view but a description of the difficulties, uncertainties and trade-offs that a practitioner is facing in order to assure consistency and accuracy of modelling results. In other terms this investigation is a sort of 'quality assurance' of the different model outputs by the systematic comparison and evaluation of results over different simulation assumptions. Finally, from a stakeholder point of view, all these issues have also much relevant implications for the interpretation of results by final users such as policy makers, local authorities and concerned residential population.

## CALPUFF VS. ADMS

ADMS-Urban v.2.2 (CERC, 2005) uses a boundary layer structure parameterisation based on the Monin-Obukhov length (LMO), and the boundary layer height (H). Distinctive modelling features can be summarised as follows: concentration distributions are Gaussian in stable and neutral conditions, but the vertical distributions is non-Gaussian in convective conditions to take account of the skewed structure of the vertical component of the turbulence; a meteorological pre-processor (Hunt *et al.*, 1981; 1988; Carruthers *et al.*, 1988) calculates the required boundary layer parameters from a variety of input data: e.g. wind speed, day time cloud cover or wind speed, surface heat flux and boundary layer height.

CALPUFF v.5.7 (Scire *et al.*, 2000; 2001) is a non-steady-state meteorological and air quality modelling system adopted by the U.S. Environmental Protection Agency (EPA, 2005) in its Guideline on Air Quality Models as the preferred model for assessing long range transport of pollutants *and on a case-by-case basis for certain specific near-field applications involving complex meteorological conditions*. Main components of the modelling system are CALMET (diagnostic 3D meteorological model), CALPUFF (air quality dispersion model), and CALPOST (post-processing of results).

In spatial terms a comparison of ADMS vs. CALPUFF outputs implies a short- against a medium-range dispersion model which is a clear violation of the assumptions regarding the applicability of each one model. But on the other hand an alternative use of ADMS vs. CALPUFF was a necessary operational trade-off in order to encompass model uncertainties associated with the complex computational domain as shortly described in the introduction (i.e. wind calms and complex orography). As will be shown later, wind calms in the modelling domain amount on annual average up to 14% of the recorded data by the meteorological surface station hereafter called Quero. This fact was clearly deploying for the use of a model fully capable of dealing with low winds: i.e. CALPUFF better than ADMS. On the other hand, considering the objective of *local* impact assessment, the use of ADMS can also be justified because of the need to evaluate impacts in the near-field and from an operational point of view because of the less input requirements. Hence the need for handling trade-offs among operational issues and modelling constraints for the problem setting and the final evaluation. To encompass shortcomings of both models under study, ADMS and CALPUFF were run under different configurations as described in Table 2 and detailed sensitivity analysis of results was performed as reported in Table 3.

### THE EMISSION SOURCE, THE POLLUTANT AND THE SIMULATION PERIOD

Table 1 contains the relevant descriptive parameters of the stack emitting pollutants from the rotary kiln of the cement plant. NOx dispersion was modelled for the year 2008 using monthly time-varying emission factors. In order to allow a more realistic comparison of results across model outputs, NOx (with no information about the ratio NO/NO2) was treated as a non-reactive pollutant with no deposition rate at the ground level.

Table 1. Descriptive parameters of the emission source and the modelled pollutant.

Parameters	Unit of measure	Stack from rotary kiln
Stack height	m	62
Stack exit diameter	m	4
Flue gas average temperature	°C	159
Flue gas average emission rate	Nm <sup>3</sup> h <sup>-1</sup>	535316
Flue gas average speed	ms <sup>-1</sup>	11.8
NOx average flow emission rate	gs <sup>-1</sup>	38.2

Modelling outputs were discussed in terms of C/E [ $\mu\text{s m}^{-3}$ ]: i.e. pollutant concentration C [ $\mu\text{g m}^{-3}$ ] over flow emission rate E [ $\text{g s}^{-1}$ ] as defined by the following simple equation (1) :

$$C / E = \left[ \frac{\mu\text{g}}{\text{m}^3} \Big/ \frac{\text{g}}{\text{s}} \right] = [\mu\text{s} \cdot \text{m}^{-3}] \quad (1)$$

### THE MODELLING DOMAIN, THE METEOROLOGICAL INPUTS AND THE MODEL CONFIGURATIONS

The computational domain for the modelling runs was defined as a square centred over the cement plant stack with a side of 6 km and a mesh size of 60 m for a total of 10.000 computational sampling grid points. Given the substantial diversity of the possible meteorological schemes serving as input for ADMS vs. CALPUFF, a discrete number of micro-meteorological input scenarios were defined as reported in Table 2.

