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Dispersion modelling of SO_2 emissions from Stanlow Refinery, Cheshire

Final report

Prepared for
Cheshire West and Chester Council

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CERC

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Contents

1 Summary

Measurement of SO_2 concentrations at Thornton-le-Moors, close to Stanlow Refinery, has revealed exceedences of the air quality objective for 15-minute SO_2 concentrations. CERC was commissioned by Cheshire West and Chester Council to carry out dispersion modelling to determine the likely extent of theses exceedences and hence to assist with defining an Air Quality Management Area.

The modelling was carried out using the ADMS 5 model (version 5.1.2) using meteorological data from the Met Office Hawarden site. The modelling took into account all sources of SO_2 emissions from the Stanlow refinery using emissions data provided by Essar. Time-varying emissions were provided for the most significant sources, with typical emissions provided for the remaining sources.

Modelling was first carried out to calculate SO_2 concentrations and the number of exceedences of the 15-minute average SO_2 concentration of 266 µg/m³ at the locations of the monitoring sites. The ADMS fluctuations option was used to take into account variations in concentration due to short time scale turbulence. Using the fluctuations option, the predicted number of exceedences agreed well with the measured data, with more than 35 exceedences per year predicted at the TLM and TLP sites and fewer than 35 at the ELT site.

Modelling of the whole area for 2013 to 2015 predicts more than 35 exceedences per year throughout Thornton-le-Moors, but not at any other residential locations.

2 Introduction

Measurement of SO_2 concentrations at Thornton-le-Moors, close to Stanlow Refinery, has revealed exceedences of the air quality objective for 15-minute sulphur dioxide (SO_2) concentrations. Where pollutant concentrations are likely to breach air quality standards, a Local Authority is required to declare an Air Quality Management Area (AQMA). CERC was commissioned by Cheshire West and Chester Council to carry out dispersion modelling to determine the likely extent of theses exceedences and hence to assist with defining the extent of an AQMA.

The modelling was carried out using the ADMS 5 dispersion model (version 5.1.2). The model inputs and the results of the dispersion modelling are described in this report.

Section 3 presents the air quality standards with which the modelled results are to be compared. Details of the assessment area, including a description of the site, are given in Section 4, along with background concentrations for the area. Section 5 describes the site layout and emissions. The meteorological data input to the modelling are described in Section 6. Section 7 sets out the results of the dispersion modelling with a discussion of the implications of the results in Section 8. Finally, a description of the ADMS model used in the assessment is given in Appendix A.

3 Air quality standards

UK air quality objectives for SO_2, set for the protection of human health, are summarised in Table 3.1. The year by which each objective is to be achieved is also shown in the table. The objectives are taken from *The Air Quality Strategy for England, Scotland, Wales and Northern Ireland*, July 2007, and are the subject of Statutory Instrument 2000 No. 928, *The Air Quality (England) Regulations 2000*, which came into force on 6th April 2000.

Table 3.1: Air Quality Objectives

	Value ($\mu g/m^3$)	**Description of standard**	**Date to be achieved**
SO_2	350	1 hour average not to be exceeded more than 24 times a year (modelled as 99.73rd percentile)	31-12-2004
	125	24 hour average not to be exceeded more than 3 times per year (modelled as 99.18th percentile)	31-12-2004
	266	15 minute average not to be exceeded more than 35 times per year (modelled as 99.9th percentile)	31-12-2005

The standards are specified in terms of the number of times during a year that a concentration measured over a short period of time is permitted to exceed a specified value. For example, the concentration of SO_2 measured as the average value recorded over a 15-minute period is permitted to exceed the concentration of 266 $\mu g/m^3$ up to 35 times per year. Any more exceedences than this during a one-year period would represent a breach of the objective.

4 Site location and surrounding area

Stanlow Refinery is located close to the banks of the Mersey, east of Ellesmere Port. The villages of Thornton-le-Moors and Elton lie to the south and east of the refinery, respectively. Figure 4.1 shows the location of the site.

Figure 4.1: Site location

4.1 Monitoring data

Concentrations of SO_2 were measured at three monitoring sites close to the refinery. The locations and details of the monitors are shown in Figure 4.2 and Table 4.1.

Figure 4.2: Site map

Table 4.1: Monitoring site details[1]

ID	Location	X	Y	Start	End
TLM	Thornton-le-Moors	344174	374461	27/06/13	12/02/15
TLP	Thornton-le-Moors	344103	374330	17/02/15	Ongoing
ELT	Elton	345642	375522	10/06/15	Ongoing

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[1] Monitoring at TLP and ELT is ongoing; only data measured up to the end of 2015 were considered in this assessment

Table 4.2 shows a summary of the monitoring data for the study period (2013 to 2015); note that as the monitoring periods at each site varied in length, the number of exceedences recorded during the monitoring period are expressed as an equivalent number of exceedences per year for comparison with the air quality standard. These exceedence-per-year values were calculated by assuming the exceedences occurred at the same rate throughout the year (for instance, for the TLP site, data were measured for 87% of the year in 2015; the recorded number of exceedences was multiplied by 1.15 to get an equivalent number of exceedences per year).

The air quality standard for 15-minute average concentrations was breached at both the TLM and TLP monitoring sites but not at the ELT site. Exceedences of the threshold of 350 µg/m³ for hourly average concentrations were recorded at both the TLM and TLP sites but there were fewer than the permitted 24 exceedences per year. No exceedences of the threshold of 125 µg/m³ for 24-hour average concentrations were recorded at any of the monitoring sites during the study period.

Table 4.2: Monitoring data summary

Averaging time	Statistic	Standard	TLM					TLP		ELT	
			2013	2014	2015	Period Total	Period Annualised	2015	Period Annualised	2015	Period Annualised
15-minute average	Exceedences of 266 µg/m³	35	32	89	6	127	79	50	59	2	4
	99.9th percentile (µg/m³)	266	325	356	404	345	345	309	309	136	136
1-hour average	Exceedences of 350 µg/m³	24	1	4	0	5	5	4	5	0	0
	99.73rd percentile (µg/m³)	350	194	232	189	219	233	200	200	107	107
24-hour average	Exceedences of 125 µg/m³	3	0	0	0	0	0	0	0	0	0
	99.18th percentile (µg/m³)	125	59	75	68	75	75	56	56	38	38

4.2 Background concentrations

Concentrations of SO_2 are dominated by local industrial emissions; background concentrations away from industrial sources are low. Measured SO_2 concentrations were obtained from two monitoring sites: the Ellesmere Port OPSIS site to the west of the refinery and Liverpool Speke to the north of the site. To avoid double counting contributions from the refinery, the minimum concentration from the two sites was taken for each hour of the modelling period.

Table 4.3: Background data

	Ellesmere Port	Speke	Combined
Average	3.9	2.5	2.0
Maximum	366.3	109.3	87.1
99.9th percentile	61.7	46.1	29.2

4.3 Surface roughness

A surface roughness length is used in the model to characterise the surrounding area in terms of the effects it will have on wind speed and turbulence, which are key components of the modelling. A surface roughness value of 1 m was used for the modelled area, to take account of the complex nature of the refinery area. A surface roughness value of 0.2 m was used for the Met Office Hawarden site. See Section 6 for information regarding the meteorological data used in the modelling.

5 Modelled stack and emissions data

5.1 Modelled stacks

SO_2 emissions were modelled from thirteen sources on site. The locations of the sources are shown in Figure 4.2 and details of the sources are given in Table 5.1.

Table 5.1: Source details

	X	Y	Height (m)	Diameter (m)
CDU3	343786	374812	75	2.65
CDU4	343951	374892	143	3.71
Secondary Processes	343639	375448	122	4.87
MP Boiler House	344204	375062	60	1.41
Platformer 3	343585	375835	120	4.52
HD Select	343840	375131	40	0.7
Ethyl Benzene Unit	343443	375268	50	1.2
Energy Recovery Plant	343786	376481	50	1.75
CO Boiler	343632	375115	80	4.14
HP Boiler House	344200	375183	155	5.02
Sulphur Recovery Unit	344387	375348	124	1.32
General Flare	344077	375458	122	2.0
Sour Flare	344077	375458	122	1.0

5.2 Emissions data

Typical and worst case emissions data were provided for each source, where available. In addition, 15-minute average temperature, velocity and emission rates were provided for the CO Boiler, HP Boiler House, Sulphur Recovery Unit, the General Flare and Sour Flare. For these sources, hourly average time-varying emissions data were used in the modelling; where data were not available, average values were used.

Table 5.2 gives a summary of the time-varying data emissions data for the CO Boiler, HP Boiler House and Sulphur Recovery Unit.

Table 5.2: Summary of time-varying emissions data

	Temperature (^{o}C)		Velocity (m/s)		Emission rate (g/s)	
	Average	Maximum	Average	Maximum	Average	Maximum
CO Boiler	168	189	10.3	13.8	103	174
HP Boiler House	153	162	6.3	7.4	80	93
Sulphur Recovery Unit	272	380	2.6	4.8	3.7	165

For the flares, 15-minute average emissions temperature and SO_2 emission rate were provided by Essar. In order to model emissions from flares, an estimate of conditions at the top of the flame is required. UK-specific guidance on modelling flares is not available; appropriate modelling parameters were calculated on an hourly basis using guidance from Ontario Ministry of Environment and Climate Change[2] and Alberta Environment and Parks. Table 5.3 gives source and emissions data for the flare.

Table 5.3: Flare emissions data

	Effective Height (m)	Effective Diameter (m)		Temperature (^{o}C)	Velocity (m/s)	Emission rate (g/s)	
		Average	Maximum			Average	Maximum
Main flare	156	2.5	14.1	1400	20	6	104
Sour flare	161	3.5	14.0	1100	20	166	2335

Table 5.4 gives emissions data for the sources for which there were no time varying data.

Table 5.4: Non-time-varying emissions data

	Temperature (^{o}C)	Velocity (m/s)	Emission rate (g/s)
CDU3[3]	235	4.7	14
CDU4	220	8.0	48
Secondary Processes	285	3.4	12
MP Boiler House	124	1.9	0.1
Platformer 3	153	2.9	13
HD Select	317	7.1	1.3
Ethyl Benzene Unit	270	4.4	0.1
Energy Recovery Plant	300	8.0	0.6

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[2] https://dr6j45jk9xcmk.cloudfront.net/documents/1444/3-7-21-air-dispersion-modelling-en.pdf

[3] CDU3 ceased operation in August 2014

5.3 Modelled buildings

Buildings close to the sources can have a significant effect on the dispersion of emissions. The modelled buildings are shown in Figure 5.1 and model input data for the buildings are given in Table 5.5.

