

Air Quality Modelling for Ireland

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ENVIRONMENTAL PROTECTION AGENCY

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- Office of Radiation Protection and Environmental Monitoring
- Office of Communications and Corporate Services

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EPA RESEARCH PROGRAMME 2014–2020

Air Quality Modelling for Ireland

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EPA Research Report

Prepared for the Environmental Protection Agency

by

Trinity College Dublin

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The EPA Research Programme addresses the need for research in Ireland to inform policymakers and other stakeholders on a range of questions in relation to environmental protection. These reports are intended as contributions to the necessary debate on the protection of the environment.

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Executive Summary

Air pollution is the primary environmental cause of premature death in the EU (EC, 2013) and the most problematic pollutants across Europe have consistently been oxides of nitrogen [e.g. nitrogen dioxide (NO_2)], particulate matter (e.g. PM_{10} , $\text{PM}_{2.5}$) and ozone (O_3). Although measurements form an important aspect of air quality assessment, on their own they are unlikely to be sufficient to provide an accurate spatial and temporal description of the pollutant concentrations for exposure assessment and moreover they cannot provide information regarding future air quality. Annex XVI of EU Directive 2008/50/EC requires Member States to “ensure that up to date information on ambient concentrations of the pollutants covered” by the Directive are “made available to the public”. This information must include actual or predicted exceedances of alert and information thresholds and a forecast for the following day of which a model is an integral part. As a result, air quality models are increasingly required for public information, air quality management and research purposes. The primary objectives of this research fellowship were to develop a calibrated air quality forecast model for Ireland capable of predicting the Air Quality Index for Health (AQIH) in each of the air quality zones in Ireland and to model the spatial variation in concentrations on a national scale.

This research project has produced three different models for NO_2 , PM_{10} , $\text{PM}_{2.5}$, O_3 and sulfur dioxide (SO_2), all of which are available for further use. These are:

1. a hybrid point-wise 48-hour forecast model;
2. a spatial model [wind sector land use regression (WS-LUR)] to produce annual mean maps of air pollution on a national scale;
3. a temporal WS-LUR model.

A comprehensive review of modelling systems carried out at the outset of this research fellowship, together with consideration of key Environmental Protection Agency (EPA) objectives, informed the direction of model development. This review is available as a separate EPA report. A priority within the EPA was to produce air quality forecasts based on the AQIH. The

AQIH is based on point-wise measurements and, in order to extrapolate these measurements to the future, statistical modelling was deemed the most suitable. The advantages of this approach were that it could be developed from first principles specific to the area of interest and completely (avoiding any reliance on a third party to supply the model or apply licensing restrictions) and the associated speed of forecast computation. Forecasts are useful only if they can be computed and made available to the public relatively quickly. Such methods also tend to be highly accurate with low bias, as they are developed site specifically, unlike large-scale deterministic models, which are often developed and tested in vastly differing domains. In particular, this method was capable of producing accurate point-wise forecasts without the need for a detailed emissions inventory. At the project outset, the emissions inventory was not of sufficient spatial resolution to make realistic point-wise forecasts in all air quality zones by deterministic means and it would have been an inefficient use of resources to base the development of forecasts on what was currently available.

Initial model development proceeded using time series analysis in conjunction with non-parametric kernel regression, with local meteorological parameters as predictor variables. A model validation study found that this technique produced an accurate forecast of O_3 and SO_2 but had a tendency to underpredict peak NO_2 and $\text{PM}_{10/2.5}$ concentrations. An analysis of air mass history using the hybrid single particle Lagrangian integrated trajectory (HYSPLIT) model was carried out, which revealed that certain air masses (primarily easterly and recirculated air) were responsible for most incidences of elevated concentrations. The results of this study were used to develop a HYSPLIT add-on for the forecast model, which operates by forecasting air mass history in real time and invoking a different forecasting methodology depending on the region of origin of the air. The ability of the hybrid point-wise model to predict daily maximum hourly NO_2 and SO_2 , 8-hourly O_3 and daily average PM_{10} and $\text{PM}_{2.5}$ was demonstrated by comparing a full year of modelled data with measured data at each of the AQIH sites. Index of agreement values ranged from a low of 0.80

for SO_2 to 0.88 for NO_2 and O_3 , whereas correlation coefficients ranged from a low of 0.69 for SO_2 to 0.82 for NO_2 . Full results of this validation study are contained in a separate report.

