Final Report **Project UKPIR15**

Final Report for SCAIL Combustion

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EXECUTIVE SUMMARY

Background

1. Under the Integrated Pollution Prevention and Control (IPPC) Directive, permits are required for combustion installations with a rated thermal input exceeding 50MW. The Directive has been transposed into the Pollution Prevention and Control (Scotland) Regulations 2000, the Pollution Prevention and Control Regulations (Northern Ireland) 2003 and the Environmental Permitting (England and Wales) Regulations 2007, and in the national legislation permits are required for combustion installations with a rated thermal input exceeding 20MW.

2. Applications for permits need to be assessed for their potential impacts on the environment including the impact of concentrations and deposition downwind of the installation.

3. There is a clear need for a simple model that could be used for 'screening' the applications to determine if the environmental impacts are likely to be a problem or not. This simple model provides an estimate of the potential deposition and air concentrations at nearby conservation (receptor) sites, from which a decision could be made whether complex dispersion and deposition modelling is needed.

4. SCAIL-Agriculture (Simple Calculation of Atmospheric Impact Limits; previously Simple Calculation of Ammonia Impact Limits, SCAIL V2.0) was developed as such a screening tool for assessing the impact of agricultural ammonia emissions.

5. SCAIL-Combustion has been developed as a partner model to SCAIL-Agriculture as a screening tool for assessing the impact of small to medium scale combustion installations (20-50MW). However, the model has been validated using much larger power stations and therefore could be used as a screening tool for any sized power station.

Meteorological Data

6. Meteorological data were collected from 78 meteorological stations across the UK. A methodology to calculate the typical metrological year from continuous five-year datasets was developed as well as a geo-statistical procedure to reduce the number of meteorological stations (to 30), whilst maintaining the spatial variability of conditions across the UK.

7. The nearest meteorological station to the emission point is selected by the screening tool.

Parameterisation of SCAIL-Combustion

8. SCAIL-Combustion uses a version of the AERMOD modelling software to calculate the dispersion of the combustion installation plume.

9. Despite the project focus being on relatively small combustion plant, the project uses atmospheric dispersion modelling methods that are applicable to a wide range of different point sources.

10. The concentration predictions of SCAIL-Combustion generally agree well with detailed modelling using AERMOD and ADMS and also measurements where monitoring data are available. In one case there was not good agreement and this

was found to be due to local meteorology differing from the nearest meteorological station selected by SCAIL-Combustion.

11. SCAIL-Combustion provides a best estimate of concentrations, therefore an additional output of “Worst Case” concentrations and deposition is also calculated by the model to put a conservative upper limit on the impact, which is useful for screening purposes.

Incorporation of SCAIL v2.0 onto the Internet

12. SCAIL-Combustion can be accessed on the internet via the SCAIL homepage. The online version of the model provides a user friendly interface with an online help system to guide the user through the operation of the model. Both SCAIL-Agriculture and SCAIL-Combustion can be accessed at: http://www.scail.ceh.ac.uk/.

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1. Background

1.1 The need for a simple model

Emissions of NO_x and SO_2 from combustion sources and their subsequent deposition to sensitive ecosystems impose an environmental burden both nationally and internationally. At a local scale the deposition of nitrogen and sulphur in the forms of nitrate (NO_3^-) and sulphate (SO_4^{2-}) can result in acidification of soils in sensitive ecosystems. The precursor gases; NO_x (= sum of NO and NO_2) and SO_2, are controlled under the UNECE and EC emissions abatement agreements of the Gothenburg Protocol by the National Emissions Ceilings Directive, the Directive on Integrated Pollution Prevention and Control (IPPC), the Pollution Prevention and Control (Scotland) Regulations 2000, the Pollution Prevention and Control Regulations (Northern Ireland) 2003 and the Environmental Permitting (England and Wales) Regulations 2007. Permits are required for combustion installations with a rated thermal input exceeding 20MW. Applications for permits need to be assessed for their potential impacts on the environment including the impact of deposition downwind of the installation. If there is the potential for deposition to have an impact on a site with a conservation designation (made or proposed) under the Conservation Regulations 1994 – known as European sites (e.g. Special Area of Conservation – SAC) – or a national Site of Special Scientific Interest (SSSI) then this potential impact needs to be considered.

Previously this could only be assessed using complex atmospheric dispersion and deposition modelling, which was both costly and time consuming. There was a clear need for a simple model that could be used for ‘screening’ the applications to determine if an environmental impact was likely. This type of screening model has already been developed for ammonia emission and deposition in the Simple Calculation of Ammonia Impact Limits (SCAIL) model, now re-named Simple Calculation of Atmospheric Impact Limits-Agriculture (SCAIL-Agriculture).

In the current project a complementary screening model, SCAIL-Combustion has been developed to provide estimates of potential environmental impacts from SO_2 and NO_x emissions on nearby conservation sites, from which a decision could be made whether complex dispersion and deposition modelling is needed.

1.2 Requirements of SCAIL-Combustion

SCAIL-Combustion calculates atmospheric concentrations and deposition rates for SO_2 and NO_x at the location of designated habitats, providing critical load/level exceedance estimates for nutrient nitrogen (N) and acidification.

The project delivers software meeting the following requirements:

1. A simple model for predicting atmospheric concentrations downwind of a point source.
2. Methods to determine deposition rates for NO_x and SO_2 (using both acidification and nutrient-N), including information for a broad range of habitat types (from information held in the Air Pollution Information System, APIS).
3. OS grid referencing in order to use data from web-based information sources for critical load and habitat information.
4. Multiple source attribution for estimating total deposition rates across the model domain.

5. A system that can be accessed by Agency staff that also provides the appropriate links to information held on APIS, UK maps and Scottish National Heritage Information (SNHi) site.
6. Information held in APIS associated with the source-attribution project for the LCP Directive (e.g., site specific critical loads data, sensitivity data and other source data associated with long-range transport).
7. Output page and export file that can be used for licence justification, including relevant information such as the model parameters, pollutants and habitat sensitivity.
8. Links to the SEPA Guidance on how to interpret the results.

2. Atmospheric modelling and selection of the appropriate methodology

Modelling methods for atmospheric dispersion and deposition are typically applied using a number of different methodologies. Three relevant types have been considered:

- Models based on simple look-up tables
- Simple Gaussian plume models of atmospheric dispersion
- Advanced Gaussian plume models

The advantages and disadvantages of each of these modelling methods for the types of source and receiving environment being considered are highlighted in the following sections.

2.1 Models based on simple look-up tables

A number of screening tools use look-up tables to calculate dispersion in the atmosphere. These include the Environment Agency (EA) H1 screening tool for environmental permitting (EA, 2008) and the SCAIL model (Theobald *et al*., 2006) used to calculate the impact of livestock units on semi-natural areas. Look-up tables are generated by running a detailed atmospheric dispersion model for a limited range of input conditions. For example, the look-up tables in the EA H1 screening tool were generated by running the ADMS model for a “worst-case” set of meteorological conditions. They provided output to show how the peak ground-level air concentration from an industrial point source varies with stack height. Likewise, Theobald *et al*. (2006) used the LADD model to calculate air concentrations downwind of near ground-level agricultural area sources (without significant buoyancy or momentum) for a range of distances with these data forming a series of curve-fits used by SCAIL-Agriculture.

This project requires the development of a modelling system which can be used to evaluate deposition and air concentrations at a range of downwind distances. This is similar to SCAIL – Agriculture, but the source characteristics have considerably more parameters than those considered by SCAIL - Agriculture (stack height, stack diameter, efflux velocity and efflux temperature). Consequently any dispersion look-up tables for such sources would be extensive. A further option would be to include calculation routines such as those considered in the HMIP D1 guidelines on discharge stack heights (HMIP, 1993) or by Briggs (1969) to evaluate effective stack heights from information on stack diameter, efflux velocity and efflux temperature. This type of system would then require a look-up table of dispersion factors from input information of downwind distance and effective stack height. However, this type of system would still require the development of computer models to deal with the plume rise calculations and the interpolation of concentration outputs.

2.2 Simple Gaussian plume models

Gaussian plume models, discussed in detail in Clarke (1979) and Pasquill and Smith (1983), are widely used to predict short-range atmospheric dispersion over distances of up to a few tens of kilometres from a source. The equation for turbulent diffusion can be solved analytically assuming steady state conditions, homogeneous turbulence, and a constant wind speed with height. The resulting equation, predicting ground-level air concentrations downwind of a surface point source in an unbounded atmosphere (that is, without the physical blocking of dispersion by an upper inversion layer), is a Fickian expression of turbulent diffusion (see Equation 1).

$$\chi\{x, y, z = 0\} = \frac{F_\chi}{2\pi \bar{u}\, \sigma_z\, \sigma_y} \exp\left(\frac{-y^2}{2\sigma_y^{\ 2}}\right) \qquad \text{(Equation 1)}$$

Where F_χ is the emission flux; σ_y and σ_z are the lateral and vertical standard deviations of the plume; and *x, y* and *z* are the downwind, crosswind and vertical positions of the receptor point along the centreline of the plume.

Simple Gaussian plume models use “turbulence typing” schemes to determine appropriate values for σ_y and σ_z following the determination of the “stability class” of the atmosphere. The separation of atmospheric stability, which has a continuous variation, into discrete stability classes was originally proposed by Pasquill (1961). In general, the stability of the atmosphere is separated into six classes ranging from A-F. These classes correspond to a range of conditions from highly unstable (A) to neutral (D) through to highly stable (F). Golder (1972) derived a relationship between the Pasquill (1961) stability classes and the Monin-Obukhov stability length (*L*) for a range of roughness lengths. Several researchers have proposed schemes for calculating σ_y and σ_z. For details, refer to the reviews of Gifford (1976) and Pasquill and Smith (1983).

Dispersion from an elevated point source, including the reflection of material at the surface and at the upper inversion layer height (*a*), can be calculated by introducing virtual source reflection terms. These reflection terms are denoted as *f* {*h,z,a*} and are shown in Equation 2. Air concentrations from elevated sources can be calculated from the product of Equations 1 and 2.

$$f\{h,z,a\} = \exp\left[\frac{-(z-h)^2}{2\sigma_z^{\ 2}}\right] + \exp\left[\frac{-(z+h)^2}{2\sigma_z^{\ 2}}\right] + \exp\left[\frac{-(2a+z+h)^2}{2\sigma_z^{\ 2}}\right] + \exp\left[\frac{-(2a+z-h)^2}{2\sigma_z^{\ 2}}\right] + \exp\left[\frac{-(2a-z+h)^2}{2\sigma_z^{\ 2}}\right] + \exp\left[\frac{-(2a-z-h)^2}{2\sigma_z^{\ 2}}\right] \qquad \text{(Equation 2)}$$

The Gaussian plume formula has several advantages over other modelling methods, including the conceptual simplicity of the method and, due to the symmetry of the plume calculations, the ease with which it can be modified to include processes such as wet and dry deposition, and plume rise. The main disadvantage of using simple Gaussian plume models (e.g., NRPB-R91 (Clarke, 1979)) is that the dispersion parameters σ_y and σ_z do not vary with height in the atmosphere. Hence such models may produce unrealistic dispersion estimates for sources released at heights significantly above ground level.

2.3 Advanced Gaussian plume models

In most industrial air quality applications, concern centres on dispersion in the planetary boundary layer (PBL), the turbulent air layer next to the earth's surface. The characteristics of the PBL are controlled by local surface friction and heating in conjunction with the overlying stratification. This layer typically ranges from a few hundred metres in depth at night up to about 2 km on hot summer days. Understanding of the PBL structure increased significantly in the 1970's through field observations, laboratory experiments and numerical simulations - summaries of which can be found in the review books of Nieuwstadt and van Dop (1982) and Venkatram and Wyngaard (1988). By the mid 1980's, scientific understanding of the PBL and new dispersion approaches had advanced sufficiently for the development of more sophisticated regulatory dispersion models.

In the USA, the Environmental Protection Agency (US-EPA) and the American Meteorological Society (AMS) developed the "AERMOD" advanced Gaussian plume model (Cimorelli et al., 2002). Whilst in the UK, the Atmospheric Dispersion Modelling System (ADMS) (Carruthers et al., 1994) was developed by Cambridge Environmental Research Consultants (CERC) through funding supplied by Her Majesty's Inspectorate of Pollution (HMIP) and a consortium of industrial sponsors.

Both ADMS and AERMOD are steady-state plume models applicable to calculating dispersion and deposition in rural and urban areas. Both models can deal with flat and complex topography (including terrain and building effects), surface and elevated releases from multiple sources and source characteristics (i.e., point, area and volume). Concentration distributions are assumed to be Gaussian in both the vertical and horizontal under stable-boundary-layer (SBL) atmospheric conditions. While under convective-boundary-layer (CBL) conditions, the distribution is assumed to be Gaussian in the horizontal and skewed in the vertical following Willis and Deardorff (1981) and Briggs (1993).

A further significant advancement was that these models apply continuous scaling (Monin-Obukhov Scaling) to characterise the PBL. These models have been widely shown to significantly improve prediction accuracy over "simple Gaussian plume models" (see Hill *et al*. (2005) for an example).

A significant advantage to the application of the AERMOD model for this project is that the source code is freely available, hence, the model can be compiled to run on most operating systems and there are no licensing requirements.

2.4 Summary

After examining the advantages and disadvantages of all of the models available the project team decided to integrate the US-EPA atmospheric dispersion modelling system AERMOD within the screening tool being developed to provide modelling of the relevant atmospheric dispersion and wet and dry deposition. The AERMOD model is well suited for such development tasks as the software has an established pedigree as state-of-the-art in modelling atmospheric dispersion from industrial sites. The use of the AERMOD model will allow the project to be fully compliant with the user requirements included in Section 1. The technical implementation report of adapting a version of AERMOD into SCAIL-Combustion and specifications for the interface and output are described in Appendix A.

3. Development of SCAIL-Combustion

Six specific modelling issues have been investigated in order to determine the most suitable model parameters to be incorporated into the SCAIL-Combustion model. The six issues are:

- The meteorological data to be used in the screening model
- Dry deposition velocities to be used in the screening model
- Atmospheric chemistry in the screening model
- Effects of orographic rain in the screening model
- Consideration of background concentrations of NO_x and SO_2 in the screening model
- Links to the Air Pollution Information System (APIS).

3.1 Meteorological data

An assessment of approaches previously used for preparing meteorological data was carried out and is summarised below. The initial approach taken to prepare meteorological data was rejected following testing and is summarised in Appendix B. An alternative approach was then developed and tested and is described below in Section 3.1.4.

3.1.1 Assessment of approach used in SCAIL-Agriculture (SCAIL v2.0)

This approach divided the UK into 15 regions. Three meteorological stations were selected from each region (according to certain criteria) and five-year wind speed and direction data were averaged for each region. Figure 1 shows the locations of the selected stations in each region. The question to be answered is: “How representative are these datasets of the meteorological conditions within the regions?” To answer this, independent meteorological datasets (i.e. from stations not used in the SCAIL-Agriculture) were compared with the ‘regional’ averages used in SCAIL-Agriculture. A comparison of the wind direction probabilities (WDP) and the mean wind speeds (MWS) of the independent datasets and the meteorological data of SCAIL-Agriculture for four UK regions are presented in Figures 2 and 3.

In the East Anglia region the independent datasets have a similar distribution of WDP, which is also similar to that used originally in SCAIL-Agriculture (red line) (Figure 2). This is probably due to the flat nature of the region. The same is true for the MWS, although the two stations on the coast (Hemsby and Weybourne) have noticeably higher wind speeds than the other stations. Within other example regions the different stations show a large variation in the distribution of WDP and MWS (Figures 2 and 3). The original SCAIL-Agriculture regional data cannot represent this variability. In conclusion, the approach used in SCAIL-Agriculture is probably adequate for flat regions of the UK e.g. East Anglia. However, this approach is not adequate for regions with complex terrain, which would apply to the majority of the UK.

Figure 1 - Locations of meteorological stations used for meteorological data in SCAIL-Agriculture, colour-coded by region. SCAIL-Agriculture was divided into 15 meteorological regions.

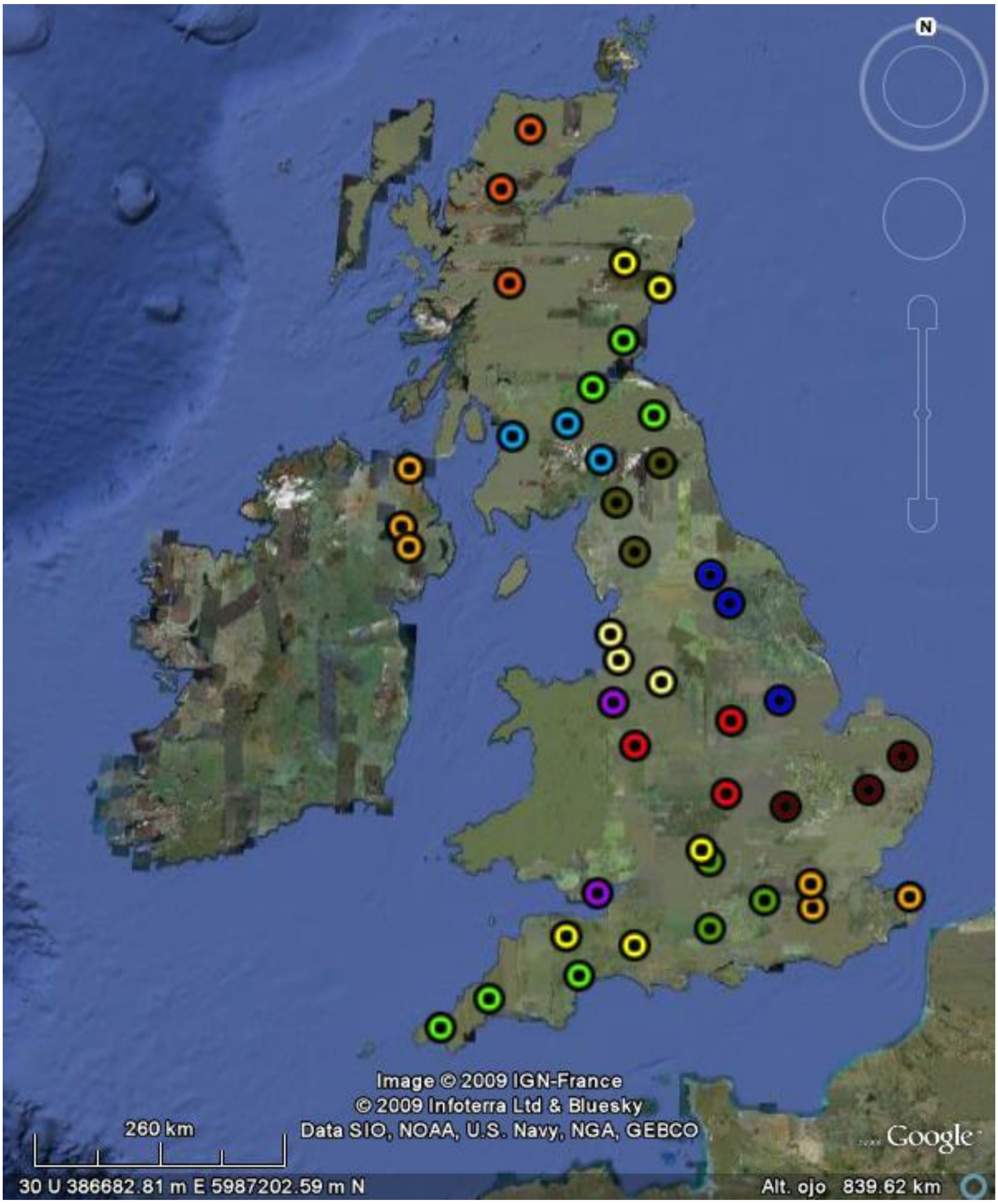


Figure 2 - Comparison of the wind direction probabilities for the period 1990-1999 at various meteorological stations for selected UK regions and the data used in SCAIL v2.0 (bold red line).

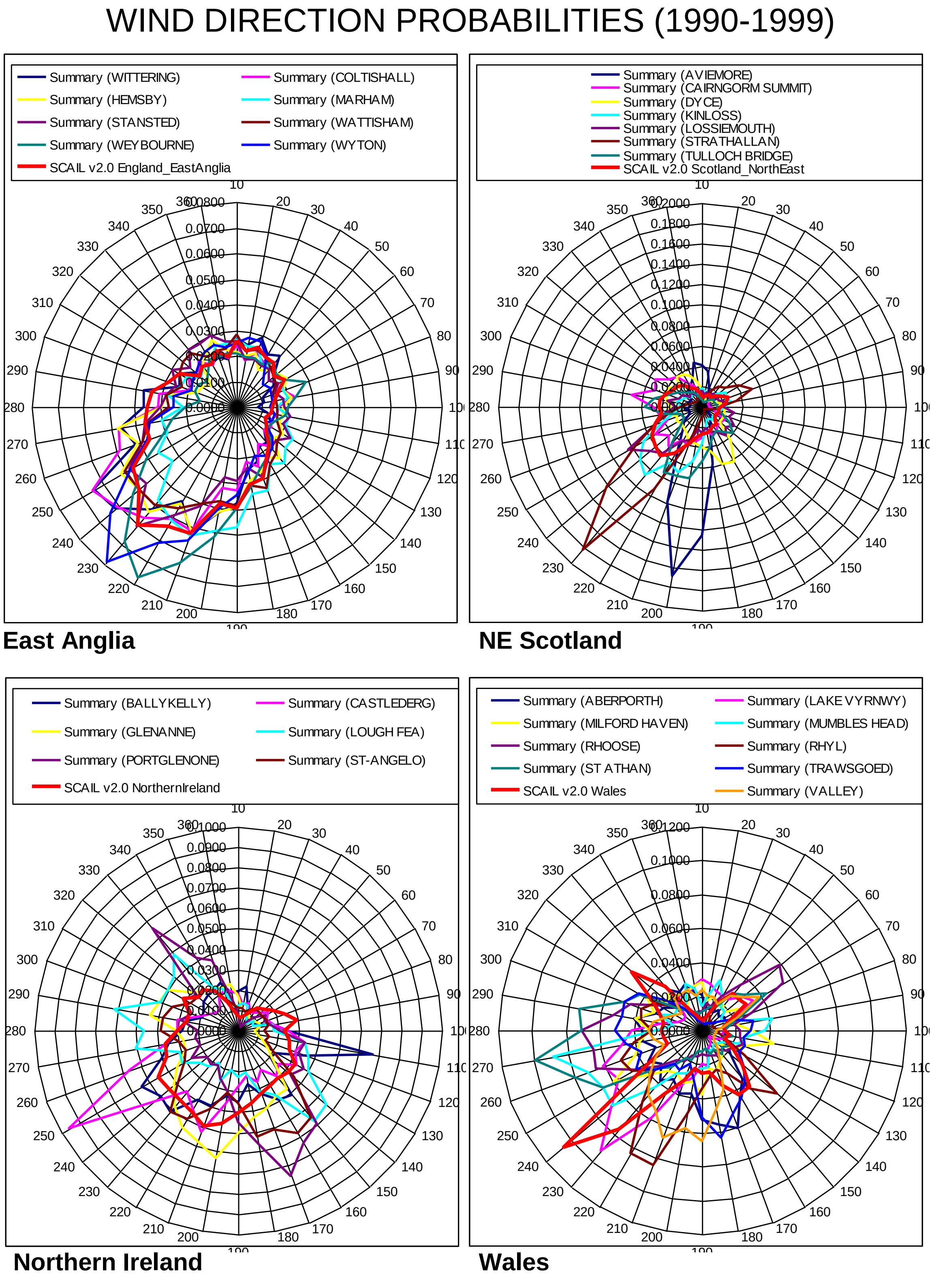
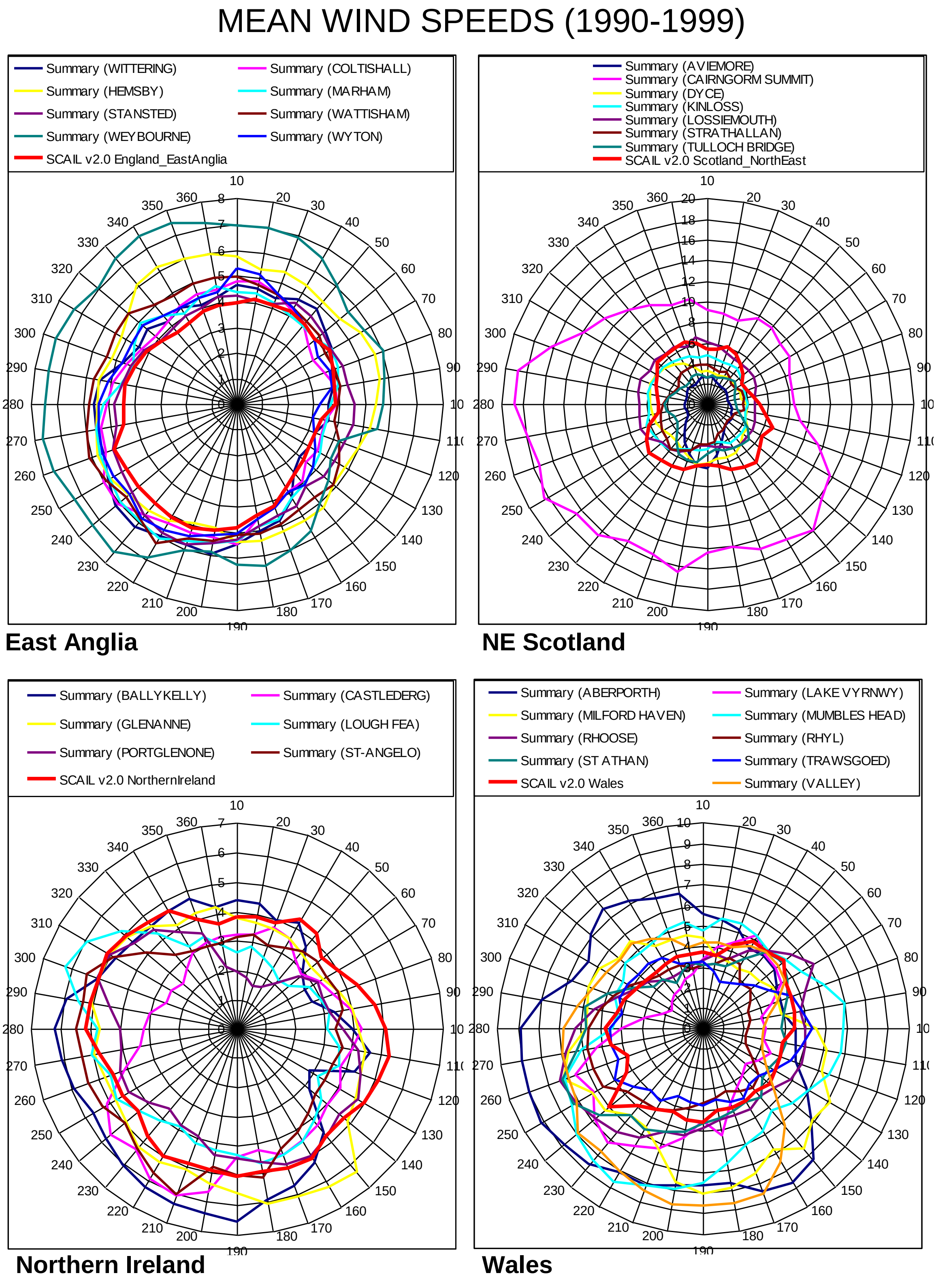


Figure 3 - Comparison of the mean wind speeds (m s^{-1}) for the period 1990-1999 at various meteorological stations for selected UK regions and the data used in SCAIL v2.0 (bold red line).



3.1.2 Typical Meteorological Year (TMY) approach

The SCAIL-Combustion screening model uses a different approach to that used in SCAIL-Agriculture, using data from a single nearby meteorological station. Detailed dispersion model assessments normally use 5 years of data from the nearest station. It is theoretically possible to prepare 5-year datasets from each UK station where the relevant variables are recorded. However, this would result in long model-run times, which are not desirable for a screening model. A simulation period of one year would reduce the screening model run-time but still provide mean annual output data. If one year of data is used then it should be a 'typical' year for that location.

What is a typical year? A typical meteorological year (TMY) should be one that best represents a longer time period (e.g. 5, 10, 50 years). A model simulation using data from a typical year should give similar mean annual output data as the mean annual output from a simulation of the longer time period. The concept of TMYs has been frequently used in building simulations, in order to assess the expected heating and cooling costs for the design of the building. More information on how datasets have been produced can be found at: http://rredc.nrel.gov/solar/pubs/tmy2/appendixa.html. A similar approach was tested for use in SCAIL-Combustion but when this approach was validated with case-study model simulations it was unable to predict the typical meteorological years satisfactorily (see Appendix B).

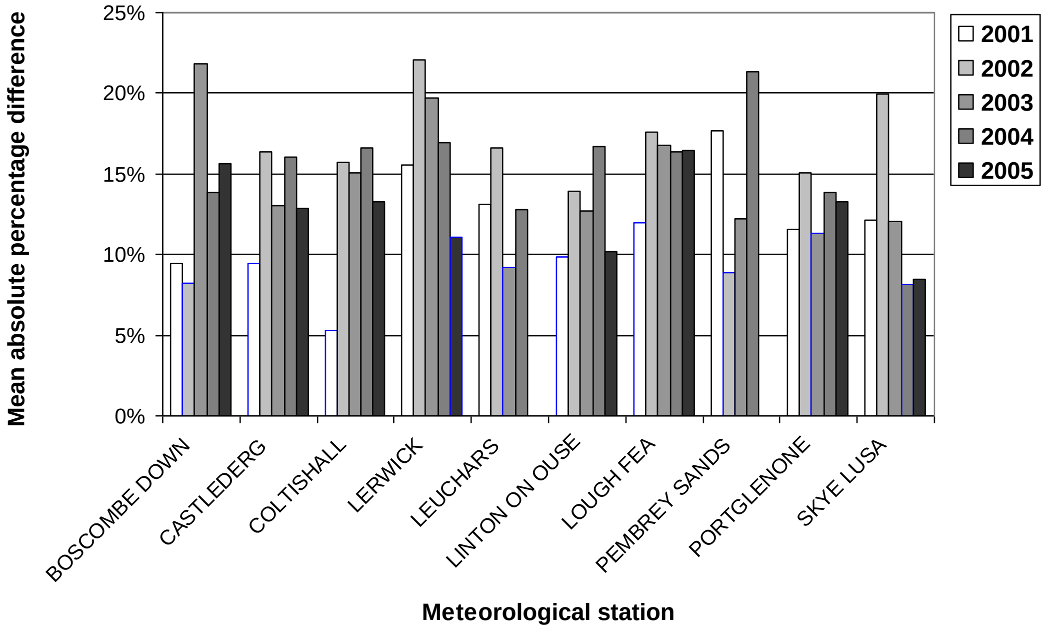
3.1.3 Atmospheric dispersion modelling for a subset of meteorological stations: comparison of modelled concentrations with the five-year average

In order to assess which year gives the most similar concentration predictions to the five-year average, dispersion modelling was undertaken using meteorological data from 10 UK stations (3 in Scotland, 3 in Northern Ireland, 3 in England and 1 in Wales). The details of the model scenarios are as follows:

- 10 Meteorological stations: Boscombe Down, Castlederg, Coltishall, Lerwick, Leuchars, Linton on Ouse, Lough Fea, Pembrey Sands, Portglenone, Skye Lusa.
- 6 Model scenarios: 2001, 2002, 2003, 2004, 2005 and 2001-2005.
- Source description: single 50 m incineration stack emitting NO_2 and SO_2 at a rate of 100 t yr^{-1}.
- Source parameters: stack diameter: 1m, exit temperature: 1000K, exit velocity: 35 m s^{-1}.
- Nine receptors: Randomly selected at distances from 2-40km in directions 0, 45, 90, 135, 180, 225, 270 and 315^o from source.

The mean absolute percentage difference between the long-term average and the annual average NO_2 and SO_2 concentrations for each year were used to determine the typical meteorological year at each receptor. Figure 4 shows these data for each of the ten meteorological datasets. Minimum values for the mean absolute percentage difference range from 5-12% for the different meteorological stations.

Figure 4 - Mean absolute percentage difference between annual predicted concentrations and five-year average values for each of the 10 meteorological validation datasets. Bars outlined in blue indicate years with lowest values for each meteorological station (i.e. the typical meteorological year).

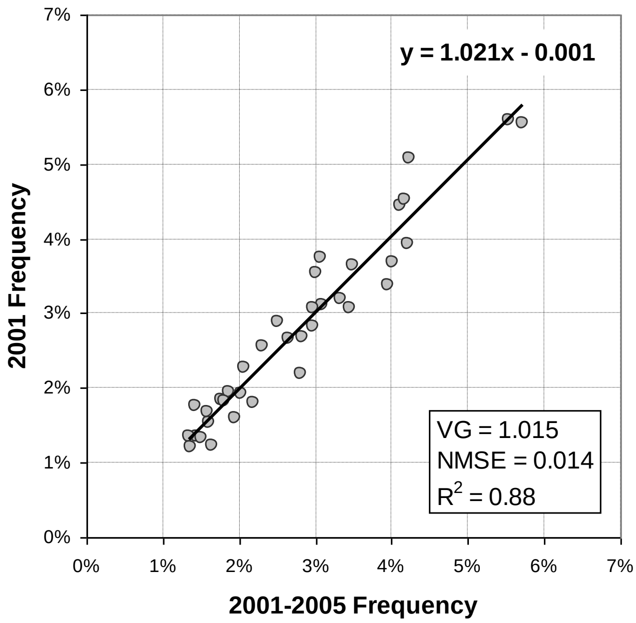


3.1.4 Wind rose similarity approach

Using the assumption that the main factor determining the inter-annual variability of concentration predictions is the annual wind direction frequency distribution, a second approach to predicting the typical meteorological year (TMY) was developed. This approach uses the similarity of the wind direction distributions for the individual years to the five-year mean as a way of predicting the typical meteorological year. The hypothesis was that the more similar the distribution for a particular year was to the five year mean, the closer the concentration predictions would be to the five-year average concentration predictions.

In order to assess the similarity of the wind direction distributions, statistical tools are needed. Three statistical performance parameters were chosen that are commonly used for model performance evaluation (see e.g. Chang and Hanna, 2005). These are geometric variance (VG), normalised mean squared error (NMSE) and the correlation parameter R^2. A perfect match between two wind direction distributions would result in VG=1, NMSE=0 and R^2=1. An example is shown in Figure 5 using the frequency distribution of the 36 wind sectors in the meteorological datasets.

Figure 5 - Comparison of the 2001 wind direction frequency distribution (36 wind sectors) with that of the long-term average (2001-2005) for the Boscombe Down meteorological data.



The performance parameters were calculated for each year and for each meteorological station. The parameter values were then compared with the mean absolute percentage differences between the annual concentration predictions (NO_2) and the five-year mean to test whether the parameter values closest to a perfect match corresponded with the years with the lowest mean absolute percentage differences in concentrations. Table 1 shows the years with the lowest mean absolute percentage difference in concentrations for each site and the corresponding performance parameter values for these years. Using the parameter values that are closest to a perfect match (i.e. VG=1, NMSE=0 and R^2=1) as a predictor of the typical meteorological year, NMSE predicts six of the ten years correctly, VG predicts eight and R^2 predicts only four correctly. From this analysis it can be concluded that VG is the most suitable performance parameter for predicting the typical meteorological year. For the two typical meteorological years that it predicted incorrectly, the difference between the mean absolute percentage difference of the actual typical meteorological year and that predicted was less than 4%.

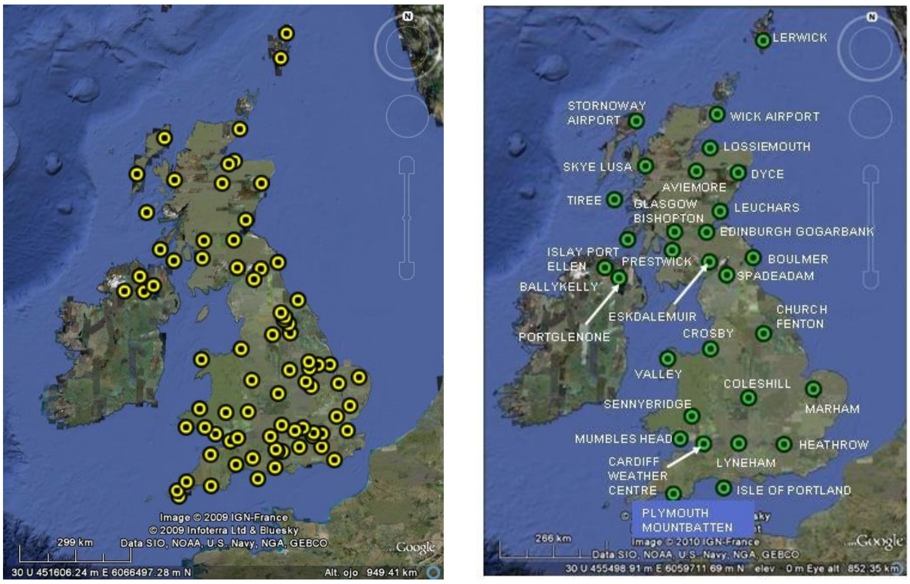
Table 1 - Years with the lowest mean absolute percentage difference from the five-year mean concentration (typical meteorological year) for each meteorological station and their performance parameter values. Values highlighted in green represent years out of the period 2001-2005 with performance parameters closest to a perfect match (i.e. the predicted typical meteorological year).

Site	Year with lowest % difference	NMSE	VG	R^2
BOSCOMBE DOWN	2002	0.020	1.019	0.839
CASTLEDERG	2001	0.029	1.028	0.856
COLTISHALL	2001	0.012	1.014	0.869
LERWICK	2005	0.036	1.050	0.773
LEUCHARS	2003	0.009	1.014	0.935
LINTON ON OUSE	2001	0.015	1.012	0.894
LOUGH FEA	2001	0.048	1.035	0.854
PEMBREY SANDS	2002	0.024	1.032	0.814
PORTGLENONE	2003	0.062	1.030	0.833
SKYE LUSA	2004	0.010	1.017	0.932

3.1.5 Meteorological station selection

A visual analysis of the distribution of the 78 suitable meteorological stations (Figure 6) shows that there are many meteorological stations that are grouped together and probably represent very similar meteorological conditions. In order to reduce the number of datasets used by SCAIL-Combustion a statistical analysis has been carried out to remove similar meteorological stations whilst maintaining the existing spatial variability across the UK. The wind direction frequency distributions of all possible pairs of stations were compared by calculating the geometric variance of the five-year distributions of the two stations. Next, all station pairs that were less than 100 km apart and had a geometric variance less than 1.5 were flagged. These criteria represented pairs of stations that were nearby and had similar wind direction frequency distributions. Furthermore tests using station pairs at the extremes of this range showed that these criteria yielded concentration predictions that would typically be within a factor of two. All station pairs were then put through an analytical procedure, which rejected all flagged station pairs (i.e. nearby stations which had similar wind direction frequency distributions) leaving a sub-set of meteorological stations which represent the UK spatial variability of wind direction distributions. The resulting sub-set contains 30 stations (including 4 stations that were requested to be included by SEPA), which are distributed as shown in Figure 6 and the details of which are included in Table C1 of Appendix C. The TMY wind roses for the 30 stations selected have also been included in Appendix C.

Figure 6 - (Left) Location of meteorological stations with hourly data of all variables necessary for SCAIL-Combustion simulations. (Right) Sub-set of 30 stations representing the spatial variability across the UK.