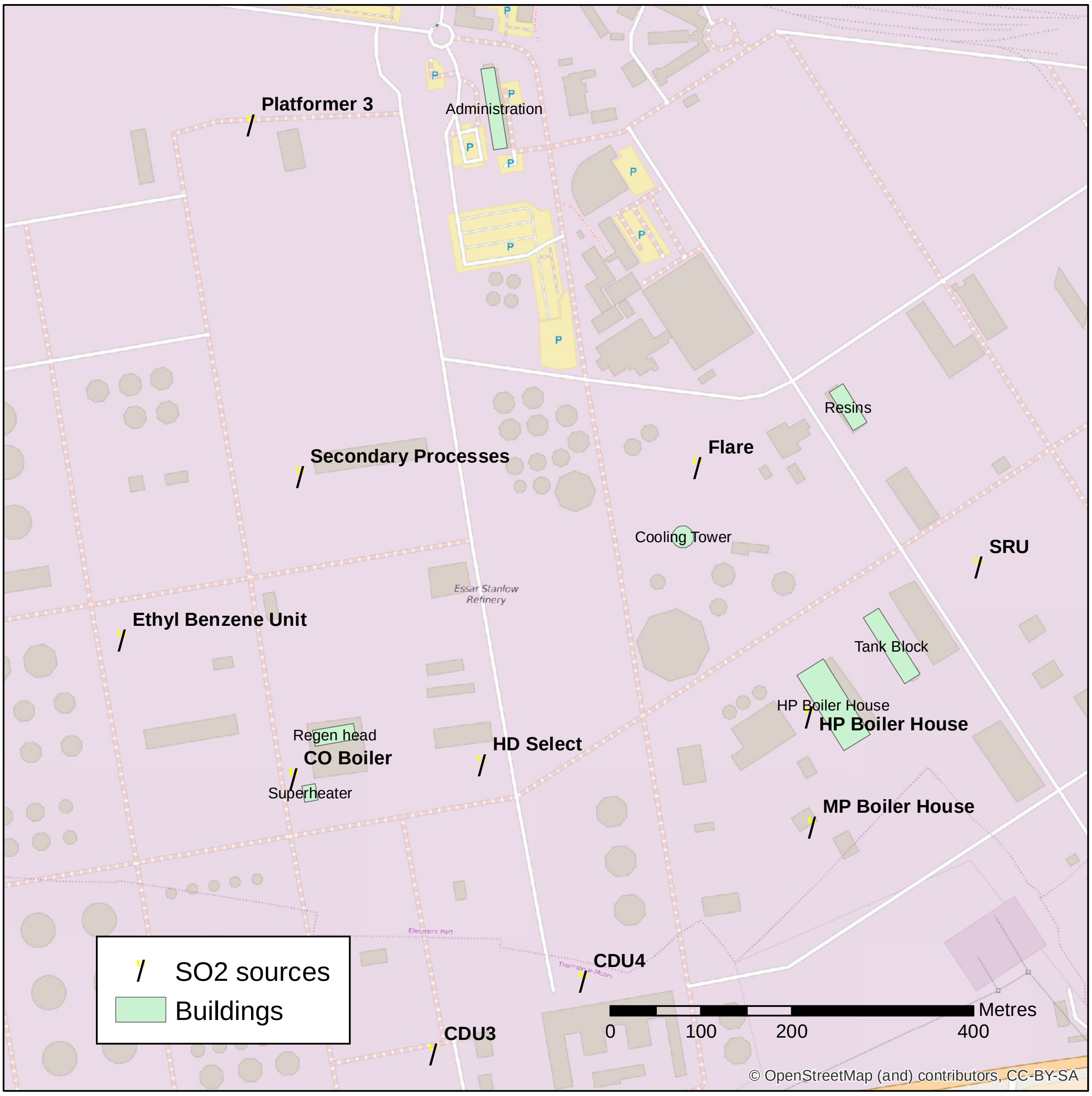


Figure 5.1: Modelled sources and buildings

Table 5.5: Modelled building data

Name	**Coordinates of building centre**		**Height (m)**	**Length (m)**	**Width (m)**	**Angle of length to north (°)**
	x	**y**				
Administration	343853	375854	43	90	15.5	171
HP Boiler House	344227	375197	28.4	98	34	148
Tank block	344291	375262	22	86	20	148
Resins	344243	375525	24	50	18	148
Superheater	343650	375100	35	18	15	170
Regen Head	343677	375164	60	46	18	80
Cooling tower	344061	375382	64	Circular: 24 m diameter		

5.4 Other sources

The Encirc site, located to the north east of the refinery, in the north of the village of Elton, is an additional source of SO_2 with the potential to have an impact on SO_2 concentrations in the area. Modelling carried out for the site by URS showed that the maximum 99.9th percentile of 15-minute average concentrations at the Thornton-le-Moors monitoring site was 9 $\mu g/m^3$, much smaller than the objective value of 266 $\mu g/m^3$.

Analysis of monitoring data shows that the peak concentrations at the Thornton-le-Moors monitoring sites occur for northerly winds, i.e. not from the direction of the Encirc site. This source was therefore not considered further in this assessment.

There are no other significant sources of SO_2 in the area.

6 Meteorological data

Modelling was carried out using hourly sequential meteorological data obtained from the Met Office Hawarden site, for the years 2013 to 2015 inclusive. The station is located approximately 13 km south east of the refinery. These data give a good representation of the meteorological conditions at the modelled location.

The hours of meteorological data used in the analysis exclude hours of calm, hours of variable wind direction and unavailable data. A summary of the data used is given below in Table 6.1. The ADMS meteorological pre-processor, written by the UK Met Office, uses the meteorological data to calculate the parameters required by the program.

Table 6.1: Summary of meteorological data used

Year	Percentage used	Parameter	Minimum	Maximum	Mean
2013	91%	Temperature (°C)	-4.7	29.6	9.9
		Wind speed (m/s)	0	16.5	3.9
		Cloud cover (oktas)	0	8	5.2
2014	89%	Temperature (°C)	-4.0	28.1	11.0
		Wind speed (m/s)	0	18.0	3.7
		Cloud cover (oktas)	0	8	5.0
2015	91%	Temperature (°C)	-4.5	28.9	10.4
		Wind speed (m/s)	0	16.5	4.0
		Cloud cover (oktas)	0	8	5.1

Figure 6.1 shows wind roses for Hawarden for the years 2013 to 2015, giving the frequency of occurrence of wind from different directions for a number of wind speed ranges.

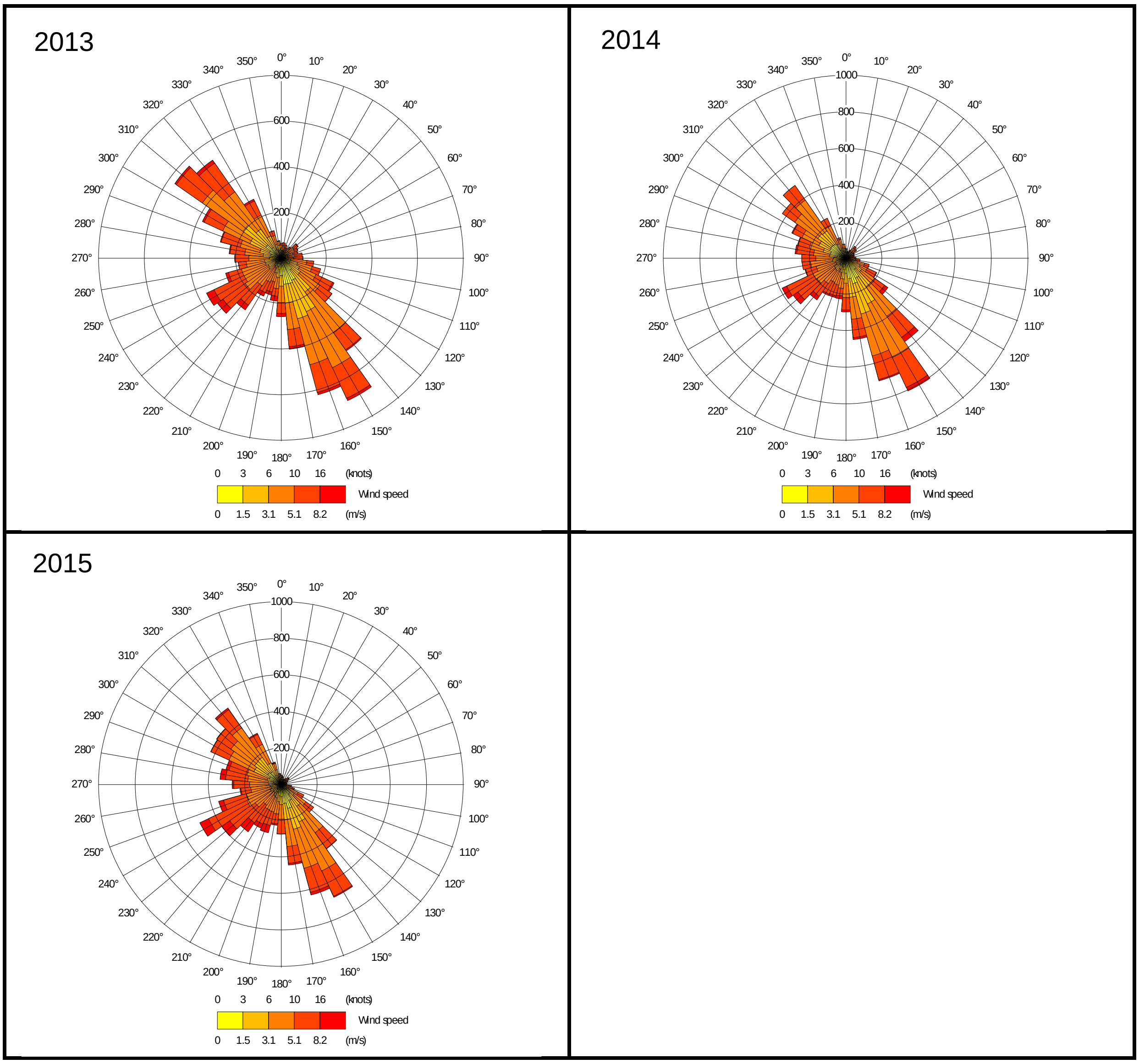


Figure 6.1: Wind roses for Hawarden, 2013 to 2015

7 Modelled concentrations

The part of the atmospheric boundary layer directly influenced by the earth's surface through surface heating or cooling and surface drag is said to be turbulent which means that, even when the prevailing meteorological conditions are constant for a significant time, the values of wind speed, wind direction and other flow field variables measured at a fixed point during short periods would not be constant.

For applications such as dispersion modelling, the period of one hour is taken as the period over which the meteorological conditions are roughly constant. Time scales less than one hour are then considered "*small*" or "*short*". Changes in meteorological conditions generally occur on time scales greater than one hour, whilst turbulent time scales are generally less than one hour.

Variations in measured concentrations over "*short*" timescales occur as a result of the turbulent fluctuations of the flow field. These variations depend on: the averaging time (variations increase with shorter averaging times); the meteorological conditions; the distance downstream from the source; and the cross-wind distance from the plume centreline.

The air quality standard for SO_2 is based on an averaging time of 15 minutes. The effect of concentration fluctuations, particularly for high stacks, is likely to be important.