The hereafter called AMDS(1) run used a single surface station Quero, located about 10 km North from the cement plant with recorded wind at 5 m height, nested into the computational domain. This station was considered as the most representative among three other possible alternatives for the area under study. A meteorological pre-processor FLOWSTAR fully integrated into the ADMS suite performed the computational flow over the complex terrain (Carruthers *et al.*, 1988).

The hereafter called CALPUFF(1) run used CALMET model to interpolate meteorological data from 10 surface stations (one of which is the same station of Quero used by ADMS(1) and 4 are synoptic) and 3 radio sounding stations in a 9 km x 8 km domain with a 250 m resolution grid.

In between of these two, a number of 'blend runs' were defined using different meteorological input scenarios, hereafter called AMDS(2) and CALPUFF(2) to CALPUFF(6), with the aim to test sensitivity of results in function of contrasting model parameterisations.

ADMS(2), CALPUFF(2) and CALPUFF(3) were all used with the same meteorological input: i.e. an extraction of micrometeorological variables as computed by the 250 m resolution CALMET grid at the stack point.

CALPUFF(2) used the similarity approach whilst CALPUFF(3) relied on the discrete approach defined by the Pasquill-Gifford dispersion coefficients. CALPUFF(4) and CALPUFF(5) both used the same classical meteorological parameters recorded by the single surface station Quero and the same micrometeorological parameters from a 1 km resolution CALMET grid but they differ from each other for the alternative description of atmospheric dispersion conditions (Pasquill-Gifford vs. similarity). For a short summary of all model runs refer to Table 2.

Figure 1 compares the wind rose and the wind class frequency distribution monitored by the surface station Quero, a few km outside the modelling domain (upper left and lower left), with the analogous data interpolated by CALMET within the modelling domain in the position level of the cement plant stack (upper right and lower right).

Data showed the same substantial patterns for both positions with most frequent winds blowing from the North West and wind calms (defined as average wind speed < 0.5 ms<sup>-1</sup>) within the range 5-14% of recorded data.

