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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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WHY USE ONE MODEL?

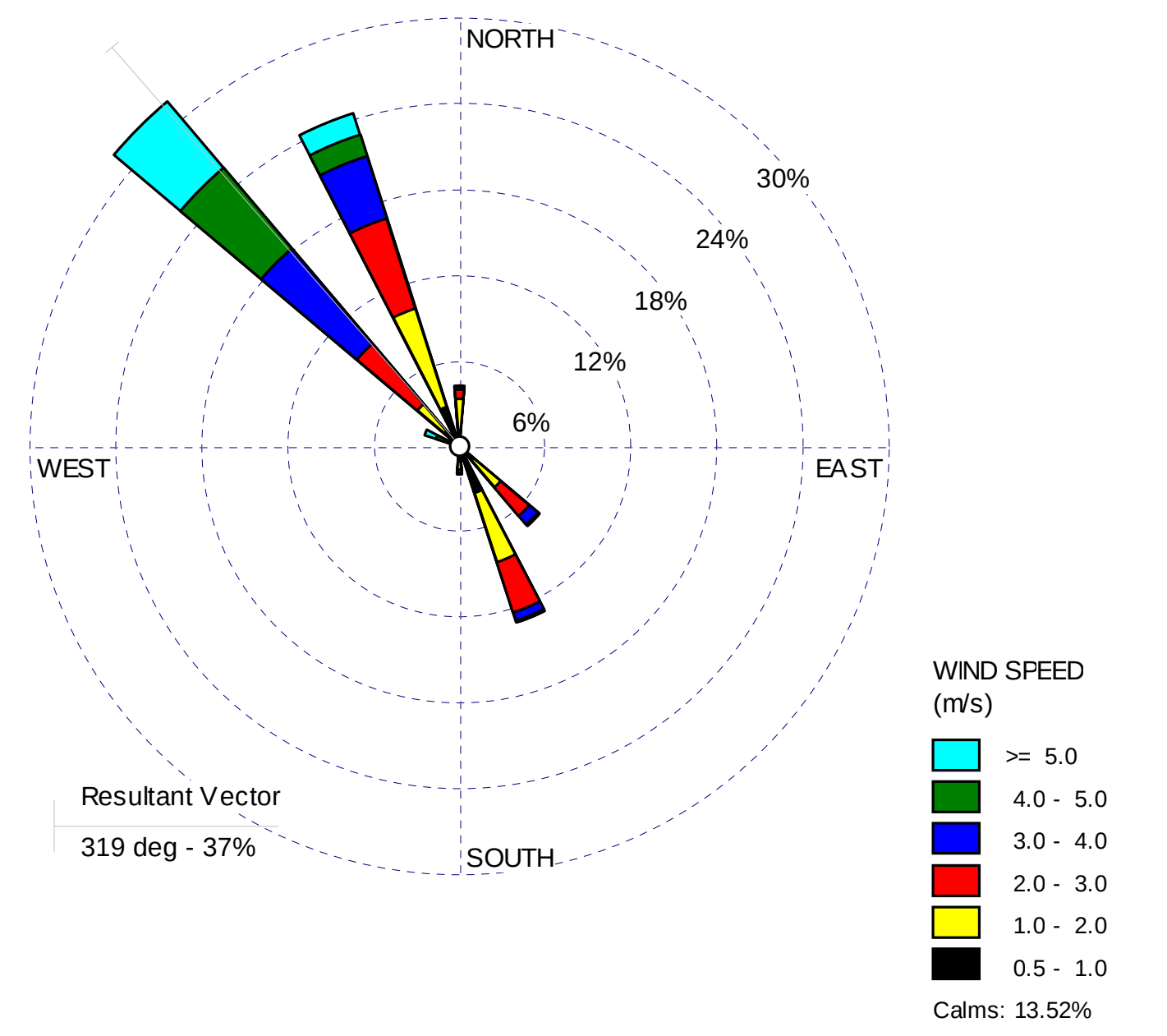
This question laid on the table until we decided to go through the environmental assessment of the facility under study by an extensive comparison of different modelling outputs.