The ADMS model includes a *fluctuations* option to take into account the variations in concentrations caused by short time scale turbulence. The model uses information about the plume and the meteorological conditions to calculate the probability that the concentration averaged over 15-minutes exceeds a threshold value. Typically, compared to the model without fluctuations (the ensemble mean model), the model predicts greater variability with a higher likelihood of both concentration peaks and concentration troughs, but similar long term averages.

One limitation of the fluctuations option is that it is not possible to take into account the effect of buildings on dispersion. Sensitivity testing determined that the effect of fluctuations is likely to be more important than the effect of buildings.

7.1 Model verification

SO_2 concentrations were calculated first at the locations of the monitoring sites for the monitoring periods. Measured and modelled concentrations were compared to verify that the model input data and assumptions were suitable for the area.

Note that both the measured and modelled data include periods of missing or invalid data; only periods where both measured and modelled data were valid were used in the verification. The data presented in this section are annual-equivalent values, as described in Section 4.1, based on the times with both valid measured and modelled concentrations. The values presented in the following tables may therefore vary slightly from those presented in Section 4.1.

Table 7.1 shows the measured and modelled 99.9th percentile of hourly average and 15-minute average concentrations, taking into account the effect of buildings on dispersion, but without using the fluctuations option. Table 7.2 shows the measured and modelled 99.9th percentile of hourly average concentrations and the number of 15-minute exceedences of the 266 µg/m³ threshold at each of the three monitoring sites, modelled without building effects but with the fluctuations option.

Table 7.1: Measured and modelled concentrations without fluctuations

	TLM		TLP		ELT	
	Measured	Modelled	Measured	Modelled	Measured	Modelled
99.9th percentile of hourly average concentrations	276	159	270	135	124	87
99.9th percentile of 15-minute average concentrations	344	168	311	142	138	91
15-minute Exceedences of 266 µg/m³	82	0	63	0	4	0

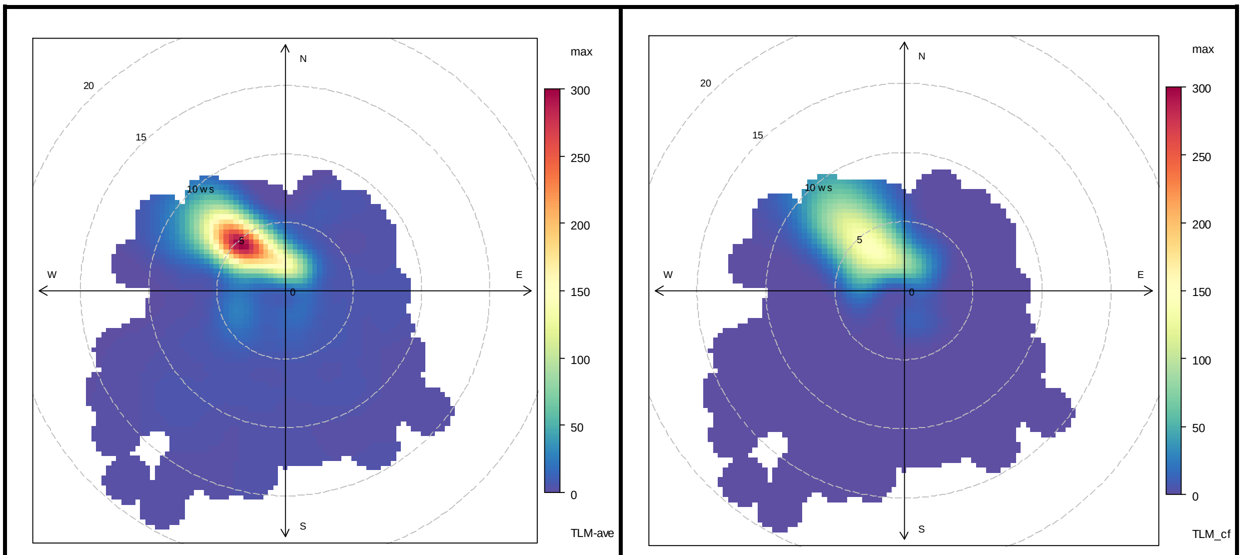
Table 7.2: Measured and modelled concentrations with fluctuations

	TLM		TLP		ELT	
	Measured	Modelled	Measured	Modelled	Measured	Modelled
99.9th percentile of hourly average concentrations	276	151	270	134	124	87
15-minute Exceedences of 266 µg/m³	82	113	63	42	4	2

The results show that while the modelled 99.9th percentile of hourly and 15-minute average concentrations are lower than the measured values, the number of predicted 15-minute exceedences of the threshold of 266 µg/m³ agrees well with the measured data when modelling including the effects of fluctuations.

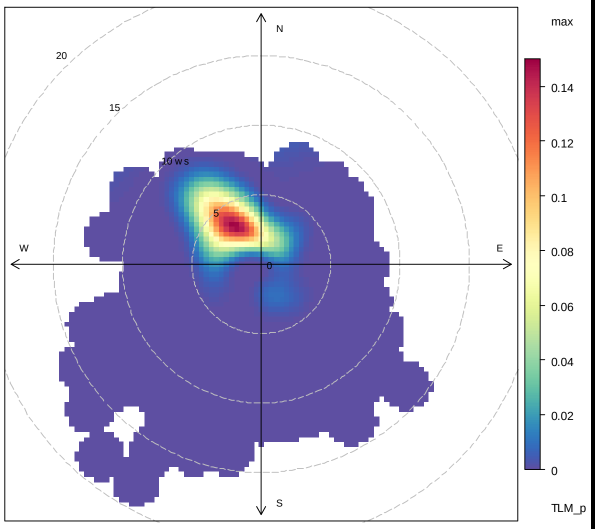
To investigate this further, polar plots of measured and modelled concentrations were produced for each monitoring site. Polar plots show how concentrations vary by wind speed and direction and can be used to help identify which sources have an influence on concentrations at the site.

Figure 7.1 to Figure 7.3 show polar plots of SO_2 concentrations at each of the three monitoring sites. The figures present, for each site: the measured maximum hourly concentration; the modelled maximum hourly concentration; and the maximum probability of the 15-minute average exceeding 266 µg/m³, for each combination of wind speed and direction.



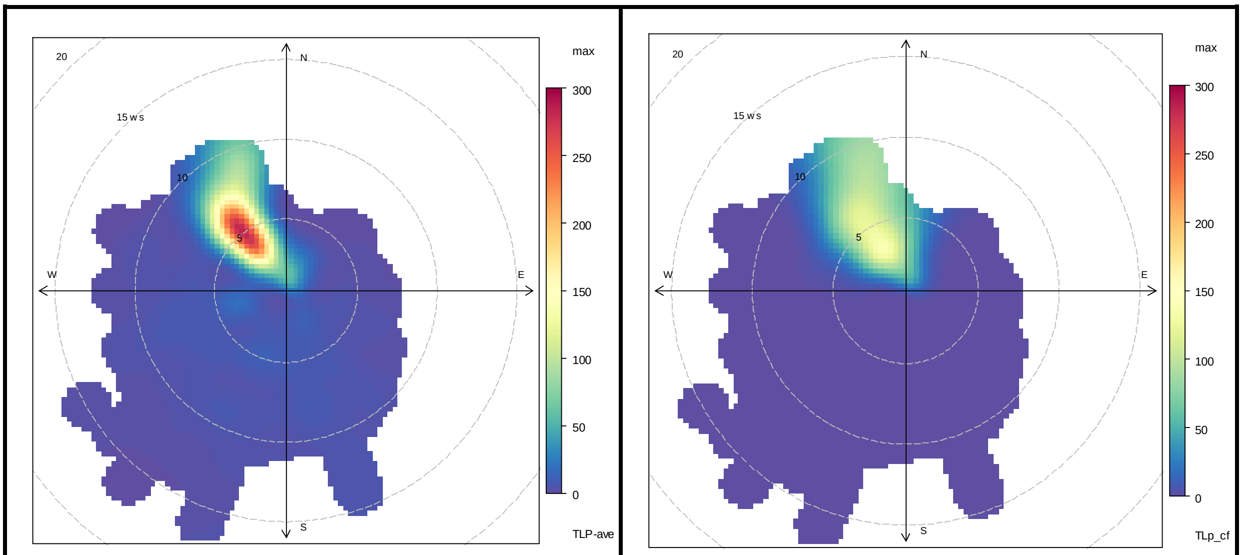
Measured maximum hourly concentrations (µg/m³)

Modelled maximum hourly concentrations (µg/m³)



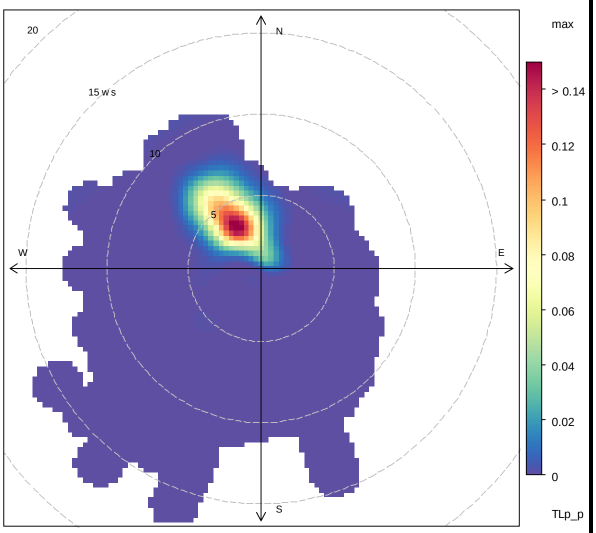
Maximum modelled probability of 15-minute average exceeding 266 µg/m³

Figure 7.1: Polar plots of SO_2 concentrations at TLM monitoring site



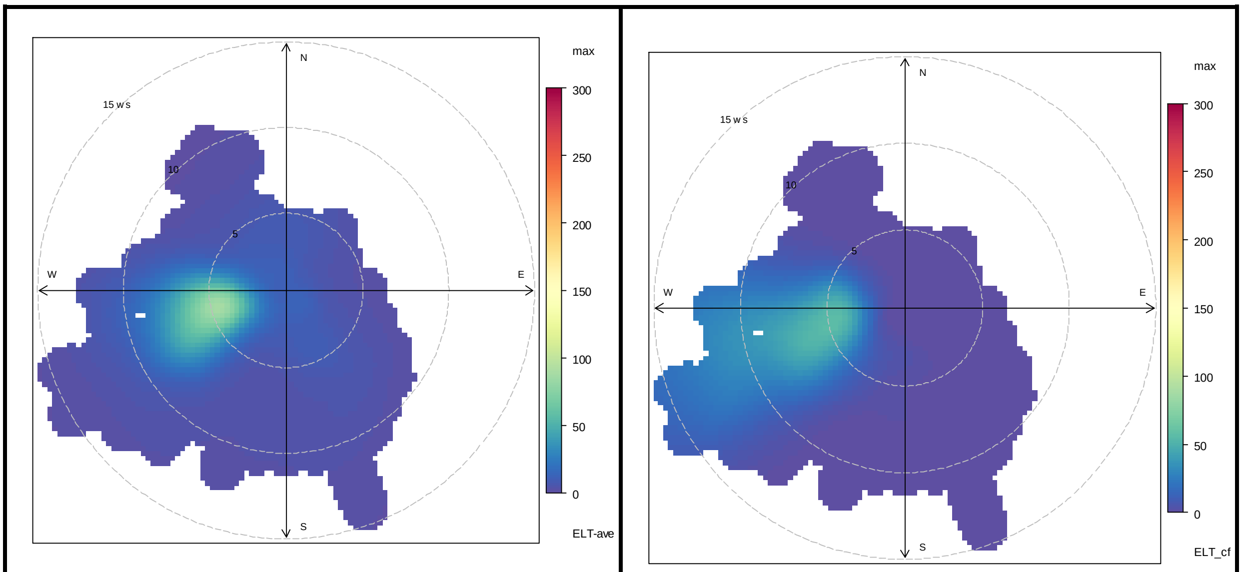
Measured maximum hourly concentrations (µg/m³)

