ADMS 6 Complex Terrain Validation
Westvaco Corporation

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1 Introduction

The Westvaco Corporation's pulp and paper mill[1] in rural Luke, Maryland is located in a complex terrain setting in the Potomac River valley [2]. A single 190 m buoyant source was modelled for this evaluation. There were 11 SO_2 monitors surrounding the facility, with eight monitors well above stack top on the high terrain east and south of the mill at a distance of 800-1500 m (**Figure 1**).

Hourly meteorological data (wind, temperature, and turbulence) were collected between December 1980 and November 1981 at three instrumented towers: the 100 m Beryl tower in the river valley about 400 m southwest of the facility, the 30 m Luke Hill tower on a 18 ridge 900 m north-northwest of the facility, and the 100 m Met tower located 900 m east-south-east of the facility on a ridge across the river.

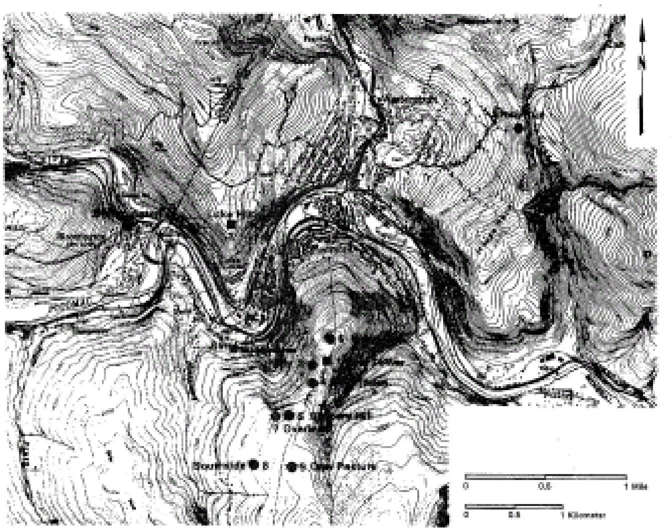

Figure 1 − Locations of SO_2 monitors and meteorological towers in the vicinity of the Westvaco Luke Mill.

The input data for the ADMS runs were taken from the AERMOD files downloaded from the United States Environmental Protection Agency website [3]. These data included the observed concentrations that have been used for comparison with the ADMS modelled concentrations.

This document compares the results of ADMS 5.2.0.0 (hereafter referred to as ADMS 5.2) with those of ADMS 6.0.0.1 (hereafter referred to as ADMS 6.0).

Section 2 describes the input data used for the model. The results are presented in Section 3 and

[1] Note that the study description and **Figure 1** have been taken directly from the document [1].

discussed in Section 4.

2 Input data

2.1 Study area

The site was located at 39.47°N. The surface roughness used varied between 0.6 and 1.3 m depending on the time of the year.

Terrain data included in the modelling covered a 6 km x 7 km area (as shown in **Figure 2**). Terrain data points were located every 160 m within this area.

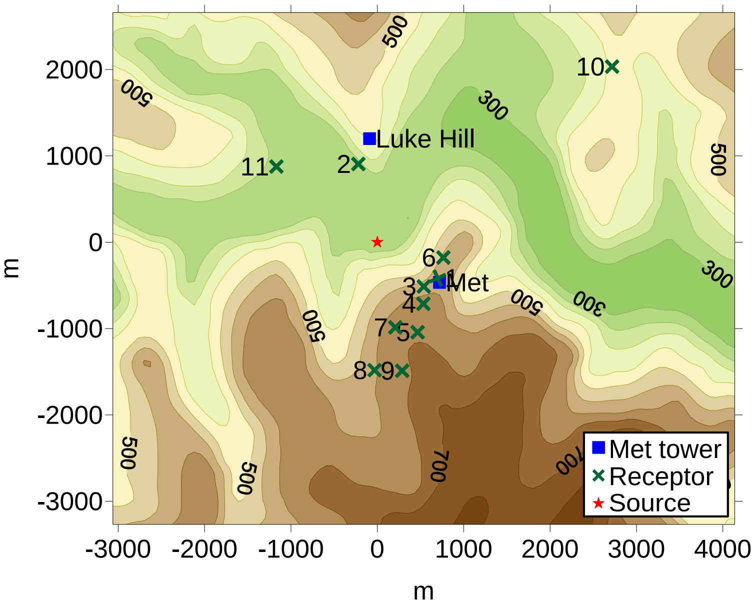

Figure 2 − Modelled terrain area around the Westvaco Corporation.

2.2 Source parameters

The source parameters are summarised in **Table 1**. Each of these sources is modelled separately for different hours. The exit velocity varied from 7.2 to 35.7 m/s, the exit temperature from 92.9 to 129.9°C and the emission rate varied from 42.8 g/s to 635 g/s.