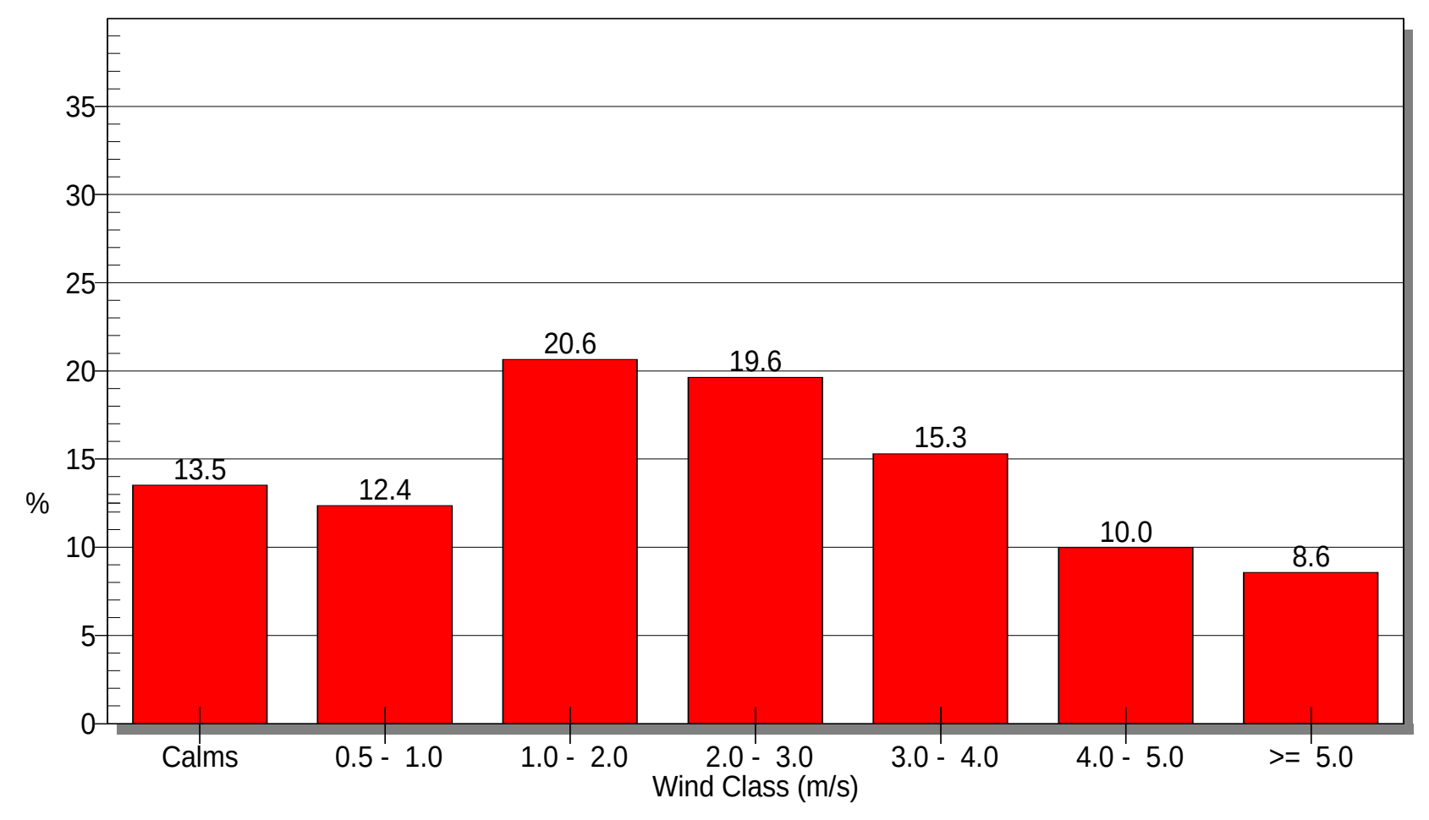
THE OBJECTIVE OF THE STUDY

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 local impacts of a cement plant in a complex domain. Therefore, this study 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 always 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. All these issues also have much relevant implications for the interpretation of results by final users and stakeholders such as policy makers, local authorities and concerned residential population.