Modelled maximum hourly concentrations (µg/m³)



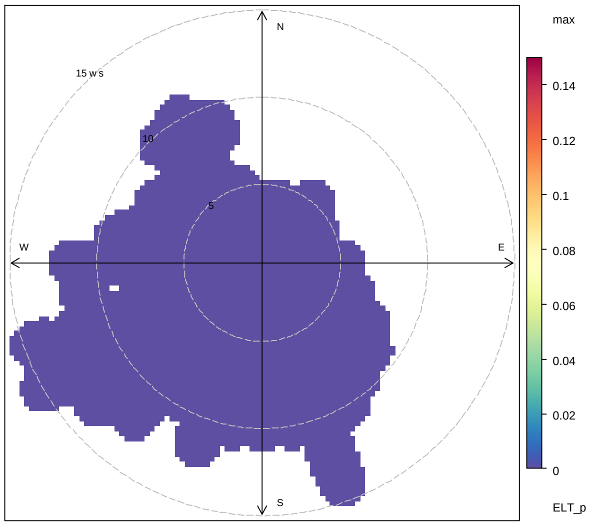
Maximum modelled probability of 15-minute average exceeding 266 µg/m³

Figure 7.2: Polar plots of SO_2 concentrations at TLP monitoring site



Measured maximum hourly concentrations (µg/m³)

Modelled maximum hourly concentrations (µg/m³)



Maximum modelled probability of 15-minute average exceeding 266 µg/m³

Figure 7.3: Polar plots of SO_2 concentrations at ELT monitoring site

The polar plots show that the maximum concentrations at TLM and TLP are measured for moderate wind speeds from the north west. For the ELT site, the maximum concentrations occur for westerly winds. The modelled concentrations at each of the three sites show the same pattern as the measured data, but at TLM and TLP, the modelled concentrations are smaller than the measured concentrations. It is likely that this is due to short-term fluctuations in concentrations; using the ADMS fluctuations option results in the modelled number of exceedences agreeing well with the measured data. The polar plots of the probability of exceeding the threshold of 266 µg/m³ have a very similar pattern to the maximum measured concentrations, indicating that the same sources are responsible for the exceedences.

7.2 Meteorological conditions during SO_2 episodes

Table 7.3 gives a summary of the meteorological conditions during the study period. For each parameter, the minimum, maximum and average values are provided for: the hours for which exceedences were measured at either the TLM or TLP monitoring sites; the hours for which the modelled probability of exceedences was greater than 1%; and the hours for which the modelled probability of exceedences was greater than 10%. The modelled exceedences occur for northerly winds, for angles between 320° and 10°; the data for all hours with wind from this direction are also presented for comparison.

The table provides data for some standard meteorological parameters but also includes data calculated by the ADMS model which characterises the behaviour of the atmosphere.

The stability of the atmosphere is calculated using two parameters: the boundary layer height and the Monin-Obukhov length (L_{MO}).

The atmospheric boundary layer is the region of the atmosphere closest to the earth's surface and is the area in which the dispersion of pollution occurs. The height of the boundary layer varies by time of the day and by meteorological conditions. The boundary layer height (h) varies from tens of metres to a few kilometres.

The Monin-Obukhov length (L_{MO}) is a measure of the relative importance of buoyancy and mechanical mixing effects. In very stable conditions it has a positive value of between 2 metres and 20 metres. In near neutral conditions its magnitude is very large, and it has either a positive or negative value depending on whether the surface is being heated or cooled by the air above it. In very convective conditions it is negative with a magnitude of typically less than 20 metres.

The stability of the atmosphere can be represented by h/L_{MO}.

- In convective conditions, h/L_{MO} is typically less than -0.3;
- In neutral conditions, h/L_{MO} is typically between -0.3 and 1; and
- In stable conditions, h/L_{MO} is typically greater than 1.

Table 7.3: Summary of meteorological conditions

		Minimum	Maximum	Average
Date	Measured exceedences	01-Feb	29-Nov	-
	Modelled probability >1%	03-Feb	19-Nov	-
	Modelled probability >10%	19-Mar	14-Sep	-
	All northerly winds	01-Jan	31-Dec	-
Hour	Measured exceedences	8:00	21:00	-
	Modelled probability >1%	8:00	18:00	-
	Modelled probability >10%	9:00	17:00	-
	All northerly winds	0:00	23:00	-
Temperature (°C)	Measured exceedences	0.3	25.5	16.6
	Modelled probability >1%	3.9	26.6	16.9
	Modelled probability >10%	8.6	26.6	18.9
	All northerly winds	0.1	26.6	12.5
Wind speed (m/s)	Measured exceedences	0.5	6.7	4.3
	Modelled probability >1%	1.0	7.2	4.1
	Modelled probability >10%	1.0	5.2	3.2
	All northerly winds	1.0	10.8	3.6
Cloud (oktas)	Measured exceedences	0	8	2
	Modelled probability >1%	0	8	3.4
	Modelled probability >10%	0	7	3
	All northerly winds	0	8	5.1
Boundary layer height (m)	Measured exceedences	50	1694	1068
	Modelled probability >1%	497	1779	1034
	Modelled probability >10%	666	1493	1026
	All northerly winds	50	1785	577
$1/L_{MO}$ (m^{-1})	Measured exceedences	-0.300	0.100	-0.007
	Modelled probability >1%	-0.083	0.000	-0.009
	Modelled probability >10%	-0.083	-0.002	-0.017
	All northerly winds	-0.115	0.100	0.009
h/L_{MO} (-)	Measured exceedences	-121.4	5.0	-6.6
	Modelled probability >1%	-96.9	0.2	-8.2
	Modelled probability >10%	-96.9	-2.6	-17
	All northerly winds	-96.9	13.6	-2.3

Figure 7.4 shows scatter plots of the day of the year and time of the day for each of the measured exceedences and for each hour with modelled probability of exceedence greater than 10%. Also shown on the same plots are the data for all northerly winds (wind angle between 320° and 10°).

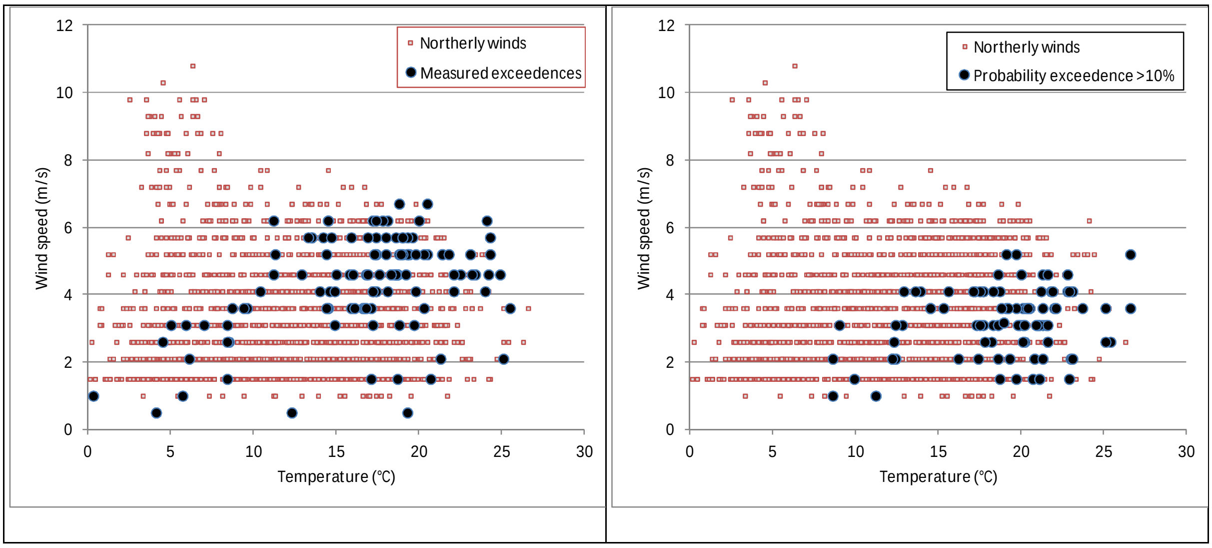


Figure 7.4: Day of year and time of day for measured exceedences (left) and modelled probability of exceedence >10% (right)

Figure 7.5 shows scatter plots of the temperature and wind speed for each of the measured exceedences and for each hour with modelled probability of exceedence greater than 10%. Also shown on the same plots are the data for all northerly winds.

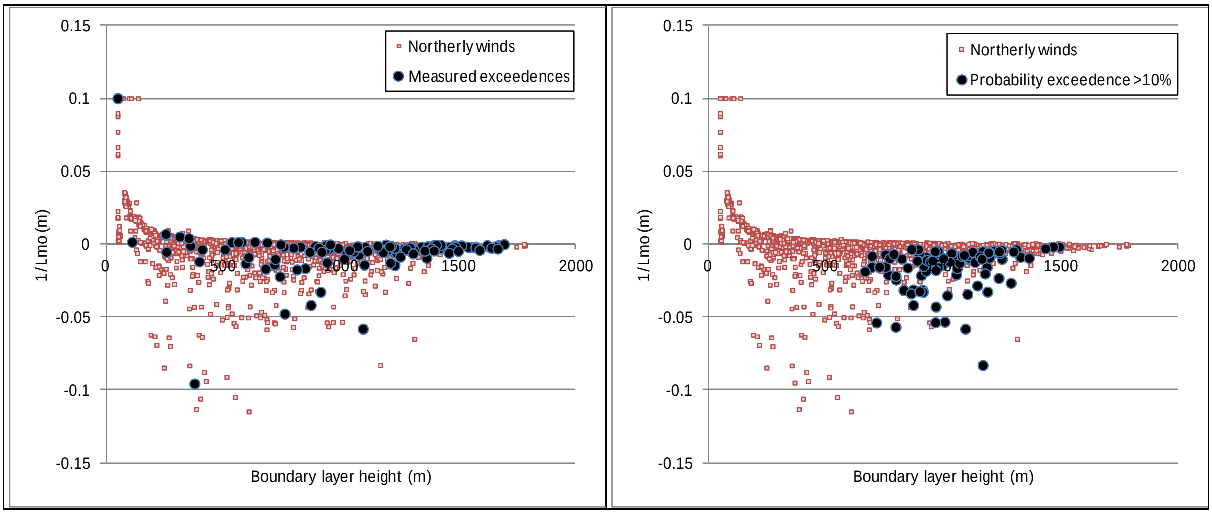


Figure 7.5: Temperature and wind speed for measured exceedences (left) and modelled probability of exceedence >10% (right)

Figure 7.6 shows scatter plots of the boundary layer height and reciprocal of the Monin-Obukhov length for each of the measured exceedences and for each hour with modelled probability of exceedence greater than 10%. Also shown on the same plots are the data for all northerly winds.