3.2 Dry deposition velocity

3.2.1 Background

Obtaining realistic estimates of the dry deposition of gases or particles from the atmosphere to the biosphere is key to understanding the transfer of pollutants from source to receptor and their subsequent impact on the environment. However, despite the importance of the deposition term in calculations to determine the impact of atmospheric pollutants on receptors, it remains a major cause of uncertainty in the source-receptor pathway, especially in areas of complex terrain or in vegetation transition zones. The SCAIL-Combustion screening tool provides estimates of pollutant concentration and fluxes at user defined distances from the source of the pollutant, allowing estimates of gas deposition velocity (V_d) using:

$$V_d = F / C_a \qquad \text{(Equation 3)}$$

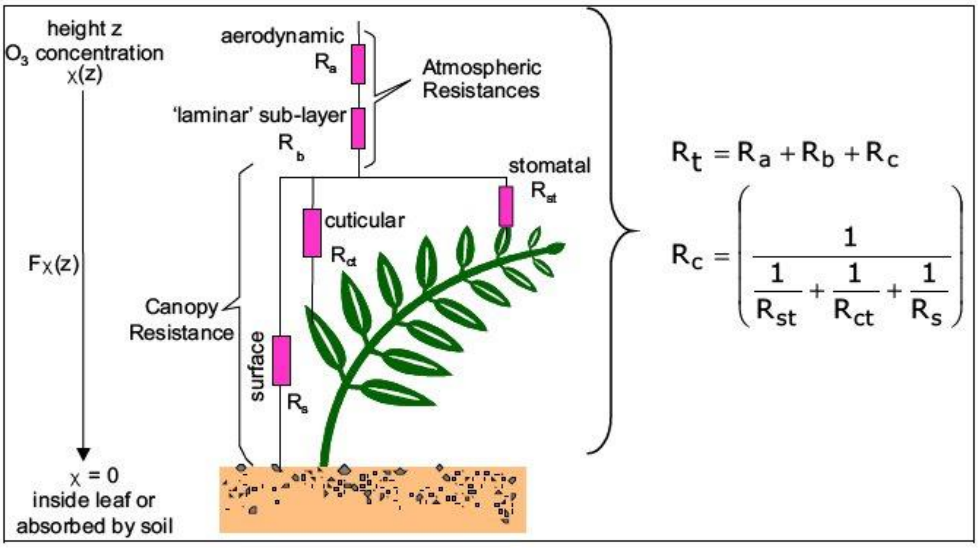
where F is the flux (µg m^{-2} s^{-1}), C_a is the atmospheric concentration of the chemical species being investigated (µg m^{-3}) and V_d is the deposition velocity (m s^{-1}).

Dry deposition of gases is an important loss process for many reactive and soluble trace gases, with the rate of deposition controlled by, (i) turbulent diffusion between the free atmosphere and the viscous boundary layer surrounding the surface, (ii) molecular diffusion of the gas molecule through the viscous boundary layer, and (iii) the physiochemical affinity of the absorbing surface for the gas molecule. This model is complicated further in crop canopies where there are three sites at which gas molecules may be absorbed, (i) plant cuticles, (ii) the walls of the sub-stomatal cavity and (iii) the soil surface (Figure 7). Consequently, V_d can be thought of as the product of a series of resistances:

$$V_d = (R_a + R_b + R_c)^{-1} \qquad \text{(Equation 4)}$$

where R_a is the aerodynamic resistance for gases, R_b is the laminar sub-layer resistance, and R_c is the total canopy resistance of the gas. R_c includes separate deposition pathways that include cuticle, stomatal and soil resistances. Because of the sensitivity of V_d to changes in vegetation type and moisture, calculations in SCAIL-Combustion to determine concentrations and fluxes are estimated using land use and season specific deposition resistance terms.

Figure 7 - Simple resistance analogy for the deposition of gaseous pollutants.



Reproduced from Fowler and Erisman (2003).

3.2.2 Model configuration

In order to establish the effects of seasonality on modelled deposition velocities, and to assess the sensitivity of SCAIL-Combustion to changes in land use, SCAIL-Combustion was configured using an arbitrary meteorological dataset. The gas deposition parameters used in SCAIL-Combustion are provided in Table 2 and the nine land use classifications and five seasonal categories used in AERMOD are provided in Table 3. Deposition velocities were calculated for a receptor site located 2 km downwind of the point source.

Table 2 - Gas deposition parameters employed in SCAIL-Combustion.

Parameter	NO_2	SO_2
Diffusivity in air ($cm^2\ s^{-1}$)	0.1361	0.1089
Diffusivity in water ($cm^2\ s^{-1}$)	1.90E-05	1.33E-05
Cuticular resistance ($s\ m^{-1}$)	9999	1
Henry's Law (Pa-m3 mol^{-1})	10132.5	82.4

Table 3 - Land use and season categories used in SCAIL–Combustion.

Land Use		Land Use	
No	**Description**	**No**	**Description**
1	Urban Land	1	Midsummer with lush vegetation
2	Agricultural Land	2	Autumn with un-harvested cropland
3*	Rangeland	3	Late Autumn after frost, no snow
4	Forest	4	Winter with snow on the ground
5	Suburban Areas, Grassy	5	Transitional spring with partial green coverage
6	Suburban Areas, Forested	6	
7	Bodies of Water	7	
8*	Barren Land, Mostly Desert	8	
9	Nonforested Wetlands	9	

* Land use classification not included in model runs to determine the sensitivity of SCAIL-Combustion to changes in land use.

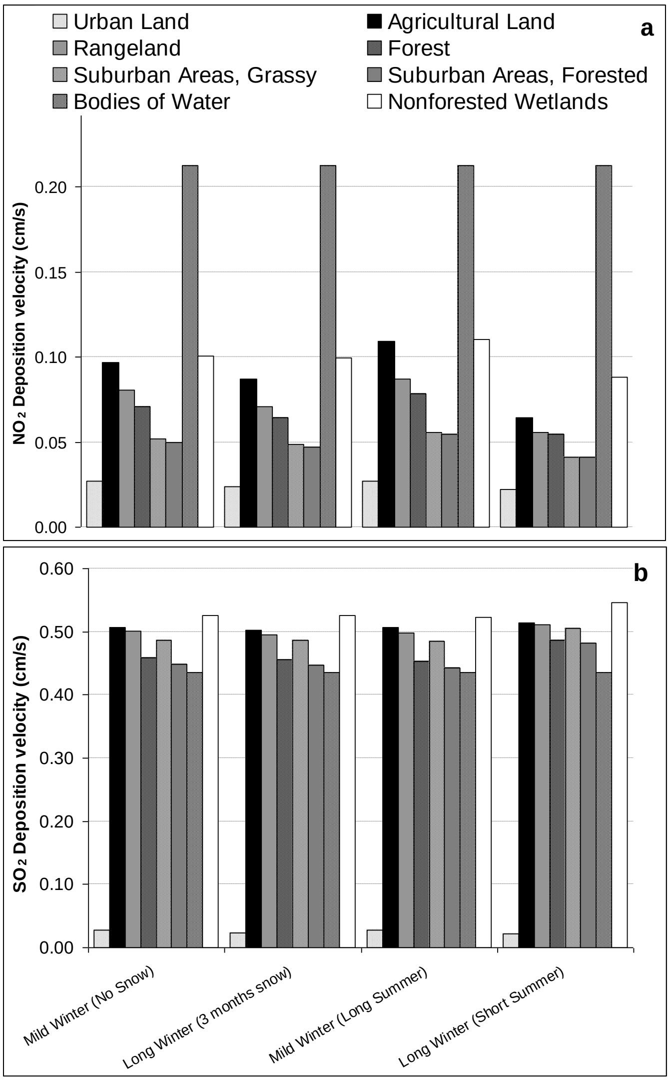
3.2.3 Model Scenarios

The effects of the different seasons and season length on model estimates of V_d for the land use classifications described in Table 3 was assessed using the following scenarios:

- Winter with no snow and three months of summer with lush vegetation
- Winter with three months of snow and three months of summer with lush vegetation
- Winter with no snow and four months of summer with lush vegetation
- Winter with four months of snow and a short summer season with two months of lush vegetation.

The results of the model runs for NO_2 and SO_2 are shown in Figure 8 and illustrate that generally, estimates of V_d for both pollutants are not sensitive to changes in season length. Overall the parameterisation for “Winter with no snow and four months of summer with lush vegetation” and “Long Winter (Short Summer)” provided the highest deposition velocities for nitrogen and sulphur, respectively. As nitrogen deposition was found to vary more with seasonal class than sulphur deposition, the “Winter with no snow and four months of summer with lush vegetation” parameterisation is recommended for application overall and has been implemented in SCAIL-Combustion.

Figure 8 - Estimates of deposition velocity with changing land use category and different seasonal scenarios. 8a shows NO_2, 8b shows SO_2.



The effect of different land use categories on model estimates of V_d was also assessed. For NO_2, model estimates of V_d were sensitive to the different land use categories with the greatest deposition velocities estimated to occur to Bodies of Water, Non-Forested Wetlands and to Agricultural Land (Figure 8a). The lowest values of V_d were to Urban Land. For SO_2 estimated V_d were greater than for NO_2 but were not as sensitive to different land uses with the greatest V_d estimated for Non Forested Wetlands, Agricultural Land, Rangeland and Suburban Grassy Areas (Figure 8b).

Mapping of AERMOD land-use types onto the 12 habitat types defined in SCAIL-Combustion that are relevant to critical loads have been implemented as shown in Table 4:

Table 4 - Mapping of AERMOD land categories to SCAIL-Combustion (and APIS) land categories

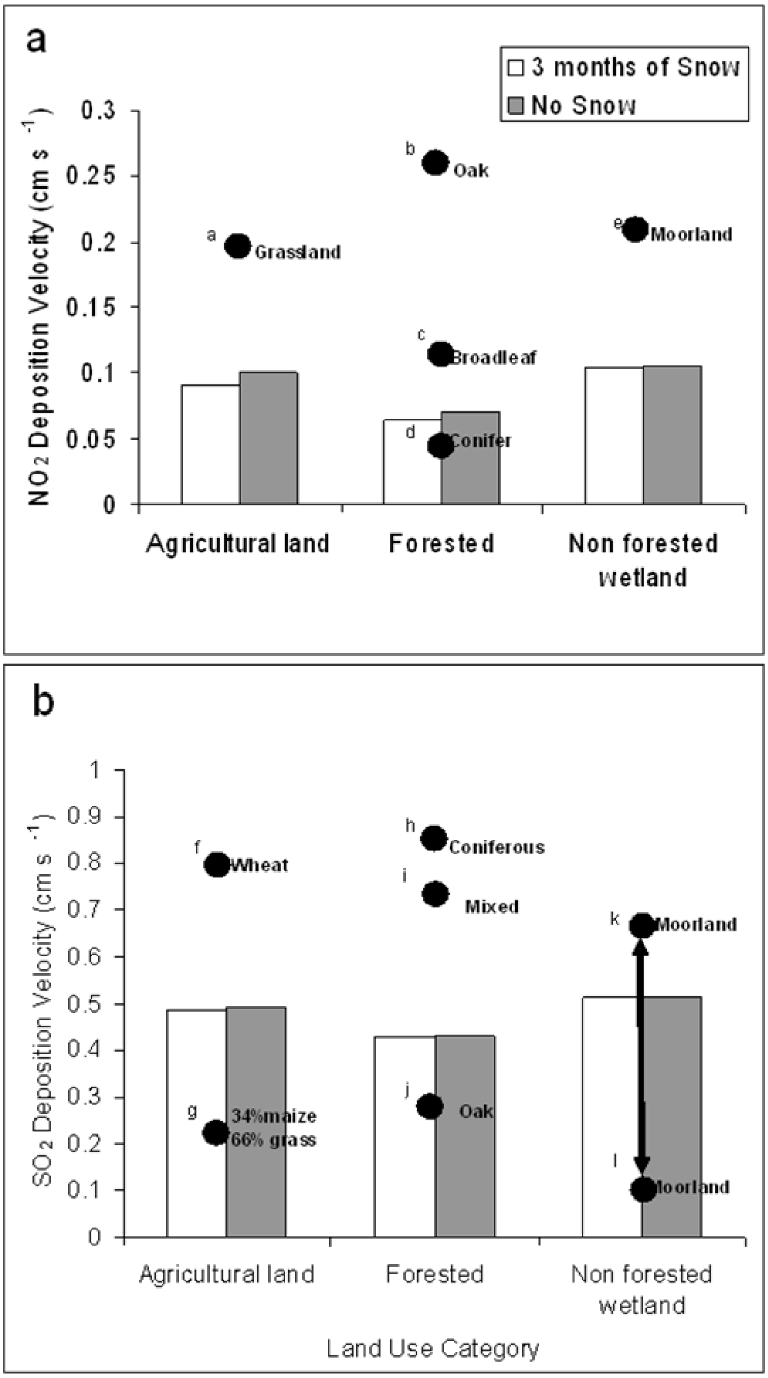
	SCAIL-Combustion	AERMOD
1	Acid grassland	Agricultural Land
2	Alkaline fens and reed-beds	Non-forested Wetlands
3	Deciduous/Coniferous woodland	Forest
4	Calcareous grassland	Agricultural Land
5	Grazing marsh	Agricultural Land
6	Limestone pavements	Urban Land
7	Lowland heathland	Non-forested Wetlands
8	Montane heaths and scrubs	Non-forested Wetlands
9	Raised bog and blanket bog	Non-forested Wetlands
10	Sand dunes	Barren Land, Mostly desert
11	Unimproved hay meadow	Agricultural Land
12	Upland heathland	Non-forested Wetlands

3.2.4 Comparison of estimated V_d with literature values

To compare V_d estimated using SCAIL-Combustion with literature values, V_d were calculated for NO_2 and SO_2 at a receptor site 2 km downwind from the stack. The land use categories chosen for the comparison were Agricultural Land, Forest land and Non-Forested Wetland. The investigation was conducted for two seasonal scenarios, one with 3 months of snow on the ground and one with no snow. The model V_d values were then compared against the literature values reviewed in Ball *et al*. (2008a).

For NO_2, modelled estimates of V_d were approximately 50% lower than reported in the reviewed literature. This was in contrast to modelled estimates of V_d for SO_2, which showed good agreement with the reported deposition velocities (Figures 9a and 9b, respectively). In order to improve the agreement between AERMOD and field data of nitrogen and sulphur deposition the reactivity parameter in the model input files was increased from its default value of 0.1 to a revised value of 0.5. This was investigated in detail and is summarised in Appendix D.

Figure 9 - a) Comparison of modelled NO_2 and b) SO_2 deposition velocity with literature values (reviewed in Ball et al., 2008a).



a. Hesterberg *et al*. (1996) – average deposition velocity of February, May, June and August
b. Puxbaum and Gregori (1998) – annual average
c & d. Hanson and lindberg (1991) – daytime conditions
e. Fowler *et al*. (1991) – daily mean
f. Fowler and Unsworth (1979) – daily mean
g. Zunckel (1999) - average deposition velocity of summer, autumn, winter and spring
h. Ferm and Hultberg (1999) – average over 5 years
i & j. Griffiths and Fowlie (2008) – annual average
k & l. Fowler *et al*. (2001) – min max values of pooled monthly data

3.3 Atmospheric chemistry

It is important to recognise that SO_2, NO and NO_2, released as "primary pollutants" from combustion plants, may react with other chemical species in the atmosphere and that these reaction processes could influence both the air concentrations of the "primary pollutants" and their subsequent atmospheric deposition. The following section considers issues of atmospheric chemistry to determine whether these need to be considered in the SCAIL-Combustion Screening model.

3.3.1 SO_2 oxidation to H_2SO_4

SO_2 oxidises in the atmosphere to H_2SO_4 via either gas phase chemistry or aqueous (heterogeneous) chemistry. The gas phase oxidation is predominately driven by the reaction with the OH radical as follows:

$$OH + SO_2 \rightarrow HSO_3 \qquad (R1)$$

$$HSO_3 + O_2 \rightarrow HO_2 + SO_3 \qquad (R2)$$

$$SO_3 + H_2O \rightarrow H_2SO_4 \qquad (R3)$$

R1 is the rate limiting step of this process and the lifetime of SO_2 (or e-folding time) is determined by the concentration of the OH radical and the second-order rate coefficient k^{II}.

SO_2 can also oxidise via aqueous phase chemistry on aqueous aerosol or in cloud droplets. SO_2 is soluble in water under conditions of pH>1. Oxidation proceeds via the following reactions:

$$SO_2 + H_2O \rightarrow H_2SO_3 \qquad (R4)$$

$$H_2SO_3 \leftrightarrow H^+ + HSO_3^- \qquad (R5)$$

$$HSO_3^- \leftrightarrow H^+ + SO_3^{2-} \qquad (R6)$$

The bisulphite (HSO_3^-) and sulphite (SO_3^{2-}) ions can react with oxidising species including ozone and peroxide to form the sulphate ion (SO_4^{2-}). The rate of loss of SO_2 and hence formation of sulphuric acid (H_2SO_4) is dependent on the concentration of ozone, hydrogen peroxide, amount of cloud water and its pH and the wind field.

The lifetime of sulphur (either in SO_2 or in sulphate aerosol) is variable according to ambient conditions, which has a significant impact on sulphate concentrations at receptor sites downwind of source. For example, under lower tropospheric conditions, approximate lifetimes of SO_2 are 31 hours with respect to the gas phase reaction (R1) and 25 hours overall with all other reaction pathways considered. The lifetime of sulphate with respect to wet deposition is ~ 80 hours, and for dry deposition > 400 hours. Gas phase reaction of SO_2 to sulphate is the dominant mechanism under atmospheric conditions where relative humidity (RH) $\leq$ 75% (i.e. when the liquid water content of the atmosphere is low) and can be approximated to a conversion rate of ~ 5% SO_2 per hour. Higher relative humidities occur frequently in the UK atmosphere; therefore aqueous phase oxidation is likely to be the dominant process. However, the aqueous phase oxidation rate is highly variable and can be up to 30% per hour (seen generally under polluted urban conditions). A more generally applicable rate is ~ 12% per hour.

3.3.3 NO_2 formation and oxidation

The atmospheric chemistry of NO_2 is more complex than SO_2, however with respect to this project, it is only necessary to consider the simplest scenarios. If more complex chemistry is required then a chemical processing module would be needed (e.g. CALPUFF or similar model). The major sink for NO_2 in the atmosphere is formation of nitric acid (HNO_3) through reactions with the hydroxyl radical:

$$OH + NO_2 \rightarrow HNO_3 \quad \text{(R7)}$$

Nitric acid can then be either dry deposited or taken up on aerosol or cloud droplets to form particulate nitrate (NO_3^-):

$$HNO_3 \leftrightarrow H^+ + NO_3^- \quad \text{(R8)}$$

Nitric acid is a weaker acid than sulphuric acid and more volatile, therefore can readily be returned to the gas phase. Note that NO_2 is also in rapid equilibrium with NO (via photolysis and reactions with O_3).

The characteristic time for conversion of NO_x to other NO_y species (NO and the sum of its atmospheric oxidation products) is 4-20 hours dependant on the point in the diurnal cycle and other atmospheric trace constituent compositions. The global atmospheric lifetime of NO_y including HNO_3 is between 1-4 days. Particulate nitrate has a lifetime in the range of 3-9 days.

3.3.4 Application in SCAIL-Combustion

The range of SCAIL-Combustion is limited to 80 km from a point source, based on the assumption of straight-line trajectories and constant meteorology implicit in the AERMOD Gaussian plume model. It should however be noted that whilst the uncertainty in Gaussian plume model predictions undoubtedly increases at distances beyond 10 km or more from a source, Lutman et al (2004) showed an encouraging agreement in annual average predictions of a Gaussian model and a more sophisticated Lagrangian particles model out to distances of almost 2000 km.

Using the approximate conversion rates of SO_2 to sulphate suggested above for wind speeds ranging from 2 ms^{-1} to ~18 ms^{-1}, a range of conversion fractions for the low (<75%) and high (>75%) RH conditions have been determined for 10 km and 80 km scenarios (Table 5). If “significant conversion” of SO_2 is set at 10%, for the 80 km scenario at low RH, conversion is significant at wind speeds less than 10 ms^{-1}; at high RH, conversion is significant at all wind speeds. For the 10 km scenario: at low RH, no wind speeds have significant conversion and at high RH only the 2 ms^{-1} scenario results in significant conversion. Figure 3 demonstrates that typically average wind speeds in the UK are of the order of 5 m s^{-1} therefore results at receptor sites within 10 km of the source are not affected by “significant conversion” of SO_2. Indeed at 80km, predictions would remain within a factor of two if SO_2 conversion were ignored. Hence it was considered unnecessary to incorporate SO_2 chemistry into SCAIL-Combustion.

For NO_x, assuming the sink is through reaction with the hydroxyl radical, the fractional chemical loss at 10km and 80 km are shown in Table 6 for different wind speed scenarios. It is noted that this is a simplification; however, it is appropriate for the scope of a simple screening tool. Under most wind speed conditions the conversion is <15% at the maximum range of SCAIL-Combustion, therefore it was considered unnecessary to incorporate NO_x chemistry into SCAIL-Combustion.

Table 5 - Conversion of SO_2 to sulphate at 10 & 80 km from source

		RH<75%		RH>75%	
Wind speed ($m.s^{-1}$)	Time (hours)	SO_2 remaining	Sulphate formed	SO_2 remaining	Sulphate formed
10 km					
2	1.4	0.93	0.07	0.84	0.16
5	0.6	0.97	0.03	0.93	0.07
10	0.3	0.99	0.01	0.96	0.04
15	0.2	0.99	0.01	0.98	0.02
20	0.1	1	0	0.99	0.01
80 km					
2	11.1	0.57	0.43	0.25	0.75
5	4.4	0.73	0.27	0.57	0.43
10	2.2	0.9	0.1	0.74	0.26
15	1.5	0.93	0.07	0.84	0.16
20	1.1	0.95	0.05	0.86	0.14

Table 6 - Chemical conversion of NO_x at 10 km and 80 km from source using only reaction with hydroxyl radical.

	10 km		80 km	
Wind speed ($m.s^{-1}$)	Time (hours)	NO_x remaining	Time (hours)	NO_x remaining
2	1.4	0.95	11.1	0.56
5	0.6	0.98	4.4	0.83
10	0.3	0.99	2.2	0.91
15	0.2	0.99	1.5	0.94
20	0.1	0.99	1.1	0.96

3.4 Wet deposition and orographic enhancement

Wet deposition is parameterised in AERMOD and will use the meteorological data supplied from the nearby weather station. In regions with hill or mountain ranges an increase in the wet deposition of gas and particles can occur. However, there is currently no orographic enhancement factor used in the AERMOD wet deposition parameterisation. In other models, e.g. FRAME and CBED (CEH), there is an enhancement factor used to increase the scavenging of gases due to excess rainfall, i.e. the amount of rainfall which is above the UK average rainfall. In the excess (“orographic”) rain fraction in these models, the concentration of the solute is doubled.

Within AERMOD, this would be the equivalent of doubling Λ (equivalent scavenging ratio) or f_{sat} (fraction of saturation) or c_L (concentration of solute in liquid phase). The orographic enhancement has been added as a factor applied to the modelled wet deposition flux, i.e.

$$F_{wg}' = \frac{R_{STN}}{Rav} F_{wg} \qquad \text{(Equation 5)}$$

where F_{wg} = modelled wet deposition flux, F_{wg}' = enhanced wet deposition flux, R_{STN} = annual rainfall at station, R_{av}= annual UK average rainfall.

Orographic enhancement factors for the UK at 5 km resolution from CEH modelling are used to account for extra wet deposition in elevated areas.

3.5 Background concentrations

The annual mean background NO_x concentration map is based on 1 km resolution national mapping data from AEA Technology and has been calculated by summing the contributions from:

- Distant sources (characterised by the rural background concentration);
- Large point sources;
- Small point sources;
- Local area sources; and
- Transportation

The area source model has been calibrated using data from the national automatic monitoring networks for 2006. At locations close to busy roads an additional roadside contribution was added to account for contributions to total NO_x from road traffic sources. This dataset is used in APIS at 1km resolution for comparison with the NO_x critical level of 30 $\mu g\ m^{-3}$.

The annual mean SO_2 concentration map for the UK is derived from interpolation of SO_2 measurements from CEH CBED data in rural locations and is reported at a resolution of 5 km. This dataset is combined with an urban and road enhancement of concentration derived from urban monitoring and emission inventory estimates.

When new stack emissions are modelled, the concentration derived from the new source can be simply added to the background to determine the total concentration. However there is more of an issue with existing stacks and accounting for their contribution to background as SO_2 and NO_x deposit over larger distances and the background in any one square will contain inputs from several upwind sources. These inputs will be highly spatially and temporally variable (particularly for SO_2).

One issue, particularly with SO_2, is that the UK emission and deposition maps change significantly on an annual basis and will continue to do so. Also, many power generation plants are not operational up to the limit of their permit. It is important therefore to use the most recently available maps.

Ideally SCAIL-Combustion should be used to look at the effect of SO_2 and NO_x emissions from new point sources (stacks). However, if an existing stack is modelled in SCAIL-Combustion then it may be appropriate to report the process contributions arising from the existing stack to SO_2 and NO_x concentrations and depositions. **Users of the model should be aware of the issue of double counting as model predictions from existing sources may be included in the estimates of background concentrations or depositions.** However, as SCAIL-Combustion is a screening tool it is appropriate to include these contributions to ensure that the model predictions are conservative. Annotations are included in the model output to identify that this has occurred and may require further consideration as part of a more detailed dispersion modelling assessment.

3.6 Links to the Air Pollution Information System (APIS)

APIS is a web-based database of air pollution information and the SCAIL-Combustion model links to the APIS database in order to access air pollution data. Scripts have been added to the output.pl file to enable the connection between the SCAIL-Combustion tool and the APIS database system. This is primarily to retrieve background concentrations and deposition based on a grid reference. It also has the ability to link into the critical loads/levels table from the APIS database with the selected habitat.

This connection to the APIS database has been tested for a number of grid references and compared with the data-table in APIS. Nitrogen and sulphur deposition were used as the pollutants for this test and, based on OS (x,y) grid coordinates, the background deposition values are displayed correctly in the SCAIL results table. Nitrogen and sulphur deposition is also dependent on the habitat type; therefore this has been taken into account in the code based on the user's habitat selection.

3.7 Summary

Meteorological data:

The SCAIL-Agriculture methodology is not adequate for elevated point sources in regions with complex terrain, which would apply to the majority of the UK. The SCAIL-Combustion screening model uses an approach that uses data from a single nearby meteorological station. The Typical Meteorological Year approach is used to derive meteorological data to best represent the long-term dataset based on the similarity of the annual wind direction distribution to the long-term average (five year). Similarity of long-term wind direction distributions of nearby stations has been used to reduce the number of meteorological stations used.

Dry deposition:

The definition of different seasonal classes did not significantly affect the AERMOD results. Therefore the class “Winter with no snow and four months of summer with lush vegetation” has been used. A scheme has been developed for mapping the land use classes used in AERMOD to those relevant for critical loads in APIS. The “reactivity factor” in AERMOD has been increased to improve agreement between the model and field dry deposition velocity data.

Atmospheric chemistry:

The effect of incorporating atmospheric chemistry into the parameterisation would be to slightly reduce deposition amounts; therefore for a screening model, where a precautionary result is acceptable, the additional complexity of considering chemistry was not required.

Wet deposition and orographic enhancement:

AERMOD does not included orographic enhancement. However a simple method to include orographic enhancement has been included in SCAIL-Combustion.

Background pollutant concentrations:

Background concentrations from the UK NO_2 and SO_2 maps, which include all current point sources are used in SCAIL-Combustion. Contributions from stacks modelled explicitly in SCAIL-Combustion should only be used to calculate total (stack+background) concentrations and deposition for ***new*** stacks.

For existing stacks the process contributions from the modelled stacks will be reported though will not be used to determine total deposition or concentration to avoid double counting.

Links to APIS

The SCAIL-Combustion model links to the APIS database in order to access air pollution data.

4. Model Validation

It is an important requirement of any air dispersion modelling assessment that the models used have been appropriately validated and can be shown to be fit-for-purpose. The selection of the AERMOD model for use in SCAIL-Combustion (as detailed in Section 2) was partially due to the extensive validation work that has been conducted with this model by the US-EPA. However, further validation trials were required to test the model for assessments in the UK and to confirm that the configurations applied in SCAIL-Combustion provided realistic results.

4.1 ADMS and AERMOD Modelling of SO_2 and NO_x

Complete validation datasets were obtained from the Environment Agency for Power Stations in the Aire Valley (Yorkshire) and Aberthaw (South Glamorgan). These datasets included ADMS model setup files, time varying stack emissions and efflux data, offsite continuous air quality monitoring data and meteorological files.

The validation process was carried out as follows:

1. Dispersion of SO_2 and NO_x emissions from three power stations within the Aire Valley (Eggborough, Drax and Ferrybridge) were modelled using AERMOD and a second widely used atmospheric dispersion model, ADMS. Modelled atmospheric SO_2 and NO_x concentrations generated with the two software packages were compared.
2. Dispersion of SO_2 and NO_x emissions from a single power station within the Vale of Glamorgan (Aberthaw power station) was modelled using AERMOD and ADMS. Modelled SO_2 and NO_x concentrations generated with the two software packages were compared.
3. Modelled SO_2 and NO_x concentrations generated for the Aire Valley and Aberthaw were compared with monitoring data collected at a network of monitoring sites.
4. SO_2 and NO_x concentrations calculated using SCAIL-Combustion were compared with monitoring data and SO_2 and NO_x concentrations modelled using AERMOD and ADMS.

The locations of the Aire Valley and Aberthaw power stations and their associated monitoring sites are summarised in Tables 7 and 8 respectively. The location of monitoring sites relative to emission sources for the Aire Valley network and Aberthaw power station are illustrated in Figures 10 and 11, respectively.

Table 7 - Power stations used in the validation exercise and their grid references

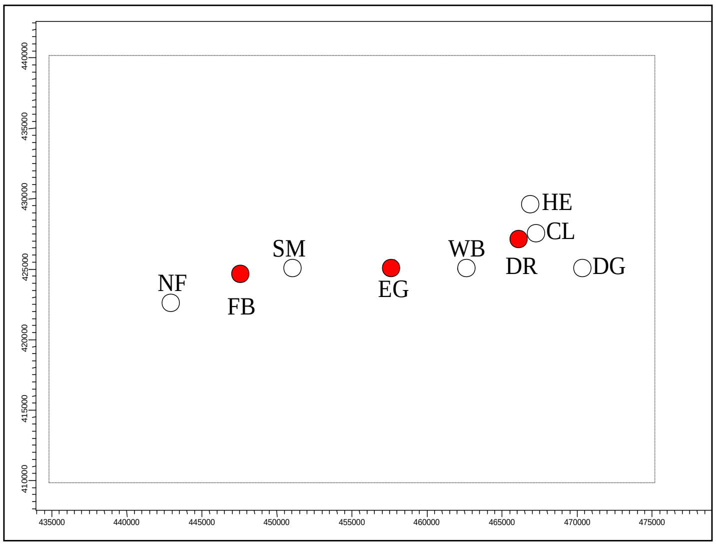
Source	Source Type	X-coord	Y-coord
Aire Valley			
Eggborough	Point	457830	425400
Drax	Point	466100	427200
Ferrybridge 1	Point	447600	424600
Ferrybridge 2	Point	447500	424600
Vale of Glamorgan			
Aberthaw	Point	302354	166311

Table 8 - SO_2 and NO_x monitoring site locations and their grid references

Monitoring Site	X-coord	Y-coord	Pollutants measured
Aire Valley			
Hemmingbrough Landing	466900	429700	SO_2, NO_x ($NO + NO_2$)
Smeathalls Farm	451200	425200	SO_2, NO_x ($NO + NO_2$)
Carr Lane*	467200	427400	SO_2
North Featherstone	442700	422700	SO_2, NO_x ($NO + NO_2$)
Westbank	462400	425000	SO_2, NO_x ($NO + NO_2$)
Downes Ground	470400	424900	SO_2, NO_x ($NO + NO_2$)
Aberthaw			
Boverton	299350	167250	SO_2, NO_x ($NO + NO_2$)
Fontygary	303350	166150	SO_2, NO_x ($NO + NO_2$)

*SO_2 only

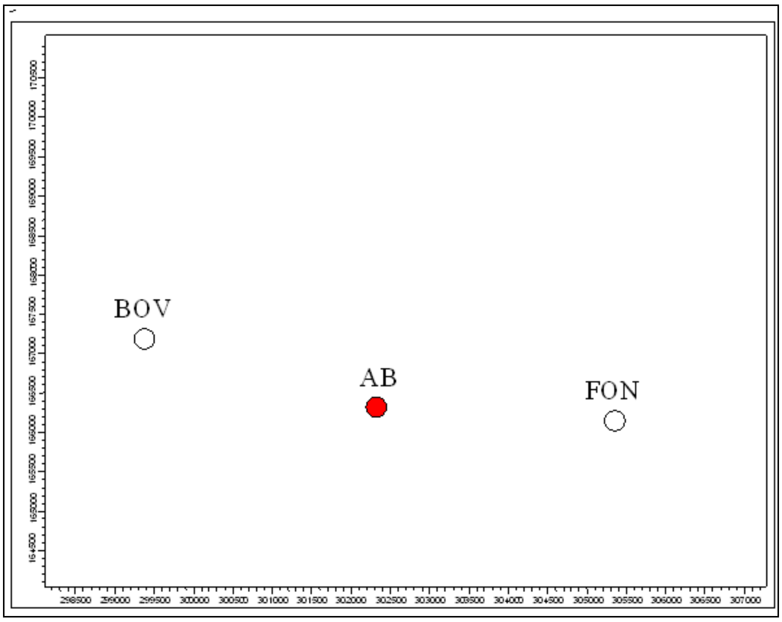
Figure 10 - Location of monitoring sites (white circles) relative to power stations (red circles) in the Aire Valley. Power stations Ferrybridge (FB), Eggborough (EG) and Drax (DR). Monitoring sites (white circles): North Featherstone (NF), Smeathalls Farm (SM), Westbank (WB), Hemmingbrough Landing (HE), Carr Lane (CL) and Downes Ground (DG).



4.1.1 Emissions Data

Emissions data were supplied by the Environment Agency in the form of ADMS format time-varying emission files, with emission rates provided in g s^{-1}. For the Aire Valley network of power stations, hourly sequential emission rates of SO_2 and NO_x were supplied for the period 1st Jan – to 31st Dec, 2003. For Aberthaw power station, hourly sequential emission rates of SO_2 and NO_x were supplied for the period 1st Jan – to 31st Dec, 2004. For the Aire Valley network, data capture ranged from 73% to 98% depending on the power Station. For Aberthaw power station, data capture was 81%.

Figure 11 - Location of monitoring sites (white circles) relative to Aberthaw power station (AB: red circle). Monitoring sites Boverton (BOV) and Fontygary (FON)



4.1.2 Monitoring Data

Within the Aire Valley, six monitoring sites measuring SO_2 and five measuring NO_x were located around Eggborough, Drax and Ferrybridge power stations, and two monitoring sites were located near Aberthaw power station. Monitoring data for the sites were supplied by the Environment Agency. For both the Aire Valley and Aberthaw power stations, monitoring sites lay in an approximately east-west configuration relative to the pollutant sources (Figures 10 and 11).

For the Aire Valley network of power stations, hourly sequential atmospheric SO_2 volume mixing ratios were provided for six locations and hourly sequential atmospheric NO_x volume mixing ratios were provided for the five locations. To allow comparison of monitored volume mixing ratios with modelled concentrations, SO_2 volume mixing ratios were converted to mass per unit volume (µg m^{-3}) according to the method outlined by the Air Quality Expert Group (AQEG, 2004). NO_x volume mixing ratios were converted to mass per unit volume according to the method outlined in TG(03) (DEFRA, 2003).

For Aberthaw power station, hourly sequential SO_2 and NO_x volume mixing ratios were available for both monitoring sites and these were processed in the same way as those for the Aire Valley.

4.1.3 Meteorology

For the Aire Valley, hourly sequential meteorological data were supplied by the Met Office for Linton-on-Ouse (Grid reference 449200, 461819), which is situated approximately 40 km north of the Aire Valley. A higher than expected frequency of calm conditions (18%) was recorded for the Aire Valley in 2003, due to the anticyclonic conditions that prevailed across the UK during this year. Nevertheless, this dataset was used here for validation purposes as monitoring data for post 2003 had a low SO_2 signal due to the introduction of flue gas desulphurisation technology. The meteorological data were converted to SAMSON format for use with AERMOD.

This was done using the ADMS to SAMSON converter available in LAKES AERMET-View.

For the Aberthaw data set, hourly sequential meteorological data were also supplied by the Met Office for St. Athan (Grid reference 300409, 167748), which is situated approximately 3 km north-west of the Aberthaw power station. This file also required conversion to SAMSON format. The frequency of calm conditions for the St. Athan meteorological dataset was 4%.

4.1.4 Modelling Domains

Modelled SO_2 and NO_x concentration data were generated using ADMS (version 4.1) and AERMOD View (version 6.2.1). For the Aire Valley, a roughness length of 0.2 m was applied to the model domain while running ADMS, which is consistent with the roughness length used in the Joint Environment Programme modelling scenarios for the Aire Valley (Brooke *et al*., 2003). A roughness length of 0.2 m was also applied to the Aberthaw modelling domain. Surface roughness is pre-defined in the land use classifications (LUC) in AERMET View. A LUC of "Cultivated Land" was selected for the Aire Valley and Aberthaw modelling domains as this is representative of the land use in these locations. The annual roughness length for this LUC in AERMOD is predefined as 0.0725 m. A separate roughness length was not assigned to the meteorological data sites as the roughness length at Linton-on-Ouse and St Athan are considered similar to the model application sites in the Aire Valley and Vale of Glamorgan. The modelling domains for the Aire Valley network of power stations and Aberthaw power station consisted of a 40 x 30 km grid and a 30 x 15 km grid, respectively. Both modelling domains had a grid resolution of 500 metres, though it should be noted that grid resolution is only relevant for contour plotting and that model predictions for specific receptors used their specific co-ordinates.

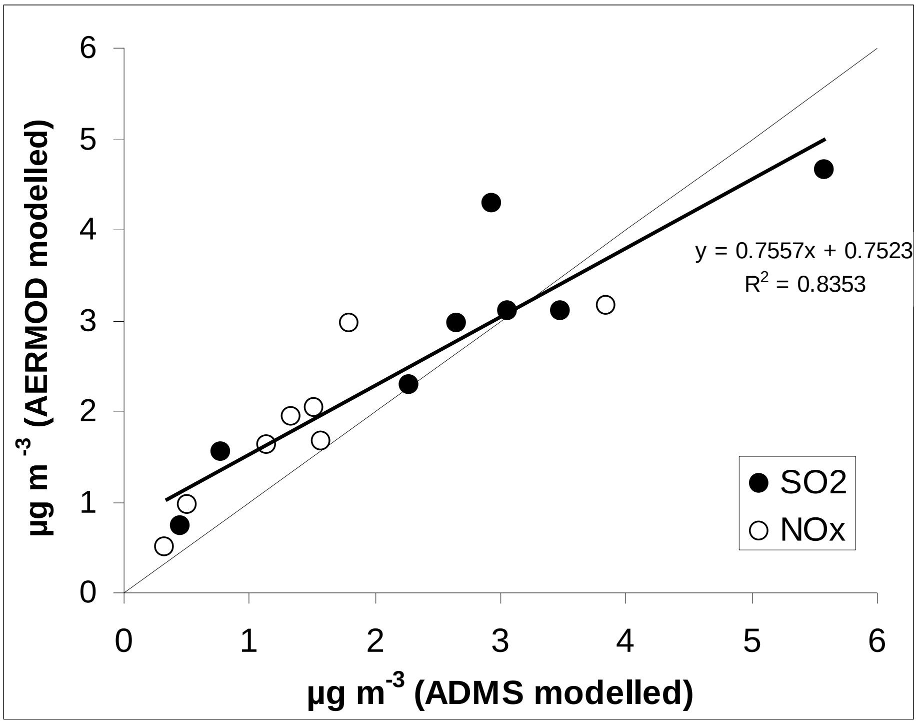
4.1.5 Results

Modelled annual average SO_2 and NO_x concentrations were derived for the Aire Valley and Aberthaw were pooled to allow comparison of AERMOD and ADMS model outputs (Figure 12). Generally good agreement was found between AERMOD and ADMS for both pollutants, with an r^2 value of 0.8 for the complete dataset. Modelled concentrations using AERMOD tended to be slightly higher than the modelled concentrations calculated using ADMS.

4.2 Monitored Concentrations

Pollution rose plots for atmospheric SO_2 and NO_x concentrations were generated using the Aire Valley and Aberthaw monitoring data, and show considerable input of pollutants at the receptor sites from sources that are not included in the modelling scenarios (Figures 13, 14 and 15).

Figure 12 - Comparison of modelled SO_2 and NO_x concentrations estimated using the atmospheric dispersion models AERMOD and ADMS. Concentrations were modelled using emissions data from the Aire Valley network of power stations and Aberthaw power station.