Source name	Pollutant	Location	h (m)	V (m/s)	T (°C)	D (m)	Q rate (g/s)
Stack	SO_2	(0,0)	189.7	varied	varied	3.36	varied

Table 1 − Source input parameters. h is the stack height, V the exit velocity, T the exit temperature, D the diameter and Q the emission rate.

2.3 Receptors

The receptor network consisted of 11 monitors located as shown in **Figure 2**.

2.4 Meteorological data

The experiment used 1 year of hourly sequential data from the 1 December 1980 to 30 November 1981.

Table 2 gives the detail of the modelled meteorological conditions. The criteria for the stability categories are as follows, where H is the boundary layer height and L_{MO} is the Monin-Obukhov length, as calculated by the model's meteorological processor:

Stable: $H/L_{MO} > 1$

Neutral: $-0.3 \leq H/L_{MO} \leq 1$

Convective: $H/L_{MO} < -0.3$

Conditions		ADMS 5.2	ADMS 6.0
Hours modelled	Stable conditions	4292 (61%)	4288 (61%)
	Neutral conditions	428 (6%)	387 (6%)
	Unstable conditions	2331 (33%)	2351 (33%)
	Total	*7051 (100%)*	*7026 (100%)*
Hours not modelled	Calm conditions	0	0
	Wind speed at 10 m < 0.75 m/s	1575	1600
	Inadequate data	134	134
	Total	*1709*	*1734*

Table 2 – Meteorological conditions. Percentage values are computed with respect to the total number of modelled hours.

The wind speeds varied from 0.3 to 14.7 m/s and the wind direction was either westerly or easterly for the majority of the study duration (see the wind rose shown in **Figure 3**). The height of the recorded wind is 30 m. The ambient temperature varied from -19.7 to 29.5°C.

The model has used a profile of wind speeds and temperature with readings at 30, 50 and 100 m; it was based on recorded wind speeds at the Luke Hill (30 m) and 'Met' (50 and 100 m) instrumented towers (see location on **Figure 2**). A correction factor is applied to wind speed data at the met. sites to account for the difference in location; this factor ranges from 60 % at 10 m to 33 % at 100 m.

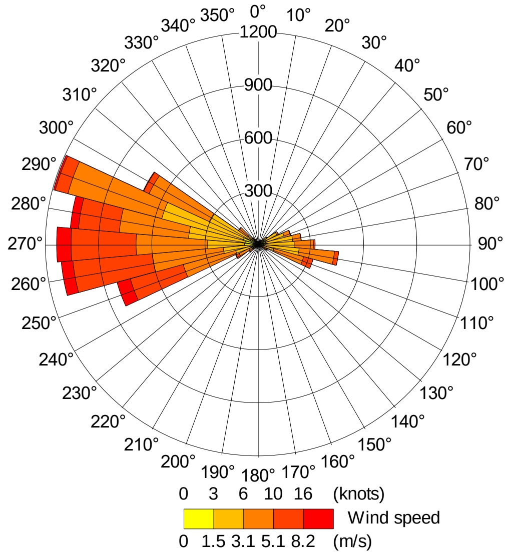

Figure 3 – Wind rose.

3 Results

Scatter plots and quantile-quantile plots of model results against observed data are presented in Section 3.1. The statistical analysis of the data is also provided in Section 3.2. The graphs and statistical analysis have been produced by the Model Evaluation Toolkit v5.2 [5].

3.1 Scatter and quantile-quantile plots

Figure 4 shows the scatter plots and quantile-quantile plots of results for hourly mean concentrations. Note that these quantile-quantile plots are *linear*; care should be exercised when comparing these plots with similar ones presented with *logarithmic* axes.