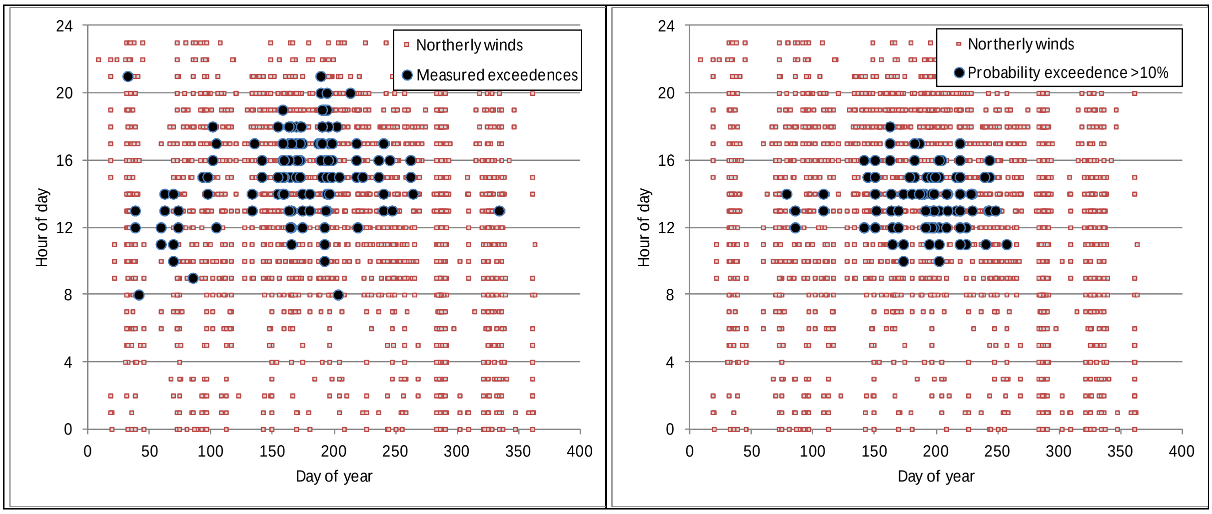


Figure 7.6: Boundary layer height and $1/L_{MO}$ for measured exceedences (left) and modelled probability of exceedence >10% (right)

For both the measured and modelled concentrations, exceedences are more likely during the day in the summer months. The majority of exceedences occur when the temperature is greater than 10°C and with wind speeds of between 2 and 6 m/s. These conditions tend to be convective (typically $h/L_{MO} < -0.3$) with boundary layer heights of between 500 and 1700 metres.

7.3 Source apportionment

Exceedences of the SO_2 concentration threshold of 266 μg/m³ are likely to be due to emissions from a combination of different sources. To investigate the relative contributions, source apportionment was carried out. Figure 7.7 shows the 99.9th percentile of 15-minute average concentrations for each source and for all sources combined. Note that these values do not take into account the fluctuations calculations. Note also that the 99.9th percentile concentration for all sources will not be the sum of the contributions from each individual sources because these will happen for different meteorological conditions.

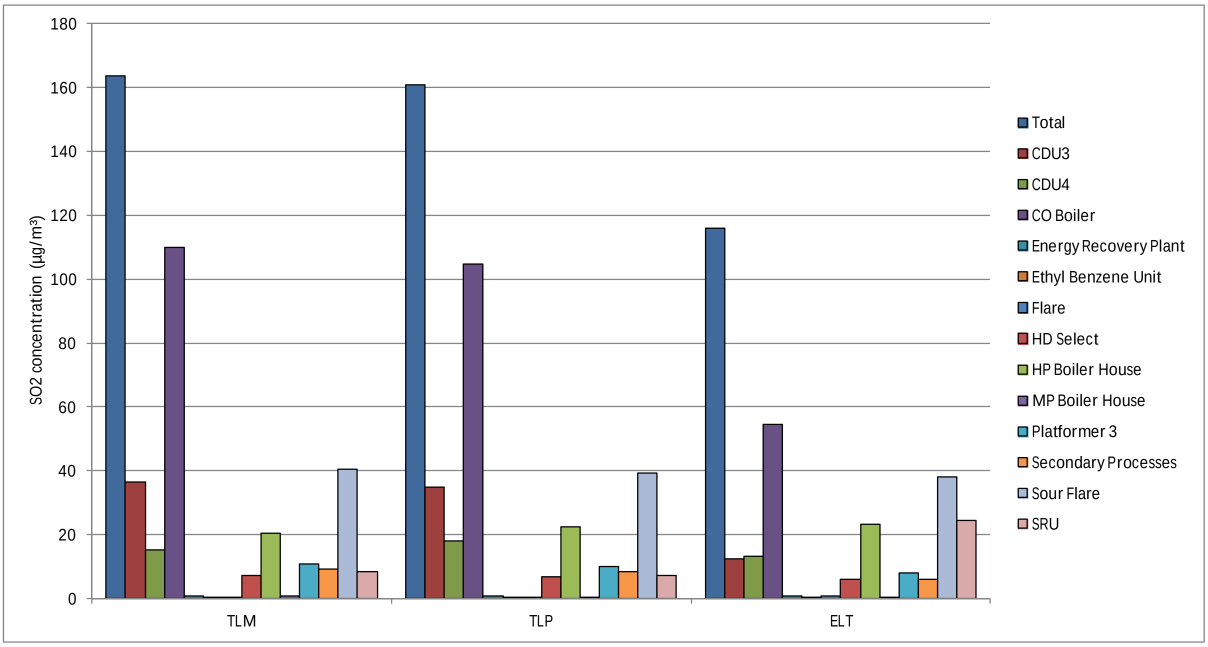


Figure 7.7: 99.9th percentiles of 15-minute average SO_2 concentrations by source type

7.4 Contour plots

The number of exceedences of the 15-minute average concentration threshold of 266 µg/m³ was calculated on a grid of output points around the refinery with a resolution of 50 metres. Figure 7.8 to Figure 7.10 show the modelled number of exceedences for the years 2013 to 2015, respectively. The air quality standard allows 35 exceedences so the areas within the 35 contour line are expected to breach the standard. Additional contour lines showing 10, 20, 70 and 100 exceedences per year are also shown to give an indication of the variability in the modelled results.

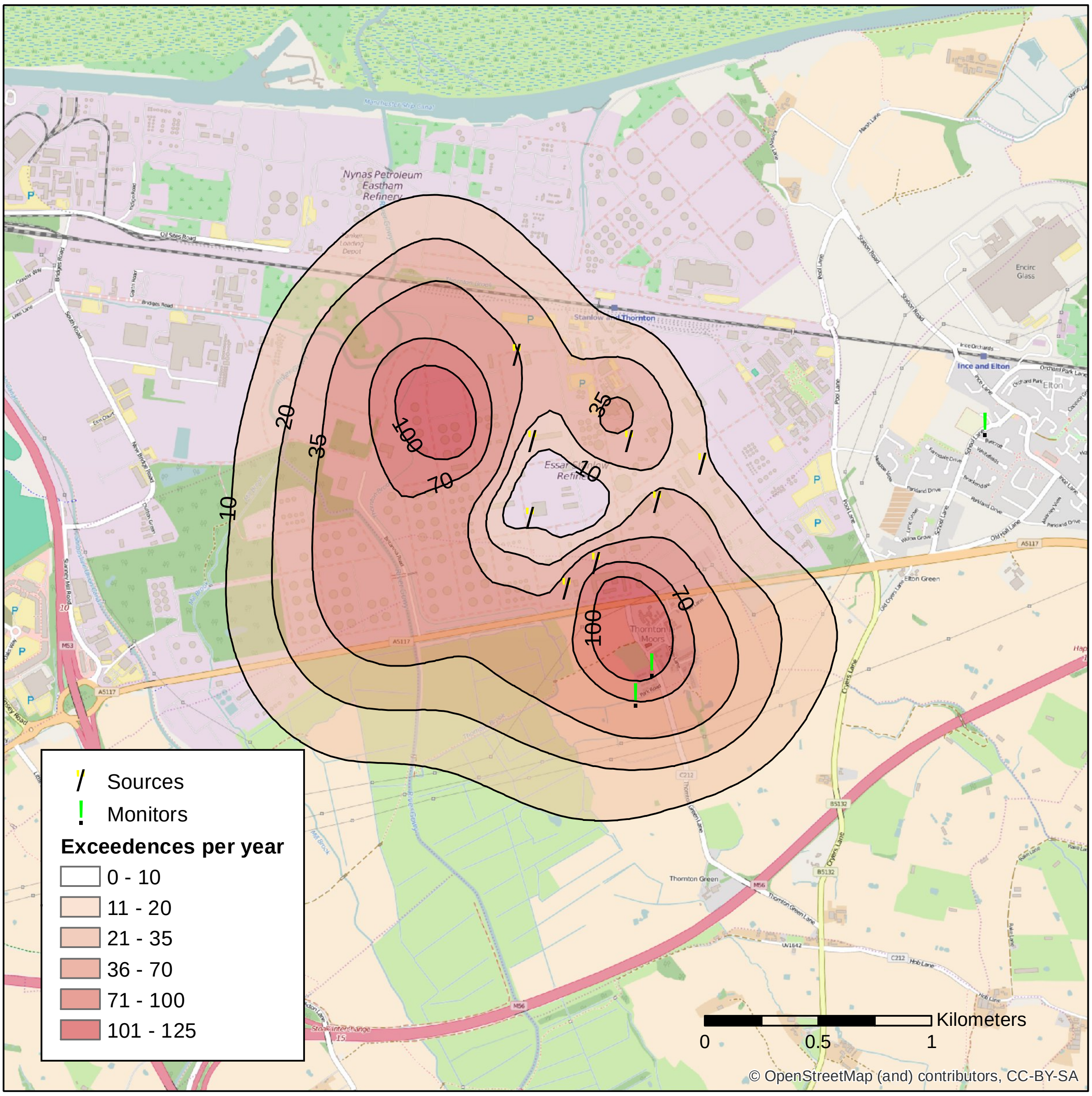


Figure 7.8: Modelled number of 15-minute exceedences of the SO_2 concentration of 266 µg/m³ for 2013