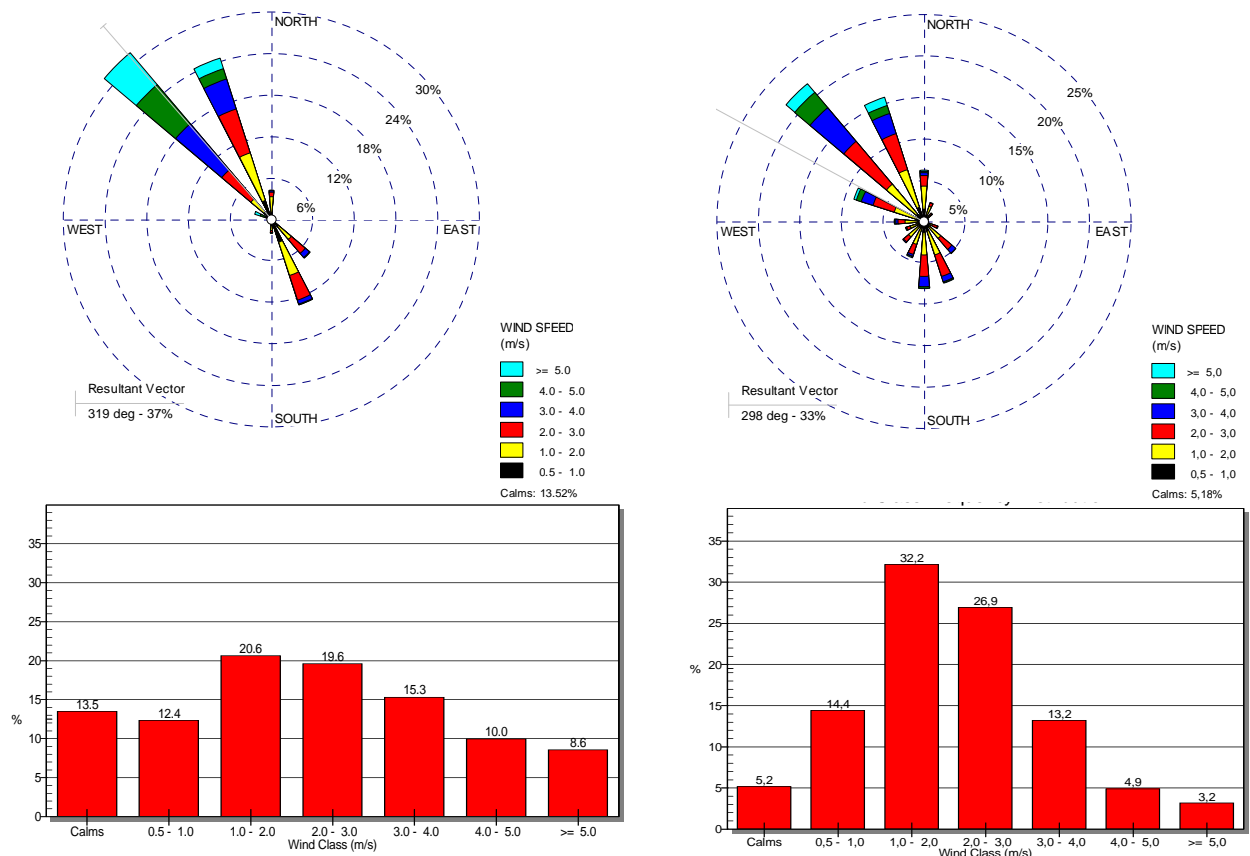


Figure 1. Wind rose and wind class frequency distribution (year 2008) respectively recorded by the meteorological surface station Quero, located about 10 km North from the cement plant with the anemometer at 5 m height (upper and lower left) and calculated by CALMET model in the position level of the cement plant stack point at 10 m height (upper and lower right); calm conditions were defined by hourly average wind speed  $< 0.5 \text{ ms}^{-1}$ .

Table 2. Short definition of the modelling configurations, micro-meteorological input scenarios and the most relevant parameters used for the different computational runs.

Model configurations	Micro-meteorological input scenarios	Relevant dispersion parametrisation
ADMS (1)	single surface station with recorded wind at 5 m height and ADMS meteorological pre-processor interpolation at 10 m height	Monin-Obukhov length (LMO) and boundary layer height (H) as computed by ADMS
ADMS (2)	1D extraction of micrometeorological variables from CALMET 3D field – 250 m resolution grid at stack point, layer 10 m	Monin-Obukhov length (LMO) and boundary layer height (H) as computed by CALMET
CALPUFF (1)	CALMET 3D field - 250 m resolution grid	Monin-Obukhov length (LMO) and boundary layer height (H) as computed by CALMET
CALPUFF (2)	1D extraction of micrometeorological variables from CALMET 3D field – 250 m resolution grid at stack point, layer 10 m	Monin-Obukhov length (LMO) and boundary layer height (H) as computed by CALMET
CALPUFF (3)	1D extraction of micrometeorological variables from CALMET 3D field – 250 m resolution grid at stack point, layer 10 m	Pasquill-Gifford (PG) (rural areas) and McElroy-Pooler (MP) dispersion coefficients (urban areas)
CALPUFF (4)	surface station with recorded wind at 5 m height + 1D extraction of micrometeorological variables from CALMET 3D field – 1 km resolution grid at the surface station, layer 10 m	Monin-Obukhov length (LMO) and boundary layer height (H) as computed by CALMET
CALPUFF (5)	single surface station with recorded wind at 5 m height + Stability Classes from Calmet 3D – 1 km resolution grid at surface station, layer 10 m	Pasquill-Gifford (PG) (rural areas) and McElroy-Pooler (MP) dispersion coefficients (urban areas)

## RESULTS AND DISCUSSION

Table 3 reports the outputs and the most relevant micro-meteorological parameters of the above defined modelling runs. Maximum C/E values (high hourly percentiles P100 and P98, respectively the 100° percentile and the 98° percentile) always occurred, as it is typical for elevated point sources, during convective conditions of the boundary layer (as showed by the

reciprocal of Monin-Obukhov Length always less than zero). Extreme C/E values were reached for very low wind or calm conditions, which are normally reported as a low accuracy condition for a typical Gaussian model (in this sense much more affecting ADMS rather than CALPUFF).