FRAMING THE ENVIRONMENTAL CONTEXT

The cement plant under study, a medium-size facility consisting of one dry-process rotary kiln with a 5-stage cyclone suspension preheather 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 in Northern East of Italy 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 diluted by fresh air)





Wind rose and wind class frequency distribution (year 2008) recorded by the meteorological surface station Quero, located about 10 km North form the cement plant with the anemometer at 5 m height.
Calm conditions were defined by hourly average wind speed < 0.5 ms^{-1}.

CALPUFF vs ADMS: BUT ARE YOU SURE ABOUT THAT?

CALPUFF is adopted by the U.S. Environmental Protection Agency 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. An alternative use of ADMS (v.2.2) vs. CALPUFF (v.5.7) was a necessary operational trade-off in order to encompass model uncertainties associated with the above given computational domain (i.e. wind calms and complex orography). Wind calms in the modelling domain amount on annual average up to 14% as recorded by the meteorological surface station 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 a strict 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 the shortcomings of both models under study, ADMS and CALPUFF were run under different configurations as described in Table 1 and detailed sensitivity analysis of outputs is reported in Table 3 and Figure 1.

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 + Stabiliy 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)

Table 1 - Modelling configurations, micro-meteorological input scenarios and the most relevant parameters used for the different computational runs.

THE SOURCE, THE POLLUTANT, THE SIMULATION PERIOD AND THE DOMAIN

Table 2 reports relevant descriptive parameters of the stack emitting pollutants from the rotary kiln. NOx dispersion was modelled for year 2008 using monthly time-varying emission factors. In order to allow a more realistic comparison of results across model outputs, NOx (with no additional information about the ratio NO/NO2) was treated as a non-reactive pollutant with no deposition rate at the ground level.

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^{3}h^{-1}	535316
Flue gas average speed	ms^{-1}	11.8
NOx average flow emission rate	gs^{-1}	38.2

Table 2 - Descriptive parameters of the emission source and the modelled pollutant.

Modelling outputs are discussed in terms of C/E [μs m^{-3}]: i.e. pollutant concentration C [μg m^{-3}] over flow emission rate E [g s^{-1}] as defined by the following simple equation:

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

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 sampling grid points.

RESULTS AND DISCUSSION

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 (Table 1).
Table 2 reports outputs and most relevant micro-meteorological parameters of these modelling runs.

Modelling configurations	Statistics	C/E spatial max [μs m^{-3}]	U [ms^{-1}]	PHI [°N]	1/LMO [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
	P99.8	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
	P99.8	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
	P99.8	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
	P99.8	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
	P99.8	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
	P99.8	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
	P99.8	2.2	0.41	67	-1.43	1967	-2809	180	270	27/06 15
	AVG	0.02	-	-	-	-	-	60	271	-

Table 2 - Modelling configurations, spatial maximum for C/E outputs with reference to 100°-, 99.8°-perc entile (P100, P99.8) 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), distance and azimuth from stack, date of occurrence for each event.

Maximum C/E values (high hourly percentiles P100 and P99.8, respectively the 100° and the 99.8° percentiles) always occurred, as it is typical for elevated point sources, during convective conditions of the boundary layer (as shown by the reciprocal of Monin-Obukhov Length always less than zero). Extreme C/E values were reached for very low or calm winds, which are normally reported as a low accuracy conditions for a typical Gaussian model (in this sense much more affecting ADMS rather than CALPUFF).

For C/E short terms 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 99.8° percentile (P99.8), as shown by CALPUFF(3) vs. ADMS(2), the difference was about 12 times larger for the latter.

For C/E long term outputs (AVG - annual average), the most contrasting values were reported by 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 2 all these 'inconsistencies' were a direct consequence of the very different atmospheric boundary layer description and pollutant dispersion parameterisation. Above mentioned cases were at the 'extreme ends' of our model comparison exercise and all others were somewhat placed in between of them.