In order to provide detail on the spatial variation of concentration levels across the country, land use regression (LUR) was recommended in the model review as the most suitable technique. This technique uses surrogate spatial indicators to explain the variation in concentration levels between monitoring points. Land cover data [Coordination of Information on the Environment (CORINE)], digital terrain model (DTM) output, road density information and population data are all factors that influence concentration levels and data that were broadly available. In contrast to most LUR studies, circular buffers were not used in the determination of spatial predictor variables. Rather, a novel sector-based approach (WS-LUR) was adopted whereby variables were calculated within eight pre-defined sectors representing the major wind directions around each monitoring site. This approach had a dual purpose. First, it accounts for the direction of influence of emission sources on air quality in a given location. Traditional LUR assumes equal influence of emissions in the area surrounding a monitoring site regardless of wind direction. This approximation may be reasonable in highly urbanised areas where emissions sources are relatively uniform in the surrounding region. However, in this study the regression was applied on a national scale and prevailing winds coupled with clear directional influence at air quality monitoring sites

meant that WS-LUR is a superior option. Second, this methodology increases the effective number of data points available for the regression analysis, resulting in a more robust final equation.

In conjunction with a second research project (2013-EH-FS-7), a set of annual mean maps within a geographic information system (GIS) environment were created and validated for each of NO_2 , PM_{10} , $\text{PM}_{2.5}$, O_3 and SO_2 . These provide a highly relevant source of information regarding spatial variation in concentration levels on a national scale, which can be used not only for exposure studies and general air quality assessment, but also as a tool to correlate emission sources and surrogates with air quality. A temporal WS-LUR model was developed for NO_2 , O_3 and PM_{10} by including hourly meteorological data in conjunction with pre-specified spatial data as predictor variables. This model has the potential to provide fast, efficient national air quality forecast maps for Ireland with minimal computational requirements.

This project has achieved key EPA objectives and has produced a fully automated and operational air quality model, which produced twice-daily forecasts of the AQIH in each air quality zone in Ireland. The stepwise approach chosen for model development allowed deliverables prior to completion of the project while minimising associated risks. The models developed as part of this fellowship form solid building blocks on which future air quality modelling studies in Ireland can be based.

1 Introduction

1.1 Overview

Air pollution as a societal concern is interlinked with other environmental, social, political and economic systems. Stakeholders for research in the field of air pollution may therefore come from diverse backgrounds but with a common interest in the impacts of air pollution. Air pollution is the primary environmental cause of premature death in the EU, accounting for 10 times the toll of road traffic accidents (EC, 2013). The most problematic pollutants across Europe have consistently been oxides of nitrogen [e.g. nitrogen dioxide (NO_2)], particulate matter (e.g. PM_{10} , $\text{PM}_{2.5}$) and ozone (O_3), whereas polycyclic aromatic hydrocarbons (PAHs) have been recently identified as pollutants of concern (EPA, 2012) and proposed new EU metrics for black carbon (BC) are under discussion (EEA, 2011). In a recent review of the evidence on the health impacts of air pollution, the World Health Organization (WHO) states that the previous causal link between $\text{PM}_{2.5}$ and adverse health impact in earlier guidelines has been strengthened by recent evidence (WHO, 2012). Both short- and long-term exposure to $\text{PM}_{2.5}$ were noted to have an adverse impact on health, even in long-term exposure studies where exposure was below the current recommended WHO annual limit of $10 \mu\text{g}/\text{m}^3$. Such findings highlight the need for the introduction of additional short-term limit values for PM to account for the health impacts of short-term but relatively high exposures, such as during commuting. These findings also further highlight the dangers of long-term exposure to PM such as from domestic fuel use. In addition, this review of recent evidence also highlights the links between exposure to NO_2 and mortality/morbidity. Such exposure is noted to be particularly elevated near roads as a result of traffic emissions. Therefore, the health impact of outdoor air pollution continues to be a global concern among the scientific community for its impacts on human health, the environment and climate change.