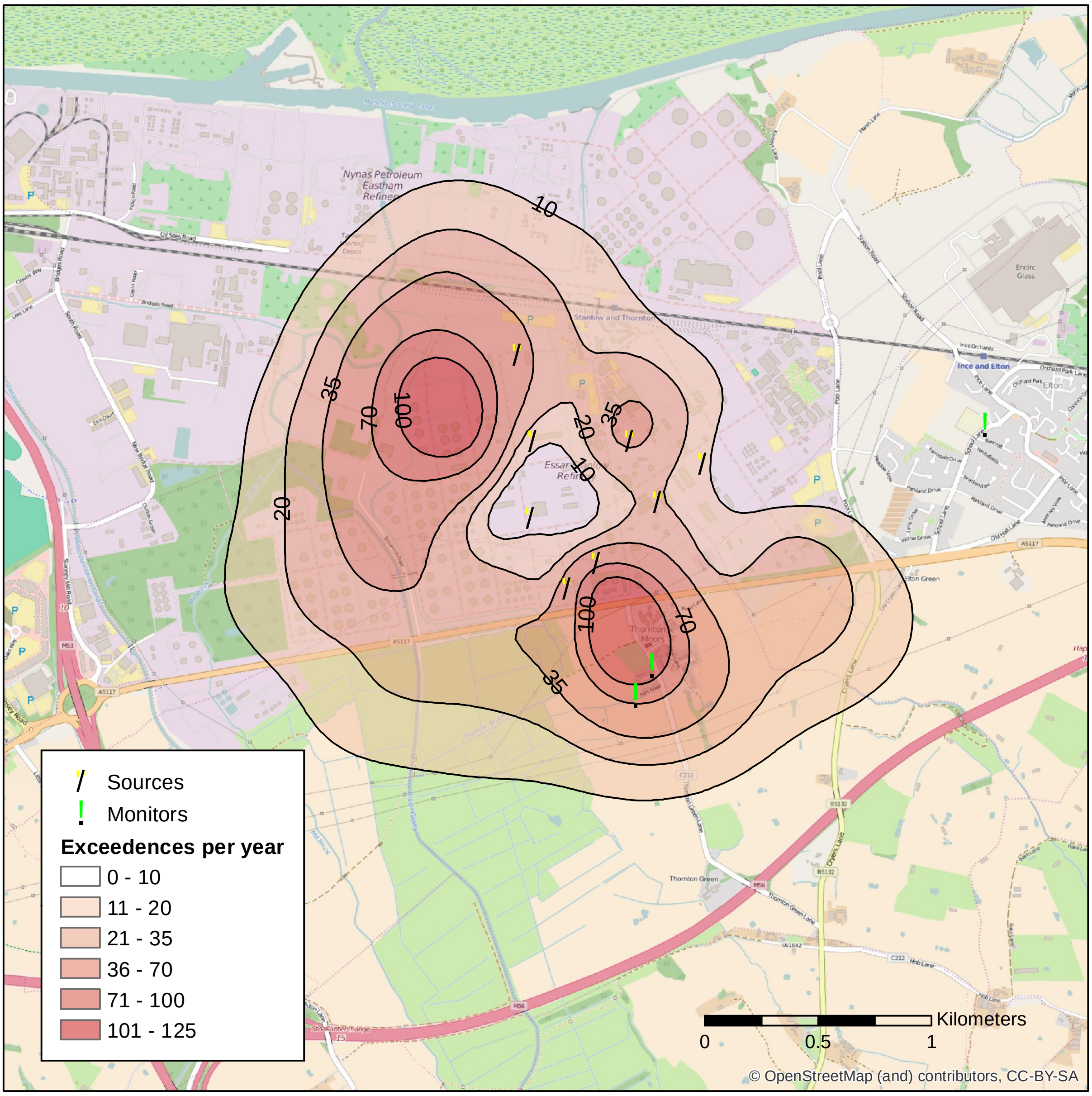


Figure 7.9: Modelled number of 15-minute exceedences of the SO_2 concentration of 266 µg/m³ for 2014

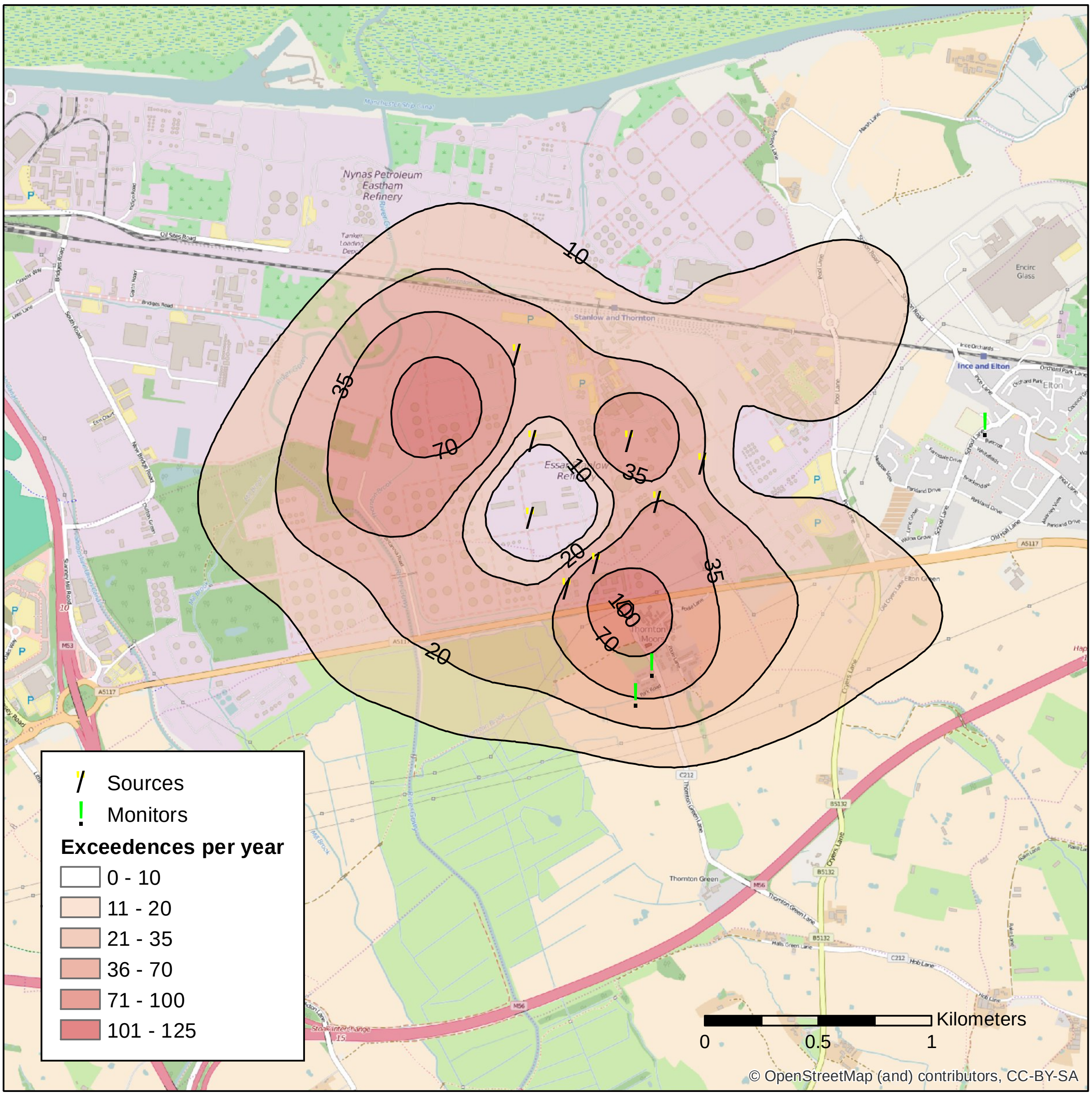


Figure 7.10: Modelled number of 15-minute exceedences of the SO_2 concentration of 266 µg/m³ for 2015

7.5 Population Exposure

When declaring an Air Quality Management Area it is required to quantify the population exposed to concentrations exceeding the air quality standard. Figure 7.11 shows the maximum modelled number of 15-minute exceedences of the SO_2 concentration of 266 µg/m³ per year for the period 2013 to 2015. Also shown are the locations of all the buildings for which more than 10 exceedences were predicted; the locations of two travellers' sites; and a public footpath at which the air quality standard also applies.

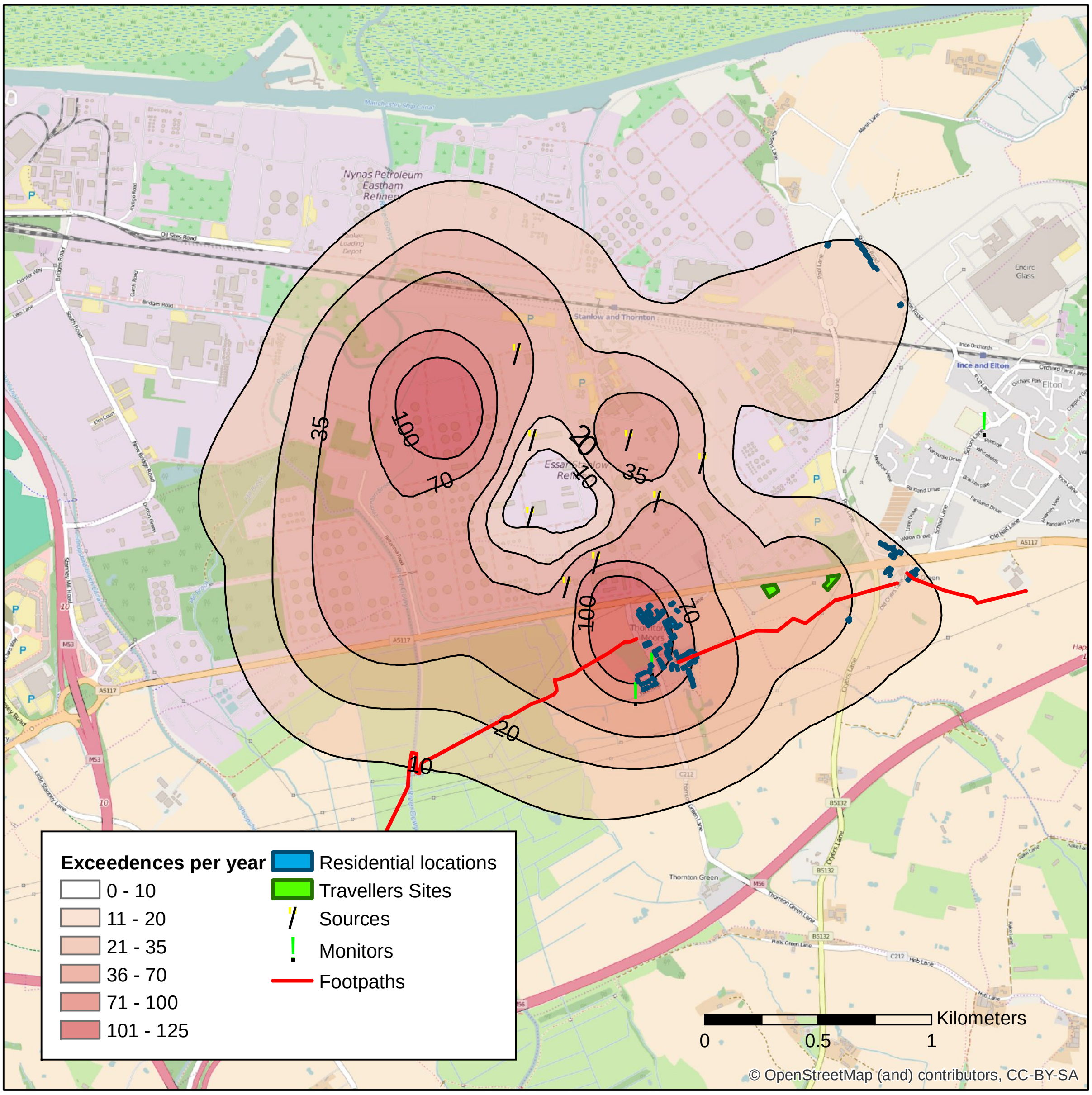


Figure 7.11: Maximum exceedences per year 2013 - 2015

Table 7.4 shows the estimated population likely to be exposed to different numbers of exceedences of the 266 µg/m³ threshold concentration per year. To estimate the population exposed, an average value of 2.4 people per household was assumed and the two travellers sites were assumed to hold a total of 50 people.