With respect to SO_2 concentrations in the Aire Valley, external sources influence the annual mean concentrations measured at the monitoring sites with significant SO_2 input into the model domain from sources located to the south east of the Aire Valley (Figure 13). This source has been identified as the Trent/Soar Valley network of power stations (Environment Agency, 2003). For Aberthaw, SO_2 pollution roses (Figure 14) show that SO_2 inputs that originate from sources not considered in the modelling exercises were low and that SO_2 concentrations at the monitoring sites were dominated by Aberthaw power station, which is approximately half way between the two monitoring sites in an east-west direction.

Interpretation of the pollution roses for atmospheric NO_x concentrations measured at the monitoring sites for both the Aire Valley network of power stations and Aberthaw power station is complex as all combustion processes in air produce oxides of nitrogen. In 2000, UK road transport accounted for approximately 50% of the total NO_x emissions, with other sources including industrial and commercial sectors as well as the electricity supply industry (AQEG, 2004). However, these figures are constantly changing and in 2007, UK road transport accounted for approximately 30% of total NO_x emissions with the contribution from the electricity generation sector estimated at 24% (CEH, 2009 draft report).

The diversity of NO_x sources is reflected in the pollution roses for both modelling domains (Figures 14 and 15), which show that atmospheric NO_x concentrations at all monitoring locations are affected by pollutant inputs that are not from the power stations. Examination of the NO_x pollution rose for the Aire Valley (Figure 15) shows that NO_x inputs at the monitoring sites occur from all directions, which is understandable given the close proximity of major roads (e.g. A1(M), M62, and M18) and large conurbations that surround the model domain. NO_x inputs at the Aberthaw monitoring sites were also influenced by sources other than Aberthaw power station

(Figure 14). Here, traffic on the M4 to the north of the monitoring sites and Cardiff to the east, as well as the docks at Barry and Cardiff, will have considerable influence on measured NO_x concentrations at the monitoring sites.

Figure 13 - SO_2 pollution roses (µg m^{-3}) for the Aire Valley network in 2003 showing significant input of SO_2 from sources located to the SE of the modelling domain. Arrows show the approximate direction of the power stations from the receptors Abbreviations; CL, DG, HE, NF, SM and WB denote the monitoring sites Carr Lane, Downes Ground, Hemmingbrough Landing, North Featherstone, Smeathalls Farm and West Bank respectively: EG, DR and FB are the power stations at Eggborough, Drax and Ferrybridge, respectively.

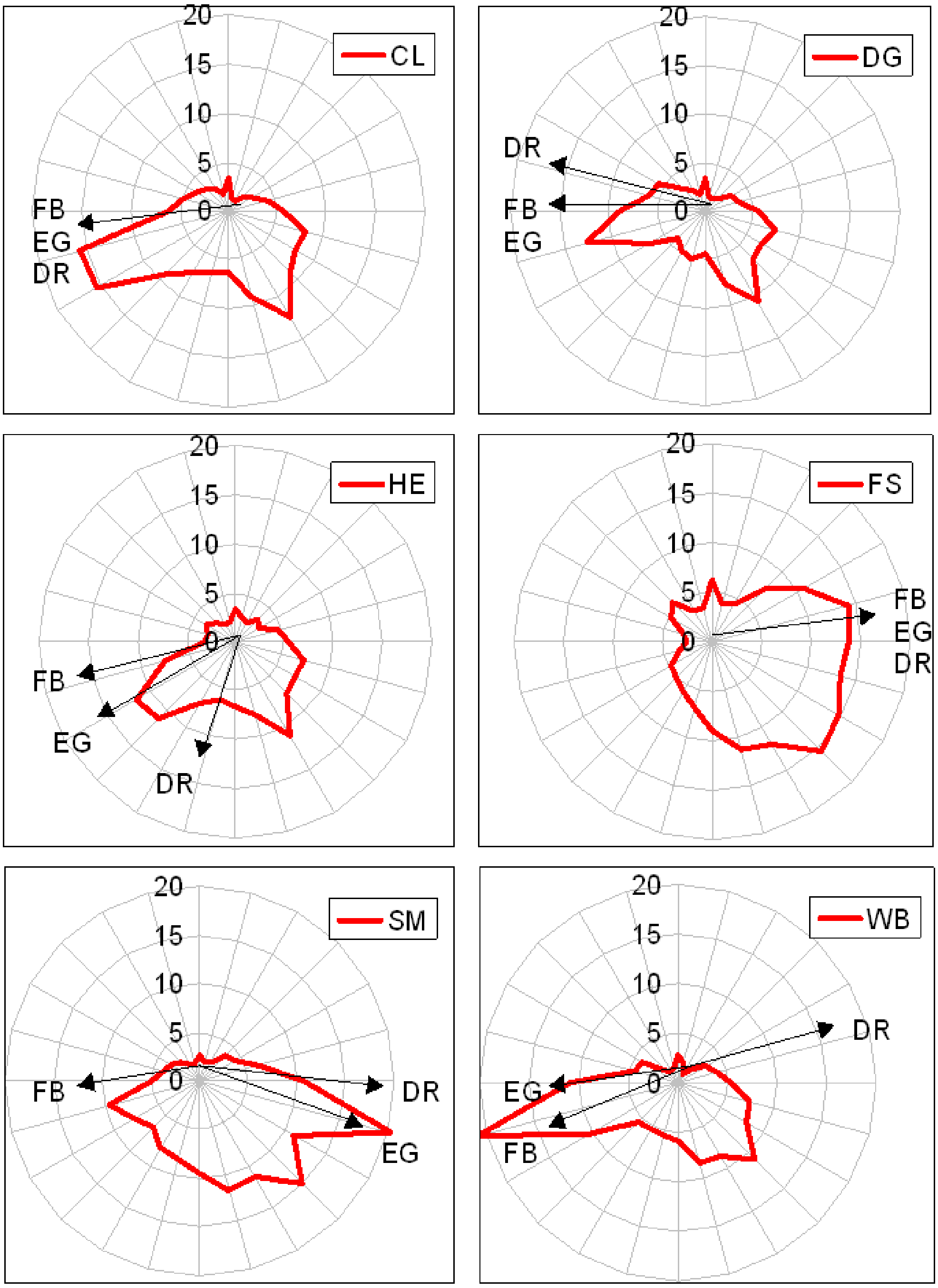


Figure 14 - SO_2 (top) and NO_x (bottom) pollution roses (μg m^{-3}) for two monitoring sites near Aberthaw power station. Arrows show the direction of Aberthaw power station from the monitoring sites. NO_x pollution roses show large input of NO_x from sources outside the modelling domain. Abbreviations; Boverton (BOV) and Fontygary (FON).

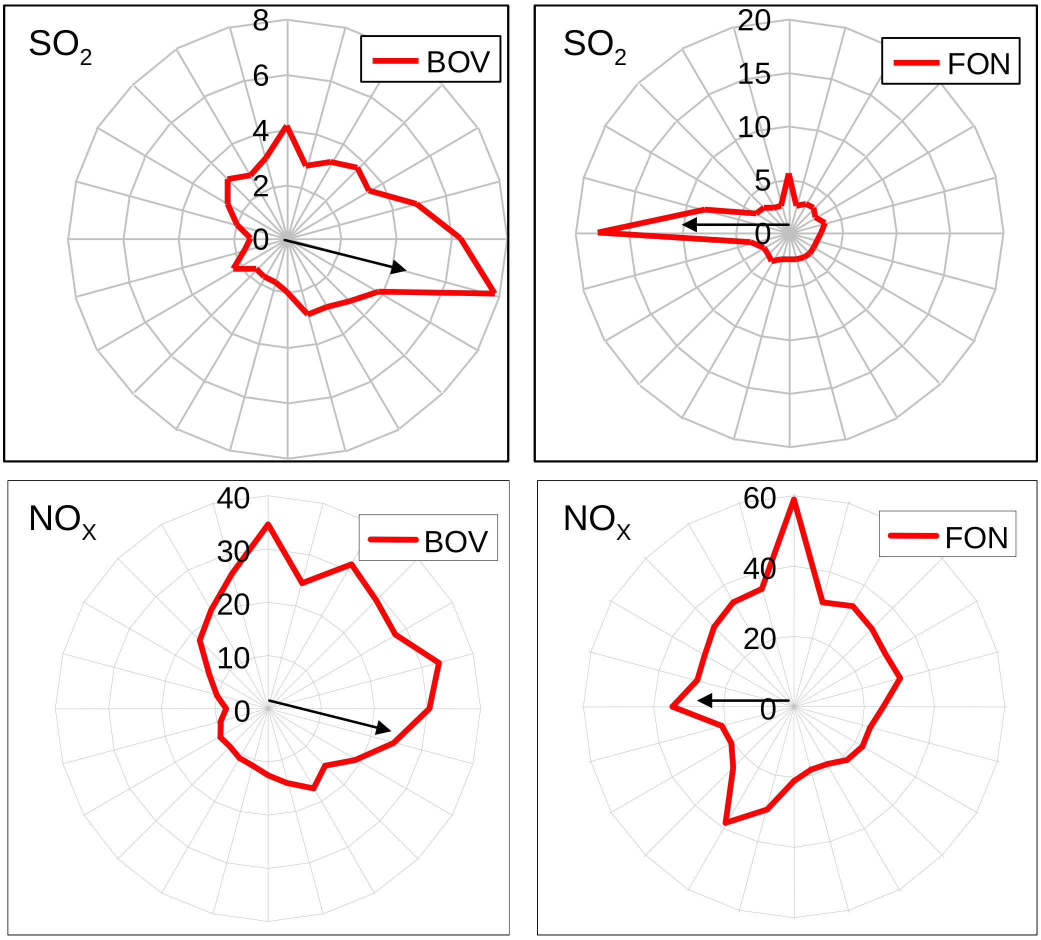
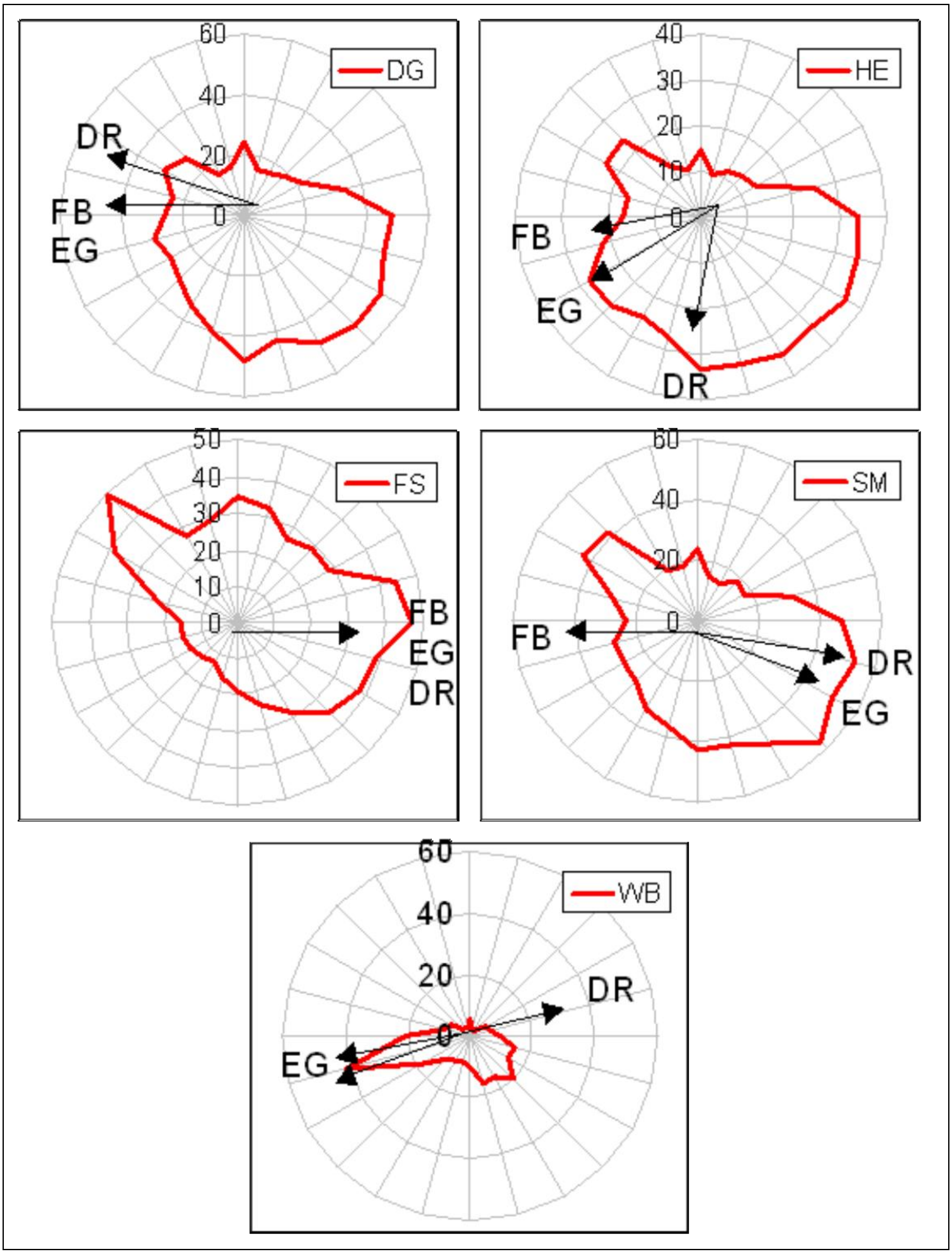


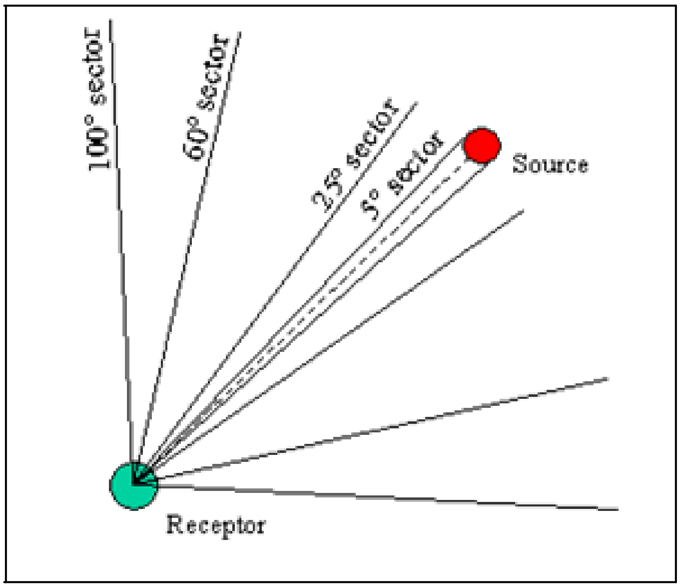
Figure 15 - NO_x pollution roses ($\mu g\ m^{-3}$) for the Aire Valley network in 2003. Abbreviations; Downes Ground (DG), Hemmingbrough Landing (HE), North Featherstone (NF), Smeathalls Farm (SM) and West Bank (WB).



4.3 Comparison of monitoring data with modelled results.

In an ideal scenario, a model will incorporate all major pollution sources and the calibration procedure acts to compensate for model inadequacy and poorly defined background contributions. In order to analyse the performance of the different modelling packages, it was necessary to remove the influence of external sources on the measured concentrations by 'sector-correcting' the monitoring data, as described by Ball *et al*. (2008b). This was achieved by calculating mean concentrations using measured data only where the wind was blowing the plume from the source to the receptor site. The calculation of mean concentrations using wind arcs ranging from 5° to 150°, increasing in increments of 5° (Figure 16), was necessary to determine the optimum sector size.

Figure 16 - Schematic of sector correction analysis. Reproduced from Ball et al. (2008b).



The Root Mean Square Error (RMSE) and the regression r^2 of the modelled vs. sector-corrected monitored data were calculated for each sector and used to determine the sector size for which optimum data compatibility could be achieved. The optimum sector size was determined where the RMSE is minimised, the r^2 is maximised, and where RMSE/r^2 is closest to zero.

For the Aire Valley SO_2 data set, the RMSE/r^2 is fairly constant above a sector size of 25°, although the r^2 is maximised and RMSE minimised at 60° (Figure 17). Consequently, an optimum wind sector size of 60° was used for the Aire Valley SO_2 data set, which resulted in good agreement between monitored and modelled data for both ADMS and AERMOD software (Figure 18), with 90 % of the data within ±25% of the monitored value.

Figure 17- Sector correction analysis for Aire Valley SO_2 data set. Vertical red line shows optimal sector size.

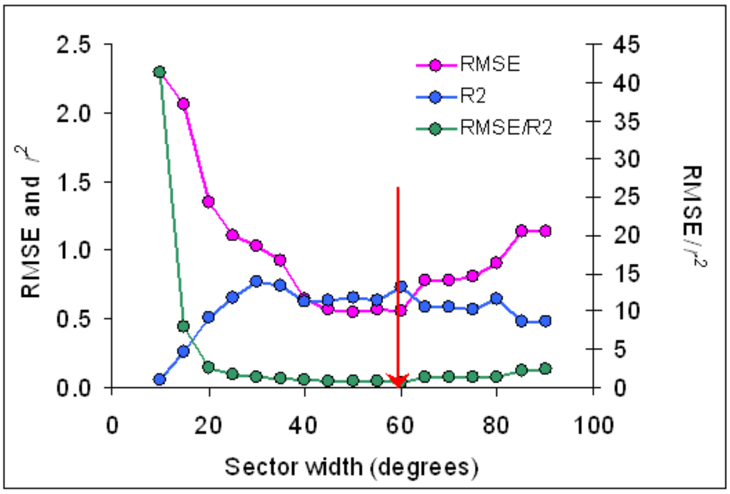
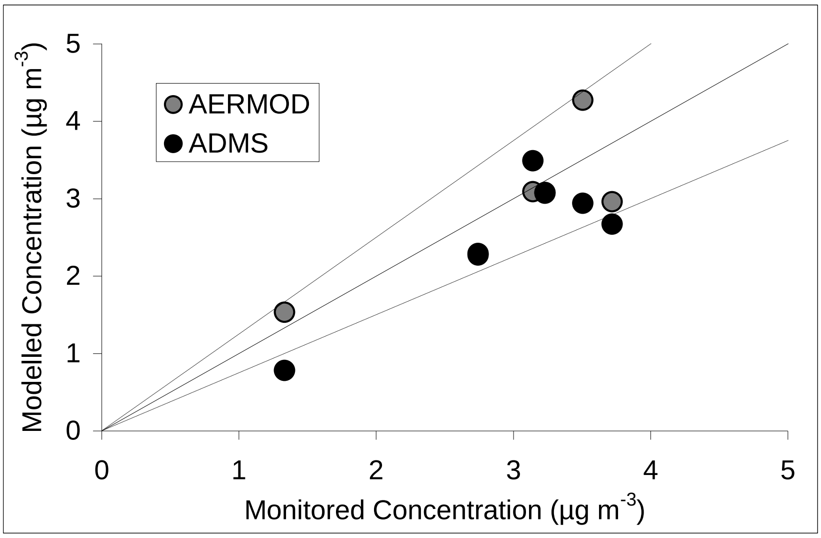


Figure 18 - Comparison of wind direction filtered SO_2 monitoring data with modelling results for the Aire Valley. (Dashed lines = ± 25% of the measured concentrations)



When considering the impact of sources other than the Aire Valley network of power stations on monitored NO_x concentrations, it was necessary to reduce the wind sector size to eliminate NO_x input from those sources not being modelled. As a consequence of attempting to screen out the high NO_x background concentration for the Aire Valley data set (Figure 15), an optimum sector size of 15° was calculated where the RMSE was low, the r^2 was high, and where RMSE/r^2 was low (Figure 19). However, even with such a small sector size, the model still tended to underestimate NO_x concentrations, although AERMOD did tend to perform better than ADMS (Figure 20).

Figure 19 - Sector correction analysis for Aire Valley NO_x data set. Vertical red line shows optimal sector size.

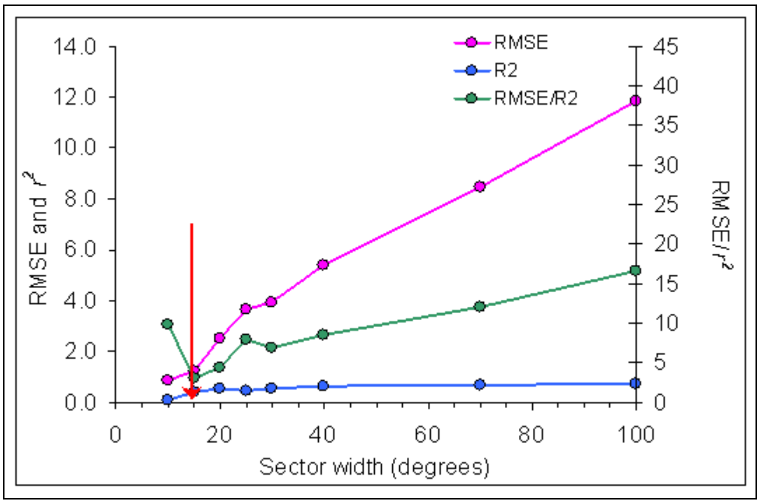
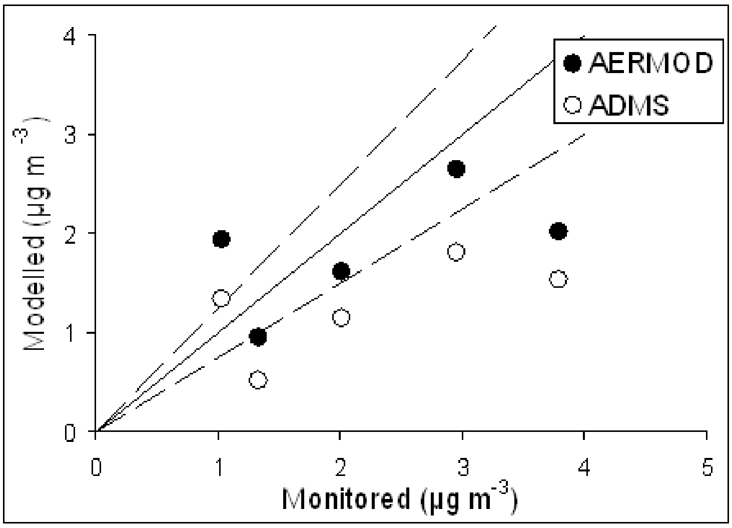
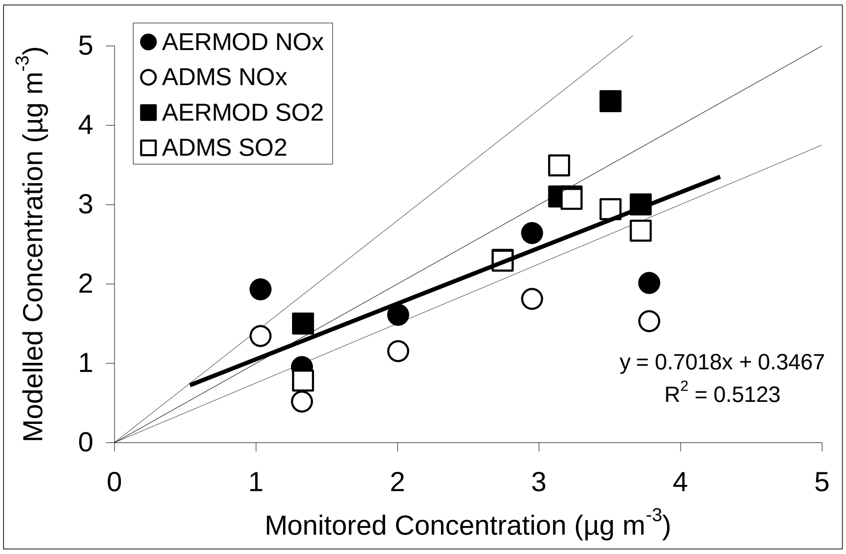


Figure 20 - Comparison of wind direction filtered NO_x monitoring data with modelling results for the Aire Valley data set. (Dashed lines = ± 25% of the measured concentration)



When the results of the two modelling packages were combined to determine the goodness of fit between the sector corrected monitoring data and all modelled results for the Aire Valley, the data showed a good correlation between modelled and monitored results (Figure 21).

Figure 21 - Comparison of wind direction filtered SO_2 and NO_x monitoring data with modelling results for the Aire Valley data set. (Dashed lines = ± 25% of the measured concentration)



For the Aberthaw data set, it was not possible to use the r^2 of the modelled vs. sector-corrected monitoring data on monitored SO_2 and NO_x concentrations as data for only two monitoring sites were available (i.e. r^2 will always equal 1). Therefore, sector correction of the Aberthaw monitoring data was carried out by analysis of the RMSE only.

For Aberthaw SO_2 concentrations, an optimum sector width of 125^o was calculated (Figure 22), whereas for NO_x concentrations an optimum sector width of 40^o was calculated (Figure 23). These values are considerably larger than those for the Aire Valley as there is a much smaller contribution from other sources at this location. To determine the goodness of fit between the sector-corrected monitoring data and modelled results, the SO_2 and NO_x concentrations modelled using AERMOD and ADMS were pooled. The results of the comparison between the sector-corrected monitoring data and the modelled data showed a strong correlation (r^2 = 0.9) (Figure 24).

Figure 22 - Root mean square of the error between wind sector-corrected monitoring data and modelled SO_2 concentrations for the Aberthaw power station dataset.

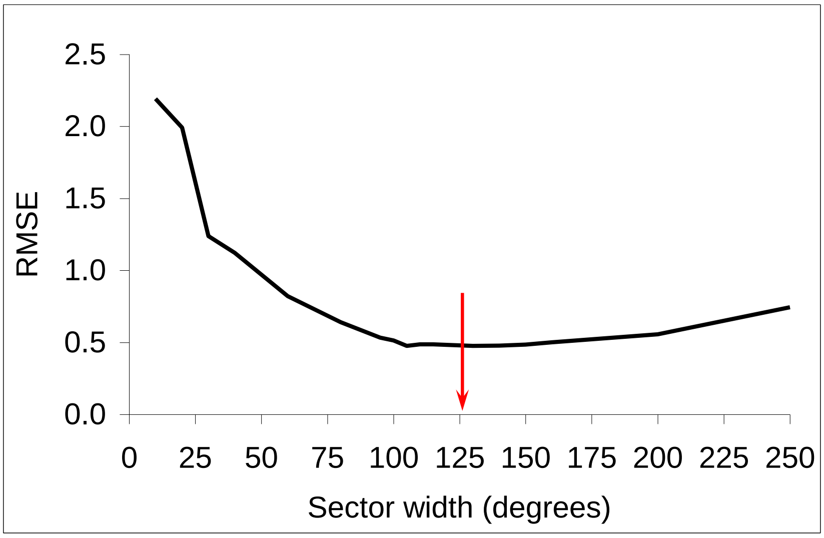


Figure 23 - Root mean square of the error between wind sector-corrected monitoring data and modelled NO_x concentrations for the Aberthaw power station dataset.

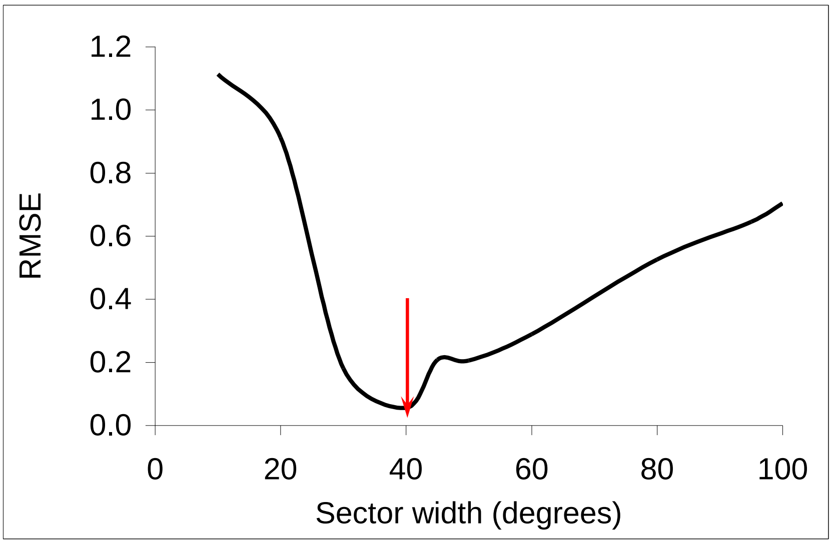
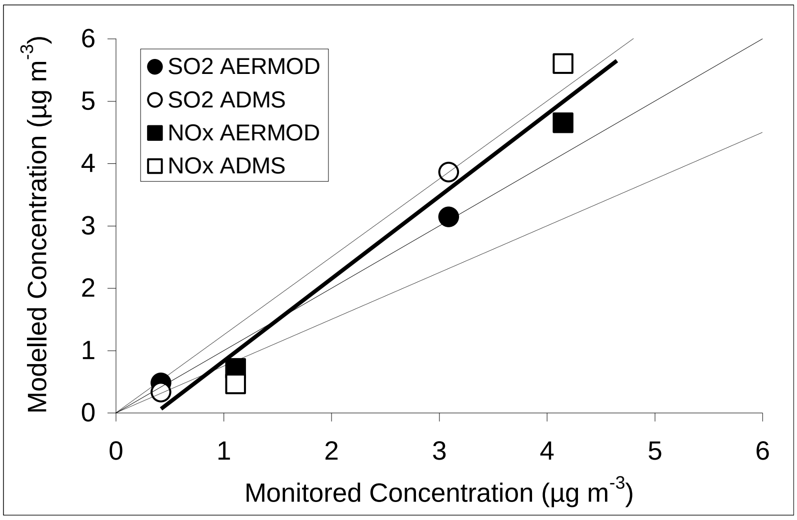


Figure 24 - Comparison of wind direction filtered SO_2 and NO_x monitoring data with modelling results for the Aberthaw power station data set. (Dashed lines = ± 25% of the measured concentration)



4.4 Validation of SCAIL-Combustion

Validation was carried out by comparison of NO_x and SO_2 concentrations modelled using SCAIL-Combustion with monitoring data, and concentrations modelled using the atmospheric dispersion modelling software AERMOD and ADMS. It is worthy of note that unlike the modelling exercises conducted for the Aire Valley and Aberthaw power stations, SCAIL-Combustion doesn't utilise meteorological data for a specific year or for a specific site. Instead, the on-line screening tool uses meteorological data for a "typical met year" selected from the nearest of one of 30 representative sites from across the UK (Section 3.1).

4.4.1 Method and general use of the SCAIL-Combustion tool

In order to run SCAIL-Combustion the input parameters are entered into the web tool. In the case of Aire Valley there are three power plants with a total of four stacks which are inputted sequentially. Once the calculation has been completed, it is easy to save the output data and then use these data within a data analysis programme e.g. Excel. For each monitoring location a SCAIL-Combustion model run was performed. The resultant output was compared with the modelled (ADMS and AERMOD) and monitored concentrations.

4.4.2 Initial modelling studies

Initial modelling studies using the Aire Valley network of power stations to validate SCAIL-Combustion showed good agreement with AERMOD and ADMS and reflected monitored SO_2 and NO_x concentrations (Figures 25 and 26, respectively). However, for Aberthaw power station, SO_2 and NO_x concentrations were underestimated for the Fontygary monitoring site (Figure 27).

It is worthy of note that the St. Athan meteorological station used for the AERMOD and ADMS modelling runs was screened out as part of the selection process when determining the TMY for SCAIL-Combustion. As a consequence of the screening process, SCAIL-Combustion used meteorological data recorded at Cardiff weather centre for the Aberthaw modelling study. The wind direction recorded at Cardiff weather centre is predominantly northeat-southwest (Appendix C), whereas the wind direction recorded at St Athan is predominantly east-west and is reflected in Figures 28a and 28b. These figures are concentration plots for SO_2 and NO_x respectively, and were generated in AERMOD using meteorological data recorded at St Athan. These figures clearly show the plume direction moving east from Aberthaw power station over the monitoring site at Fontygary.

To investigate if differences in meteorology between the TMY used in SCAIL-Combustion and the St Athan meteorological dataset used in AERMOD and ADMS are the reason for SCAIL-Combustion underestimating downwind concentrations of NO_x and SO_2 at Fontygary, a series of SCAIL-Combustion runs using a grid resolution of 1 km were carried out for 20 points around the source and receptor. It was found that using the TMY in SCAIL-Combustion, placed the plume to the north of the monitoring site (Figure 29 and 30), which accounts for the underestimation of pollutant concentrations at this site.

To address this uncertainty in modelling NO_x and SO_2 concentration with SCAIL-Combustion, a new modelling methodology was derived that would take account of variations in local wind directions. Also, one of the requirements for SCAIL-Combustion is that it should provide a precautionary screening assessment of combustion plants, with more detailed assessments being required on at-risk sites. Therefore a further modification was required to ensure that conservative results were achieved.

Figure 25 - Comparison of SCAIL-Combustion (SCAIL-C) model runs for SO_2: Aire Valley monitoring sites against AERMOD and ADMS. (Dashed lines represent ±25% of the measured concentration

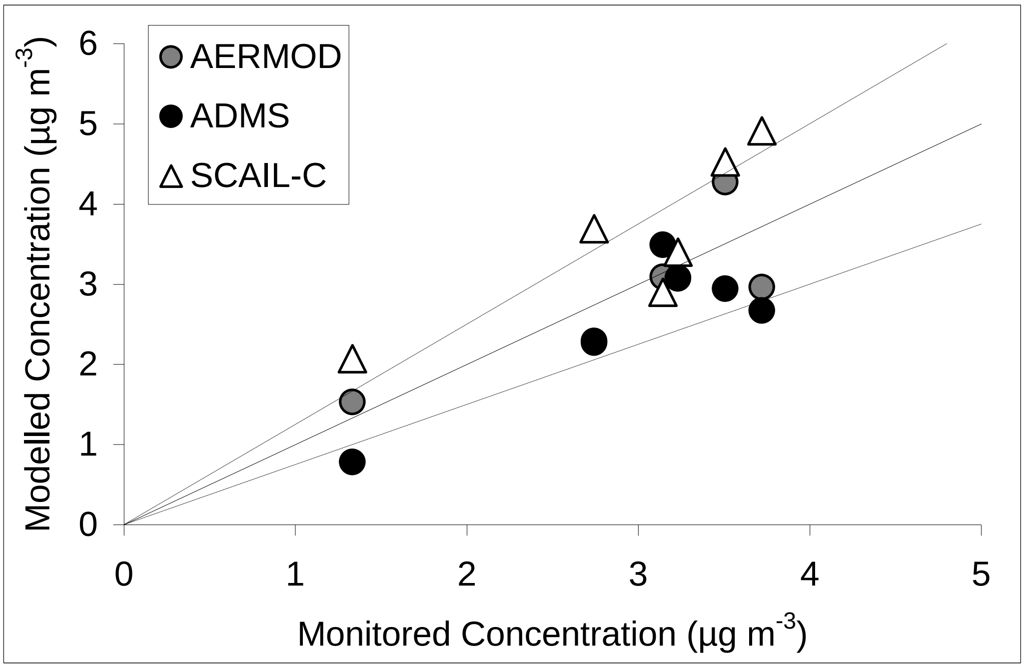


Figure 26 - Comparison of SCAIL-Combustion (SCAIL-C) model runs for NO_x: Aire Valley monitoring sites against AERMOD and ADMS. (Dashed lines represent ±25% of the measured concentration)

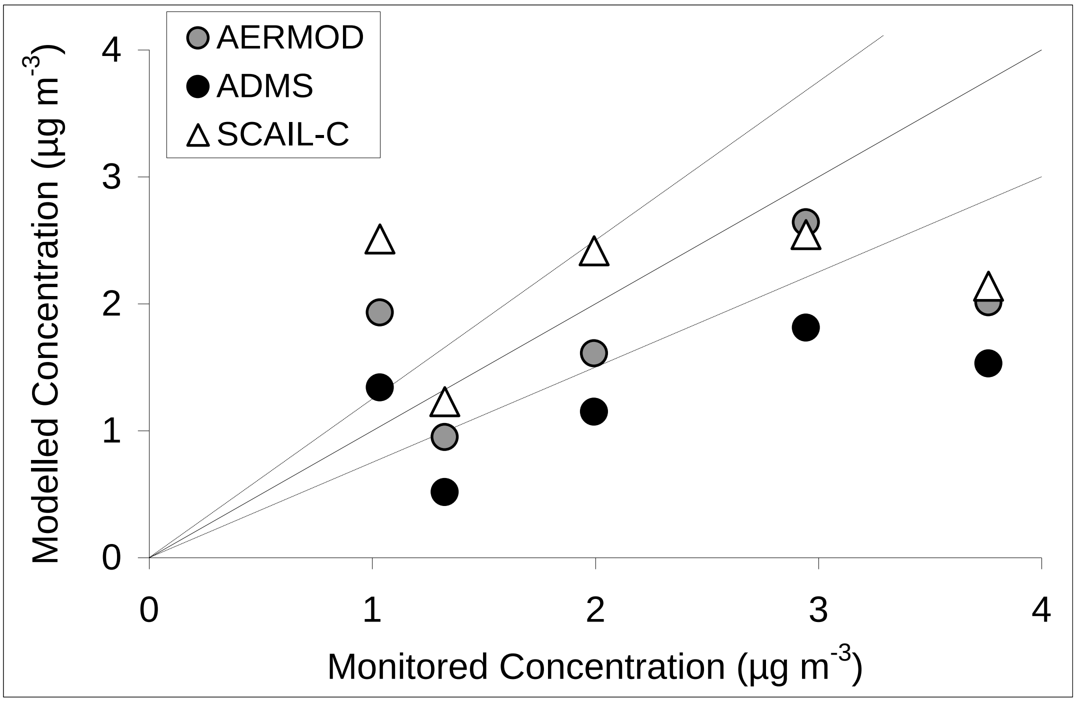


Figure 27 - Comparison of SCAIL-Combustion (SCAIL-C) model runs for SO_2 and NO_x: Aberthaw monitoring sites against AERMOD and ADMS

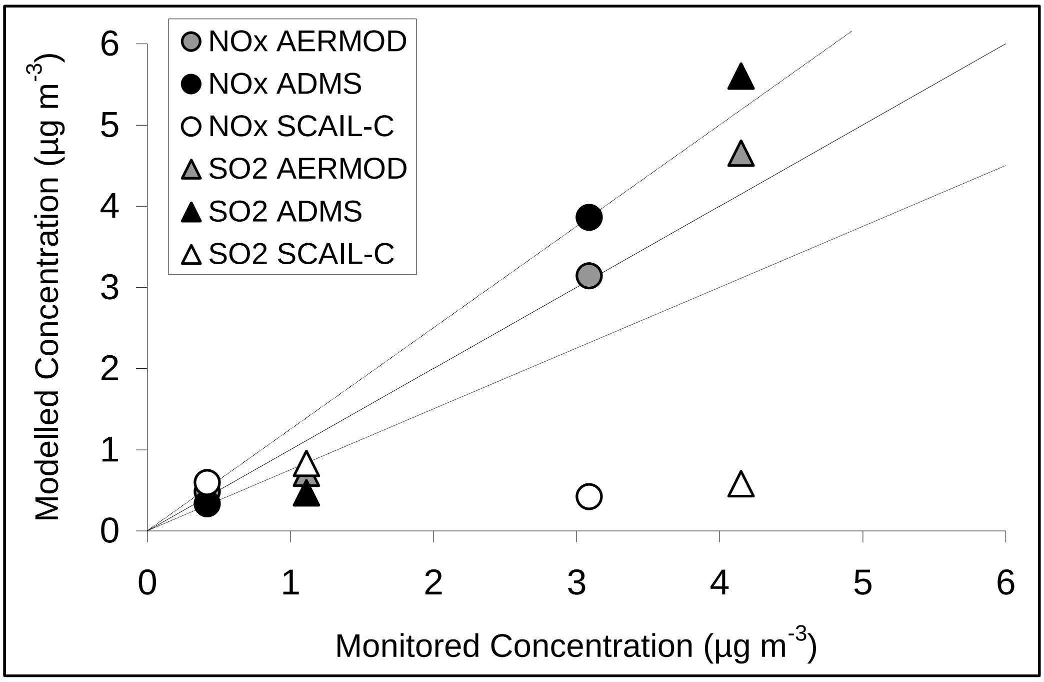
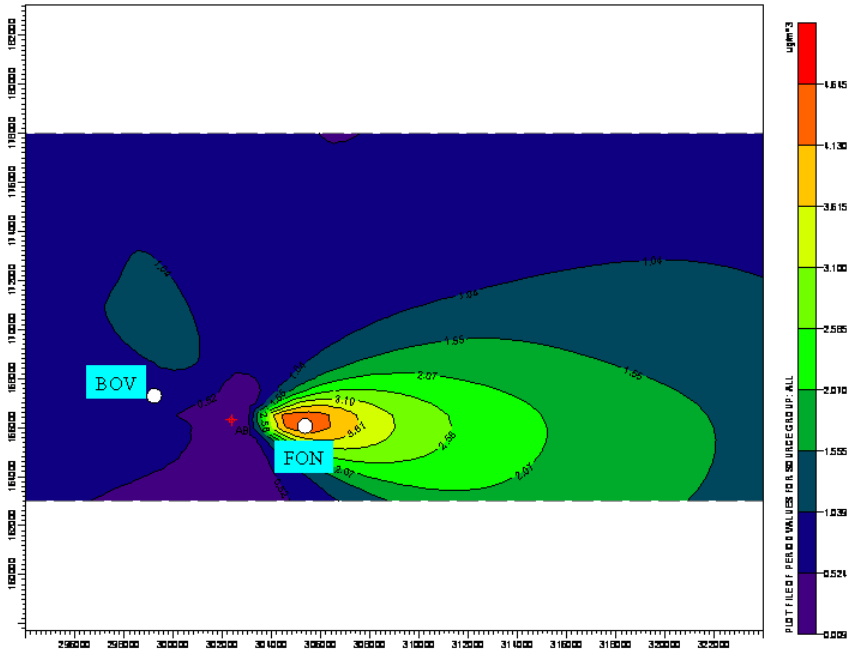


Figure 28 - Annual average SO_2 (top) and NO_x (bottom) concentrations for the Aberthaw power station modelled using AERMOD. Aberthaw power station (Red cross). Monitoring sites (white circles): Boverton (BOV), Fontygary (FON).