Concerning C/E short term outputs (hourly averages), the most contrasting values were accounted for the 100° percentile (P100) referring to ADMS(1) vs. CALPUFF(1) comparison, with an estimate of about 17 times larger for the second model configuration; for the 98° percentile (P98), as shown by CALPUFF(3) vs. ADMS(2), the difference was about 12 times larger for the latter. Regarding C/E long term outputs (AVG - annual average), the most contrasting values are from the comparison of CALPUFF(3) vs. ADMS(2) for which the difference was up to 50 times larger for the second model configuration. As evident by Table 3 all these 'inconsistencies' were a direct consequence of the very different atmospheric boundary layer description and the pollutant dispersion parameterization. Above mentioned cases were at the 'extreme ends' of our model comparison exercise and all other cases were somewhat placed in between of them.

Beside this, many other aspects of interest are evident by examining data reported in Table 3:

- ADMS(1) vs. ADMS (2): ADMS experienced a very different output in terms of both P100 and P98 (the difference is obviously less evident for the annual average); the maximum C/E value (P100) increased dramatically from ADMS(1) to ADMS(2) showing how the model was very sensitive to alternative meteorological inputs;
- CALPUFF(1) vs. CALPUFF(2) vs. CALPUFF(4) on one side and CALPUFF(3) vs. CALPUFF(5) on the other: CALPUFF resulted not so sensitive to 3D vs. 1D dimensioning of the meteorological inputs (i.e. single surface station or a 3D field) yet it was much more sensitive to the dispersion coefficient parametrizations; the use of Pasquill-Gifford parameters leads to 'diluted' values of a factor of 10 both for high percentiles (P100, P98) and annual average (AVG);
- ADMS(1) vs. CALPUFF(3) showed that the second model converged upon the first with the use of Pasquill-Gifford parameters; on the contrary, ADMS(2) vs. CALPUFF(1) experienced how the first model 'forced' into the use of the micrometeorological parameters as computed by CALMET was in good agreement with the 'extreme' C/E outputs of the second.

Table 3 Modelling configurations, spatial maximum for C/E outputs with reference to 100°-, 98°-percentile (P100, P98) and annual average (AVG) for year 2008, micro-meteorological parameters (U = wind speed, PHI = wind direction, 1/LMO = reciprocal of Monin-Obukhov Length, H = boundary layer depth, Z0 = roughness length), distance and azimuth from stack, date of occurrence for each event.

Modelling configurations	Statistics	C/E spatial max [ $\mu\text{s m}^{-3}$ ]	U [ $\text{ms}^{-1}$ ]	PHI [ $^{\circ}\text{N}$ ]	1/LMO [ $\text{m}^{-1}$ ]	H [m]	H/LM	Distance from stack [m]	Azimuth from stack [degrees]	Date of event [dd/mm hh]
ADMS (1)	P100	2.6	0.59	309	-0.31	1348	-422	231	130	22/09 13
	P98	1.8	1.72	123	-0.06	2000	-124	504	334	23/04 11
	AVG	0.2	-	-	-	-	-	782	138	-
ADMS (2)	P100	30.2	0.75	317	-9.34	966	-9022	53	206	10/09 13
	P98	15.8	0.75	301	-6.53	1453	-9488	93	56	01/08 12
	AVG	0.5	-	-	-	-	-	149	352	-
CALPUFF (1)	P100	44.1	0.39	350	-3.09	497	-1538	86	315	17/05 08
	P98	8.8	0.37	325	-0.45	1365	-608	240	180	23/09 16
	AVG	0.1	-	-	-	-	-	366	351	-
CALPUFF (2)	P100	33.9	0.14	224	-1.67	279	-465	216	56	18/11 10
	P98	11.4	0.42	320	-2.50	730	-1825	247	166	14/01 14
	AVG	0.2	-	-	-	-	-	247	346	-
CALPUFF (3)	P100	3.5	0.33	355	-10.00	1257	-12573	494	166	05/06 15
	P98	1.3	0.21	25	-10.00	685	-6849	190	162	18/10 11
	AVG	0.01	-	-	-	-	-	119	180	-
CALPUFF (4)	P100	30.0	0.19	122	-1.25	300	-375	216	304	21/09 10
	P98	11.7	0.50	131	-0.27	1717	-464	255	315	30/08 18
	AVG	0.3	-	-	-	-	-	268	333	-
CALPUFF (5)	P100	5.6	0.12	117	-10.00	1238	-12378	135	297	19/04 13
	P98	2.2	0.41	67	-1.43	1967	-2809	180	270	27/06 15
	AVG	0.02	-	-	-	-	-	60	271	-