Table 7.4: Estimated population exposed to 15-minute exceedences of 266 µg/m³

No. exceedences per year	Residential properties	Travellers sites	Total population
10	113	2	321
20	71	2	220
35	71	0	170
70	60	0	144
100	32	0	77

8 Discussion

The air quality standard for 15-minute average SO_2 concentrations is 266 µg/m³, not to be exceeded more than 35 times per year. Monitoring of SO_2 concentrations near the Stanlow refinery has measured more than 35 exceedences per year.

Dispersion modelling of emissions from all sources of SO_2 on the Stanlow refinery site was carried out to determine the extent of the exceedences and hence to assist with defining an Air Quality Management Area.

The modelling was carried out using the ADMS dispersion model (version 5.1.2). The modelling used the fluctuations option which takes into account short time scale turbulence which, compared to the model without fluctuations, predicts greater variability with a higher likelihood of both concentration peaks and troughs.

One limitation of the fluctuations option is that it is not possible to take into account the effect of buildings on dispersion. However, for the case being considered here, sensitivity test have shown that the effect of fluctuations is more important than the effect of buildings.

The predicted number of exceedences at the monitoring sites agreed well with the measured data. More than 35 exceedences were predicted at the TLM and TLP sites and fewer than 35 exceedences were predicted at the ELT site, in accordance with the monitoring data.

Modelling was carried out for the years 2013 to 2015 to predict the extent of the exceedences. More than 35 exceedences per year were recorded throughout the village of Thornton-le-Moors but did not extend to any other residential areas. Decreasing the number of exceedences to 20 per year takes in the two travellers' sites to the east of Thornton-le-Moors, and decreasing it further to 10 exceedences takes in the western end of the villages of Elton and Ince.

APPENDIX A: Summary of ADMS 5

ADMS, the Atmospheric Dispersion Modelling System, has been developed to make use of the most up-to-date understanding of the behaviour of the lower levels of the atmosphere in an easy-to-use computer modelling system for atmospheric emissions. This allows the impacts of emissions from industrial and other facilities to be thoroughly investigated as part of an environmental assessment or for other regulatory purposes. The following is a summary of the capabilities and validation of ADMS 5. More details can be found on the CERC web site at www.cerc.co.uk.

The core model calculates the average concentration arising from an emission for a given meteorological condition (for example, wind speed and direction), taking account of plume rise and stack downwash where required. The emission may be released from a single source or from a number of sources. In addition, ADMS is able to:

- calculate long-term concentration statistics, typically for a period of one year, for direct comparison with air quality standards and objectives;
- take into account the often very significant effects that a nearby building can have on the dispersion of emissions;
- model the chemical conversions that occur in the atmosphere between nitric oxide (NO), nitrogen dioxide (NO_2) and ozone (O_3);
- include background concentrations in concentration statistics;
- allow for the effects of complex terrain and changes in surface roughness on wind speed and direction, and on the levels of turbulence in the atmosphere;
- determine the quantities of an emission deposited to the ground by both dry and wet deposition processes;
- include the decay of radioactive emissions and determine the gamma dose at a location received from passing material;
- report the extent to which a moist plume will be visible;
- model sources over the sea, such as oil platforms, using special calculations of surface roughness and heat fluxes; and
- output temperature, relative and/or specific humidity, as well as exceedences of temperature and/or humidity thresholds and simultaneous exceedences of temperature and humidity threshold values.

More details of these processes are given below.

ADMS runs in Windows 8, Windows 7, Windows Vista and XP environments. It has been developed by CERC in conjunction with the UK Meteorological Office and the Department of Mechanical Engineering at the University of Surrey. In its earlier stages, ADMS was developed with contributions from a number of sponsors, including the Environment Agency (originally under HMIP), the Health and Safety Executive and a number of the successor companies of the CEGB.

Dispersion Modelling

ADMS uses boundary layer similarity profiles in which the boundary layer structure is characterised by the height of the boundary layer and the Monin-Obukhov length, a length scale dependent on the friction velocity and the heat flux at the ground. This has significant advantages over earlier methods in which the dispersion parameters did not vary with height within the boundary layer.

In stable and neutral conditions, dispersion is represented by a Gaussian distribution. In convective conditions, the vertical distribution takes account of the skewed structure of the vertical component of turbulence. This is necessary to reflect the fact that, under convective conditions, rising air is typically of limited spatial extent but is balanced by descending air extending over a much larger area. This leads to higher ground-level concentrations than would be given by a simple Gaussian representation.

The formulation of ADMS means that, for a given meteorological condition, as well as determining average concentrations the model is also able to provide statistical information on concentration fluctuations. This can be particularly important in applications such as, for example, determining whether or not a dispersing material exceeds flammability or odour detection thresholds.

Emissions

Buoyant emissions, and those with vertical momentum, rise in the atmosphere after emission. This movement, which is referred to as *plume rise*, also results in additional dilution and can result in the emission penetrating the top of the atmospheric boundary layer and being lost from the local area. These effects are included in the modelling using an integral solution of the conservation equations for the plume's mass, momentum and heat. The possibility of entrainment behind the stack, known as *downwash*, which can lower the effective height of the emission, is also included in the calculation.

ADMS can also model emissions represented as:

- lines – for linear sources;
- areas – to represent situations where a source can best be represented as uniformly spread over an area, such as evaporation from an open tank;
- volumes – to represent situations where a source can best be represented as uniformly spread throughout a volume, such as fugitive emissions from a factory complex; and
- jets – to represent situations where emissions are not emitted vertically upwards.

Presentation of Results

For most situations ADMS is used to model the fate of emissions for a large number of different meteorological conditions. Typically, meteorological data are input for every hour during a year or for a set of conditions representing all those occurring at a given location. ADMS uses these individual results to calculate statistics for the whole data set. These are usually average values, including rolling averages, percentiles and the number of hours for which specified concentration thresholds are exceeded. This allows concentrations to be calculated for direct comparison with air quality limits, guidelines and objectives, in whatever form they are specified.

Results can be presented as numerical values at specified locations. In addition, by calculating concentrations over a grid of locations, results can be presented graphically as concentration contours or isopleths. This can be done using the ADMS-Mapper, and is also facilitated by a link with GIS[4] ESRI ArcGIS.

Complex Effects - Buildings

A building or similar large obstruction can affect dispersion in three ways:

1. It deflects the wind flow and therefore the route followed by dispersing material;
2. This deflection increases levels of turbulence, possibly enhancing dispersion; and
3. Material can become entrained in a highly turbulent, recirculating flow region or cavity on the downwind side of the building.

The third effect is of particular importance because it can bring relatively concentrated material down to ground-level near to a source. From experience, this occurs to a significant extent in more than 95% of studies for industrial facilities.

The buildings effects module in ADMS has been developed using extensive published data from scale-model studies in wind-tunnels, CFD modelling and field experiments on the dispersion of pollution from sources near large structures. It operates out to a distance of about 30 building heights from the building and has the following stages:

(i) A complex of buildings is reduced to a single rectangular block with the height of the dominant building and representative streamwise and crosswind lengths.
(ii) The disturbed flow field consists of a recirculating flow region in the lee of the building with a diminishing turbulent wake downwind, as shown in Figure A1.
(iii) Concentrations within the well-mixed recirculating flow region are uniform and based upon the fraction of the release that is entrained.
(iv) Concentrations further downwind in the main wake are the sum of those from two plumes: a ground level plume from the recirculating flow region and an elevated plume from the non-entrained remainder.

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[4] Geographical Information System