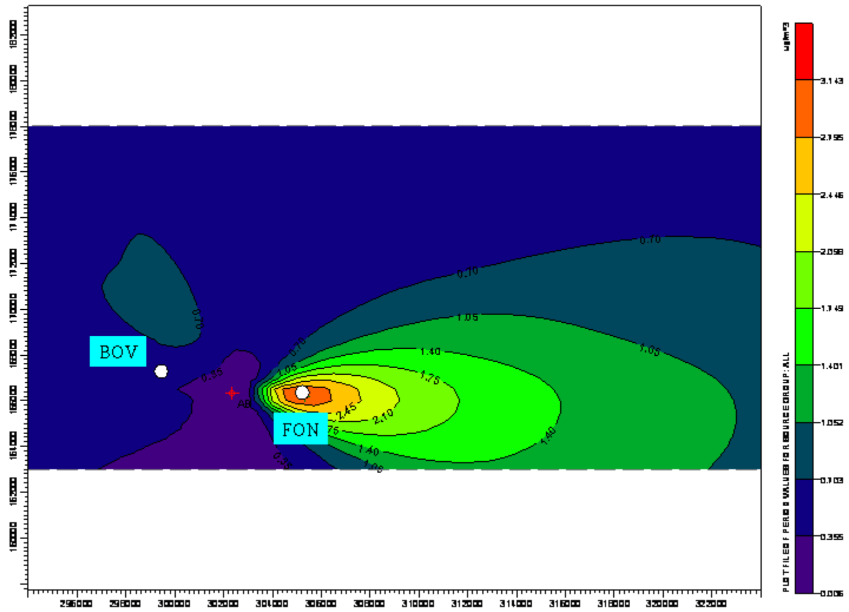


Figure 29 - SCAIL-Combustion concentration field for NO_x at 1 km resolution between the Aberthaw power station and the Fontygary monitoring site.

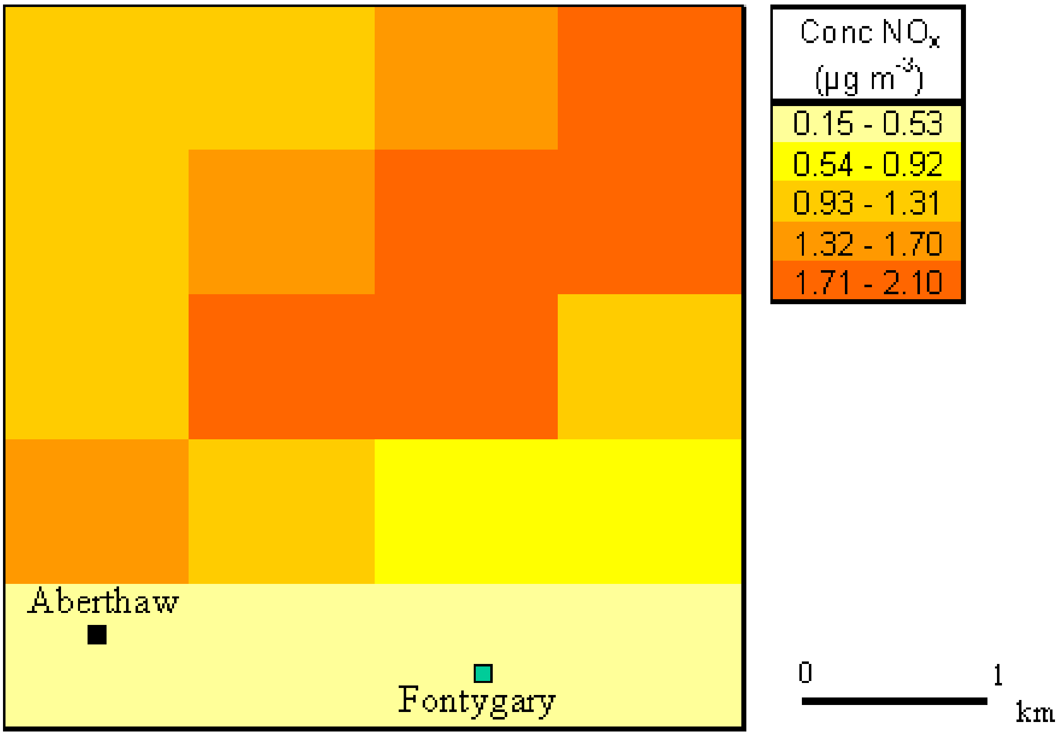
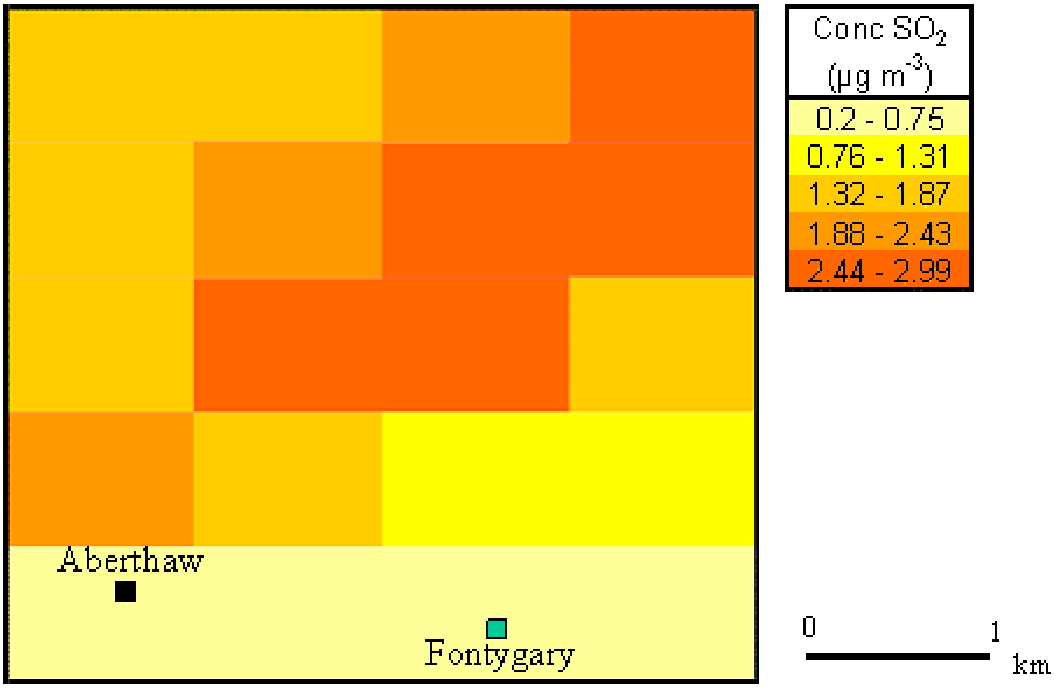


Figure 30 - SCAIL-Combustion concentration field for SO_2 at 1 km resolution between the Aberthaw power station and the Fontygary monitoring site.



4.4.3 Modified SCAIL methodologies

Two additional criteria were addressed when constructing the tool to ensure that the model would be able to produce conservative assessments and therefore not under-estimate a potential exceedance at a specific site. These criteria were: (a) that the results from SCAIL-Combustion relate to the upper percentiles of measurement data; and (b): to account for the variations in local wind conditions.

The data from the validation studies conducted using the AERMOD model (noting that SCAIL-Combusion uses AERMOD as its dispersion kernel) were used to identify a suitable correction factor to ensure that modelled data reflected the upper 90th percentile of monitoring data. Ratios of the measured to modelled (AERMOD) data were determined for SO_2 and NO_x from both the Aire Valley and Aberthaw studies. A cumulative probability distribution was constructed of these ratios and a log-normal distribution was fitted to the data (shown in Figure 31). The ratio of measured to modelled data corresponding to the 90th percentile (the top 10% of data) of 1.6 was calculated as the correction factor.

The validation study for Aberthaw highlighted that local variations in wind direction, due to either local topography or annual climatic variations, could result in the SCAIL-Combustion tool underpredicting impacts on specific sites. Consequently an option was provided that rotates the location of habitat to be in the prevailing wind direction from the combustion plant. This methodology ensures that the downwind distance does not change and also uses the midpoint of groups of sources (see Figure 32). It should be noted however, that the method works best when sources are in reasonably close proximity. For situations where a large number of sources are being modelled across a wide geographical area the modeller should use the actual source position as applied through the “realistic met” option. Furthermore, consideration should also be made whether to upload local meteorological data, if such data are available.

Figure 31 - Probability distribution function derived from the Aire valley and Aberthaw model validation data using the AERMOD predictions. Points show the validation data, solid line shows a log normal distribution fit to the data and dashed lines show the ratio corresponding to the 90th percentile.

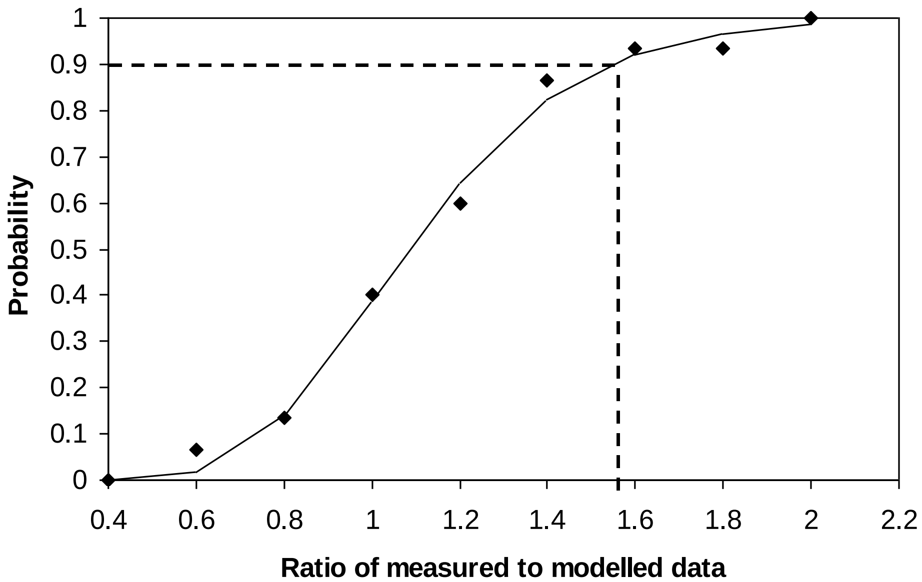
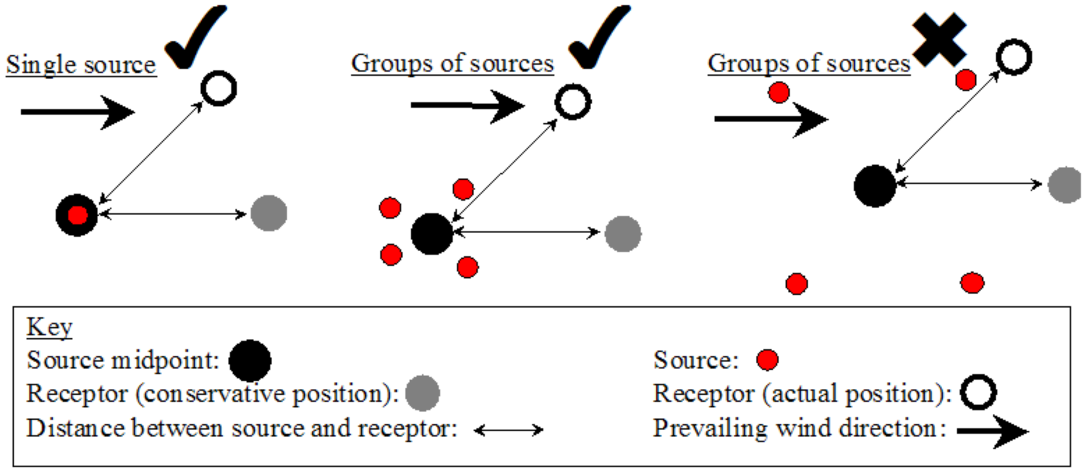


Figure 32 - Schematic showing the methodology used to determine the "conservative met" assumptions in SCAIL-Combustion illustrating situations where the method can and cannot be reasonably expected to work well.



4.4.4 Evaluation of the modified methodology: Aire Valley

Figure 33 shows the concentration of SO_2 modelled using the refined methodology in SCAIL-Combustion and is compared with monitoring results and concentrations estimated using AERMOD and ADMS. Using the refined methodology in SCAIL-Combustion to model SO_2 concentrations at receptor sites in the Aire valley has resulted in a more pessimistic estimate of the effect of emission on the environment. Modelled SO_2 concentrations are more conservative than in previous modelling exercises and now overestimate the atmospheric concentration of SO_2 at the receptor location, a result that is desirable for a screening tool.

Similar results were also observed when using the refined methodology in SCAIL-Combustion to model NO_x concentrations at the receptor locations (Figure 34). Here, NO_x concentrations are also more conservative than in the previous modelling exercise with majority of results greater than their monitored values.

The result of using the conservative methodology to ensure that local variations in wind direction in the Aire valley are taken into account is compared in Table 9. These results show that generally using the "Conservative Met" option to ensure that the receptor is always in the prevailing wind resulted in more pessimistic estimates of pollutant concentrations and nitrogen and acid deposition. However, in one instance (the impact of Drax power station on the receptor located at Westbank), using the Conservative Met option as opposed to using the "Realistic Met" option did result in lower estimates of pollutant concentrations, which highlights that this method works best when sources are in reasonably close proximity (see Figure 32).

Figure 33 - Comparison of SCAIL-Combustion (SCAIL-C) model runs for SO_2: Aire Valley monitoring sites against AERMOD and ADMS. (Dashed lines represent ±25% of the measured concentration)

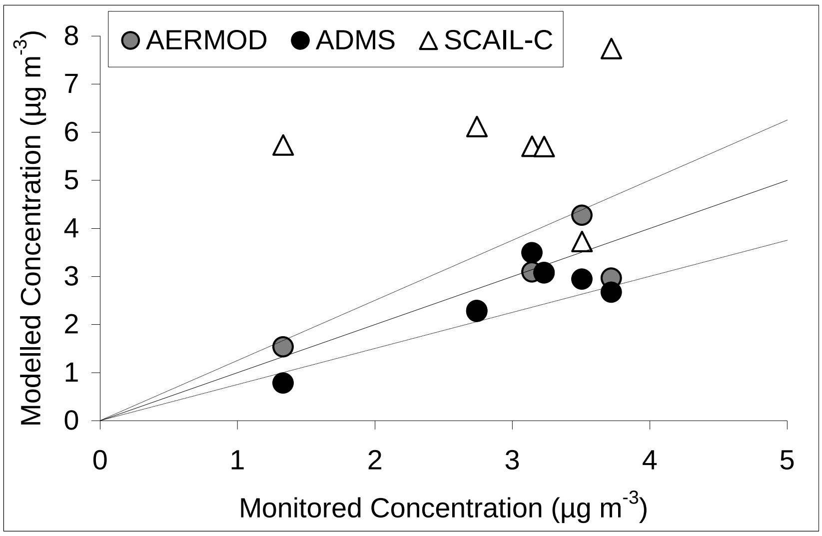
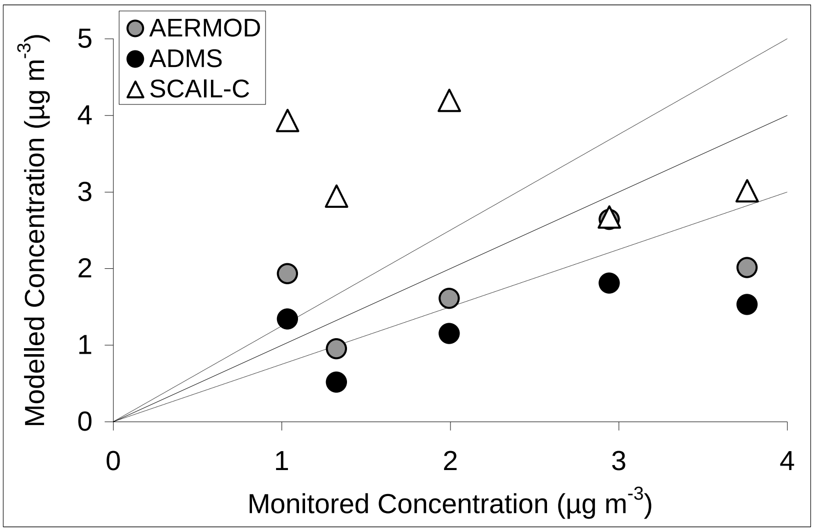


Figure 34 - Comparison of SCAIL-Combustion (SCAIL-C) model runs for NO_x: Aire Valley monitoring sites against AERMOD and ADMS. (Dashed lines represent ±25% of the measured concentration)



4.4.5 Evaluation of the modified methodology: Aberthaw

Figure 35 shows the results of implementing the refined modelling methodology in SCAIL-Combustion and compares SCAIL-Combustion results with monitored concentrations and AERMOD and ADMS modelling results. The initial modelling study for the upwind monitoring site at Boverton (Figure 27) showed good agreement between modelled and monitored NO_x and SO_2 concentrations. Figure 35, shows that using the modified methodology in SCAIL-Combustion resulted in more conservative estimates of NO_x and SO_2 concentrations at this site.

Using the new methodology also resulted in an increase in modelled NO_x and SO_2 concentrations at the downwind receptor at Fontygary. In the previous modelling exercise, SCAIL-Combustion underestimated modelled atmospheric concentrations of NO_x and SO_2 at this location, which has been attributed to differences between the meteorology for Cardiff weather station (used in SCAIL-Combustion) and the meteorology experienced at the monitoring locations. Using the new methodology has resulted in a marked improvement on initial modelling results with modelled NO_x and SO_2 concentrations for this receptor now comparable with the monitored concentrations. The result of using the conservative methodology to ensure that local variations in wind direction are taken into account for monitoring sites near Aberthaw power station is shown in Table 10.

Figure 35 - Comparison of SCAIL-Combustion (SCAIL-C) model runs for NO_x and SO_2: Aberthaw monitoring sites against AERMOD and ADMS. (Dashed lines represent ±25% of the measured concentration).

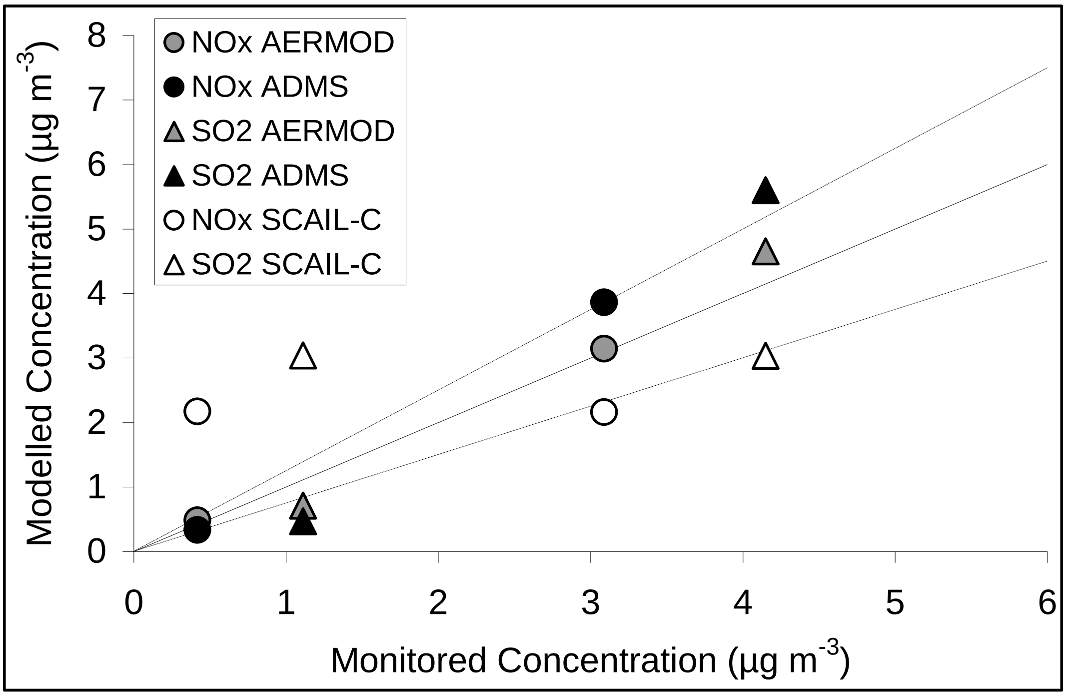


Table 9 - Summary of Results from SCAIL-Combustion Runs for Aire Valley Monitoring Sites

Monitoring Site	Source No.	Source Name	New or Existing	NO_x (t/a)	SO_2 (t/a)	Realistic Dep N (kg/ha)	Conservative Dep N (kg/ha)	Realistic Conc NO_x (μg/m3)	Conservative Conc NO_x (μg/m3)	Realistic Conc SO_2 (μg/m3)	Conservative Conc SO_2 (μg/m3)	Realistic Dep Acid (kEq H+/ha)	Conservative Dep Acid (kEq H+/ha)
Downes Ground	1	Eggborough	Existing	17925	52007	0.25	0.25	0.96	0.96	2.8	2.8	0.21	0.21
Downes Ground	2	Drax	Existing	65893	46232	0.55	0.66	2.0	2.3	1.4	1.6	0.13	0.16
Downes Ground	3	Ferrybridge 1	Existing	10540	19850	0.11	0.11	0.44	0.43	0.82	0.81	0.064	0.062
Downes Ground	4	Ferrybridge 2	Existing	11424	22816	0.11	0.11	0.47	0.46	0.92	0.90	0.071	0.069
Total						**1.02**	**1.13**	**3.87**	**4.15**	**5.94**	**6.11**	**0.475**	**0.501**
Carr Lane	1	Eggborough	Existing	17925	52007	0.25	0.30	0.94	1.1	2.7	3.2	0.20	0.24
Carr Lane	2	Drax	Existing	65893	46232	0.11	0.23	0.40	0.87	0.28	0.61	0.026	0.051
Carr Lane	3	Ferrybridge 1	Existing	10540	19850	0.10	0.12	0.42	0.48	0.78	0.89	0.058	0.069
Carr Lane	4	Ferrybridge 2	Existing	11424	22816	0.11	0.12	0.44	0.50	0.87	0.99	0.064	0.076
Total						**0.57**	**0.77**	**2.2**	**2.95**	**4.63**	**5.69**	**0.348**	**0.436**
Smeathalls Farm	1	Eggborough	Existing	17925	52007	0.17	0.015	0.67	0.056	1.9	0.16	0.13	0.011
Smeathalls Farm	2	Drax	Existing	65893	46232	0.27	0.33	1.0	1.2	0.73	0.85	0.063	0.075
Smeathalls Farm	3	Ferrybridge 1	Existing	10540	19850	0.35	0.18	1.2	0.69	2.2	1.3	0.18	0.099
Smeathalls Farm	4	Ferrybridge 2	Existing	11424	22816	0.35	0.19	1.2	0.72	2.4	1.4	0.19	0.11
Total						**1.14**	**0.715**	**4.07**	**2.666**	**7.23**	**3.71**	**0.563**	**0.295**
Westbank	1	Eggborough	Existing	17925	52007	0.47	0.47	1.6	1.6	4.7	4.7	0.37	0.37
Westbank	2	Drax	Existing	65893	46232	0.32	0.31	1.2	1.1	0.83	0.80	0.071	0.070
Westbank	3	Ferrybridge 1	Existing	10540	19850	0.15	0.14	0.59	0.57	1.1	1.1	0.085	0.082
Westbank	4	Ferrybridge 2	Existing	11424	22816	0.16	0.15	0.62	0.60	1.2	1.2	0.094	0.091
Total						**1.1**	**1.07**	**4.01**	**3.87**	**7.83**	**7.8**	**0.62**	**0.613**
North Featherstone	1	Eggborough	Existing	17925	52007	0.095	0.30	0.40	1.1	1.1	3.3	0.071	0.24
North Featherstone	2	Drax	Existing	65893	46232	0.18	0.22	0.70	0.83	0.48	0.58	0.042	0.049
North Featherstone	3	Ferrybridge 1	Existing	10540	19850	0.11	0.12	0.43	0.48	0.80	0.90	0.055	0.069
North Featherstone	4	Ferrybridge 2	Existing	11424	22816	0.12	0.13	0.45	0.51	0.89	1.00	0.061	0.077
Total						**0.505**	**0.77**	**1.98**	**2.92**	**3.27**	**5.78**	**0.229**	**0.435**
Hemmingbrough Landing	1	Eggborough	Existing	17925	52007	0.25	0.29	0.92	1.1	2.7	3.2	0.19	0.24
Hemmingbrough Landing	2	Drax	Existing	65893	46232	0.49	0.25	1.7	0.95	1.2	0.67	0.11	0.056
Hemmingbrough Landing	3	Ferrybridge 1	Existing	10540	19850	0.099	0.12	0.41	0.47	0.76	0.88	0.057	0.068
Hemmingbrough Landing	4	Ferrybridge 2	Existing	11424	22816	0.10	0.12	0.43	0.50	0.85	0.98	0.063	0.075
Total						**0.939**	**0.78**	**3.46**	**3.02**	**5.51**	**5.73**	**0.42**	**0.439**

Table 10 - Summary of Results from SCAIL-Combustion Runs for Aberthaw

Run	Source Name	New or Existing	NO_x (t/a)	SO_2 (t/a)	Realistic Dep N (kg/ha)	Conservative Dep N (kg ha/yr)	Realistic Conc NO_x (µg/m3)	Conservative Conc NO_x (µg/m3)	Realistic Conc SO_2 (µg/m3)	Conservative Conc SO_2 (µg/m3)	Realistic Dep Acid (kEq H+/ha)	Conservative Dep Acid (kEq H+/ha)
Boverton	Aberthaw	Existing	23826	33420	0.20	0.86	0.95	3.5	1.3	4.9	0.092	0.41
Fontygary	Aberthaw	Existing	23826	33420	0.14	0.86	0.67	3.5	0.93	4.9	0.067	0.41
Total					**0.34**	**1.72**	**1.62**	**7**	**2.23**	**9.8**	**0.159**	**0.82**

4.5 Case study

A case study was conducted for a Combined Heat and Power (CHP) Plant in Scotland. This power station has a thermal input of 44 MW and therefore is within the anticipated range of operating stations that SCAIL-Combustion should be applied. Unfortunately, monitoring data were not available for the Power Station, so an intercomparison with the predictions of the ADMS and AERMOD models was used to provide an assessment of the uncertainty in the modelling results. Input data used in the modelling assessment are shown in Table 11. The model automatically selected the closest meteorological station, which was Lossiemouth.

Table 11 - Input parameter values for the CHP plant used in the case study.

Parameter	Value	Units
Stack Location	NH716701	National Grid
Exit Temperature	150	°C
Efflux Velocity (m/s)	22	m/s
Flow Rate (m^3/s)	103000	Nm^3/hr
Stack Height	36	m
Stack Diameter	1.6	m
NO_x Concentration	300	mg /Nm^3
SO_2 Concentration	200	mg/Nm^3
NO_x Emission	271	Tonnes/year
SO_2 Emission	181	Tonnes/year

The “SNHI Habitat check” function on the SCAIL-Combustion website was used to load the Scottish National Heritage SiteLink Database. The “Map Search” function within the SNHI website was used to identify sensitive habitat sites within approximately 10 km of the case study Power station. The MultiMap website was then used to locate the nearest point on the habitat site to the case study power plant. A list of ten identified locations is included in Table 12.

Table 12 - Locations of potentially sensitive habitats around the case study CHP. Distances are expressed to the case study CHP plant.

Location	SCAIL Habitat Type	NGR	X (OS)	Y (OS)	Distance (m)
Cromarty Firth 1	Sand dunes	NH740700	274050	870050	2436
Cromarty Firth 2	Sand dunes	NH7106740	271050	867450	2734
Cromarty Firth 3	Sand dunes	NH686691	268650	869150	3121
Morangie Forest	Deciduous/Coniferous woodland	NH683738	268350	873850	4953
Kinrive-Strathroy	Deciduous/Coniferous woodland	NH694753	269450	875350	5656
Loch Achnacloich	Alkaline fens and reedbeds	NH667736	266750	873650	6008
Braelangwell Wood	Deciduous/Coniferous woodland	NH688631	268850	863150	7503
Norvar	Deciduous/Coniferous woodland	NH635699	263550	869950	8067
Rosemarkie to Shandwick coast	Sand dunes	NH777642	277750	864250	8494
Struie Channels	Deciduous/Coniferous woodland	NH673781	267350	878150	9088

Model predictions using the ADMS and AERMOD models are shown in Figure 36 and illustrate an excellent agreement between the models with all predictions agreeing within +/- 50%. An intercomparison of SCAIL-Combustion, run using “realistic” and “conservative” meteorological assumptions, with ADMS and AERMOD is shown in Figure 37. The results show that SCAIL-Combustion predicted higher concentrations than either ADMS or AERMOD by between factors of 1.01-1.67 and 2.6 –11.7 depending on whether “realistic” or “conservative” meteorological assumptions were made. The over-predictions are expected as the tool is designed to provide a precautionary screening assessment for the combustion plant.

Figure 36 - Intercomparison of AERMOD and ADMS for habitats surrounding the case study CHP Plant

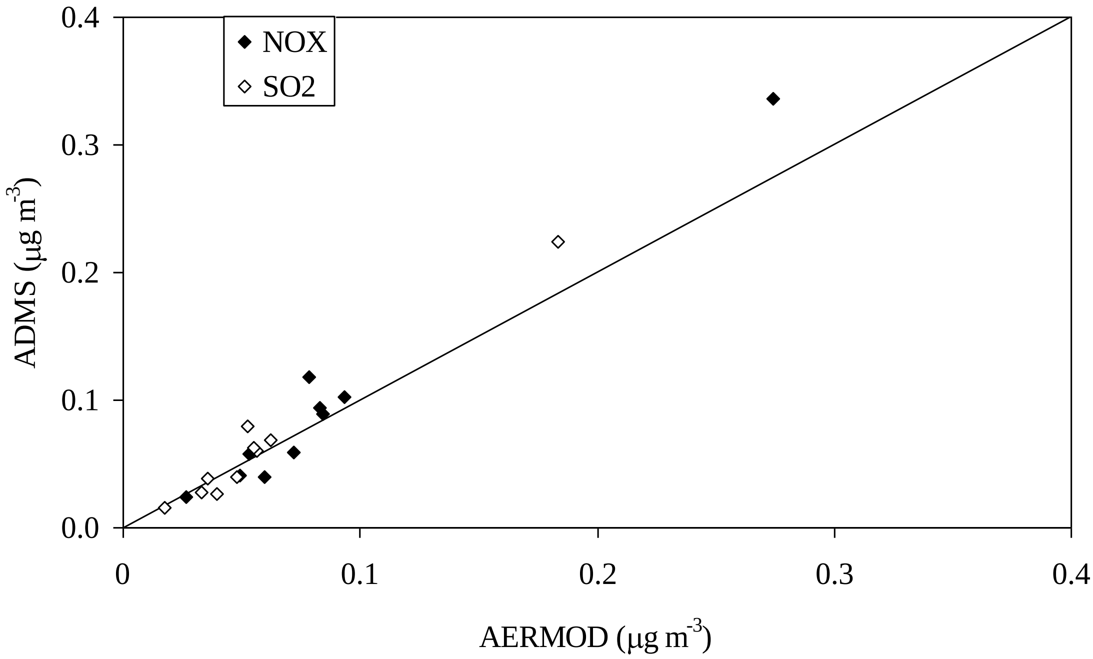
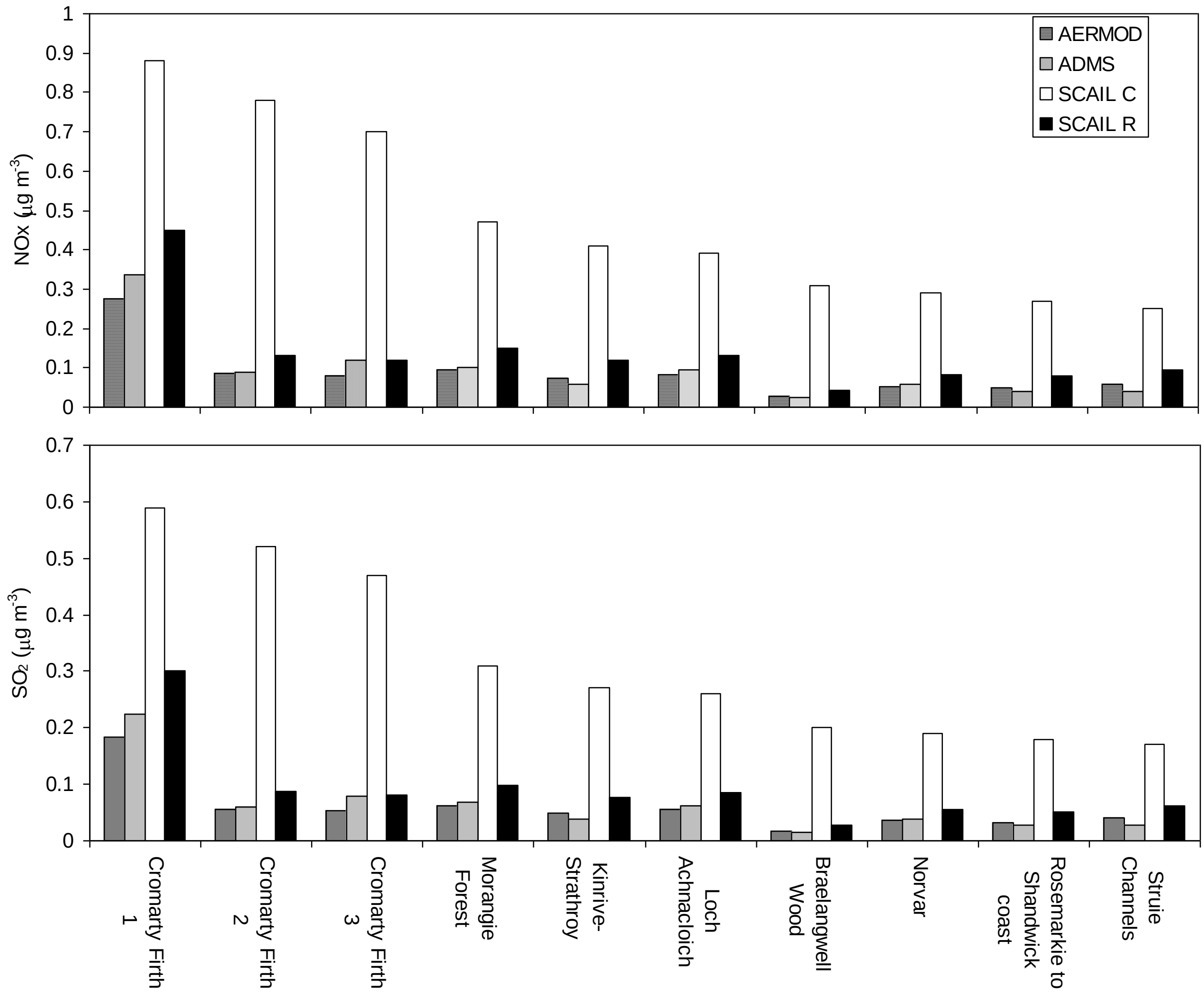


Figure 37 - Intercomparison of AERMOD, ADMS and SCAIL-Combustion for habitats surrounding the case study CHP plant (C denotes conservative meteorology and R denotes realistic meteorology for SCAIL-Combustion).



The SCAIL combustion tool was run in “conservative” mode to provide an initial screening assessment for the case study CHP plant. As previously mentioned, this mode of SCAIL-Combustion ensures that the receptor is in the prevailing wind direction, accounting for the potential effects of local wind fields and therefore is likely to provide higher concentrations than when the actual geographical position of the receptor site is considered. The results of the assessment are shown in Table 13.

Concentrations of NO_x and SO_2 (shown in Table 13) were all considerably lower than the respective environmental standards of 30 µg m^{-3} and 20 µg m^{-3}. Nitrogen fluxes were also all predicted to be below the relevant critical loads, however critical loads for acid deposition were exceeded at two sites: Loch Achnacloich and Norvar. It should be noted however that at both sites the contribution from the case study CHP plant was considerably less than 10% of the critical load (5.4 %: Loch Achnacloich; 1.4 % Norvar) and that the exceedance of the critical loads were due to other “background” sources. SCAIL-Combustion was re-run using the “realistic” meteorology mode whereby the actual geographical positions of the sites are considered. The results from this assessment are listed in Table 14 and show that the case study CHP plant contributed less than 2% of the critical load for acid deposition at Loch Achnacloich and less than 0.5% of the critical load at Norvar.

Table 13 - Results from SCAIL-Combustion using “conservative” meteorology for the habitat sites identified at case study CHP plant. Exceedances of the relevant standards are shown in grey.

Receptor name	NO_x ($\mu g\ m^{-3}$)		SO_2 ($\mu g\ m^{-3}$)		Deposited N (kg ha^{-1})			Deposited Acid (kEq H+ ha^{-1})		
	CHP Plant	CHP plant + Background	CHP Plant	CHP plant + Background	CHP Plant	CHP plant + Background	Critical Load	CHP Plant	CHP plant + Background	Critical Load
Cromarty Firth 1	0.88	0.88	0.59	1.09	0.10	5.10	20	0.02	0.49	N/A
Cromarty Firth 2	0.78	0.78	0.52	1.72	0.09	4.59	20	0.02	0.51	N/A
Cromarty Firth 3	0.70	3.50	0.47	1.17	0.08	5.68	20	0.02	0.57	1.50
Morangie Forest	0.47	2.37	0.31	0.71	0.05	9.95	15	0.02	0.87	1.27
Kinrive-Strathroy	0.41	2.21	0.27	0.47	0.05	8.45	15	0.02	0.81	0.95
Loch Achnacloich	0.39	2.29	0.26	0.66	0.05	5.35	35	0.02	0.52	0.35
Braelangwell Wood	0.31	2.21	0.20	0.40	0.03	11.33	15	0.01	0.98	1.23
Norvar	0.29	2.89	0.19	0.79	0.03	8.53	15	0.01	0.81	0.78
Rosemarkie to Shandwick coast	0.27	2.17	0.18	0.48	0.03	4.63	20	0.01	0.44	0.75
Struie Channels	0.25	1.85	0.17	0.37	0.03	8.43	15	0.01	0.80	1.28

Table 14 - Results from SCAIL-Combustion using "realistic" meteorology for the habitat sites identified near to the case study CHP plant. Exceedances of the relevant standards are shown in grey.