Figure 2 depicts the average hourly profiles of H/LMO (boundary layer depth (H) times the reciprocal of Monin-Obukhov Length) used by the five modelling configurations with the similarity theory approach: i.e. ADMS(1), CALPUFF(1),(2),(4); data comparison showed the substantially different description of the boundary layer conditions in function of the alternative model computational approaches and their relative micro-meteorological variables used as input.

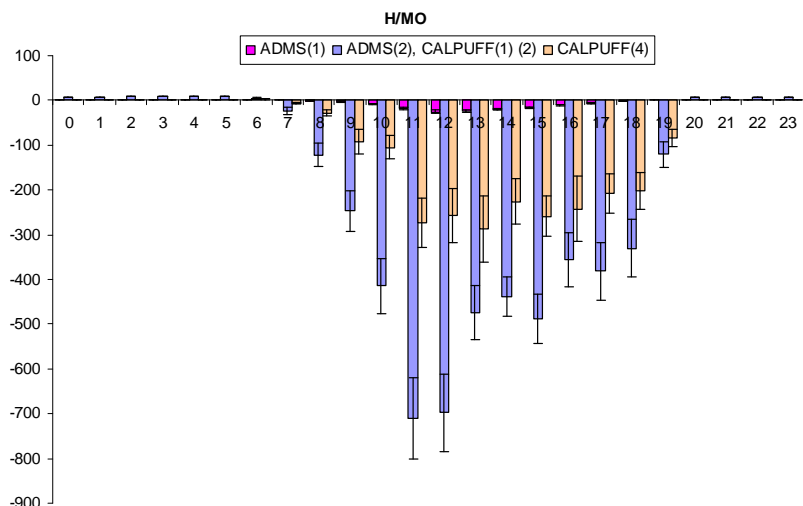


Figure 2. H/LMO = boundary layer depth (H) times the reciprocal of the Monin-Obukhov Length (1/LMO): comparison of the average hourly profiles among the different modelling configurations using the similarity theory approach; error bars are indicating the standard error of the mean.

Finally, although both models (ADMS and CALPUFF) were much sensitive to alternative meteorological inputs and relative dispersion parametrizations, some computational configurations were in good agreement within a factor of two in terms of C/E outputs. An important final caveat was identified: sensitivity analysis is a key issue in the ‘tailoring’ of the ‘optimal model configuration’ for a given computational domain. One possible solution to overcome these model limitations was the method we have here briefly envisaged: i.e. the cross-checking of one model results against the other (by possibly considering at least one more ‘advanced model’ for some specific features but with the same overall finalities).

### Lessons learned

A number of issues arise when selecting and applying a model or a set of models for environmental impact assessment and related regulatory activities which are including: the selection of a model from multiple possibilities, the level of expertise, the model assumptions and its range of applicability, the cost and the availability of the model, the adaptability of the model; and the data availability. All models come with specific assumptions and application limitations and understanding these issues is critical because they define a specific application range for a given model and computational domain.

Model practitioners should be fully aware of the boundary within which a model can be properly used and they should refrain or refuse to use it when a major assumption within the model is directly violated or is close to being violated. A possible way forward in such cases it to set up experiments that always foreseen the parallel use of two or more models possibly run in a series of standard configurations.

Effective decision making will require providing policy makers, stakeholders and local concerned population with more than a single pollutant distribution for a model output but with a full insight of the degree of uncertainty of the same.

Models are tools providing input into decisions rather than truth-generating machines. Direct implications of this finding are clear: although policy makers may desire a clear and unique answer, models are best considered to be just one of the multiple sources of input into the complex regulatory process. The challenge then is to properly communicate model results and improve the understanding of policy makers about the capabilities and limitations of the model results.

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