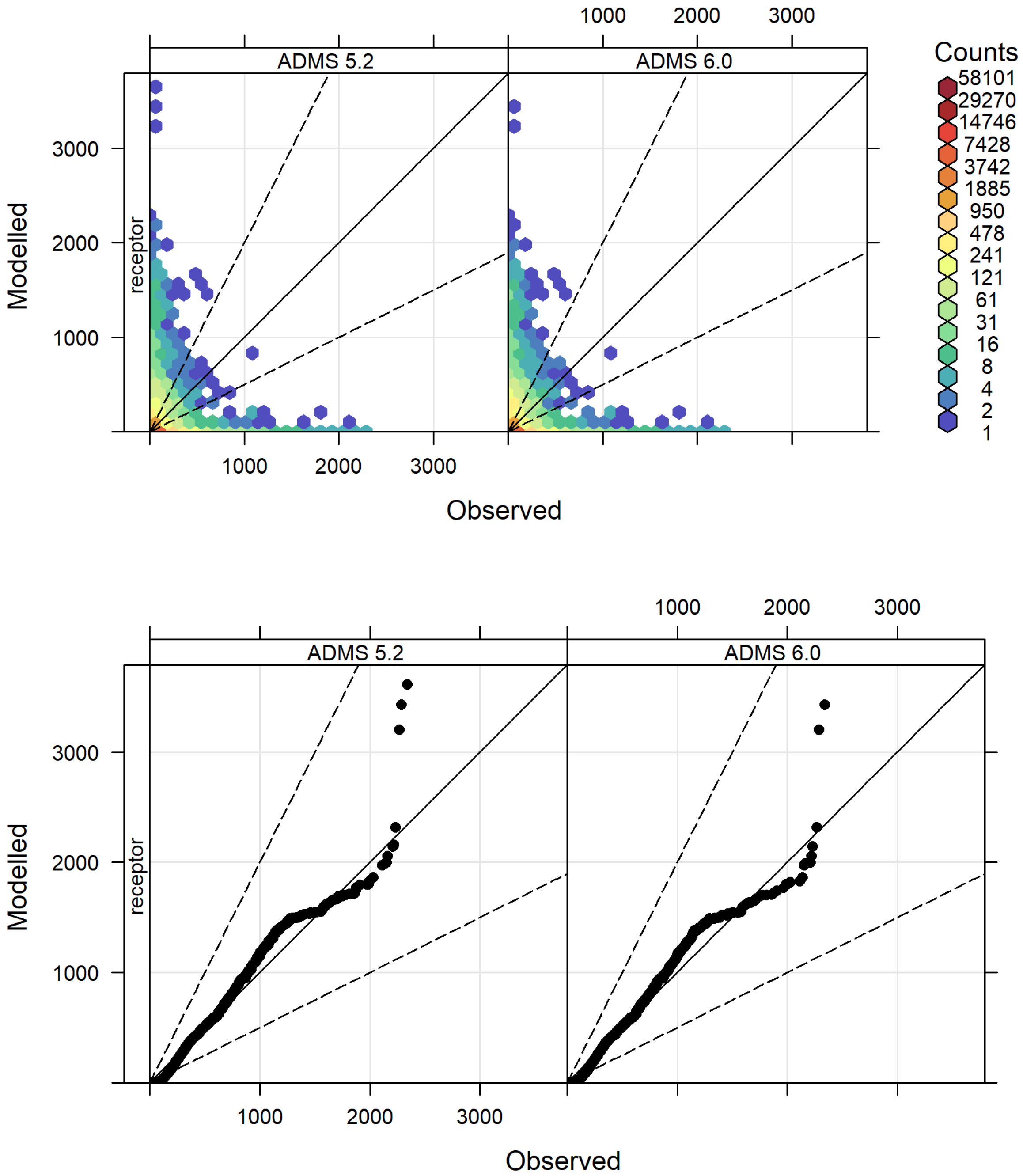

Figure 4 − Scatter plots and quantile-quantile plots of ADMS results against observed data (ug/m³).

3.2 Statistics

Table 3 compares compares the modelled and observed maximum 1-hour, 3-hour and 24-hour average concentrations at the receptor points. **Table 4** compares the corresponding robust highest concentrations, where this statistic is defined by:

$$\text{robust highest concentration} = \chi(n) + (\chi - \chi(n))\ln\left(\frac{3n-1}{2}\right),$$

where n is the number of values used to characterise the upper end of the concentration distribution, χ is the average of the $n-1$ largest values, and $\chi(n)$ is the n^{th} largest value; n is taken to be 26, as in Perry et *al*. [4].

Statistics	Data	Concentrations (ug/m³)											Mean M/O ratio
		P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	
1-hour maximum	Observed	1909	496	1601	2290	2341	2269	2234	2210	1859	468	533	-
	ADMS 5.2	3202	629	3613	1346	1175	3427	947	856	670	173	460	0.93
	ADMS 6.0	3202	629	2142	1234	1175	3427	947	856	670	247	460	0.85
3-hour maximum	Observed	1741	290	1344	1583	1564	1979	1684	1286	1045	409	533	-
	ADMS 5.2	1394	210	1204	524	780	1740	407	467	317	123	271	0.53
	ADMS 6.0	1394	210	865	524	780	1853	407	438	317	190	314	0.53
24-hour maximum	Observed	554	89	369	351	617	346	1164	399	336	94	455	-
	ADMS 5.2	738	44	305	159	133	1345	96	93	158	36	69	0.78
	ADMS 6.0	772	50	337	168	138	1345	97	88	158	50	75	0.81

Table 3 − Observed (O) and modelled (M) maximum concentrations (ug/m³) per receptor point, and the mean ratio of modelled/observed values for each statistic.