Receptor name	NO_x ($\mu g\ m^{-3}$)		SO_2 ($\mu g\ m^{-3}$)		Deposited N (kg ha^{-1})			Deposited Acid (kEq H+ ha^{-1})		
	CHP Plant	CHP plant + Background	CHP Plant	CHP plant + Background	CHP Plant	CHP plant + Background	Critical Load	CHP Plant	CHP plant + Background	Critical Load
Loch Achnacloich	0.13	2.03	0.09	0.49	0.02	5.32	35	0.007	0.51	0.35
Norvar	0.08	2.68	0.06	0.66	0.01	8.51	15	0.003	0.80	0.78

5. Validation Conclusions

Atmospheric SO_2 and NO_x concentrations for the Aire Valley network of power stations and Aberthaw power station in the Vale of Glamorgan were estimated using the atmospheric dispersion modelling tools AERMOD and ADMS. Atmospheric pollutant concentrations estimated using both software packages showed good agreement. Also, when modelled concentrations were compared against wind sector-corrected monitoring data to remove the effects of other emission sources, both AERMOD and ADMS were able to closely predict atmospheric concentrations of the pollutants at the monitoring locations. In conclusion, the validation of AERMOD for use as a dispersion modelling tool in SCAIL-Combustion has been successful, as it has been shown that AERMOD reproduces atmospheric concentrations of pollutants that are comparable with estimates produced using the widely used atmospheric dispersion model, ADMS. More importantly, it has been shown here that AERMOD can produce atmospheric pollutant concentrations that are comparable with monitored data.

SCAIL-Combustion was also run to determine atmospheric concentrations of NO_x and SO_2 at receptor sites in the Aire Valley and at locations close to Aberthaw power station. Initial modelling studies showed that SCAIL-Combustion was able to reproduce atmospheric concentrations that were comparable with other modelling packages and with monitoring data for seven out of eight monitoring locations. However, for use as a screening tool, it was necessary to produce a new model methodology for SCAIL-Combustion that allows more conservative estimates of the impact of combustion sources on the environment. The new methodology now employed in SCAIL-Combustion has resulted in more conservative estimates of NO_x and SO_2 concentration for seven out of the eight receptor sites investigated in the Aire valley and the Vale of Glamorgan and more realistic estimates of pollutant concentrations for the site where pollutant concentrations were previously underestimated

It is concluded that SCAIL-Combustion is fit for purpose as an on-line screening tool to assess the impacts of SO_2 and NO_x emissions from small to medium sized combustion sources on sensitive habitats.

6. Overall Conclusions

- SCAIL-Combustion has been developed as a screening tool to assess the impact of NO_x and SO_2 emissions from small to medium size combustion plants on designated habitats;
- The atmospheric dispersion model AERMOD, which is used within SCAIL-Combustion was validated using data for Power Stations in England and Wales and shown to provide similar estimates to another regulatory dispersion model ADMS;
- The concentration predictions of SCAIL-Combustion were engineered to represent the upper 90^{th} percentile of those that may be monitored and modelling methodologies were included to account for localised wind flows;
- Data from the Air Pollution Information System were incorporated into SCAIL-Combustion to accurately account for background concentrations and critical loads;
- SCAIL-Combustion is hosted alongside SCAIL-Agriculture and can be accessed at http://www.scail.ceh.ac.uk.

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APPENDICES

Appendix A Architectural Design Specification

Interface Design

The interface of SCAIL-Combustion was developed with its users in mind. It is predicted that the users will include pollution regulators, planning officers and conservation officers, all with an interest in assessing ecosystems and the impacts from combustion sources. It has been anticipated that the range of computer literacy will be diverse and so the system has been designed to suit all competencies. The main aim of SCAIL-Combustion is to make it simple with step-by-step instructions guiding the user how to input the relevant information. The input screen was also designed to include inputs likely to be included on a permit application for a combustion plant. The system can account for multiple sources and calculates a total critical load exceedance at the edge of the protected habitat for all of the sources entered.

Input screen

Figure A1 shows the SCAIL-Combustion input form. Here the user adds the relevant information to obtain a deposition estimate for the habitat from a series of sources. Information that is entered includes:

Project details:

Project notes (Input Field): The user inputs details on the sources to be modelled and the type of run being carried out, e.g. 'worse case' or 'realistic'. This information is copied onto the output screen and also to any output files saved.

Project Run Mode (Select Box): The user selects 'Conservative Met' or Realistic Met'.

Location details:

Country (Select List): The user selects the relevant country for the location of the Combustion plant. The model uses this selection to link to the correct series of meteorological stations. The user does have the option to enter site specific meteorological data by clicking the 'Upload Local Met Data' button, however, this option is for expert users only.

Habitat Type (Select List): The user selects a relevant habitat type that matches the protected habitat in question. These habitats are based on the APIS habitat classification system and a critical load is associated with each one. The habitat details can be checked by clicking on the 'SNHi Habitat check' button.

Habitat Grid Reference (Input Field): The user enters the grid reference of the habitat, which is required in order to obtain the background nitrogen and sulphur deposition to the site. The background data comes from the APIS database. The grid reference can be entered either as Landranger (e.g.NJ692258) or OS x,y, co-ordinates (e.g. 345665,456755) in meters. The location of the habitat can be checked by clicking on the 'Verify Location' button. This will use the grid reference entered and look up the location on www.multimap.com. For Northern Ireland only x,y, co-ordinates in meters can be entered but the multimap lookup function cannot be used.

Background Levels and Habitat Impact Limits: The user can click the 'Check Background Levels' button to link to the APIS site and check the background levels for the Grid Reference entered.

Emission / source details:

Source: The user will be able to enter a maximum of 20 combustion sources/plants.

Source Name (Input Field): The user enters the Name of the Combustion Plant being modelled.

New or existing (Select list): The user selects 'new' or 'existing' from the drop down list. Ideally SCAIL-Combustion should be used to look at the effect of SO_2 and NO_x emissions from new point sources (stacks). However, if an existing stack is modelled in SCAIL-Combustion then it may be appropriate to report the process contributions arising from the existing stack to SO_2 and NO_x concentrations and depositions. Users of the model should be aware of the issue of double counting as model predictions from existing sources may be included in the estimates of background concentrations or depositions. However, as SCAIL-Combustion is a screening tool it is appropriate to include these contributions to ensure that the model predictions are conservative. Annotations are included in the model output to identify that this has occurred and may require further consideration as part of a more detailed dispersion modelling assessment.

Number of stacks: The user cannot manually change this box. The model updates the number of stacks automatically as new stack data is added. A maximum of ten stacks are permitted per source.

Stack (Select List): The user can only add additional stacks once all inputs for the previous stack have been entered. A maximum of 10 stacks are permitted per source.

Stack Height (Input Field): The user enters the stack height in metres.

Stack inner diameter (Input Field): The user enters the stack inner diameter in metres.

Stack Gas Temperature (Input Field): The user enters the stack gas temperature in degrees Celsius (^oC).

Stack gas velocity (Input Field): The user enters the stack gas velocity in metres per second ($m\ s^{-1}$).

SO_2 Emission rate (Input Field and Select Box): The user enters the SO_2 emission rate in tonnes per year ($t\ a^{-1}$ (default)), kilograms per day ($kg\ d^{-1}$) or grams per second ($g\ s^{-1}$). If the user has emission rates in normalised metres cubed per second ($Nm^3\ s^{-1}$) or milligrams per normalised metre cubed ($mg\ Nm^{-3}$) the ‘Emission Calculator’ button can be used to convert these to an emission rate. An error trapping system has been incorporated to prevent non-expert users entering unrealistically high emission rates.

NO_x Emission rate (Input Field and Select Box): The user enters the NO_x emission rate in tonnes per year ($t\ a^{-1}$ (default)), kilograms per day ($kg\ d^{-1}$) or grams per second ($g\ s^{-1}$). If the user has emission rates in normalised metres cubed per second ($Nm^3\ s^{-1}$) or milligrams per normalised metre cubed ($mg\ Nm^{-3}$) the ‘Emission Calculator’ button can be used to convert these to an emission rate. An error trapping system has been incorporated to prevent non-expert users entering unrealistically high emission rates.

Stack Grid Reference (Input Field): The grid reference of the stack is required to calculate the distance of the stack to the habitat site being examined. The grid reference can be entered either as Landranger (e.g.NJ692258) or OS x,y, co-ordinates (e.g. 345665,456755) in meters. The location of the stack can be checked by clicking on the ‘Verify Location’ button. This will use the grid reference entered and look up the location on www.multimap.com. For Northern Ireland only x,y, co-ordinates in meters can be entered but the multimap lookup function cannot be used.

Notes Box (Input Field): The user enters information about the Sources and Stacks being considered in the current model run. This information is copied onto the output screen and also to any output files saved.

Submit buttons: There are four submit buttons –

- ‘Load Input Data’ allows the user to load previously saved input files;
- ‘Calculate’ takes the user to the results page;
- ‘Save input data’ allows the user to save the parameters entered into the input screen. If required the user can enter any saved input files back into SCAIL-Combustion or directly into AERMOD; and,
- ‘Clear Form’ clears the form but more importantly it deletes sources that have already been entered. It is used for setting up a completely new query.

Throughout the form filling the user can consult the guidance notes by clicking on the info button (?). Figure A2 shows an example of this. These are quick notes and information that compliment the fuller user guide document.

It should be noted that the application of AERMOD used does not include the option to include the influence of site buildings on plume dispersion as detailed building data are unlikely to be readily available and as building effects are only of significance in close proximity to the site. A simple assessment of the downwind distance that site buildings affect dispersion can be made as the lesser of 10W or 10H where W and H are the width and height of the site building or building group respectively. Consequently a generic estimate of the minimum distance that the predictions of the model may be considered representative would be of the order of 100 - 500m. The upper distance that the model predictions may be considered representative can be determined by the time-of-flight of the plume. AERMOD uses discreet 1-hour meteorological periods hence for typical UK wind speeds a dispersing plume may be estimated to travel 10-30 km per hour. Although the model may be used at a range of downwind distances users should note that the uncertainties of the modelling approach may be higher than usual when the distances selected are either less than 500 m or greater than 30 km.

Results Page

The results page provides a simple table of all the sources that have been added with a deposition contribution from each source (see Figure A3). The type of run (Conservative Met. or Realistic Met.) is displayed along with the degrees that the receptor is off the plume centre line if 'Conservative Met." is selected. Any notes the user has entered on the input page are also displayed along with the meteorological station that SCAIL-Combustion has used to calculate the results.

A breakdown of the total deposition to the habitat is given together with the background deposition taken from the APIS database and based on the grid reference supplied by the user on the form. The critical level/load based on the habitat type is provided. A critical level/load exceedance (total deposition - critical level/load) is then calculated and displayed for NO_x, SO_x, N Deposition and Acid Deposition. A positive value indicates an exceedance.

The user will be able to click the 'help' button to show a simple guidance note on how to interpret the data written by SEPA. The output page also provides a link to the appropriate SEPA/EA contacts if further information is required.

Development and programming

SCAIL-Combustion has been designed for the web using standard html and the scripts have been written using a mixture of Perl, Javascript Php and SQL. The database that holds the background deposition and concentrations, and the critical load information for each habitat, are stored in the APIS Oracle database.

The AERMOD model (version 07026) has been recompiled using a Linux Fortran Compiler to run off the CEH server currently used to host SCAIL - Agriculture. Text-format AERMOD input files have been created using data entered into the user interface using a suitable scripting language. Meteorological input data for 30 sites have been included within the model along with an option for expert users to include site-specific data. All the input data entered by the user into the interface is appended to the AERMOD input file, thus allowing the user the option to load a saved data set which is compatible with stand-alone versions of the AERMOD executable file.

The model is hosted on a virtual server (Linux server). The system uses session id's to store and pass information between the client browser and the server, for example, as stacks are added or in calculating the results. User inputs into the web-form are validated using the Javascript client-side language.

The system has undergone a series of testing phases.

Figure A1 - SCAIL – Combustion Input Screen

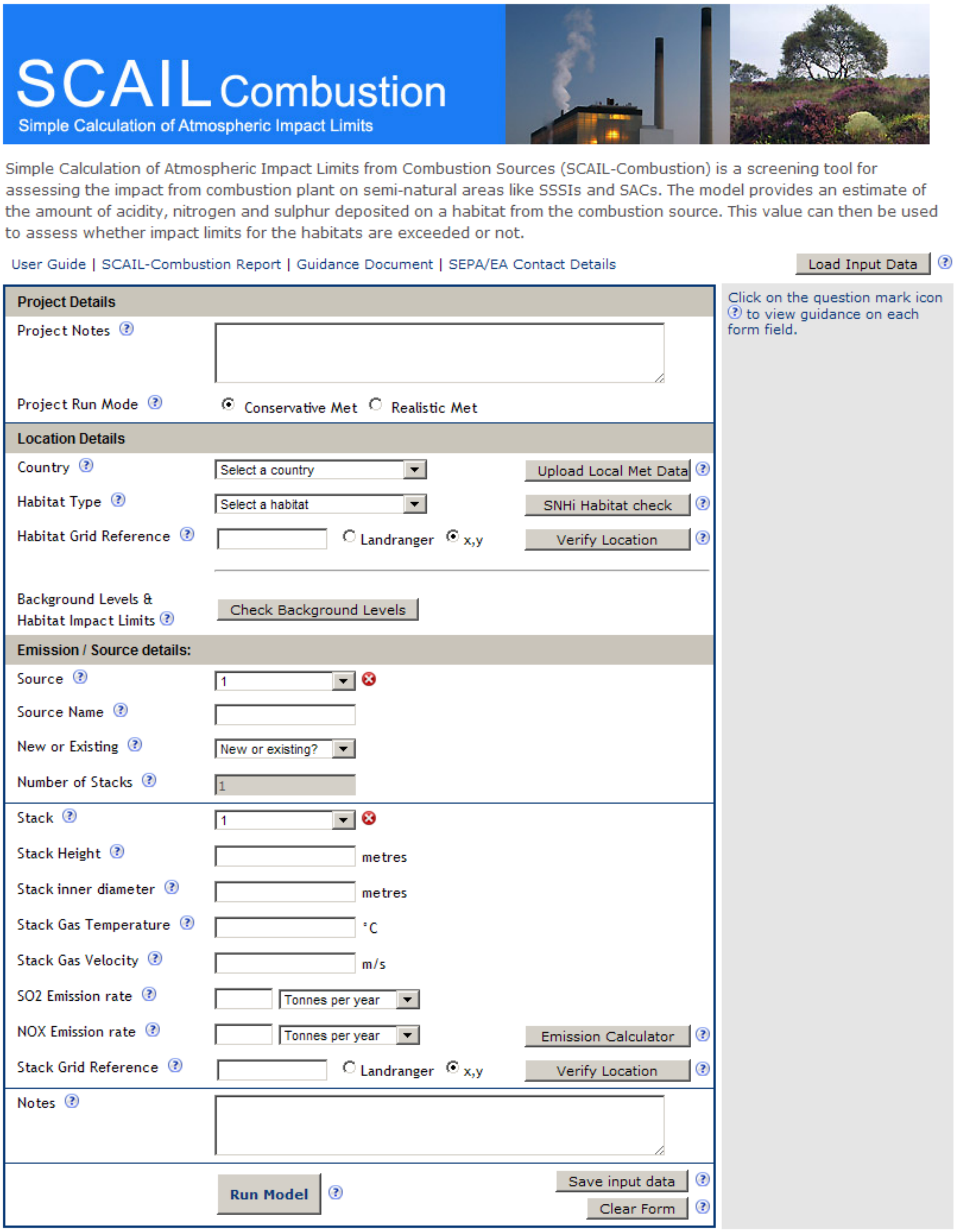


Figure A2 - Example of the info button. Users can gain guidance on an input field by clicking on the info button (?). The guidance text is displayed on the right.

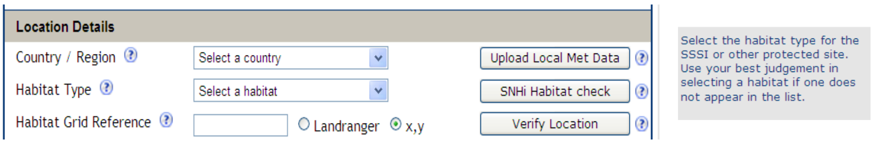
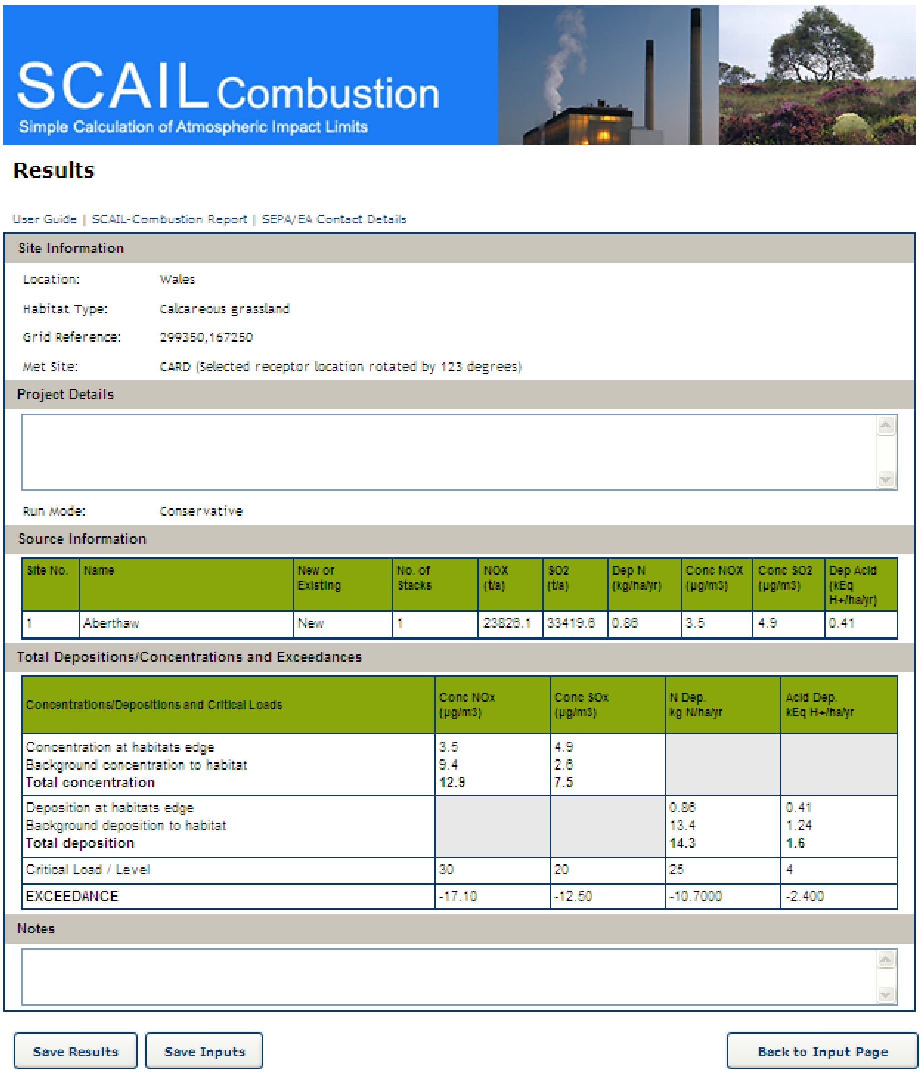


Figure A3 - SCAIL – Combustion Output Screen



Results

User Guide | SCAIL-Combustion Report | SEPA/EA Contact Details

Site Information

Location: Wales

Habitat Type: Calcareous grassland

Grid Reference: 299350,167250

Met Site: CARD (Selected receptor location rotated by 123 degrees)

Project Details

Run Mode: Conservative

Source Information

Site No.	Name	New or Existing	No. of Stacks	NOX (t/a)	SO2 (t/a)	Dep N (kg/ha/yr)	Conc NOX (µg/m3)	Conc SO2 (µg/m3)	Dep Acid (kEq H+/ha/yr)
1	Aberthaw	New	1	23826.1	33419.6	0.86	3.5	4.9	0.41

Total Depositions/Concentrations and Exceedances

Concentrations/Depositions and Critical Loads	Conc NOx (µg/m3)	Conc SOx (µg/m3)	N Dep. kg N/ha/yr	Acid Dep. kEq H+/ha/yr
Concentration at habitats edge Background concentration to habitat **Total concentration**	3.5 9.4 **12.9**	4.9 2.6 **7.5**		
Deposition at habitats edge Background deposition to habitat **Total deposition**			0.86 13.4 **14.3**	0.41 1.24 **1.6**
Critical Load / Level	30	20	25	4
EXCEEDANCE	-17.10	-12.50	-10.7000	-2.400

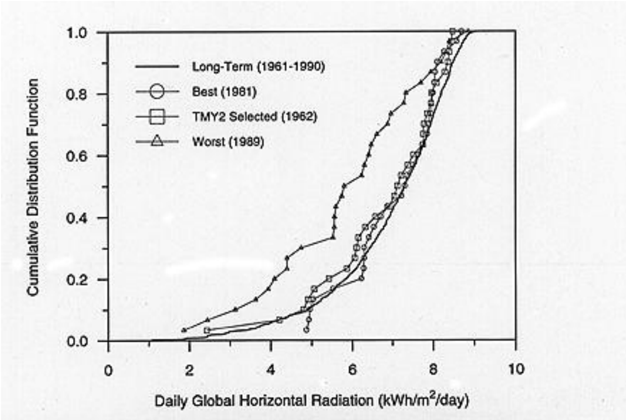
Notes

Save Results | Save Inputs | Back to Input Page

Appendix B Initial typical meteorological year (TMY) approach

The approach used for the initial typical meteorological year calculations (called the Sandia method) calculates the cumulative value of a variable (e.g. global radiation) for all years in the long-term dataset (cumulative distribution function: CDF) during a whole month and compares this with the long-term average value (see Figure B1 for an example).

Figure B1 - Example cumulative distribution functions (CDFs) for global radiation for June in Boulder, Colorado (taken from: http://rredc.nrel.gov/solar/pubs/tmy2/figA-1.html)



The comparison of the individual years with the long-term average (for the selected month) is done using Finkelstein- Schafer (FS) statistics (Finkelstein and Schafer, 1971):

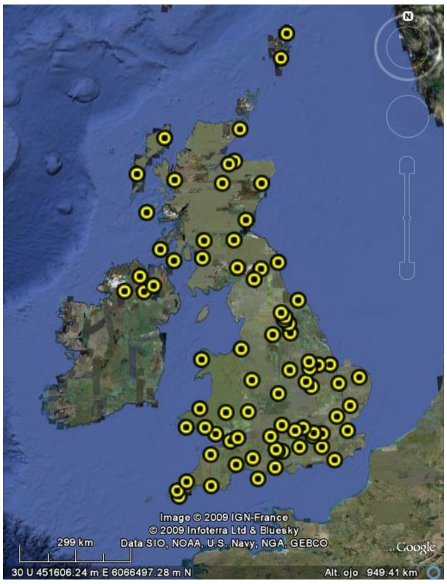
$$FS = \left(1/n\right)\sum_{i=1}^{n}\delta_i \ , \qquad \text{(Equation B1)}$$

where δ_i is the absolute difference between the long-term CDF and the candidate month CDF and n is the number of daily readings in a month. This type of statistic is more suitable for meteorological variables compared with e.g. normalised mean square error because it recognises the cumulative effect of environmental variables e.g. if the beginning of a month is cooler than the long-term average but the end of the month is warmer, then meteorological processes (such as pollutant dispersion) averaged over the month may be similar. The Sandia method then joins together ‘typical’ months to produce the typical meteorological year (with some smoothing for the month boundaries) that best represents the long-term dataset.

TMY for SCAIL-Combustion

The SAMSON pre-processor, which is used to prepare the meteorological data for SCAIL-Combustion requires hourly values of the following variables: air temperature, wind speed, wind direction, precipitation, cloud cover and relative humidity. A review of UK meteorological data reveals that the number of meteorological stations that record hourly values for all of these variables (over the period 2001-2005) is 78 (Figure B2). The suggested approach for SCAIL-Combustion is to prepare a typical meteorological year (TMY) for each of these locations for the period 2001-2005. Applying the Sandia method to data from 78 stations would be a big task and one outside of the scope of this project. Therefore a simpler method has been applied (based on monthly mean values instead of daily values) to select one year of continuous real data that best represents the meteorological conditions for that location during the period 2001-2005.

Figure B2 - Location of meteorological stations with hourly data of all variables necessary for SCAIL-Combustion simulations.



An Excel macro was developed to calculate FS statistics of the CDFs from the mean monthly values of air temperature, wind speed, precipitation, cloud cover and relative humidity. The values of FS for each year were then normalised (by dividing by the largest value for that location) to give a normalised values between 0 and 1.

Wind direction, one of the most important variables for pollutant dispersion, had to be processed differently. This is because wind direction is not a simple scalar quantity (such as air temperature) that can be summed cumulatively. The approach used for wind direction was to identify the three most frequently occurring wind directions for each month of each year and compare this with the three most frequently occurring wind directions over the 2001-2005 period. The 'score' for each year is then simply the number of wind directions the year datasets have in common with the long-term dataset.

To obtain the TMY for each location, the normalised FS values (NFS) were combined with the wind direction score. The NFS value for wind speed was multiplied by two to give it double the weighting of the other variables (air temperature, cloud cover, relative humidity and precipitation) due to its importance for pollutant dispersion. The final value for each year of data for each location was calculated as:

$$TMY_{score} = \frac{2 \cdot NFS_{ws} + NFS_{at} + NFS_{cc} + NFS_{rh} + NFS_{p}}{WD_{score}}; \qquad \text{(Equation B2)}$$

where the suffixes wd, at, cc, rh and p refer to wind direction, air temperature, cloud cover, relative humidity and precipitation respectively and WD_{score} is the number of 'top three' wind directions in common with the long-term dataset (averaged over all 12 months). The year with the lowest value of TMY_{score} is taken as the TMY for that location.

Results of the TMY calculations

Figure B3 shows the year with the lowest NFS value (for wind speed, air temp, cloud cover, relative humidity and precipitation) or WD_{score} for each station (x axis) i.e. these are the 'typical' years for the individual variables (during the period 2001-2005 inclusive). There is significant scatter between the different stations for most of the variables although for air temperature the NFS value is lowest (i.e. the annual data are most similar to the 5-year mean) for 2004 for the majority of the stations. Figure B4 shows the years with the lowest TMY_{score} values for all of the stations (i.e. the typical years according to Equation B2). Interestingly, the application of Equation B2 results in 2004 being the typical year for the majority of the stations (75%). This may be partly due to the influence of the air temperature statistics but there must also be some other factors contributing. These are preliminary calculations since the weighting of the variables in Equation B2 is arbitrary. These can be refined by running the atmospheric dispersion model for a subset of meteorological stations for each of the 5 years and comparing the output concentrations with the 5-year average. This will provide an opportunity to calibrate the weightings of the different variables.

Figure B3 - Year with the lowest NFS value (for wind speed, air temp, cloud cover, relative humidity and precipitation) or WD_{score} for each station (x axis). These represent the 'typical' years for the individual variables.

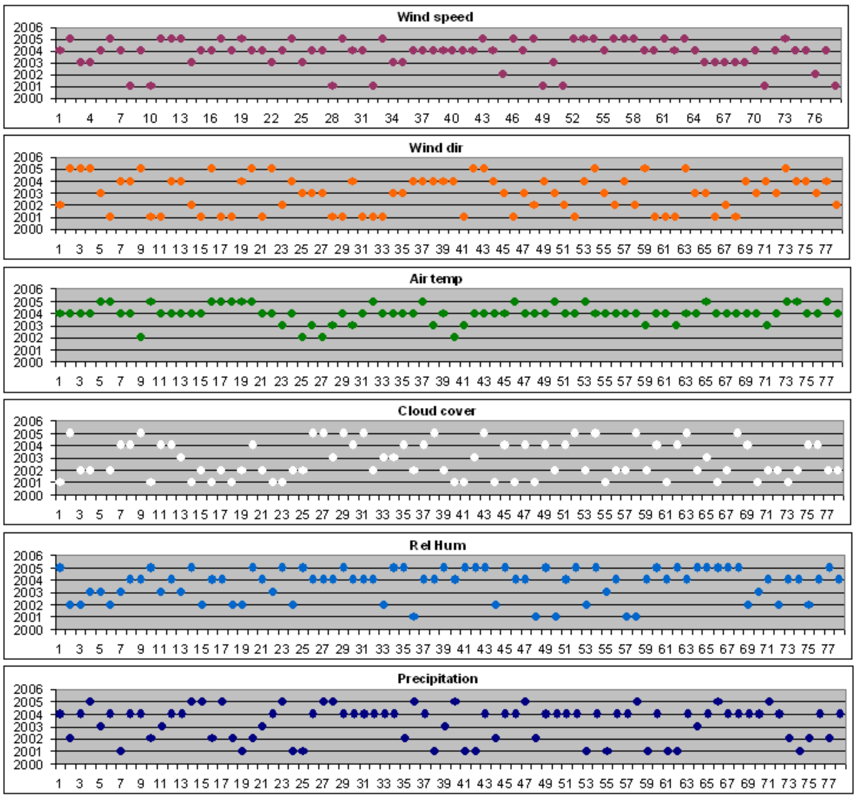
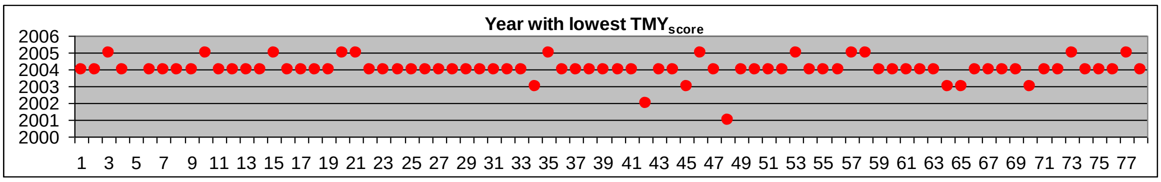


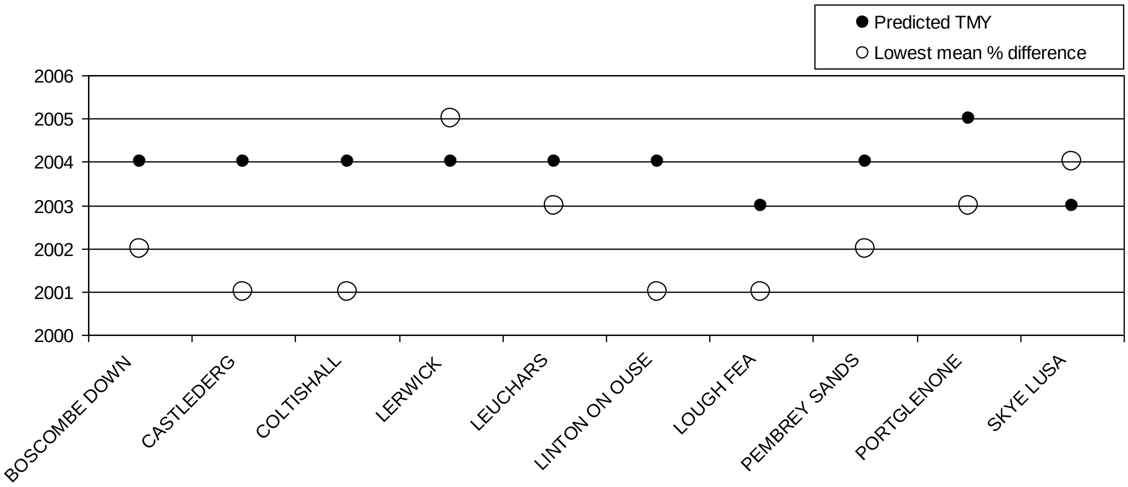
Figure B4 - Years with the lowest TMY_{score} values for all of the stations (i.e. the typical years according to Equation B2).

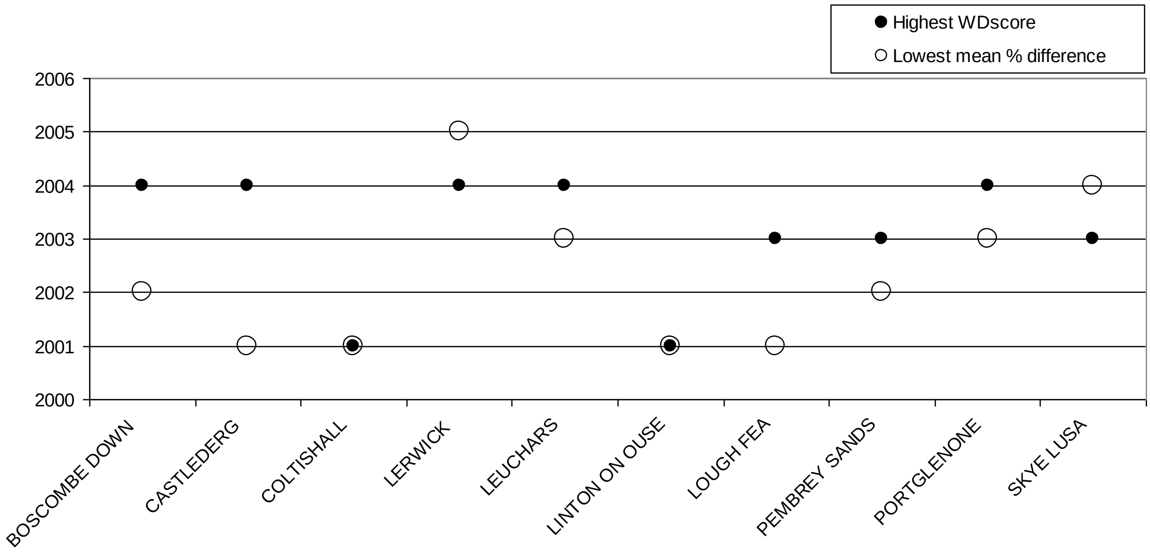


Validation of the TMY approach

The approach described above was validated by comparing the results of the model simulations described in Section 3.1.3 with the predicted TMYs. The absolute percentage difference between the model concentration prediction (for NO_2) for each individual year and the five-year average was calculated for each year and each receptor. The year with the lowest percentage difference (averaged over all receptors) was then compared with the predicted TMYs to test the TMY approach. Figure B5 shows that the TMY approach did not correctly predict the simulation year with concentration predictions most similar to the five year mean for any of the ten validation sites. An analysis of the individual terms in Equation B2 shows that none of them can be used to predict the year with concentration predictions most similar to the five year mean. The term which can be used to predict the most years with the lowest percentage difference is WD_{score}. However, the years predicted by WD_{score} only agree with years with the lowest percentage difference for two of the ten sites i.e. this term can only predict one fifth of the years with the lowest percentage difference. In conclusion, this TMY approach is not suitable for predicting the simulation years that predict the most similar concentrations to the five year mean.

Figure B5 - Years with the highest WD_{score} values for the ten validation sites and the year which gave the lowest percentage difference between the individual year and the five-year average NO_2 concentrations.





Appendix C Typical Meteorological Year Wind Roses

Table C1 - Details of meteorological sites included in SCAIL-Combustion.