As a member of the EU, Ireland is required to demonstrate compliance with a number of EU limit values encompassing NO_2 , PM, sulfur dioxide (SO_2), lead, benzene, carbon monoxide, O_3 , arsenic, cadmium, nickel and benzo[a]pyrene. Challenges

facing Ireland in meeting its obligations under the EU directives include reductions of nitrogen oxides (NO_x) in traffic-impacted areas [noted to be a significant contributor to air pollution in Ireland (McGettigan *et al.*, 2000) and targeted by plans such as the *Dublin Regional Air Quality Management Plan for Improvement in Levels of Nitrogen Dioxide in Ambient Air Quality* (Dublin City Council *et al.*, 2010)], reduction of $\text{PM}_{2.5}$ by 10% between 2010 and 2020 (EU, 2008) and reducing emissions from domestic solid fuel systems, which contribute to high levels of PM and PAHs in towns and cities (EPA, 2012).

1.2 Air Quality Modelling and Policy Relevance

Although measurements form an important aspect of air quality assessment, on their own they are unlikely to be sufficient to provide an accurate spatial and temporal description of the pollutant concentrations and, as a result, models are often needed (Moussiopoulos, 1997). Government departments, agencies and local authorities increasingly rely on air pollution models for decision-making in relation to air quality, traffic management, urban planning and public health and, consequently, the community that uses these models is becoming larger and more diverse (Vardoulakis *et al.*, 2002). EU Council Directive 2008/50/EC (EU, 2008) states that “A combination of measuring and modelling techniques” may be used to assess ambient air quality where levels over a representative period are below a level lower than the limit value. The Directive goes on to state that “the sole use of modelling or objective estimation techniques for assessing levels may be possible” where levels are below a specified level. The transposition of this into Irish law has resulted in the recognition of modelling as an assessment technique under the Air Quality Standards Regulations Act, 2002 (DEHLG, 2002) in certain circumstances; “where the levels of pollutants are below the lower assessment threshold, modelling or objective assessment techniques may be used solely to assess ambient air quality, except in agglomerations in the case of sulphur dioxide and nitrogen dioxide” and “where fewer than five years’

data are available, measurement campaigns of short duration during the period of the year and at locations likely to be typical of the highest pollution levels may be combined with results obtained from emission inventories and modelling.” The use of modelling in other situations where concentrations may approach or exceed limit values is also emphasised in EU Directive 2008/50/EC (EU, 2008), which states that “Where possible modelling techniques should be applied to enable point data to be interpreted in terms of geographical distribution of concentrations. This could serve as a basis for calculating the collective exposure of the population living in the area.”

Air quality models are an important aspect of air quality management and have two primary functions in this regard. First, they can be used to provide predictions of air quality in both the near future (48 hours) and more distant future (years). Annex XVI of EU Directive 2008/50/EC (EU, 2008) requires Member States to “ensure that up to date information on ambient concentrations of the pollutants covered” by the Directive are “made available to the public”. This information must include actual or predicted exceedances of alert and information thresholds and a forecast for the following day, of which a model is an integral part. The provision of air pollution forecasts requires the development of a suitable air quality model.

Second, air quality modelling improves our knowledge regarding the spatial variation in pollutant concentrations and the identification of the concentration gradient and peak location. The need for caution when assessing air quality based on sampling networks alone and the importance of a spatial approach has long been emphasised (Muschett, 1981; Greenland and Yorty, 1985). Anticipating and managing changes in pollutant concentrations relies on an accurate representation of the current and future chemical state of the atmosphere. Numerical models capable of simulating the chemistry and transport of constituents in the atmosphere have, over the last number of years, been developed for the analysis and forecast of transboundary transport of photo-oxidant pollutants.

An air quality model (like any model) is a representation of reality in which a number of parameters are used to calculate a result and it can be conceptual, empirical or process oriented. The more

physical processes that are included in the model, the more comprehensively it will generally be able to describe reality. However, increasing the inputs and processes leads to high demands on the quantity and quality of information needed to drive the models (EEA, 2011). Traditionally, monitoring has been the primary means of assessing air pollution levels but it can provide only real-time information at best and cannot provide the spatial coverage of modelling. However, it must be noted that model results are based on their input data and some models require extensive data that may be unreliable or difficult to obtain consistently. The accuracy of any model is dependent on the quality of the input data coupled with the ability of the model to represent real world chemical and physical responses.