Statistics	Data	Robust Highest Concentrations (ug/m³)											Mean M/O ratio
		P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	
1-hour RHC	Observed	2192	490	2055	1893	2588	2511	2434	2286	2341	434	585	-
	ADMS 5.2	2972	372	2229	990	887	2426	780	559	748	219	382	0.64
	ADMS 6.0	2801	443	1846	892	918	2433	783	567	764	251	401	0.64
3-hour RHC	Observed	1602	290	1344	1583	1564	1979	1684	1286	1045	409	533	-
	ADMS 5.2	1437	140	1085	681	549	1876	404	248	373	137	224	0.50
	ADMS 6.0	1431	165	950	641	550	1889	410	244	378	184	235	0.51
24-hour RHC	Observed	503	93	384	379	490	438	600	292	316	93	181	-
	ADMS 5.2	551	28	284	152	91	908	64	43	79	37	73	0.55
	ADMS 6.0	556	32	274	153	93	923	65	42	80	49	68	0.57

Table 4 – Observed (O) and modelled (M) robust highest concentrations (RHC) per receptor point, and the mean ratio of modelled/observed RHC for each statistic (number of points = 26).

4 Discussion

The scatter and quantile-quantile plots (**Figure 4**) show relatively good agreement between modelled and observed concentrations. The scatter plots compare predicted and measured concentrations at a particular location at a particular time, i.e. an (x,t) pairing. The quantile-quantile plots compare the distribution of predicted and measured concentrations during the period having abandoned the (x,t) pairing. Predicting the distribution of concentrations accurately is relevant to calculations for permitting purposes, where the comparison with air quality limits is more important than accurately predicting a time series of concentrations at each location. The latter is a harder task.

The pollutant monitored for this study is SO_2. There are a number of issues with using SO_2 as a tracer, which include:

- The detection limits of monitors are usually of the order of 16 µg/m³, and concentrations below these are set to one-half of the limit. This leads to considerable inaccuracy when modelled concentrations are low.

- SO_2 is released from other sources. If estimates of these background concentrations are not available, then the model will underestimate concentrations, particularly long-term averages.

The issue with missing background pollutant data can be investigated by inspecting monitored concentration values when all sources are downwind of the receptors. When this is done, it is clear that there are significant levels of background SO_2 present during this study. Comparisons between modelled and observed annual average concentrations are not presented in this report due to the issues with monitor detection limits and background data.

The predictions of maximum concentrations and robust highest concentrations presented in **Tables 3** and **4** show good model performance considering the complexity of the domain modelled. The model has a tendency to predict slightly lower maximum concentrations than those observed. However, this apparent underestimate of observed maximum concentrations is a usual feature of a model that has been developed to represent the ensemble mean i.e. a model that neglects turbulent fluctuations.

There has been a slight change in how the Model Evaluation Toolkit calculates the data averaged over multiple hours in the version used to process data for this report, which leads to slight differences between the data for ADMS 5.2 and observed data presented here and in the previous validation document comparing ADMS 5.1 to ADMS 5.2. The data presented in this study (i.e. ADMS 5.2 vs ADMS 6.0) use the same version of the Toolkit and so are consistent with each other.

Consideration of the scatter and quantile-quantile plots shows that the concentrations predicted by ADMS 5.2 and ADMS 6.0 are very similar. The statistics presented in **Tables 3** and **4** show no clear trend, with ADMS 6.0 performing slightly better than ADMS 5.2 in some cases and slightly worse in others in terms of modelled-to-observed-ratio. There has been a change to the meteorological processor, in which the solar elevation angle is calculated at the middle of the hour rather than the end of it, which is having some effect in daylight hours.

5 References

[1] Paine, R.J, Lee, R.F, Brode, R, Wilson, R.B, Cimorelli, A.J., Perry, S.G., Weil, J.C., Venkatram, A, and Peters, W., 1998: *Model Evaluation Results for AERMOD (draft)*. United States Environmental Protection Agency.

[2] Strimaitis, D. G., R. J. Paine, B. A. Egan and R. J. Yamartino, 1987: *EPA Complex Terrain Model Development: Final Report*. Contract No. 68-02-3421, United States Environmental Protection Agency, Research Triangle Park, North Carolina.

[3] United States Environmental Protection Agency website, *Model Evaluation Databases*. https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models

[4] Perry, S. G., Cimorelli, A. J., Paine, R.J., Brode, R.W., Weil, J.C., Venkatram, A., Wilson, R.B., Lee, R.F, & Peters, W.D. 2005: AERMOD: A Dispersion Model for Industrial Source Applications. Part II: Model Performance against 17 Field Study Databases. *J. Appl. Met.* **44**, pp 694-708.

[5] Stidworthy A, Carruthers D, Stocker J, Balis D, Katragkou E, and Kukkonen J, 2013: *MyAir Toolkit for Model Evaluation*. 15th International Conference on Harmonisation, Madrid, Spain, May 2013.