Station	Name (Short)	Station Grid	Station X Coordinate (m)	Station Y Coordinate (m)	Station Elevation (m)	Wind Direction (degrees)
AVIEMORE	AVIE	OS	289652	814315	228	210
BALLYKELLY	BALL	IRL	263400	423800	4	110
BOULMER	BOUL	OS	425300	614200	23	250
CARDIFF WEATHER CENTRE	CARD	OS	318200	176100	52	230
CHURCH FENTON	CHUR	OS	452818	438027	8	270
COLESHILL	COLE	OS	421090	286940	96	200
CROSBY	CROS	OS	329940	400570	9	150
EDINBURGH GOGARBANK	EDIN	OS	316100	671400	57	250
ESKDALEMUIR	ESKD	OS	323500	602600	242	190
GLASGOW BISHOPTON	GLAS	OS	241788	671073	59	210
HEATHROW	HEAT	OS	507700	176700	25	210
ISLAY PORT ELLEN	ISLA	OS	132900	651300	17	140
ISLE OF PORTLAND	ISLE	OS	367798	69251	52	250
LERWICK	LERW	OS	445392	1139664	82	170
LEUCHARS	LEUC	OS	346800	720900	10	260
LOSSIEMOUTH	LOSS	OS	321249	869822	6	250
LYNEHAM	LYNE	OS	400629	178255	145	210
MARHAM	MARH	OS	573700	309100	21	210
MUMBLES HEAD	MUMB	OS	262700	187000	32	270
PLYMOUTH MOUNTBATTEN	PLYM	OS	249219	52714	50	90
PORTGLENONE	PORT	IRL	299100	403100	64	330
SENNYBRIDGE NO 2	SENN	OS	289408	241777	307	230
SKYE LUSA	SKYE	OS	170593	824888	18	210
SPADEADAM NO 2	SPAD	OS	364700	573000	285	250
STORNOWAY AIRPORT	STOR	OS	146443	933104	15	190
VALLEY	VALL	OS	230885	375849	10	210
DYCE	DYCE	OS	387810	812800	62	170
PRESTWICK RNAS	PRES	OS	236902	627653	10	250
TIREE	TIRE	OS	99900	744600	10	190
WICK AIRPORT	WICK	OS	336490	952230	30	150

Figure C1 - Aviemore Wind rose for 2001

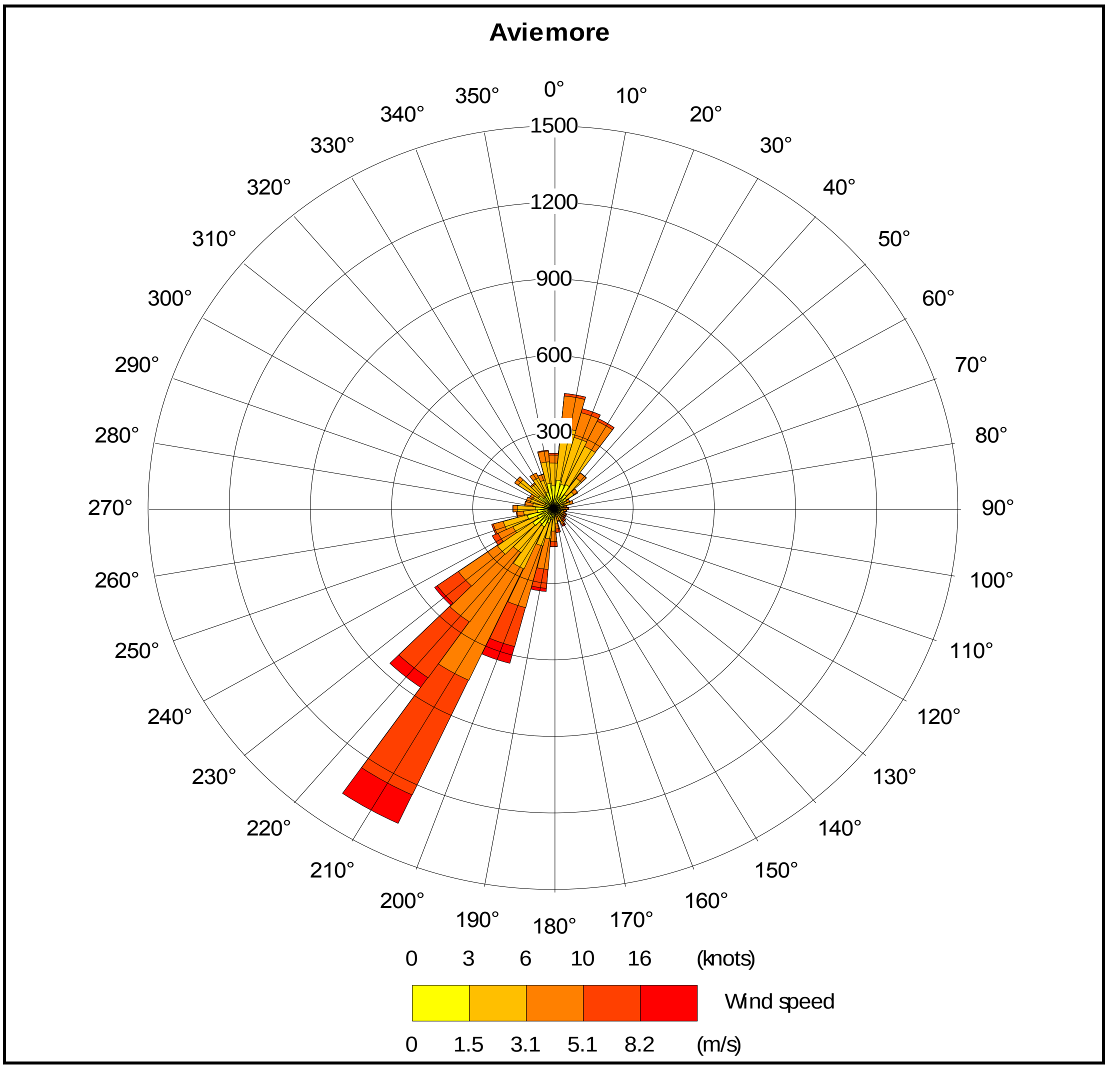


Figure C2 - Ballykelly Wind rose for 2001

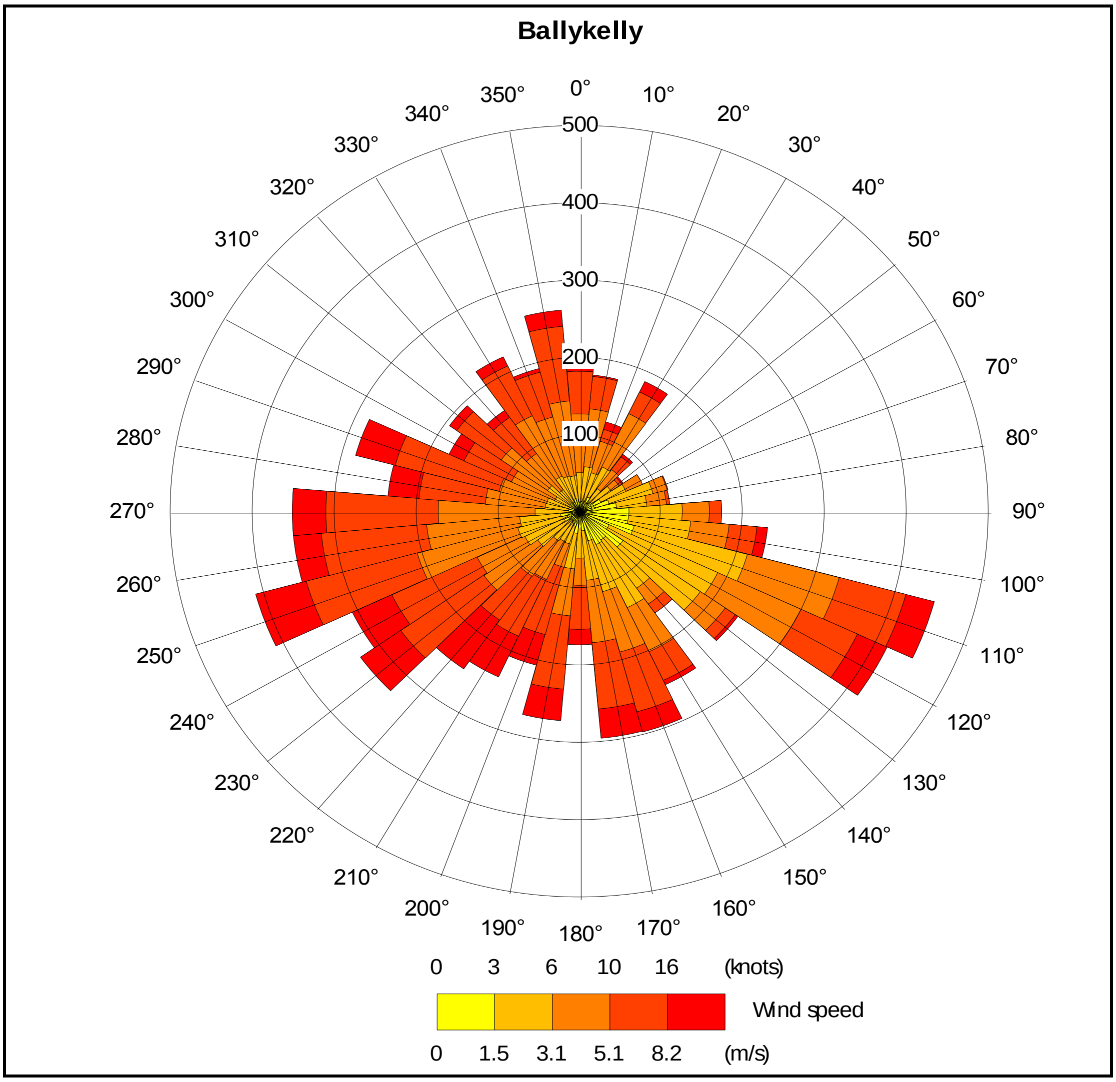


Figure C3 - Boulmer Wind rose for 2004

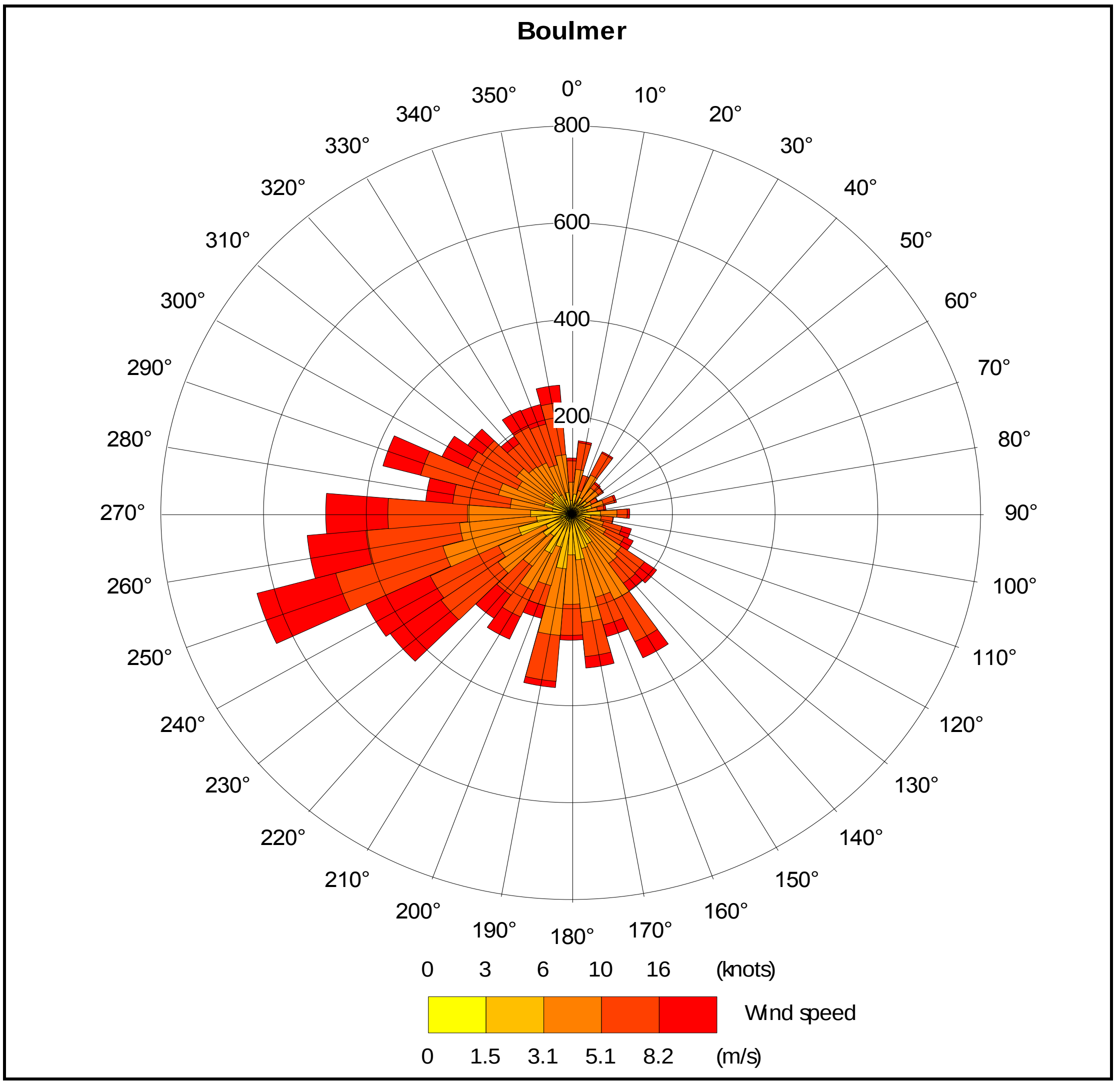


Figure C4 - Cardiff Weather Centre Wind rose for 2003

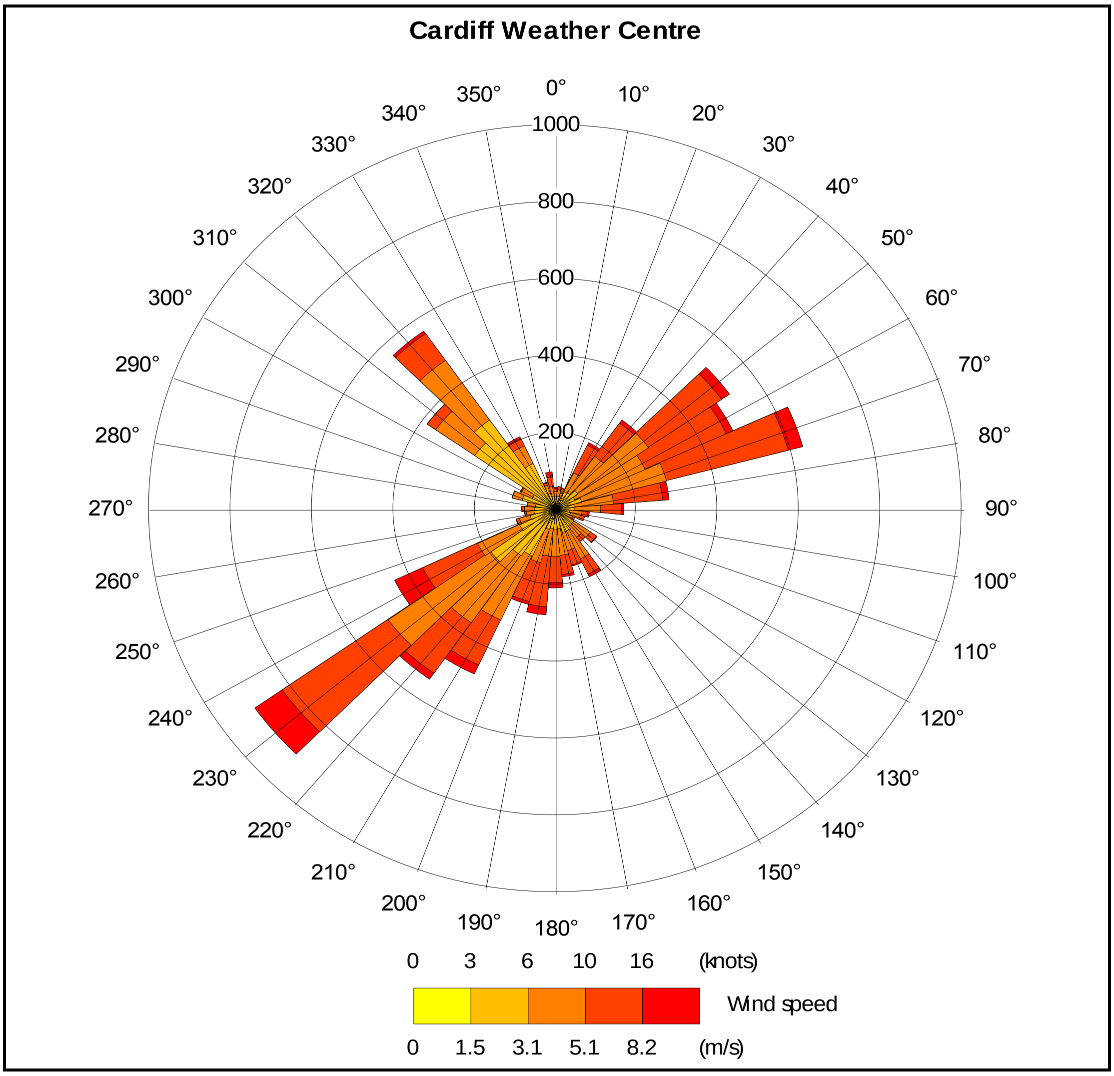


Figure C5 - Church Fenton Wind rose 2003

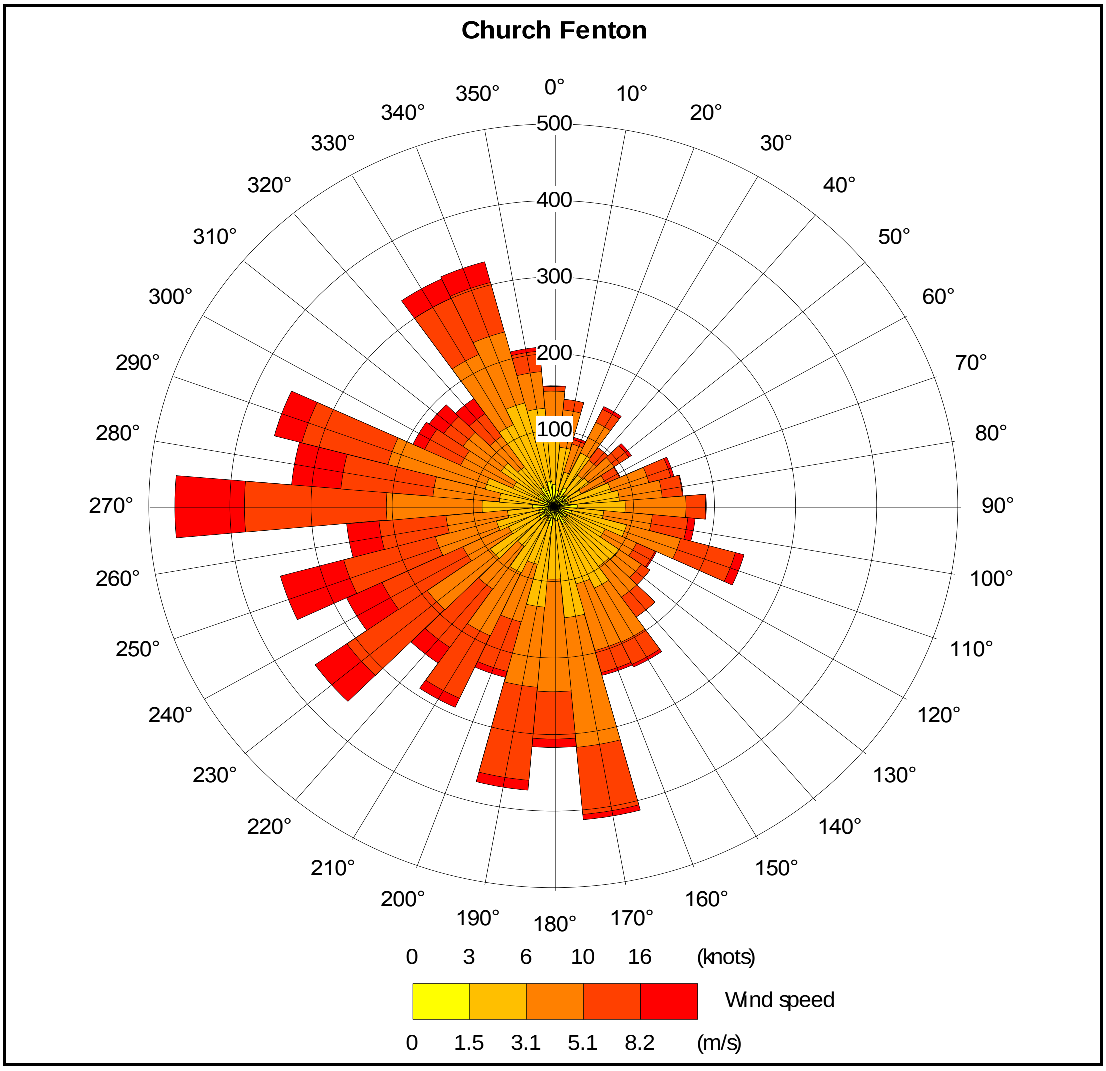


Figure C6 - Coleshill Wind rose for 2001

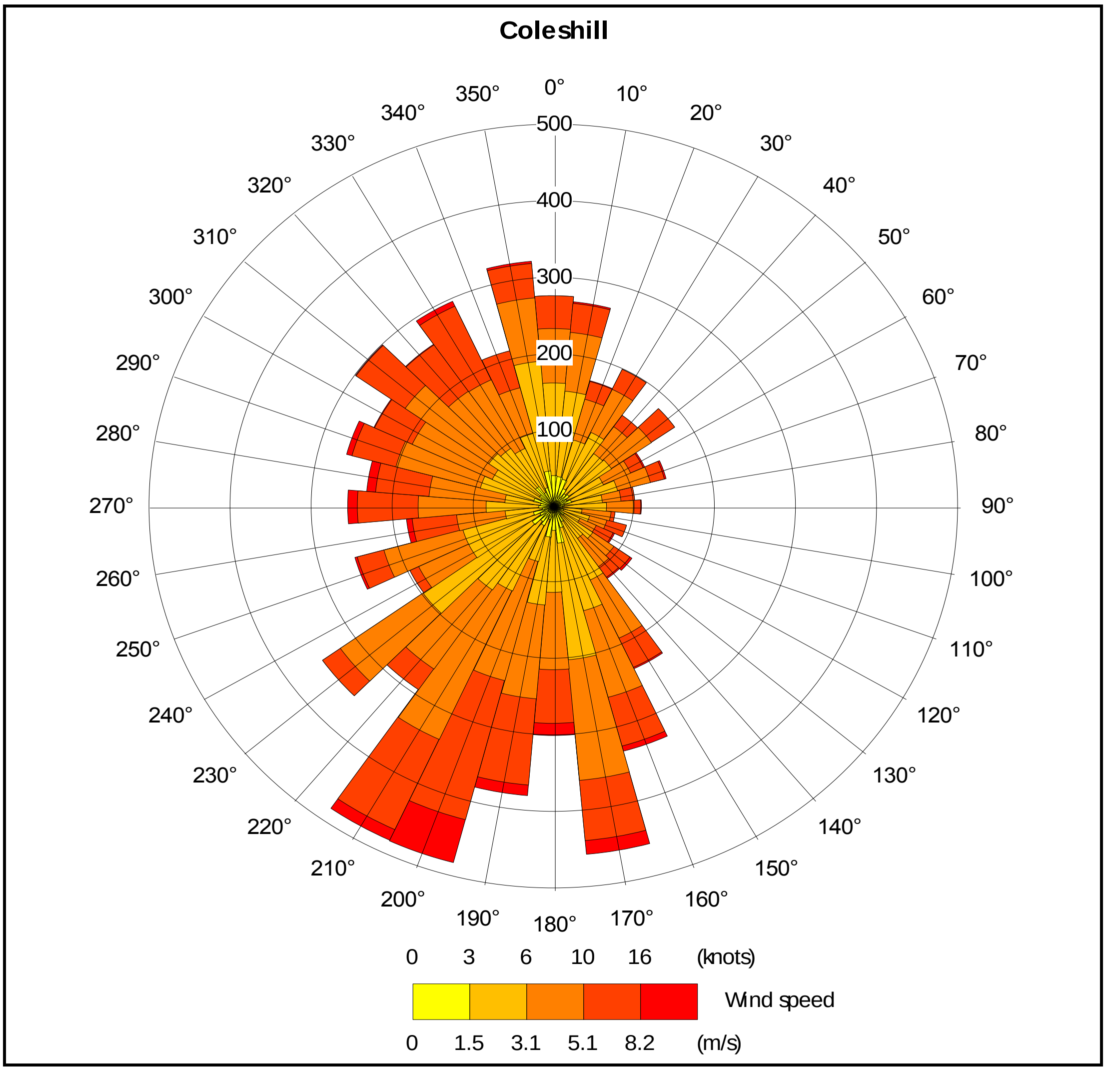


Figure C7 - Crosby Wind rose for 2001

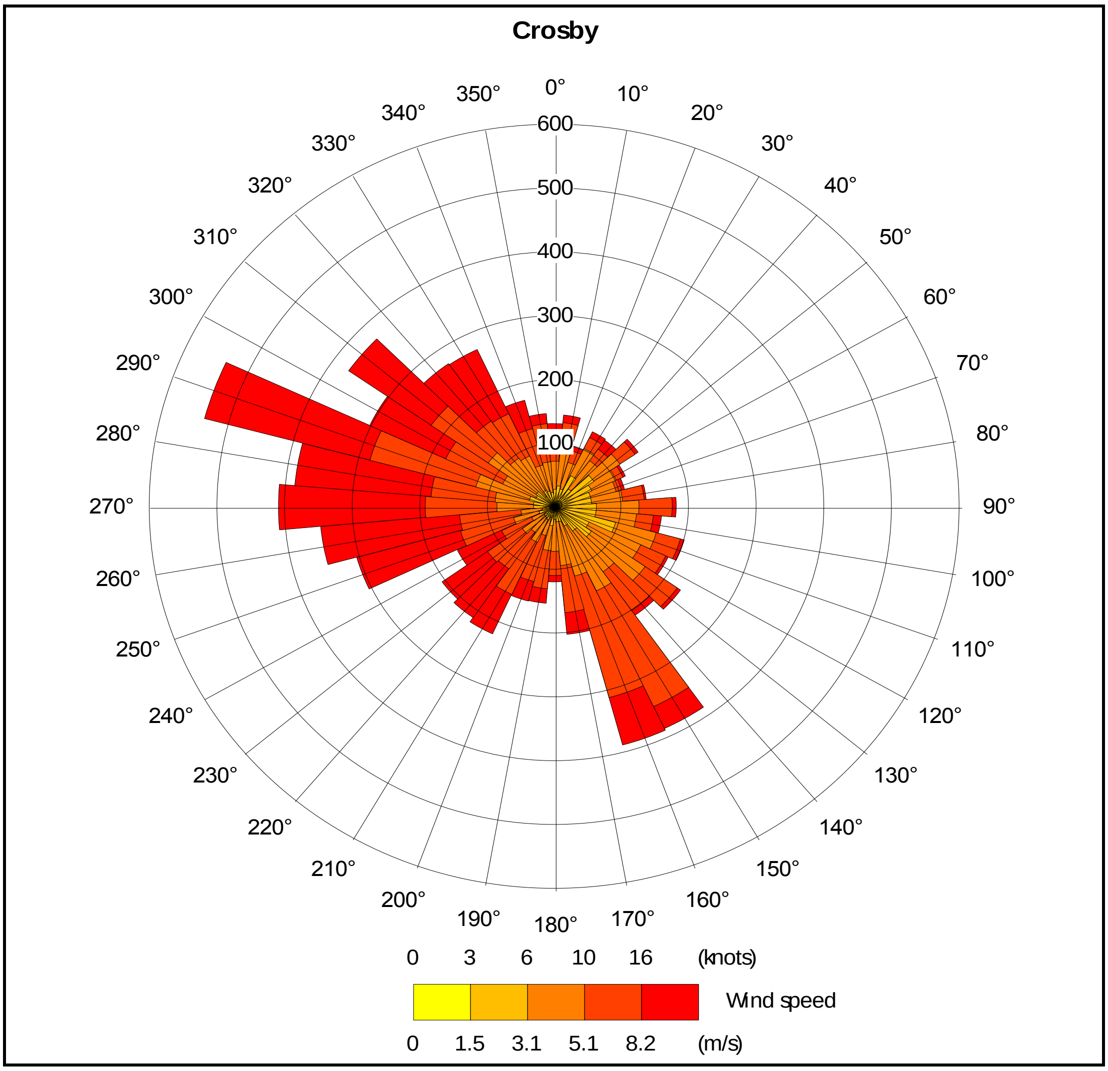


Figure C8 - Edinburgh Gogarbank Wind rose for 2003

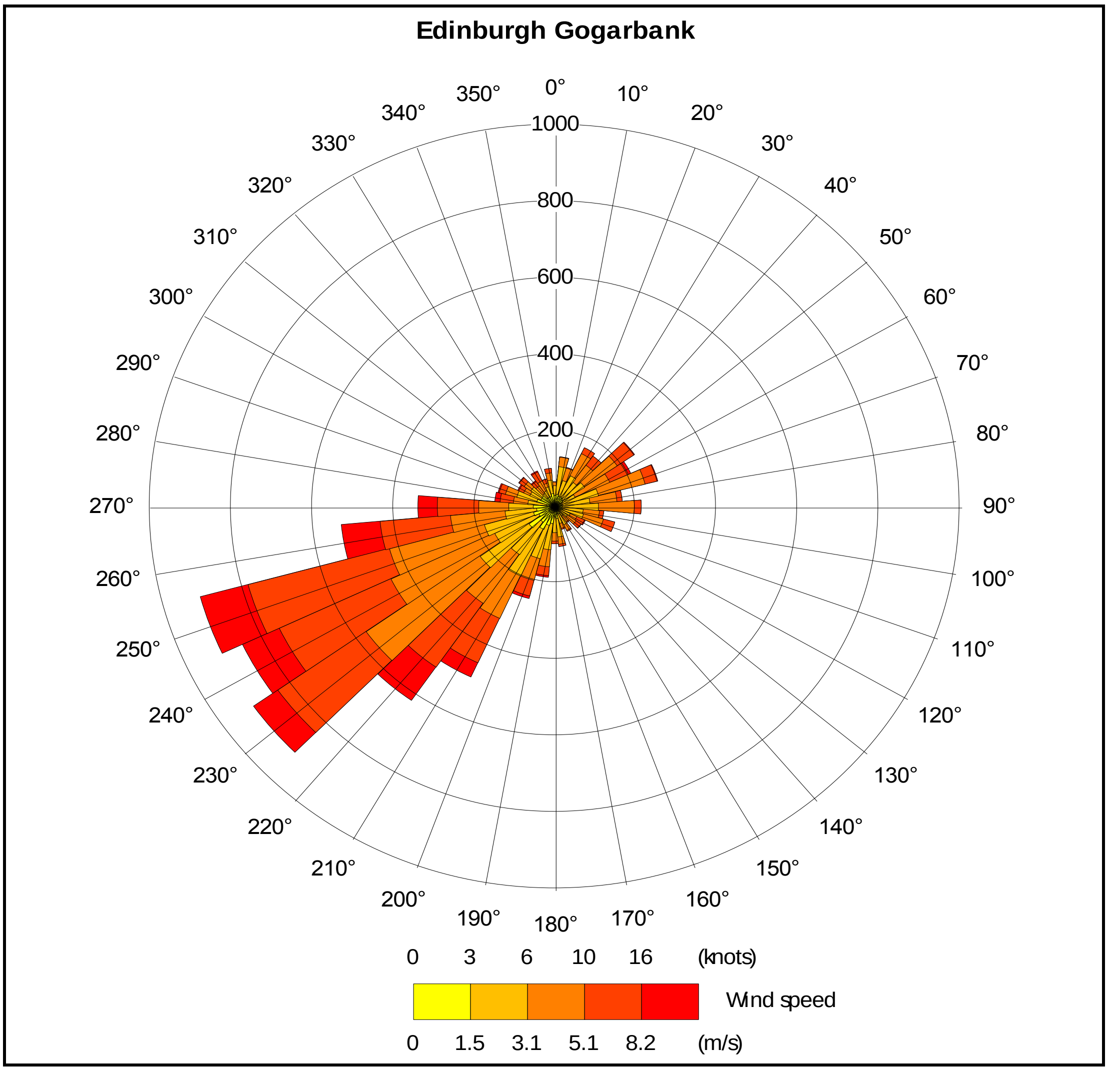


Figure C9 - Eskdalemuir Wind rose for 2004

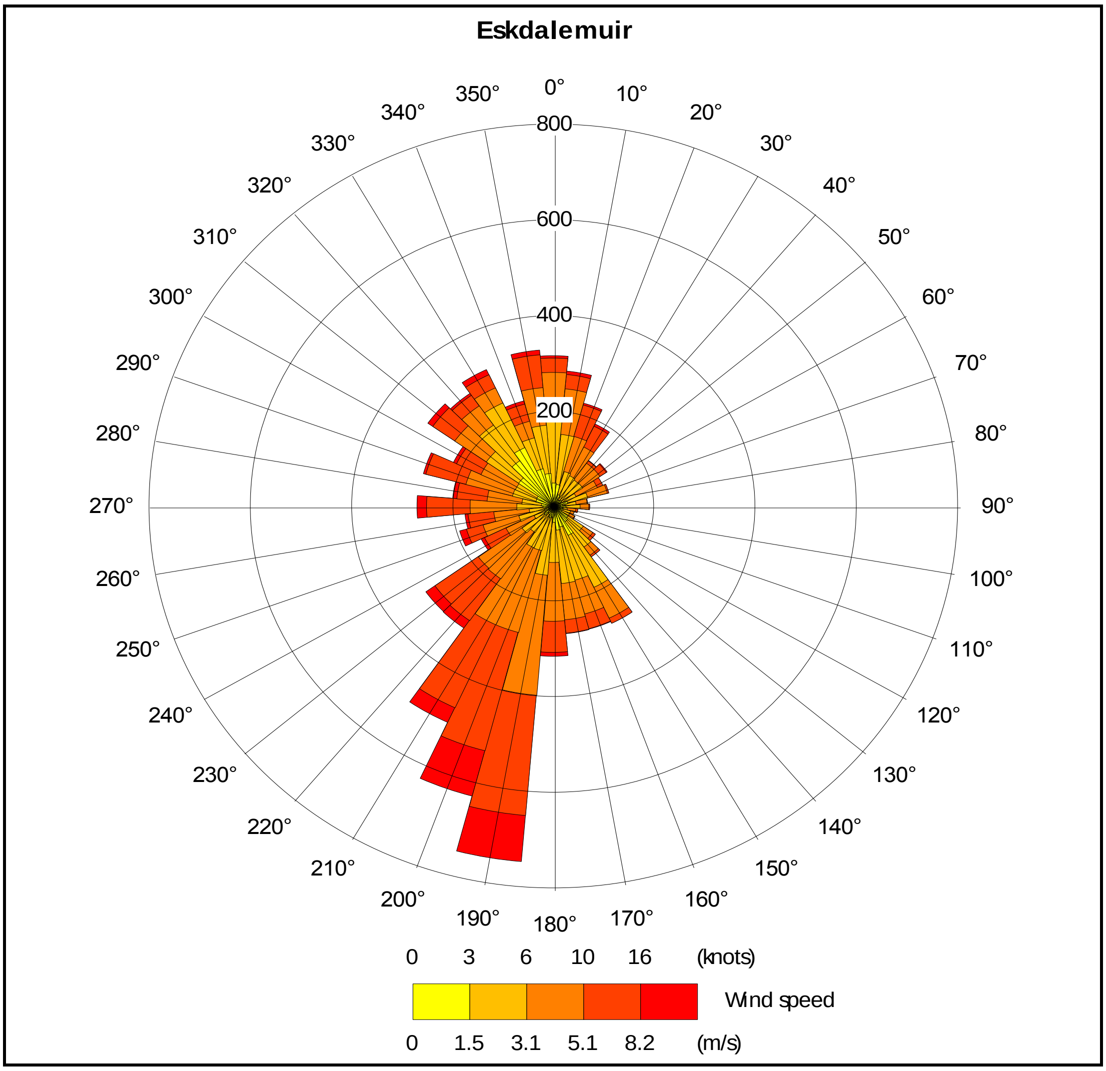


Figure C10 - Glasgow Bishopton Wind rose for 2001.