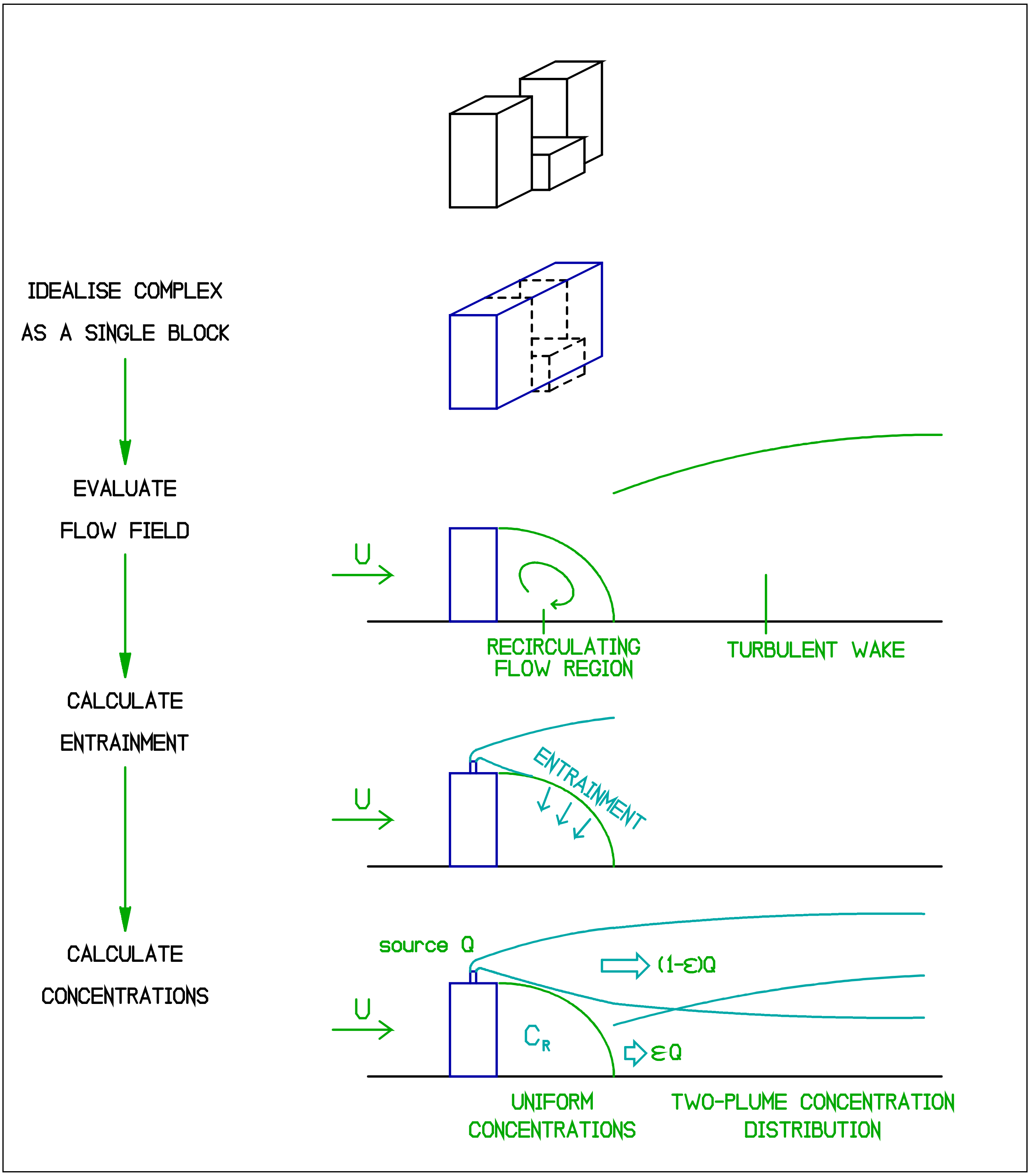

Figure A1: Stages in the modelling of building effects

Complex Effects – NO_x Chemistry

Nitrogen oxides (NO_x) emitted from combustion processes are typically only 5% to 10% nitrogen dioxide (NO_2), with the remainder as nitric oxide (NO). After emission, the NO combines with the ozone (O_3) present in the atmosphere to increase the proportion of NO_2. The key features of the two processes involved can be represented by:

(1) $NO + O_3 \rightarrow NO_2$
(2) $NO_2 + h\nu \rightarrow NO + O_3$

where the role played by oxygen (O and O_2) has been omitted for clarity and $h\nu$ represents ultra violet radiation. Both of these reactions, which can proceed relatively rapidly, are modelled by ADMS, which only allows the second reaction to occur in daylight. Other reactions that involve O_3 and NO_2, such as those with Volatile Organic Compounds (VOCs), have not been included because their reaction times are significantly longer. They would not have any significant effect on concentrations arising from specific industrial emissions.

Complex Effects – Terrain and Roughness

Complex terrain can have a significant impact on wind-flow and consequently on the fate of dispersing material. Primarily, terrain can deflect the wind and therefore change the route taken by dispersing material. Terrain can also increase the levels of turbulence in the atmosphere, resulting in increased dilution of material. This is of particular significance during stable conditions, under which a sharp change with height can exist between flows deflected over hills and those deflected around hills or through valleys. The height of dispersing material is therefore important in determining the route it takes. In addition areas of reverse flow, similar in form and effect to those occurring adjacent to buildings, can occur on the downwind side of a hill.

Changes in the surface roughness can also change the vertical structure of the boundary layer, affecting both the mean wind and levels of turbulence.

The ADMS Complex Terrain Module models these effects using the wind-flow model FLOWSTAR. This model uses linearised analytical solutions of the momentum and continuity equations, and includes the effects of stratification on the flow. Ideally hills should have moderate slopes (up to 1 in 2 on upwind slopes and hill summits, up to 1 in 3 in hill wakes), but the model is useful even when these criteria are not met. The terrain height is specified at up to 66,000 points that are interpolated by the model onto a regular grid of up to 256 by 256 points. The best results are achieved if the specified data points are regularly spaced. FLOWSTAR has been extensively tested with laboratory and field data.

Regions of reverse flow are treated by assuming that any emissions into the region are uniformly mixed within it. Material then disperses away from the region as if it were a virtual point source. Material emitted elsewhere is not able to enter reverse flow regions.

Deposition

Material in a plume that is close to the ground can be lost to the ground by dry deposition. This process is included in ADMS by using a gravitational settling velocity for particles, and a deposition velocity based on aerodynamic, sub-layer and surface-layer resistance values for gases. The concentration profile within a dispersing plume is then adjusted to take account of the losses at the surface. Dry and wet deposition parameters can be varied spatially, to take into account changes in land use across the modelled area.

Wet deposition is included via a washout coefficient to control the quantity of material incorporated into rain. In addition, for SO_2 and HCl emitted from point sources, the 'Falling Drop' model is available, which includes the kinetics of the uptake of gases, as well as the thermodynamics and chemistry of the dissolution of gases in raindrops.

Radioactivity

For radioactive releases ADMS calculates the transformations within the plume of one isotope into another by radioactive decay. ADMS can also determine the gamma dose received at a location from a dispersing plume.

Visible Plumes

For moist emissions ADMS determines the section of the plume where the liquid water content is sufficient for the plume to be visible. This allows statistics of the frequency and lengths of visible plumes to be calculated.

Fluctuations

ADMS models short time-scale fluctuations calculating the probability distributions of pollutant concentrations; probabilities of exceedence of specified threshold; and the range of concentrations for averaging times as little as a second. The module has application where estimates of the occurrence of peaks of concentration over short averaging times are important (e.g. odours, 15-minute air quality objective for SO_2). This module takes into account variations due both to turbulence, and changes in meteorology

Data Comparisons – Model Validation

The individual components of ADMS, for example the Buildings Module, have been developed using published scientific data and each component extensively tested to ensure that it provides reliable results. In addition, a very large number of studies have been performed on the accuracy of ADMS for point source emissions.

Among other validation studies, ADMS output has been compared with three flat terrain data sets known as Kincaid, Indianapolis and Prairie Grass, which are available from the US Modellers Data Archive. Each of these datasets has been generally accepted as containing enough measurements of sufficient quality for meaningful validation.

Further details of ADMS and model validation, including a full list of references, are available from the CERC web site at www.cerc.co.uk.

APPENDIX B: Additional contour plots

This section presents the contour plots from Section 7, presented on a scale expressing the annual exceedences of the 15-minute average concentration threshold of 266$\mu g/m^3$ as a percentage of the 35 allowed exceedences per year, allowing uncertainty in the model results to be taken into account. The number of exceedences of the 15-minute average concentration threshold of 266 $\mu g/m^3$ was calculated on a grid of output points around the refinery with a resolution of 50 metres. Figure B.1 shows the maximum modelled number of 15-minute exceedences of the SO_2 concentration of 266 $\mu g/m^3$ for the years 2013 to 2015. Also shown are the locations of all the buildings for which more than 10 exceedences were predicted; the locations of two travellers' sites; and a public footpath at which the air quality standard also applies.

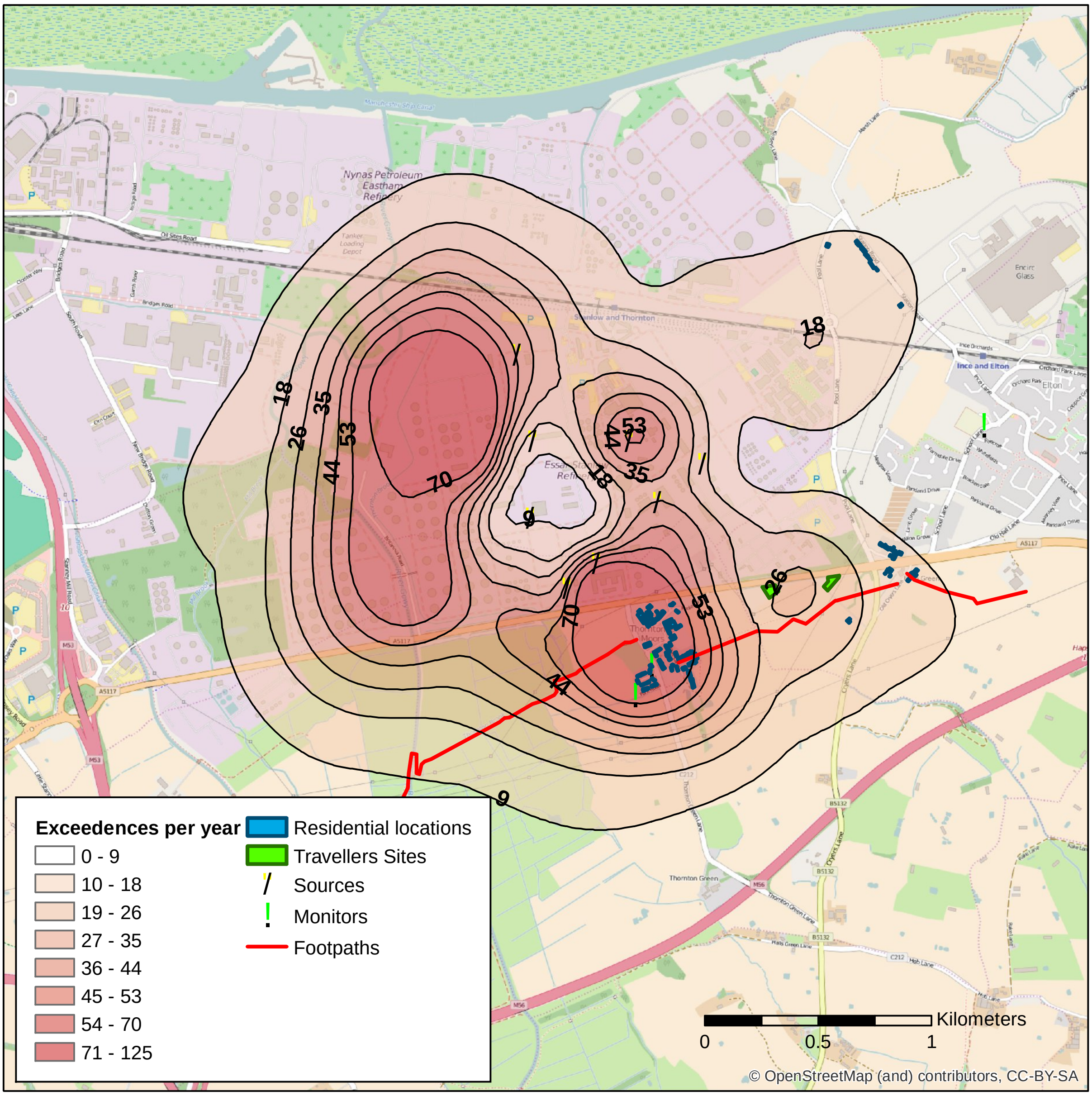

Figure B.1: Maximum exceedences per year 2013 - 2015