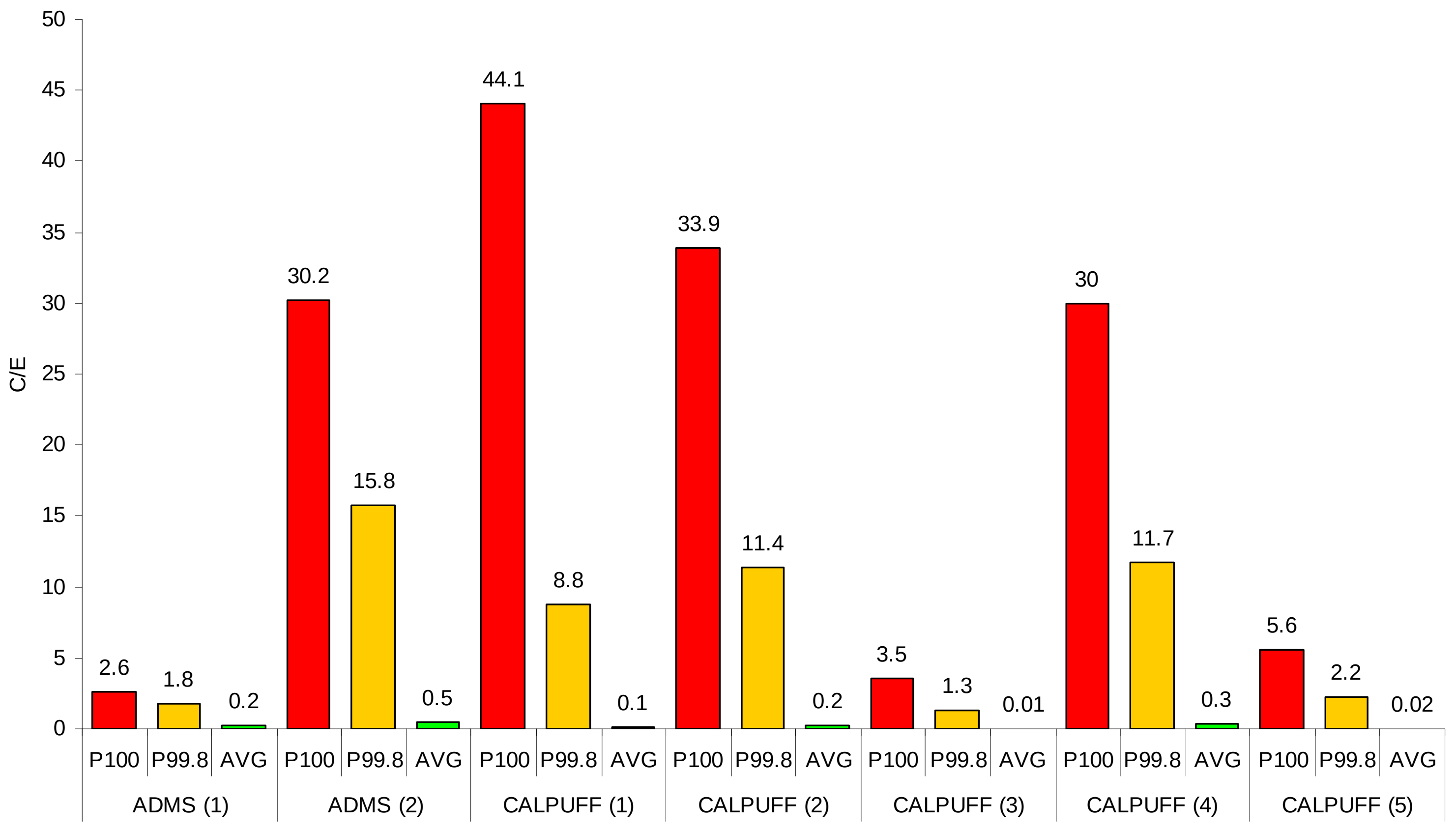


Figure 1 – Comparison of modelling outputs: P99.8 (99.8° percentile), P100 (100° percentile) and AVG (ann ual average) for the different computational runs as reported in Table 1.

Many other aspects of interest are evident by looking at Figure 1:

- ADMS(1) vs. ADMS (2): ADMS experienced a very different output in terms of both P100 and P99.8 (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 extremely 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 parameterisations; the use of Pasquill-Gifford parameters leads to 'diluted' values of a factor of 10 both for high percentiles (P100, P99.8) 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.

FINAL CONCLUSIONS AND LESSONS LEARNED

Although both models (ADMS and CALPUFF) were much sensitive to alternative meteorological inputs and relative dispersion parameterisations, 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 'tailoring' the 'optimal model configuration' for a given computational domain.
One possible solution to overcome single model limitations was the method we have here briefly envisaged: i.e. the cross-checking of one model results against the other.
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.