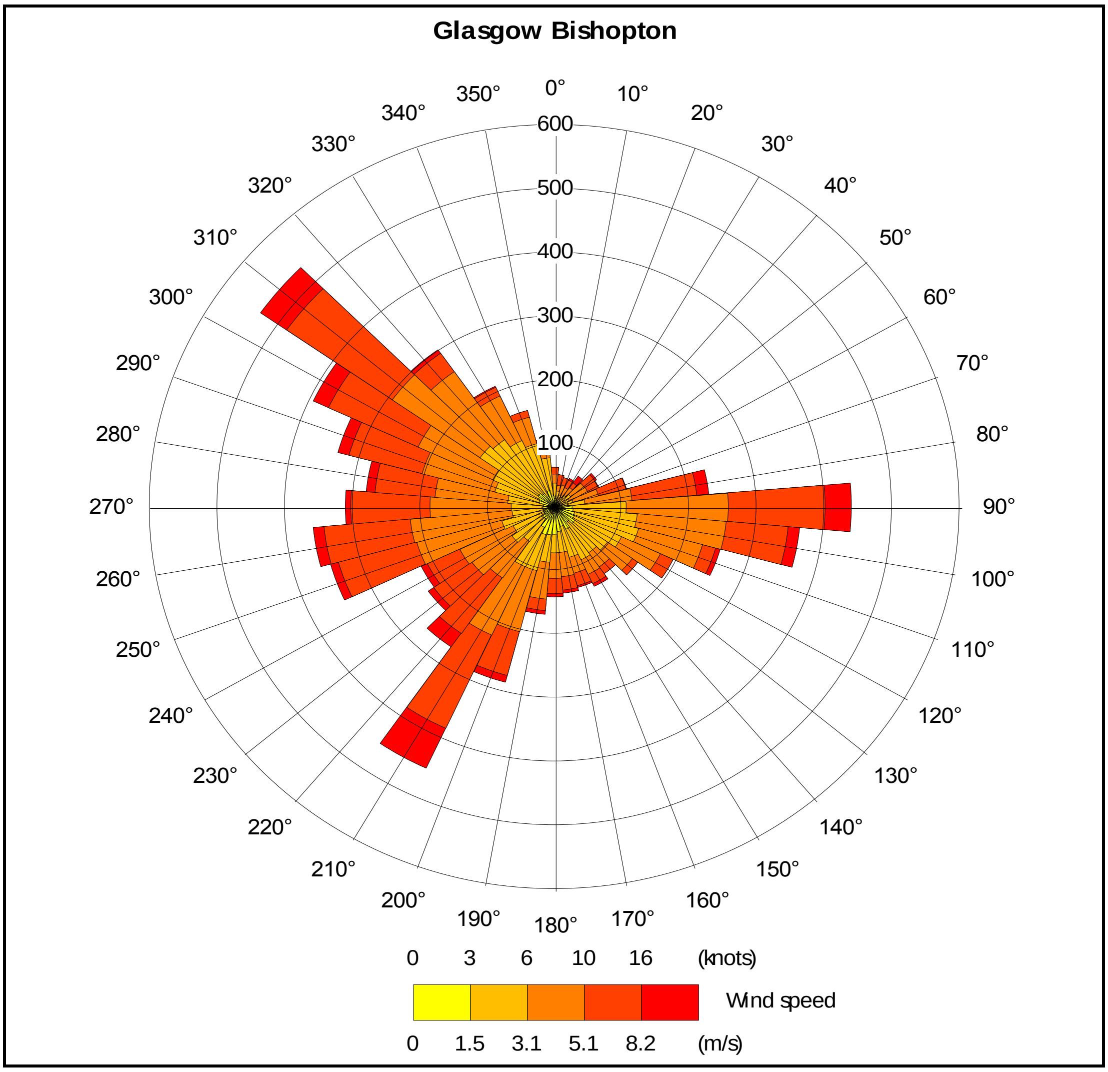


Figure C11 - Heathrow Wind rose for 2001

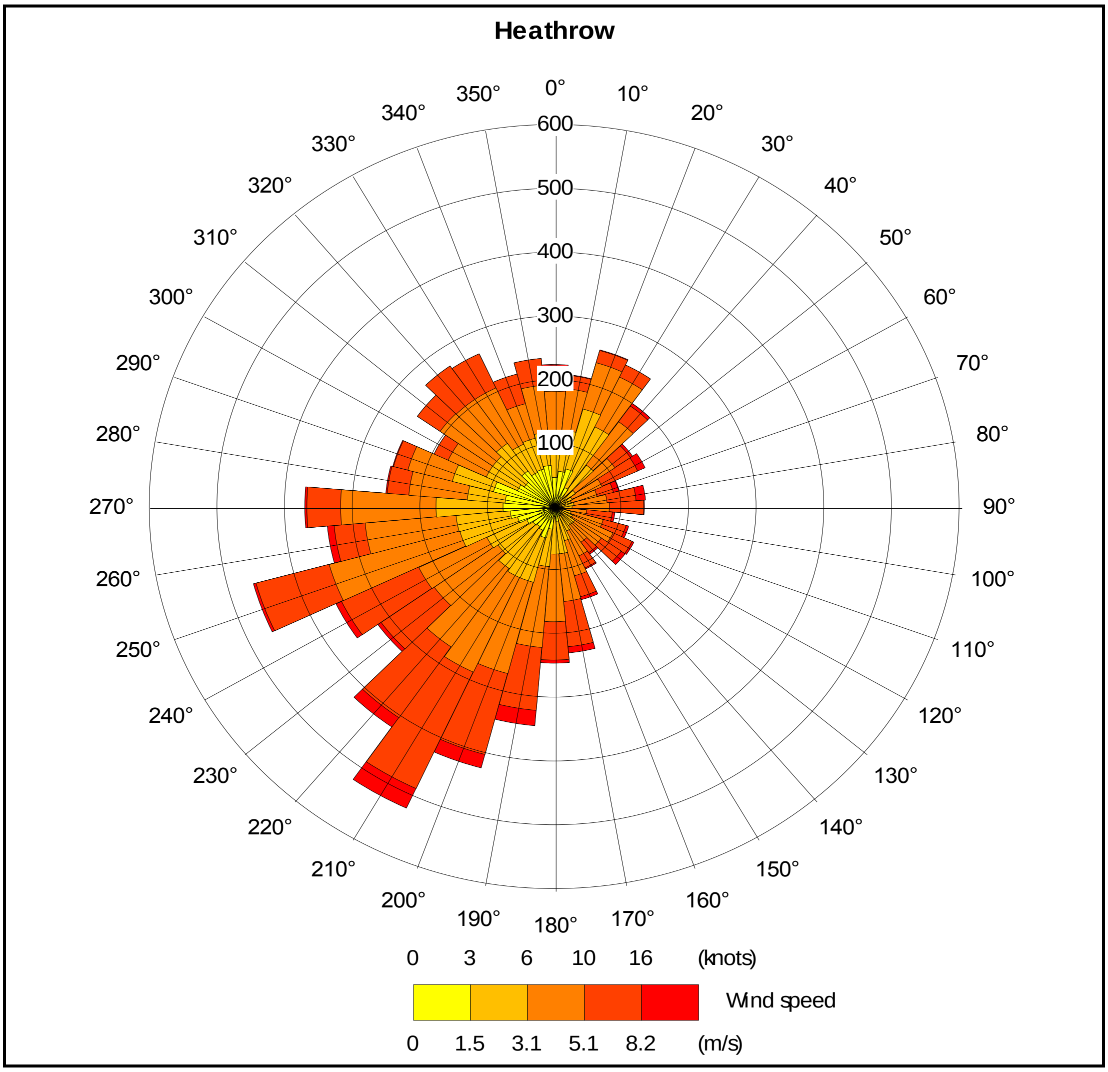


Figure C12 - Islay Port Ellen wind rose for 2005

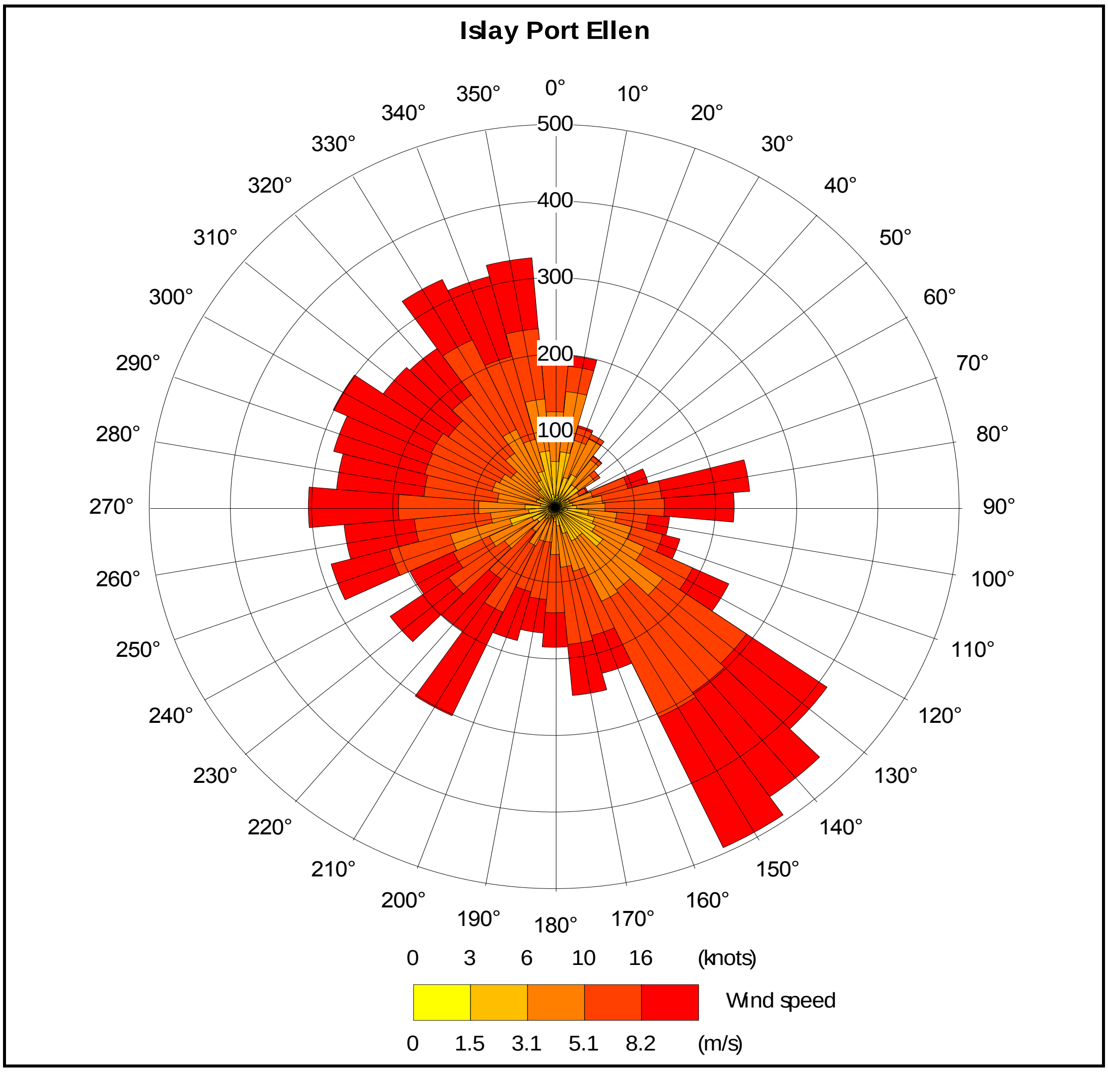


Figure C13 - Isle of Portland wind rose for 2001

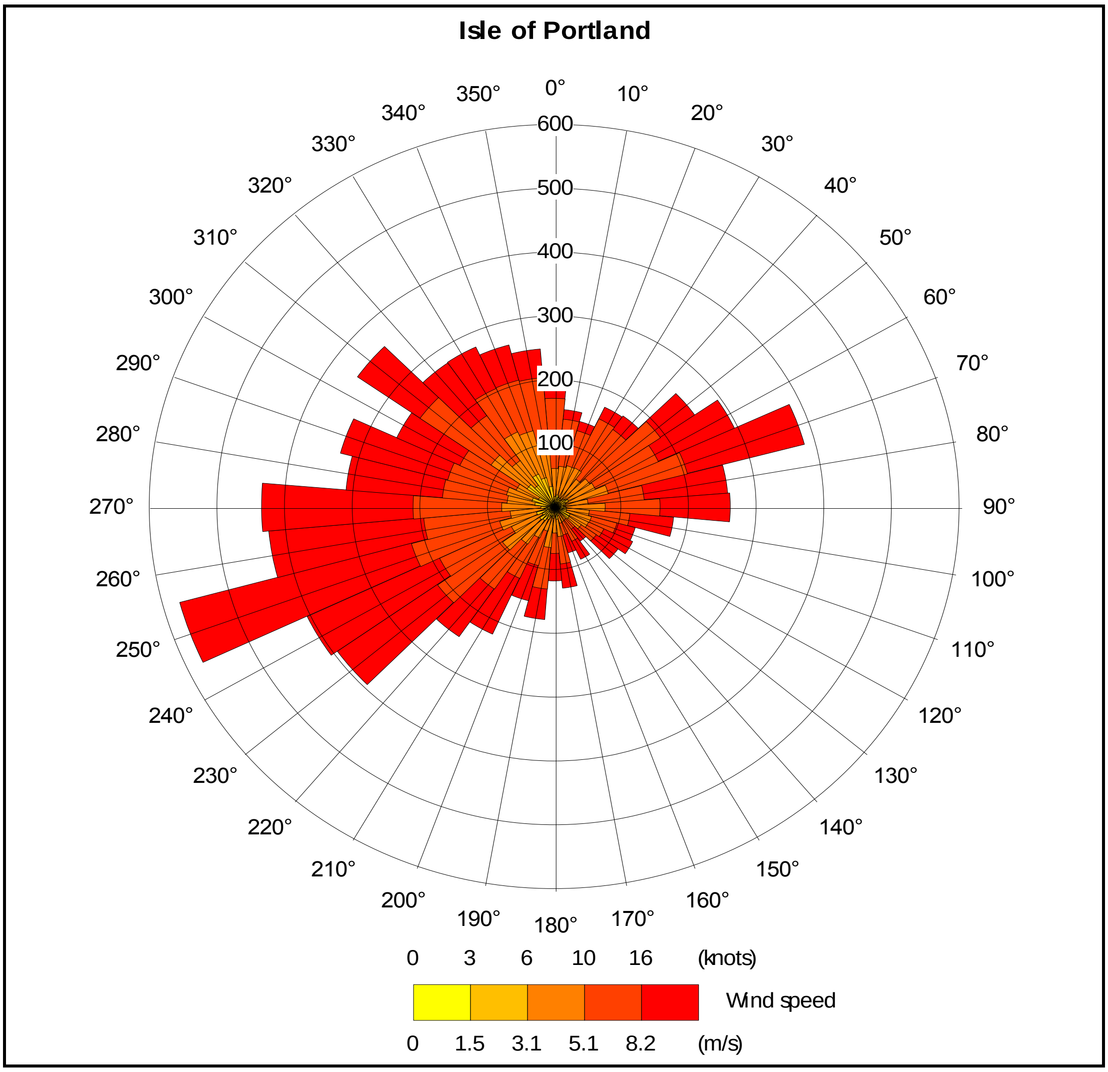


Figure C14 - Lerwick wind rose for 2005

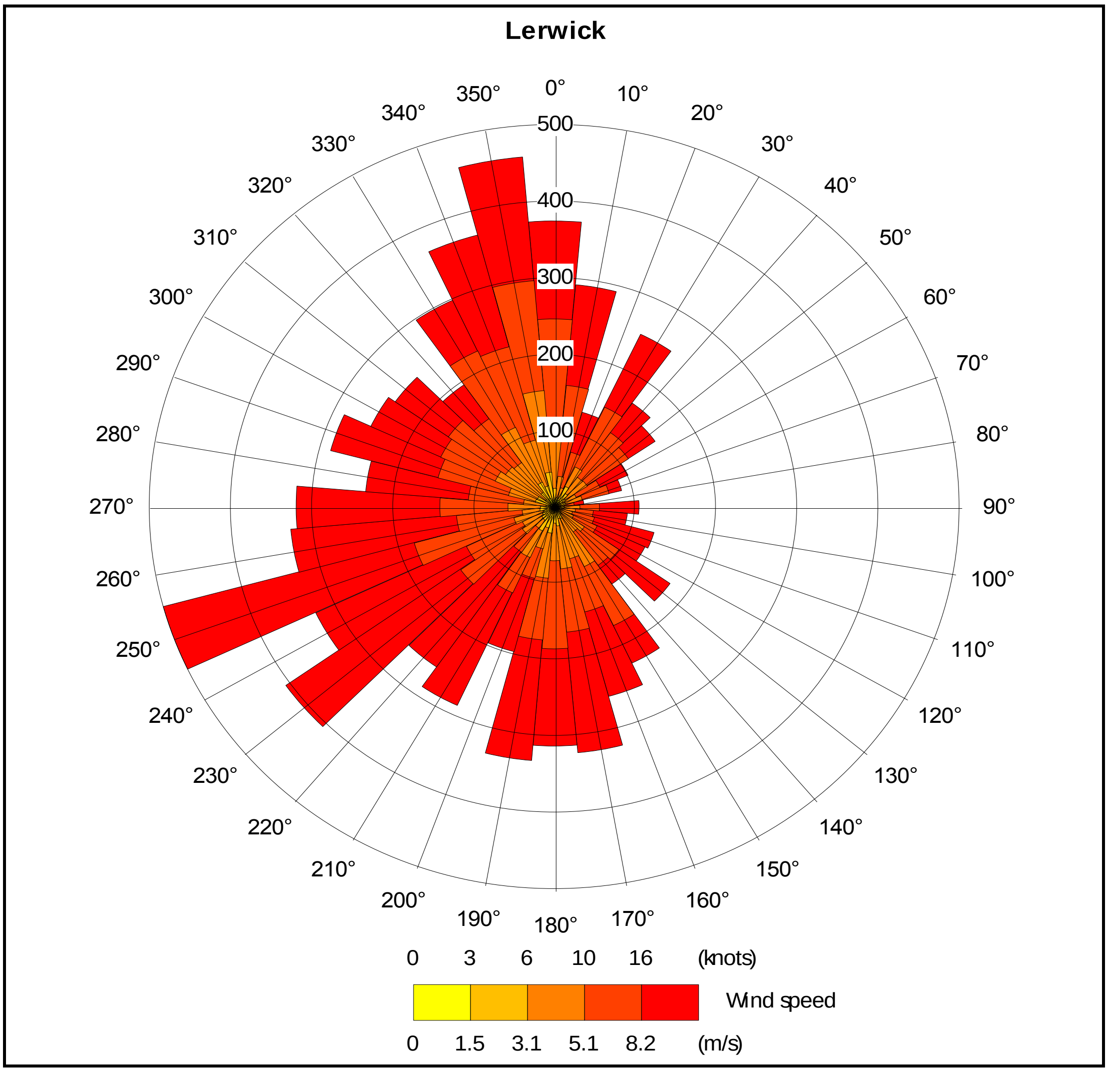


Figure C15 - Leuchars wind rose 2003

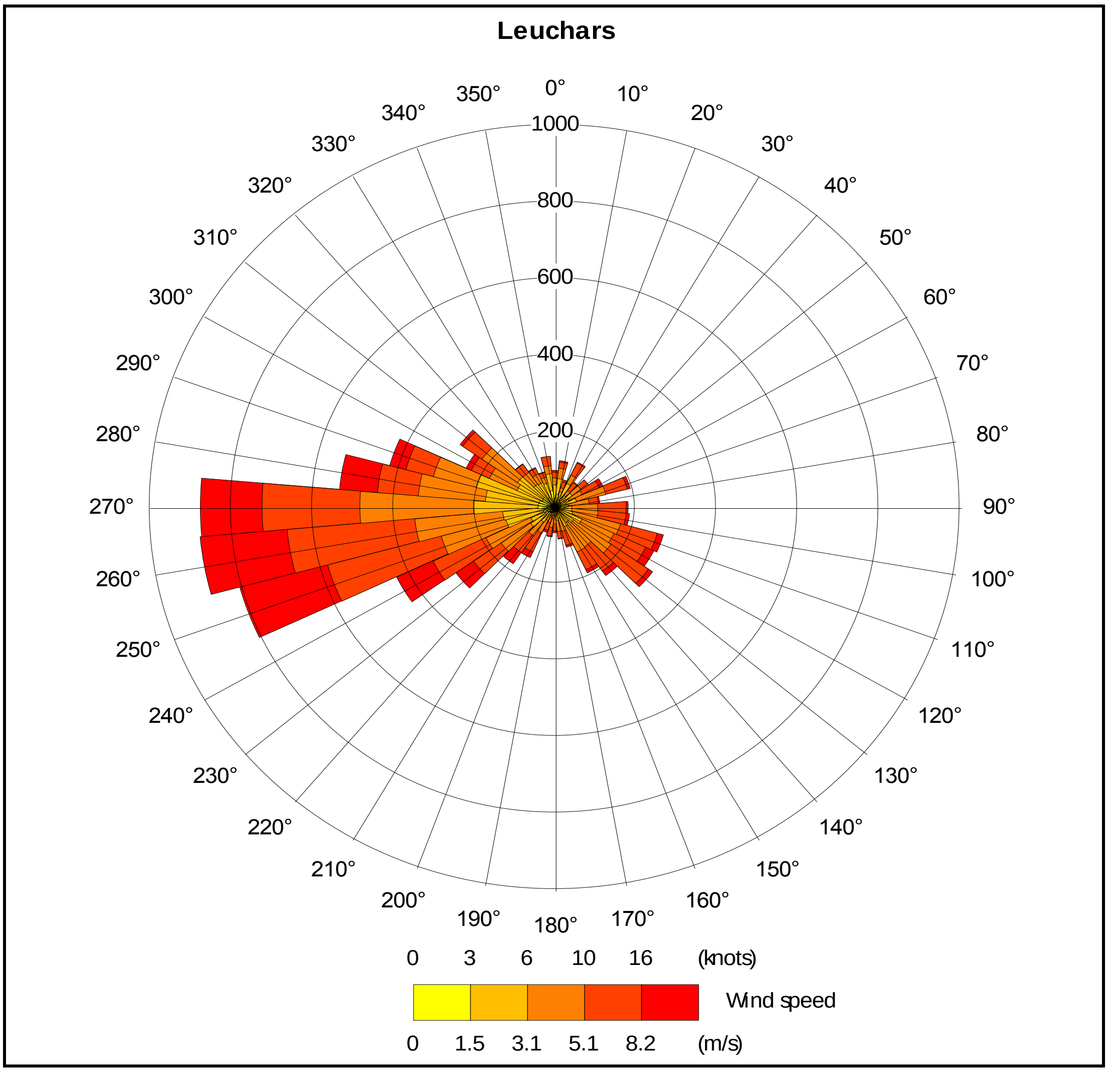


Figure C16 - Lossiemouth wind rose 2004

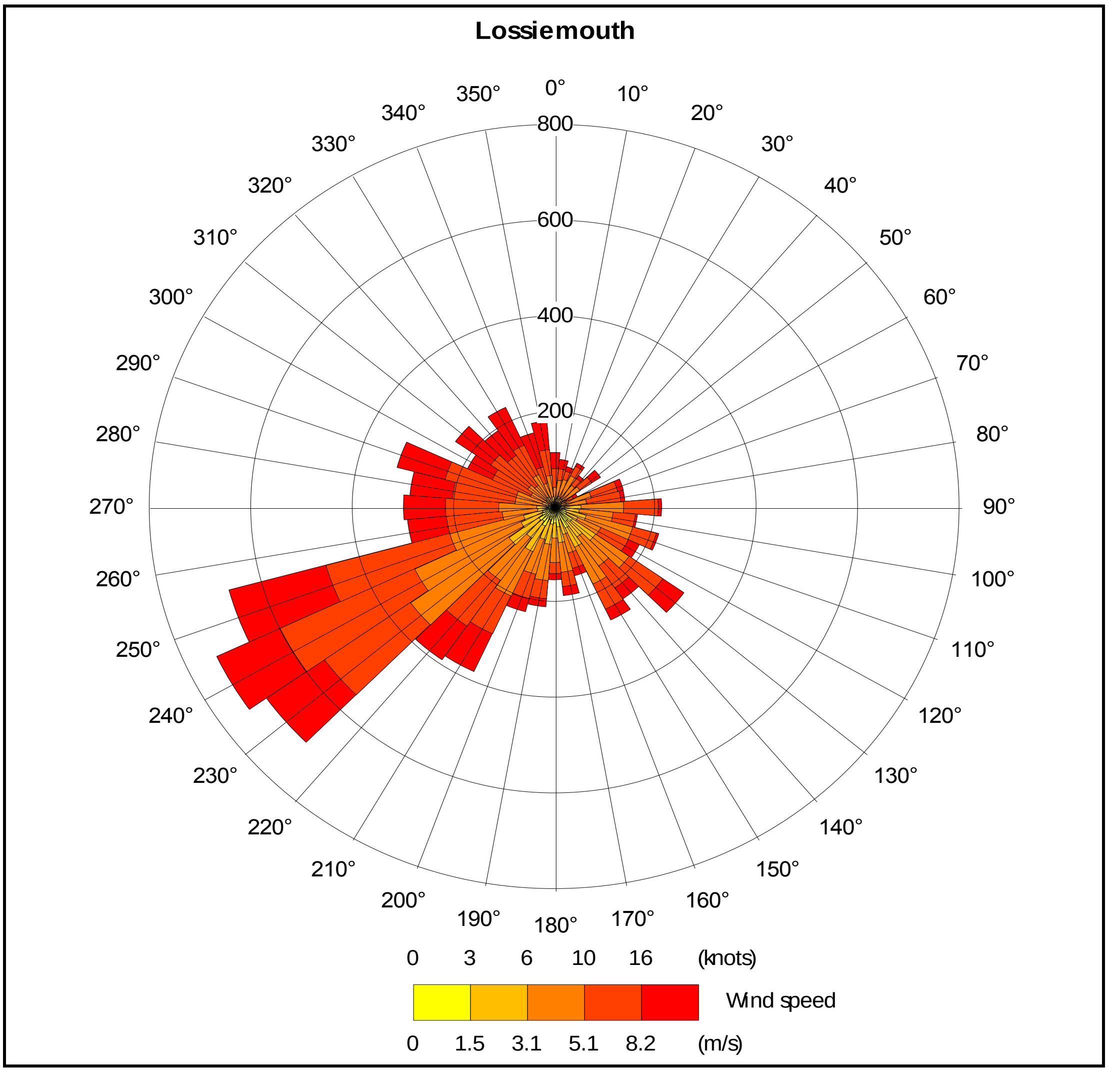


Figure C17 - Lyneham wind rose for 2002

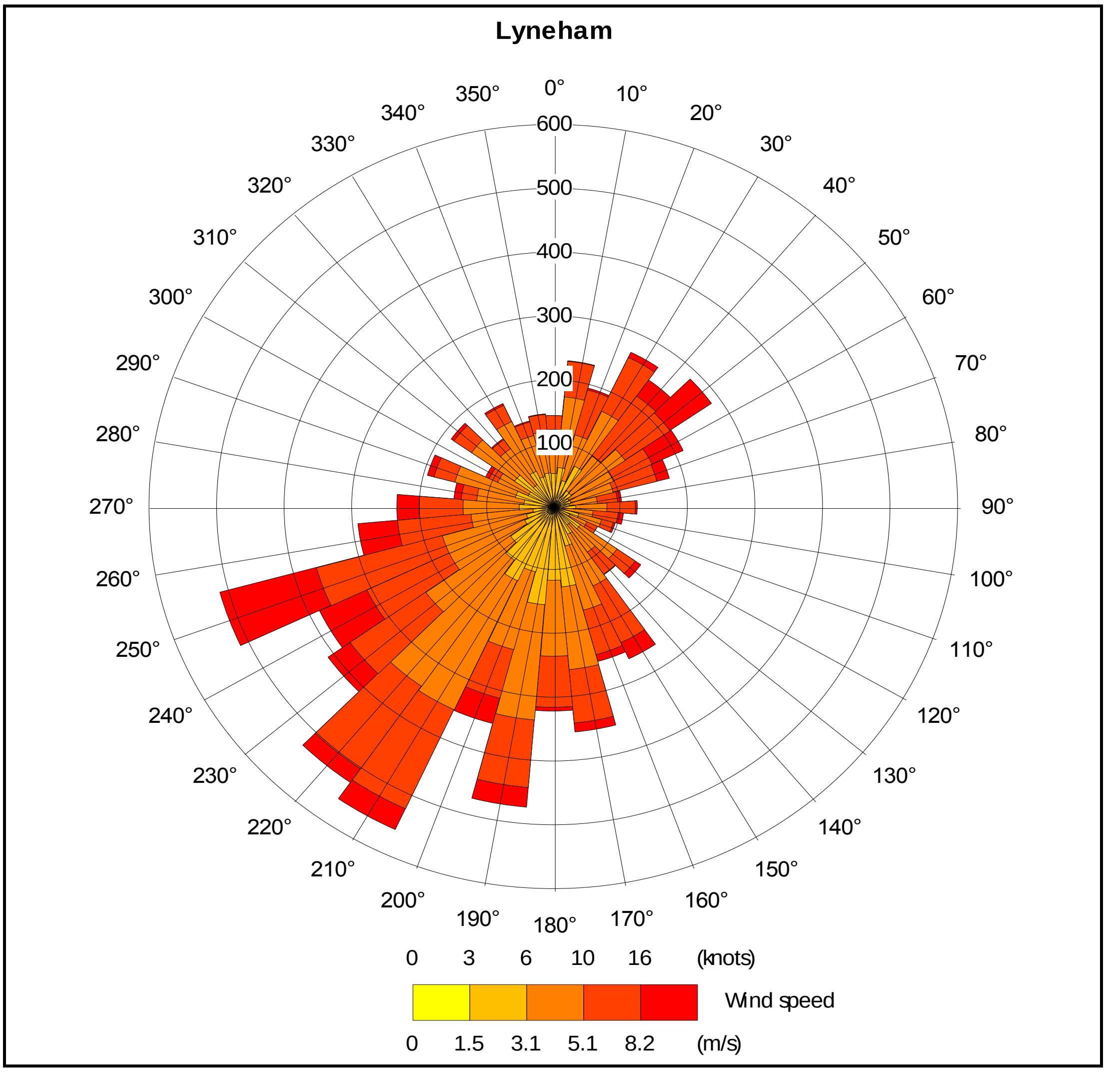


Figure C18 - Marham wind rose for 2001

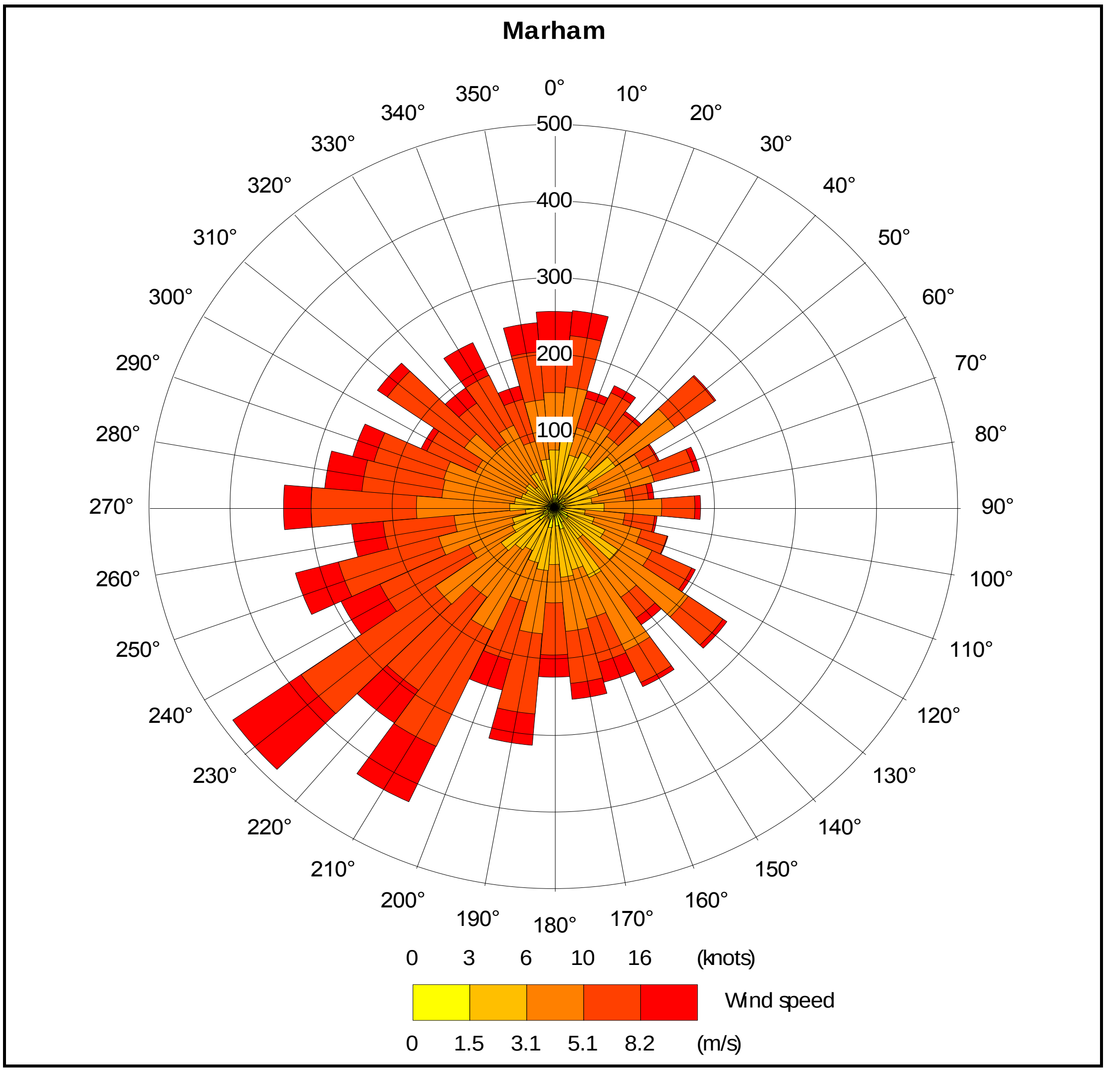


Figure C19 - Mumbles Head wind rose for 2001

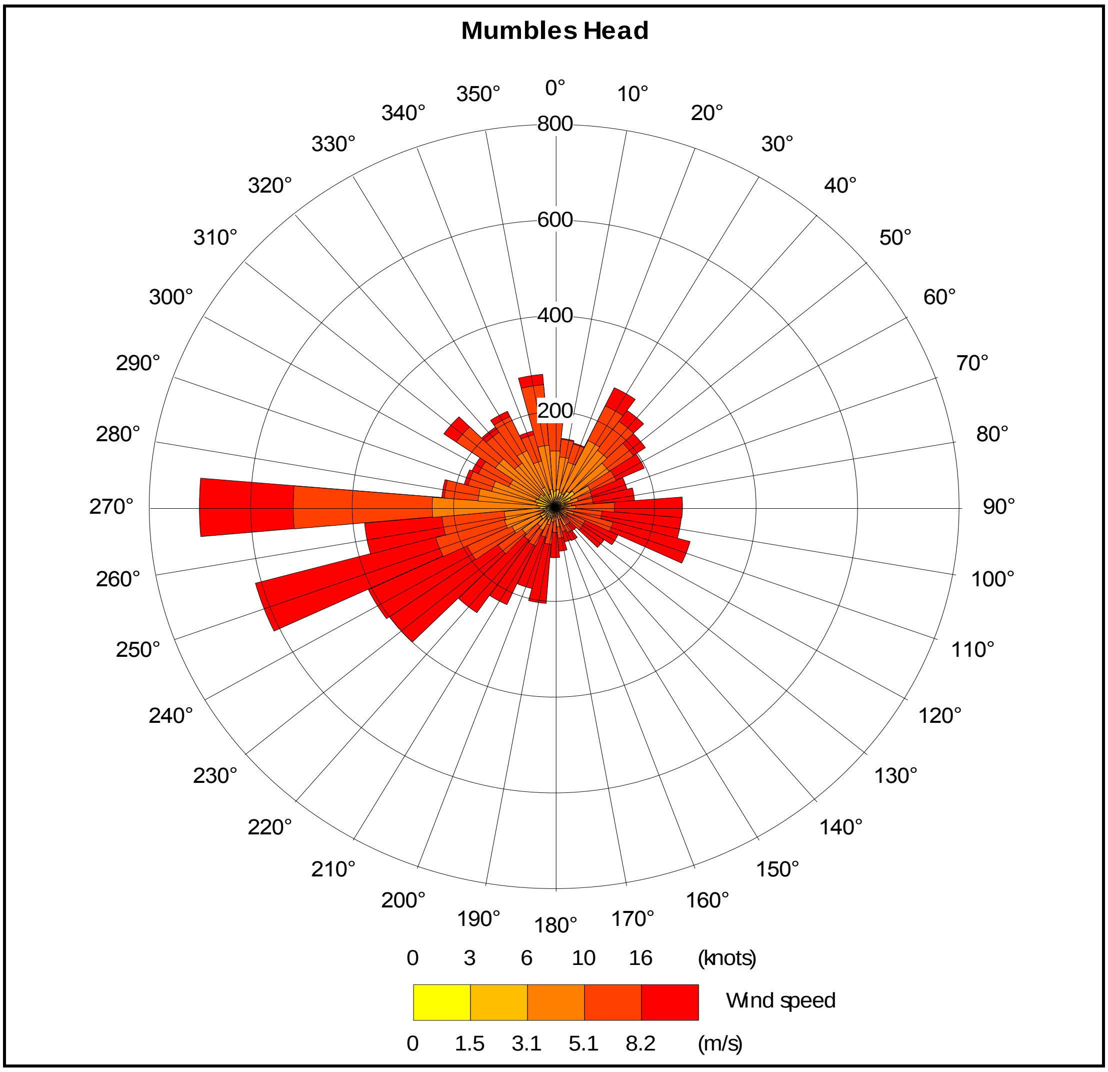


Figure C20 - Plymouth Mountbatten wind rose for 2001

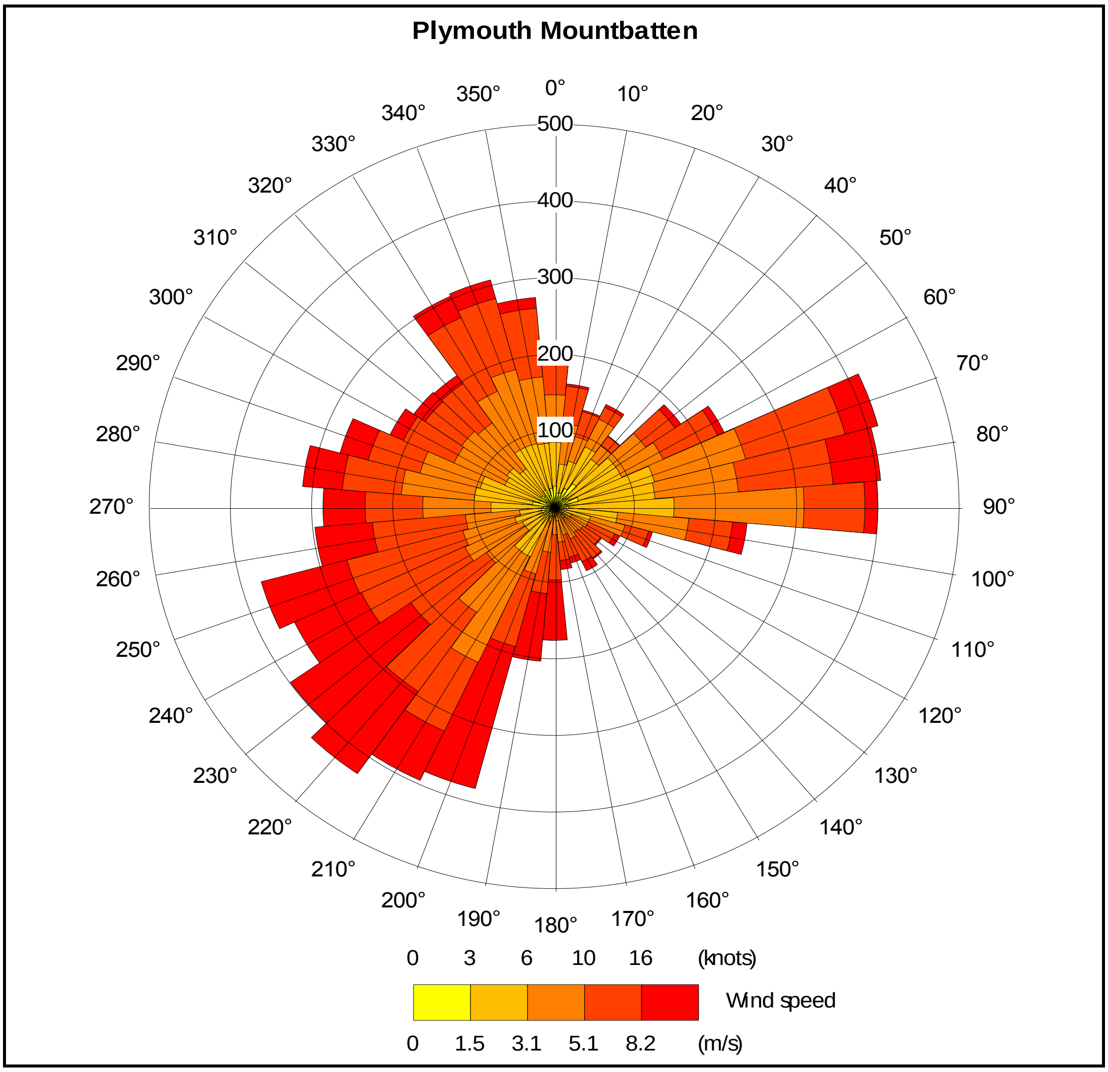


Figure C21 - Portglenone wind rose for 2002

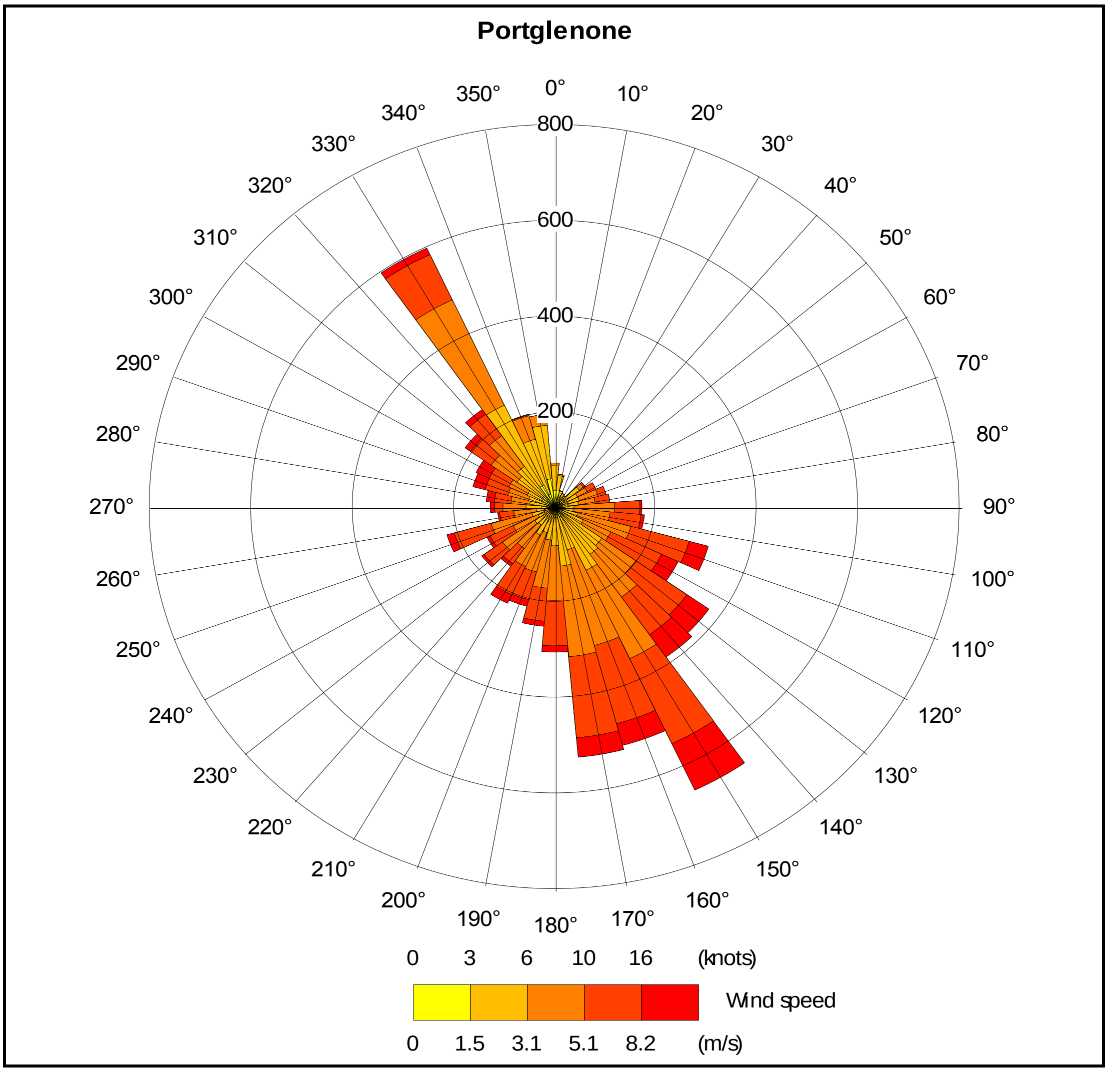


Figure C22 - Sennybridge wind rose for 2001

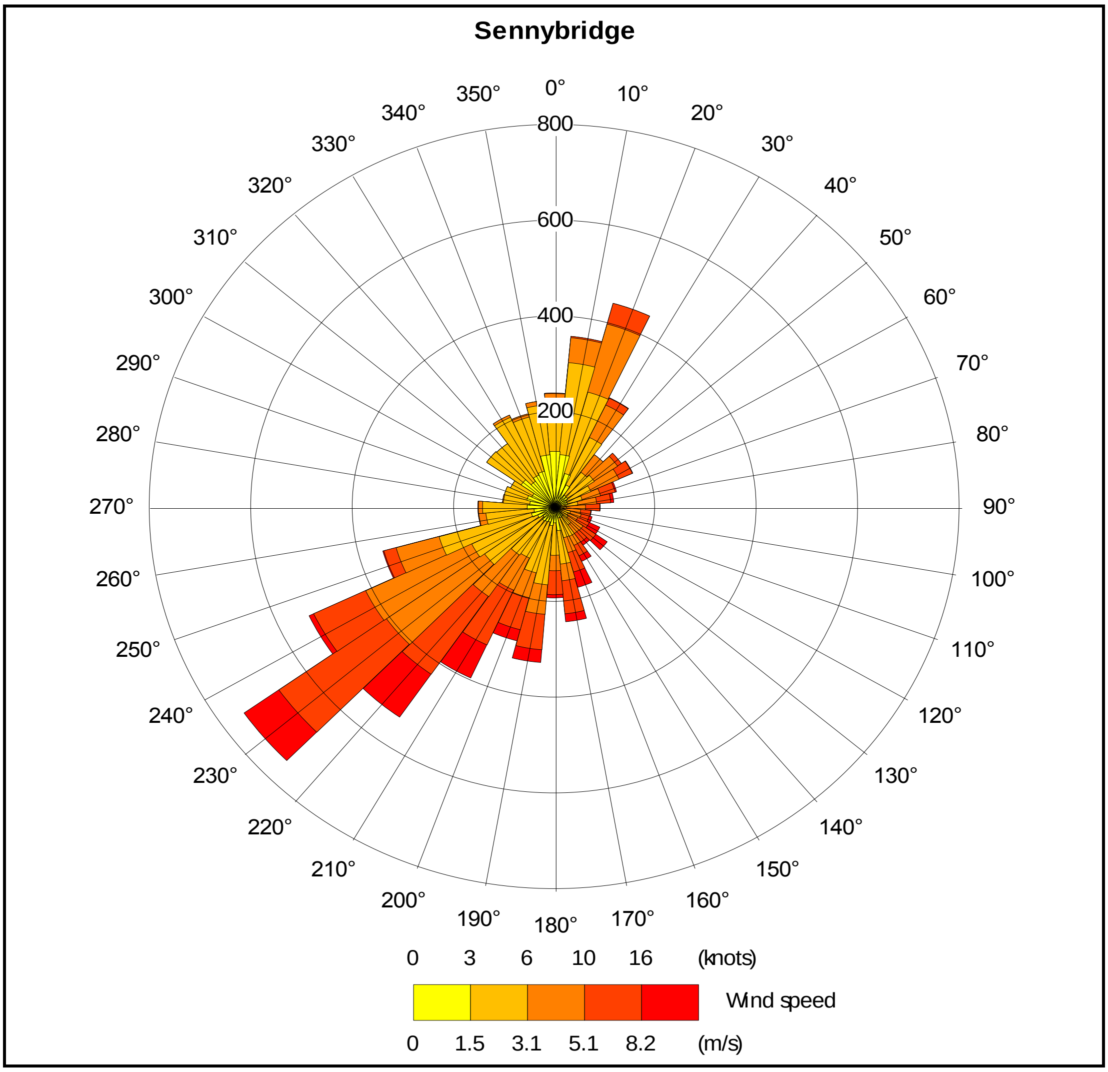


Figure C23 - Skye Lusa wind rose for 2004

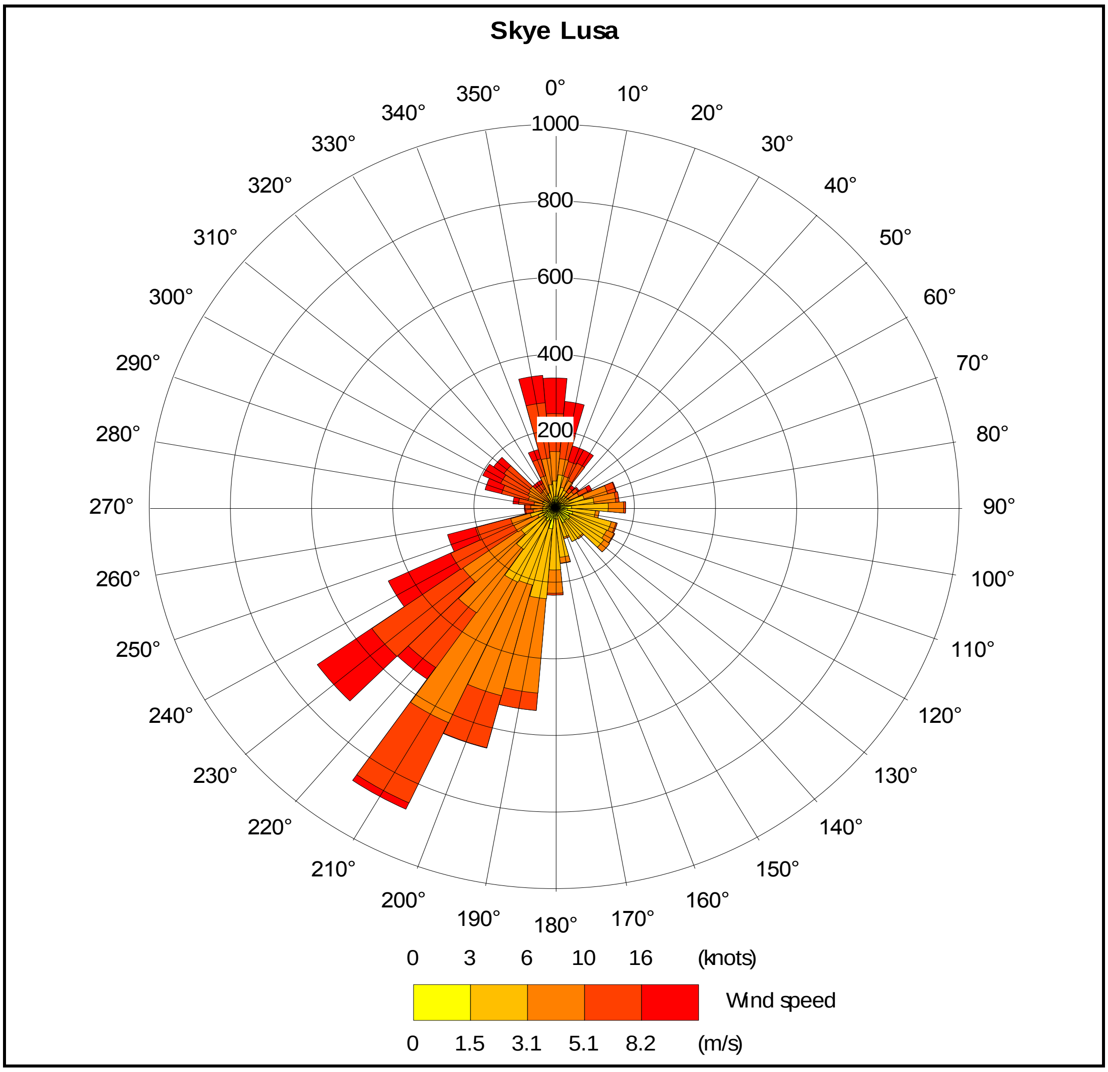


Figure C24 - Spadeadam wind rose for 2001

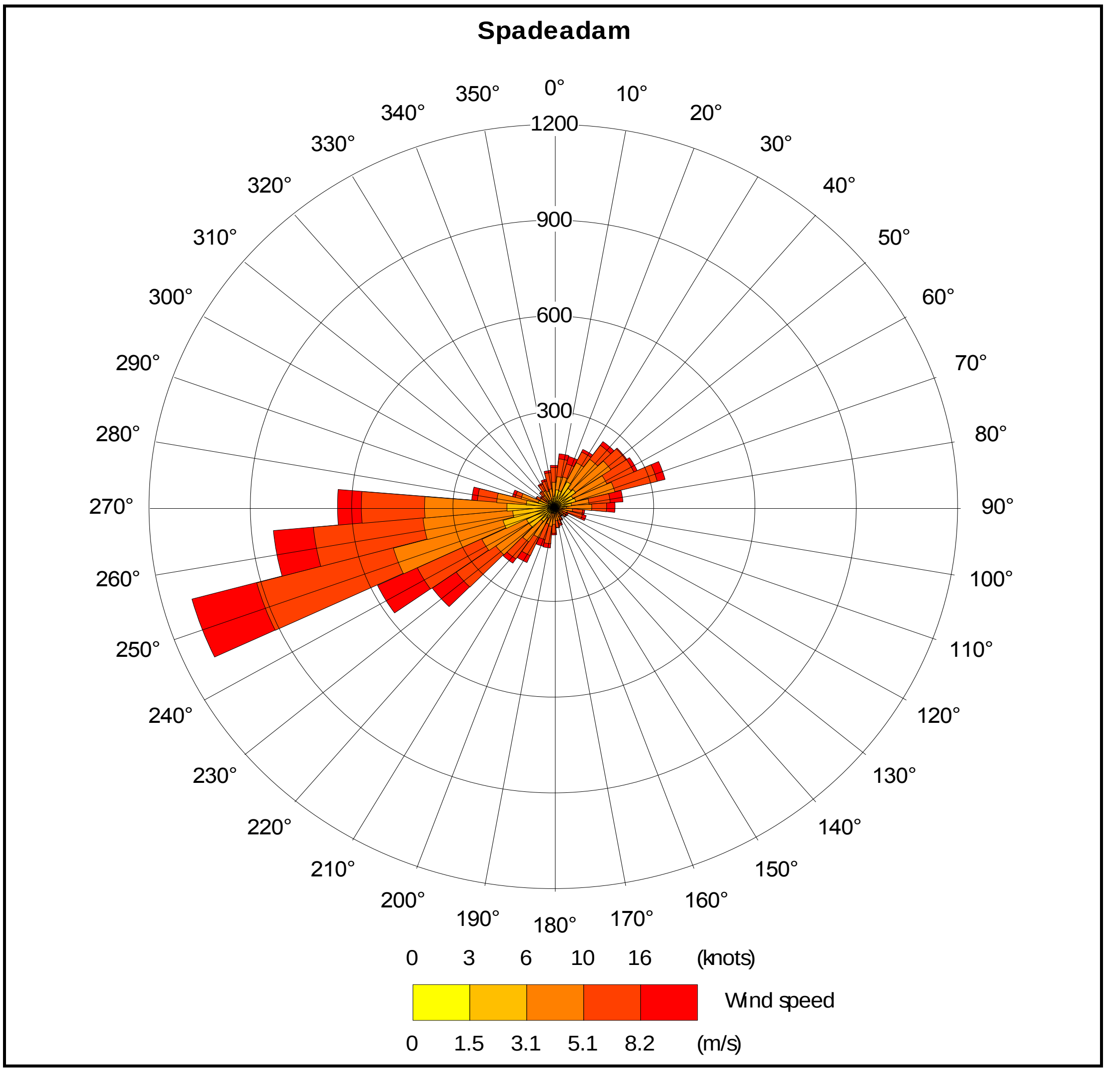


Figure C25 - Stornoway Airport wind rose for 2005

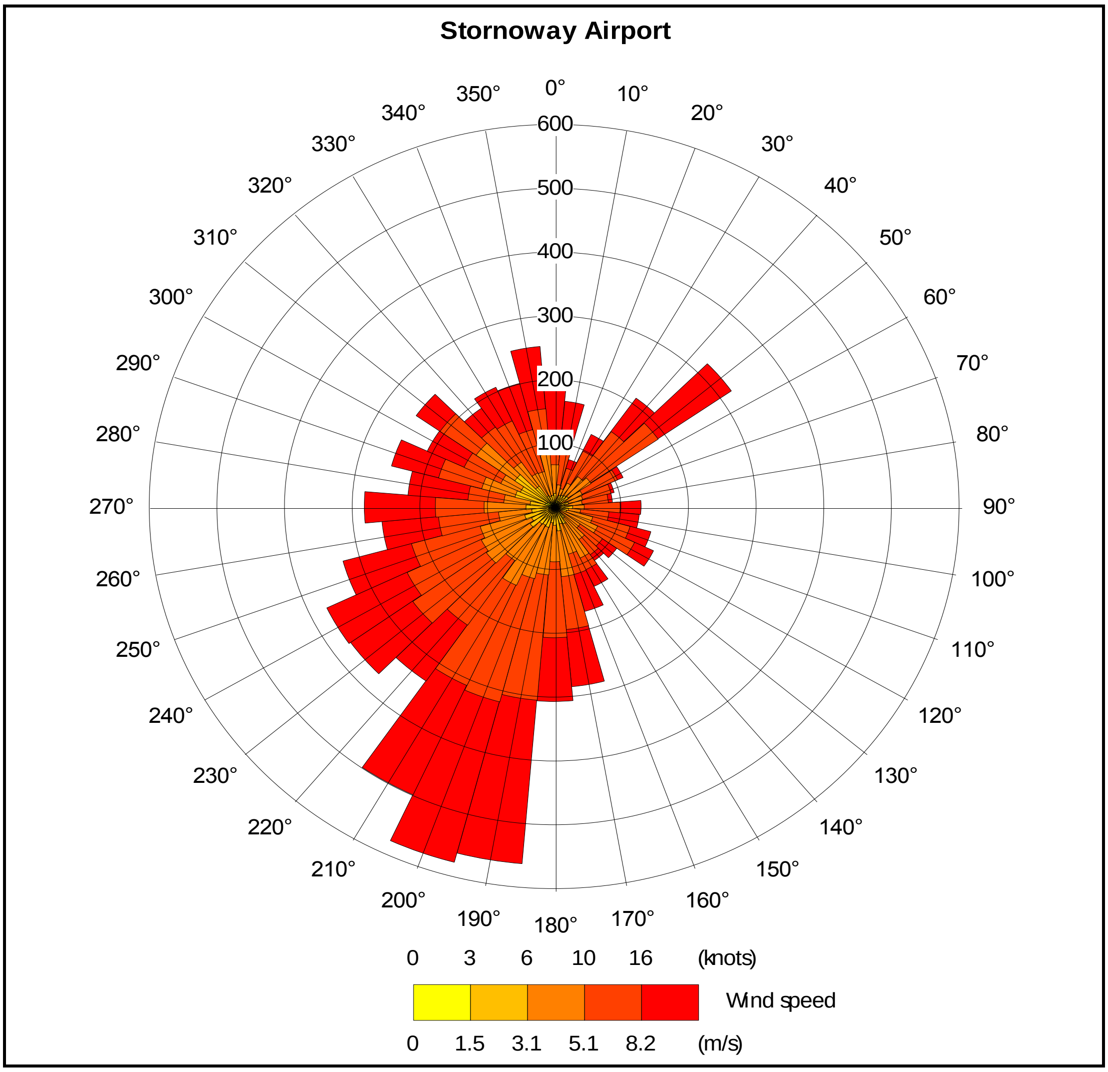


Figure C26 - Valley wind rose for 2001

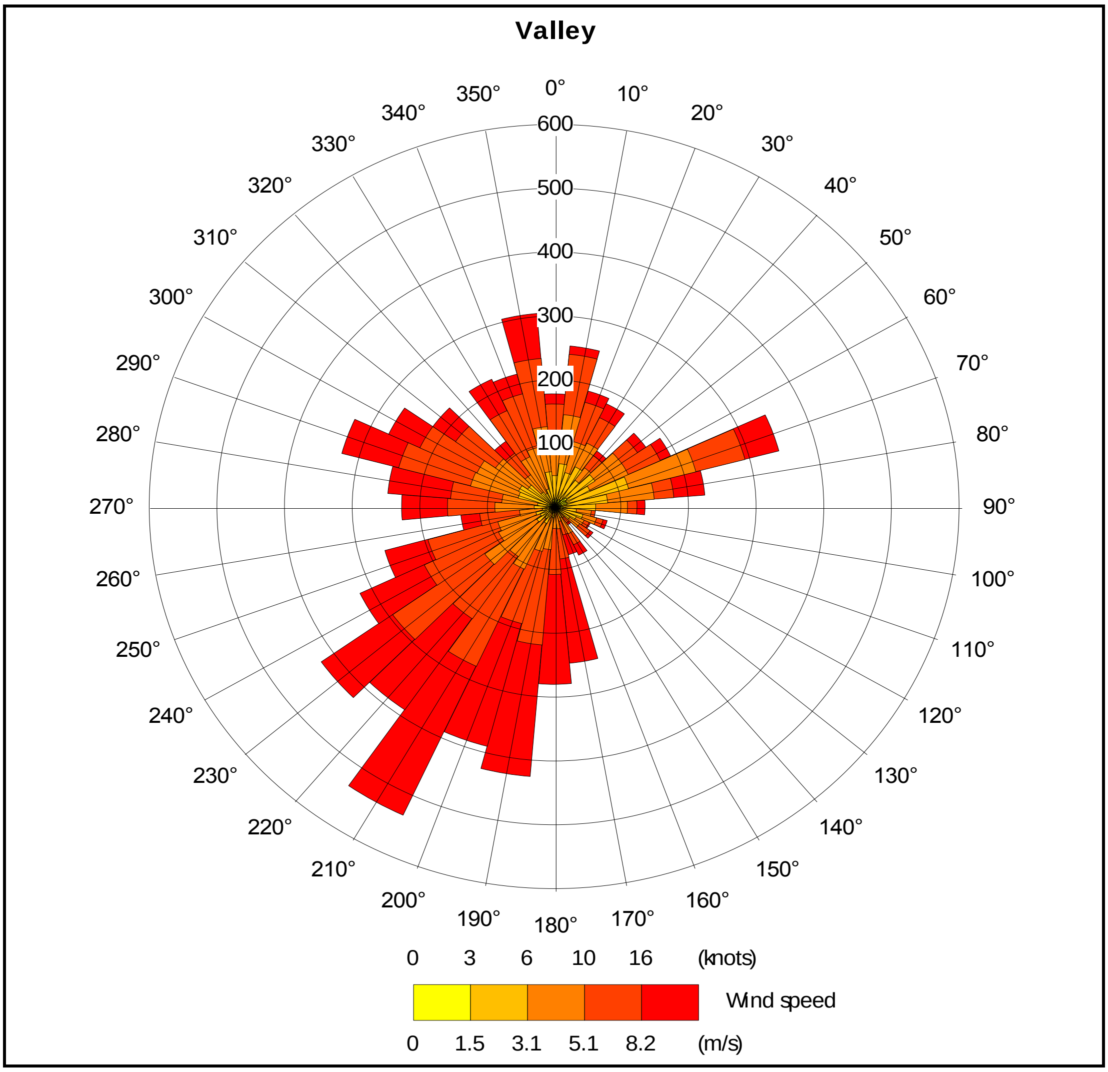


Figure C27 - Dyce wind rose for 2001

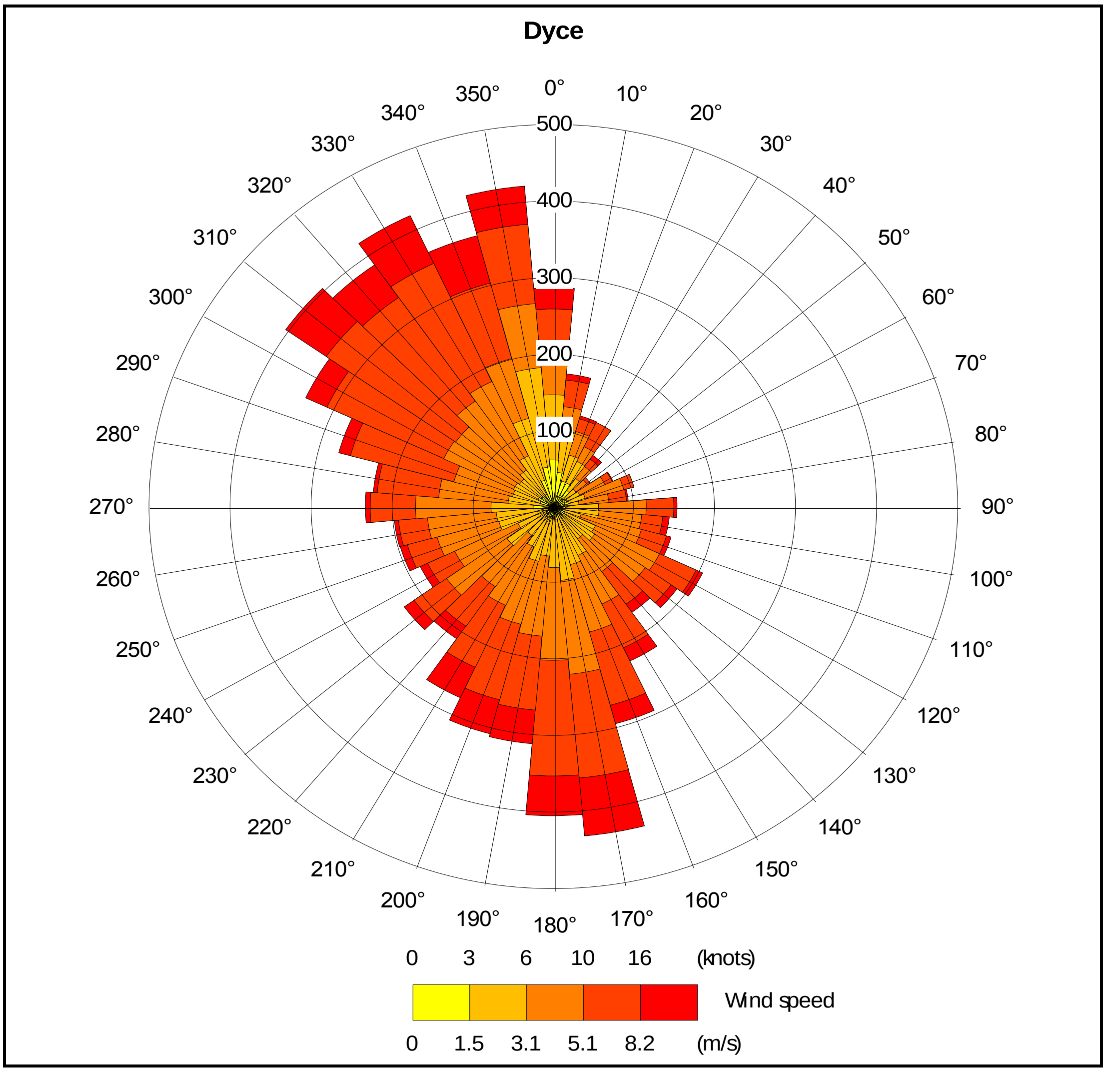


Figure C28 - Prestwick RNAS wind rose for 2005

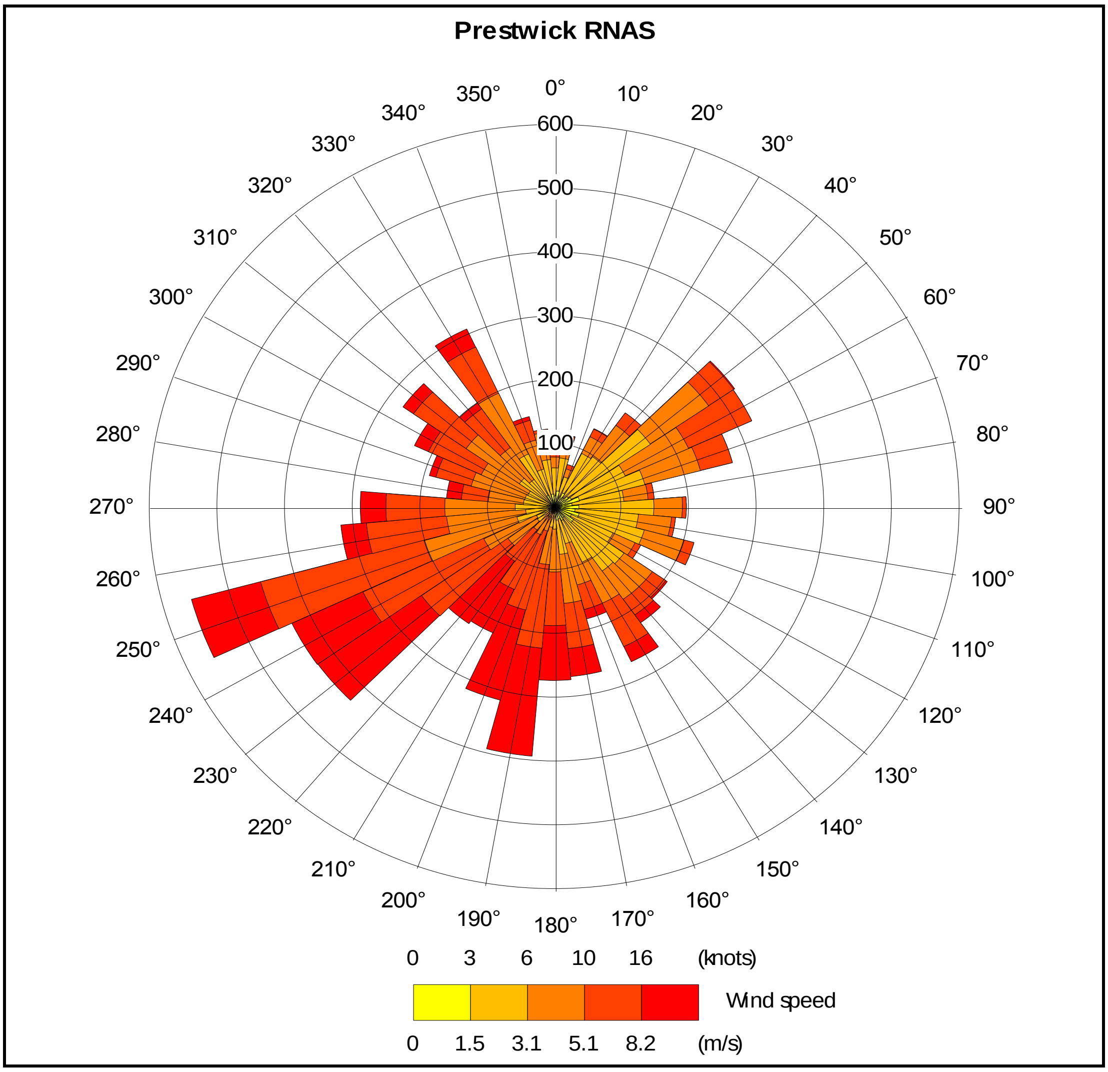


Figure C29 - Tiree wind rose for 2005

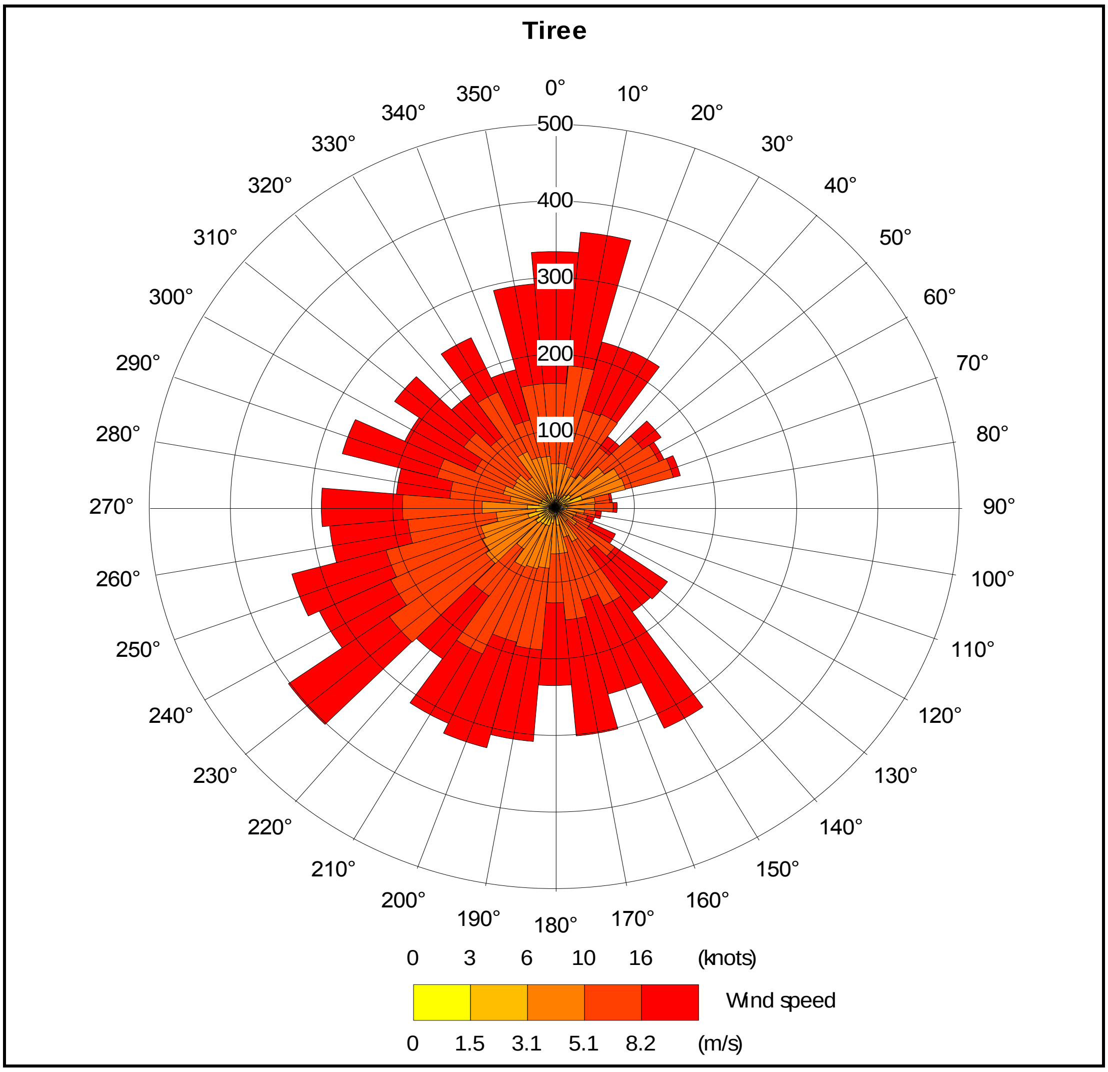
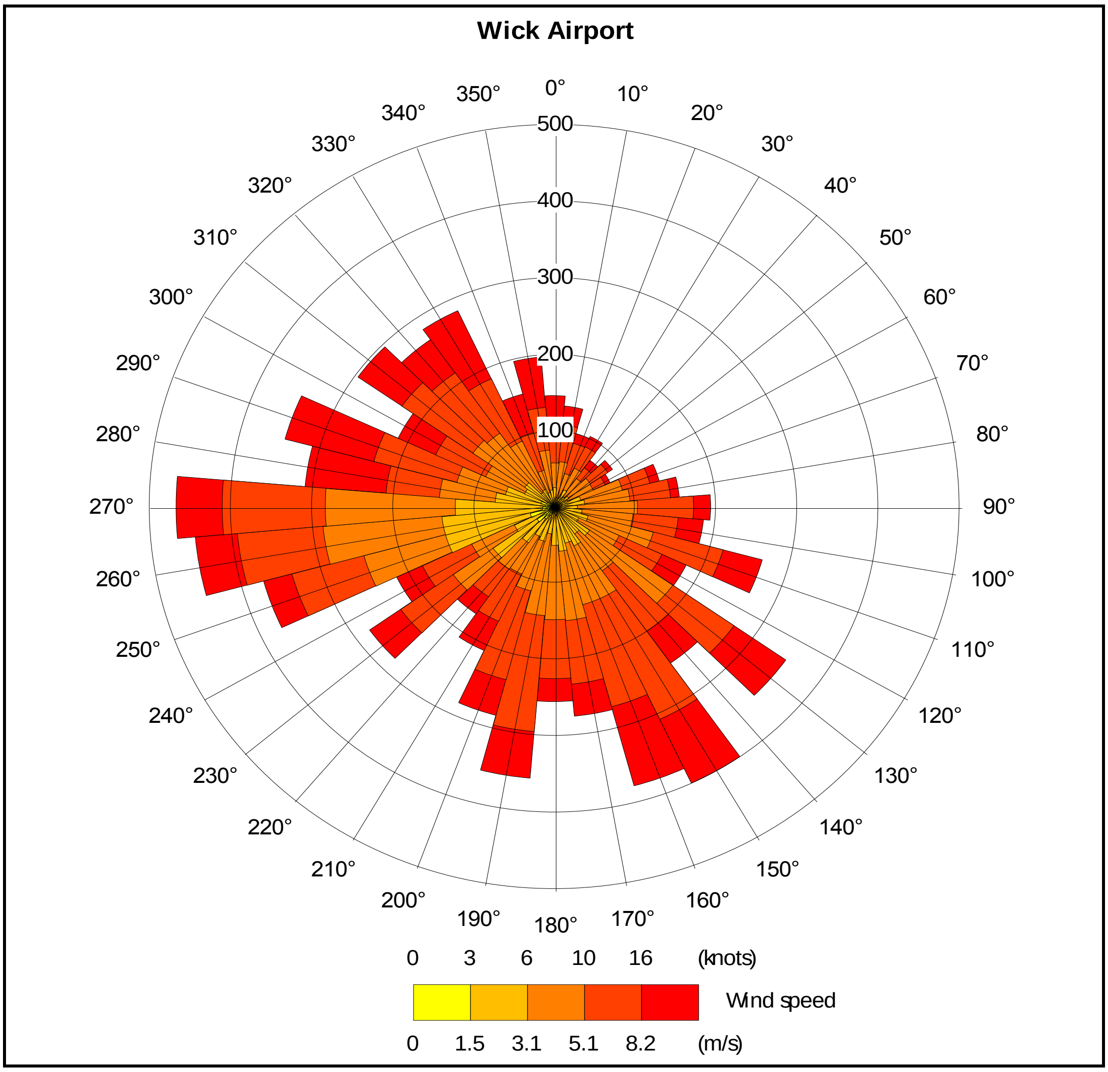


Figure C30 - Wick Airport wind rose for 2001



Appendix D New gas reactivity factor sensitivity analysis and validation

The sensitivity of the model deposition velocities to gas reactivity parameters has been investigated and the operation of the working SCAIL-Combustion model tested against the Aire Valley and Aberthaw data sets.

Sensitivity Study

Introduction

In UKPIR15 Interim Report 2 (Model Configuration), time averaged SO_2 and NO_2 deposition velocities were calculated using the SCAIL-Combustion output for a receptor site located downwind from a point source using Equation D1:

$V_d = F/C_a$ (Equation D1)

where F is the flux (µg m^{-2} s^{-1}), C_a is the atmospheric concentration of the chemical species being investigated (µg m^{-3}) and V_d is the deposition velocity (cm s^{-1}). It should be noted that the SCAIL–Combustion screening tool provides estimates of SO_2 and NO_2 pollutant concentration by calculating deposition velocities on an hourly basis using a complex resistance model.

In the main report, time averaged V_d, calculated using SCAIL-Combustion, were compared with literature values reported in Ball *et al.* (2008) for different land use classifications (LUC). The LUC chosen for the comparison were Agricultural Land, Forest land and Non-Forested Wetland. For NO_2, it was found that modelled estimates of V_d using SCAIL-Combustion were approximately 50% lower than reported in the reviewed literature. As a result, the nitrogen flux will be underestimated, atmospheric concentrations at downwind receptor locations will be overestimated and the impact of the combustion source on its surroundings will be underestimated. This result was in contrast to modelled estimates of V_d for SO_2, which showed good agreement with the reviewed literature. In order to increase the V_d for NO_2, it was recommended that the reactivity parameter in the SCAIL-Combustion input file be increased.

This section summarises the result of a sensitivity study to determine the effects of different gas reactivity factors on estimated deposition velocities for a range of land use classifications before comparing the new modelled V_d with literature values. The land use classifications used in this sensitivity analysis were:

- Urban Land;
- Agricultural Land;
- Forest;
- Suburban Grassy;
- Suburban Forest;
- Bodies of Water; and
- Non-forested Wetland.

Land use classifications

Gas deposition velocities for five LUC were reviewed and literature values compared with the new model estimates for this parameter. The LUC reviewed included:

- Urban Land;
- Agricultural Land;
- Forest;
- Bodies of Water; and
- Non-forested Wetlands.

Methodology

Within the model code of the SCAIL-Combustion input file, there is an optional gas deposition factor keyword available on the control pathway for use with gas dry deposition algorithms, which allows the modeller to override default values for this parameter. Therefore, in order to reduce the disparity between the modelled V_d for NO_2 and reviewed literature values, the optimum gas reactivity factor was calculated that would increase modelled NO_2 deposition velocity while having negligible effect on SO_2 deposition. This was done by increasing the gas reactivity factor from its current value of 0.1 to 0.5 in increments of 0.1. Modelled V_d were then compared with literature values for the LUC described above.

SCAIL-Combustion was configured for a single 50 m incineration stack emitting NO_2 and SO_2 at a rate of 100 tonnes per year. The diameter of the stack was one metre and the pollutants were emitted at a velocity of 35 m s^{-1}. Deposition velocities were calculated for a receptor site 2 km from the source. The gas deposition values employed in the model are supplied in Table D1.

Table D1 - SCAIL – Combustion Gas deposition parameters.

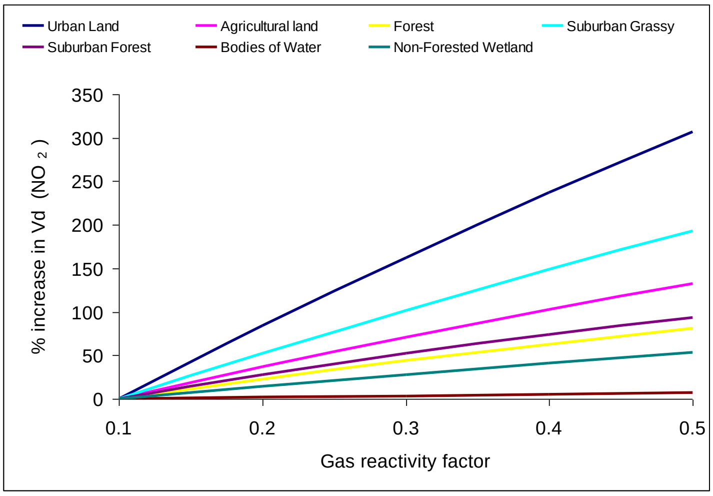
Parameter	NO_2	SO_2
Diffusivity (air) ($cm^2\ s^{-1}$)	0.1361	0.1089
Diffusivity (water) ($cm^2\ s^{-1}$)	1.90E-05	1.33E-05
Cuticular resistance ($s\ m^{-1}$)	9999	1
Henry's Law ($Pa\text{-}m^3\ mol^{-1}$)	10132.5	82.4

Results

NO_2 Sensitivity

The results of changing the gas reactivity factor on NO_2 deposition velocities are illustrated in Figure A1 and show that the sensitivity of V_d depends on the LUC being modelled. The least sensitive LUC was "Bodies of Water", which had an increase in V_d of only 7% when the gas reactivity factor was changed from 0.1 to 0.5. The most sensitive LUC was "Urban Land", where the V_d increased by approximately 300% across the same range of gas reactivity factors.

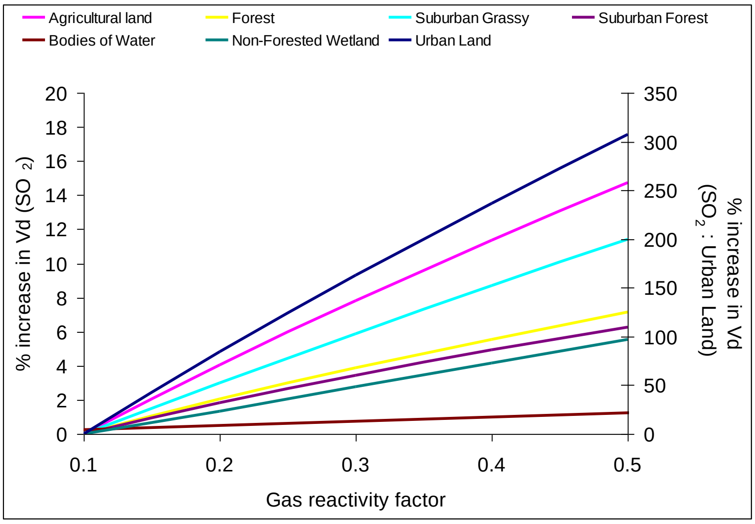
Figure D1 - Percentage change in *Vd* (NO_2) as a function of gas reactivity factor



SO_2 Sensitivity

Generally, the sensitivity of SO_2 deposition velocity to changes in the gas reactivity factor was low except for "Urban Land". Here, the value of V_d also increased by approximately 300% across a range of gas reactivity factors of 0.1 to 0.5. For the other LUC, an increase in the gas reactivity factor from 0.1 to 0.5 resulted in an increase in the value of V_d between 3% and 15% (Figure D2).

Figure D2 - Percentage increase in V^d (SO_2) as a function of gas reactivity factor and land use category (LUC). Note: values for Urban Land plotted on separate axis.



Comparison of modelled V_d with literature values

SO_2 and NO_2 deposition velocities calculated from modelled concentrations and fluxes using SCAIL-Combustion are compared with literature values in Table D2. The comparison showed that using a gas reactivity factor of 0.5 increased the deposition velocity of NO_2 to levels that are comparable with the literature values for the five LUC reviewed here. With respect to SO_2, because the percentage increase in V_d was generally small, using a gas reactivity factor of up to 0.5 did not increase V_d for this pollutant outside the range of the literature reviewed.

With respect to "Urban Land ", literature values for V_d of gaseous pollutants are often low, likely due to an increase in boundary layer resistance because of a reduction in modelled green leaf area. However, estimates of V_d calculated in the initial study were very low and the high percentage increase in V_d for this land use classification has resulted in closer agreement between literature and modelled values. The new V_d calculated here using a gas deposition factor of 0.5 is in the range of deposition velocities reported for stone surfaces (Table D2).

Table D2 - Comparison of modelled and literature values for the deposition velocity (in cm s^{-1}) of NO_2 and SO_2 for four land use classifications

Land use category	Pollutant	Literature deposition velocity	Gas reactivity factor				
			0.1	0.2	0.3	0.4	0.5
Urban Land	NO_2 *	0.05 – 0.09	0.025	0.046	0.065	0.084	0.101
	SO_2 **	0.02 – 0.23	0.025	0.046	0.065	0.084	0.101
Agricultural Land	NO_2	0.2 – 2.0	0.092	0.126	0.157	0.186	0.214
	SO_2	0.1 – 1.5	0.487	0.507	0.525	0.542	0.56
Forest	NO_2	0.03 – 3.5	0.065	0.079	0.093	0.105	0.117
	SO_2	0.16 – 0.89	0.427	0.436	0.444	0.451	0.458
Bodies of water	NO_2	0.3 – 0.8	0.213	0.216	0.220	0.224	0.228
	SO_2		0.44	0.438	0.441	0.444	0.448
Non-Forested	NO_2	0.2	0.104	0.119	0.133	0.147	0.160
Wetlands	SO_2	0.08 – 2.2	0.513	0.520	0.527	0.535	0.542

* V_d to cement structures (Gravenhorst and Bottger, 1983)
** V_d to dolomite/marble (Coburn *et al*., 1993)

Conclusion

Increasing the reactivity factor to 0.5 improves the agreement between SCAIL-Combustion and measurement data and is recommended for implementation in the model.