1.3 Objectives

The overarching aim of this research was to develop an air quality model for Ireland that could be implemented to produce short-term forecasts of the pollutants outlined in the Clean Air for Europe (CAFE) Directive (EU, 2008), particularly targeting NO_x, PM₁₀, PM_{2.5}, SO₂ and O₃. The model would furthermore be used to anticipate pollution episodes, to aid local and regional air quality management and for further research into population exposure. There were a number of specific objectives, including:

1. review the applicability of current models and previous relevant studies relating to forecasting air quality levels in Ireland and internationally;
2. assess the applicability of existing models to Ireland;
3. participate in relevant EU initiatives on modelling;
4. build, analyse and contribute to emissions data on a local and regional scale;
5. develop a geographic information system (GIS)-based statistical model to determine the spatial variation in background concentration levels of pollutants on a national scale at short and long temporal resolutions;
6. develop a calibrated air quality forecast model for Ireland.

Such a model needs to be capable of being run routinely with minimum resource requirements.

Routine air quality forecasts are of high importance from public health, air quality management and scientific perspectives. Densely populated areas and urban locations would benefit significantly from air quality forecasting as the population can be warned and emergency control measures adopted in advance of pollution episodes. These forecasts would necessarily be 24–72 hours in advance.

1.4 EU Initiatives

Within Europe no single body has assumed formal responsibility for the development and use of particular models in specific circumstances. In contrast, the USA has adopted a more structured approach whereby the US Environmental Protection Agency cites regulatory models for specific uses. This means that model development has been structured, transparent and fully documented (Williams *et al.*, 2010). Within the EU the development of models has mainly been driven by the Convention on Long-range Transboundary Air Pollution (CLRTAP), the European Commission and the CAFE programme. The CAFE Directive (EU, 2008) sets out performance criteria that the model should satisfy but the choice of model is not indicated. As a result, individual European countries have adopted a wide range of approaches to modelling their air quality depending on their main objectives, available resources and previous results. The Forum for Air Quality Modelling in Europe (FAIRMODE) is a concerted effort to bring together air quality modellers and harmonise modelling on a European scale. Although models can be used to demonstrate compliance with EU limit values, no direction on which model to use is given by the Commission.

There are a number of EU initiatives whereby European air quality modellers run models for the whole European domain both in real time and retrospectively. The Monitoring Atmospheric Composition and Climate (MACC)/Copernicus programme generates ensemble forecasts on a twice-daily basis, which are made available to the public via an air quality map of Europe online. MACC-Interim Implementation (II) has the overall objective of delivering reliable operational products and information that support research, European environmental policy and the development of user-specific downstream services.

1.5 Air Quality Index for Health

The Air Quality Index for Health (AQIH) was developed by the Air Quality Health Information Working Group, comprising members from the Environmental Protection Agency (EPA), Met Éireann, the Department of the Environment and the Health and Safety Executive (HSE). The index is currently used by the EPA to provide information to the public about air quality in each of six air quality zones across Ireland in real time. It is measured on a scale from 1 to 10 (“good” to “poor”), representing the level of air pollution. The index for each pollutant is calculated separately using set concentration ranges. The AQIH is based on the worst index of the five pollutants assessed. Alongside the index itself additional information is provided regarding the health effects of air pollution and health advice to follow when using the AQIH. A priority for this fellowship, as indicated by the EPA at the outset of this project, was to produce forecasts of the AQIH. As these forecasts are necessarily produced on a daily or twice-daily basis for public information, practical considerations such as computing requirements, speed of computation and ease of operation influenced the direction of the work.

1.6 Context

This report provides an overview of major work areas completed as part of the research fellowship. The research project itself has produced some key, tangible outputs. Primarily, it has produced the first fully operational air quality forecast model for Ireland. Model development has been carried out by the research fellow from first principles meaning that no licensing restrictions apply. The fellow has developed a modelling system that runs automatically twice daily to produce 24- and 48-hour forecasts of NO₂, PM₁₀, PM_{2.5}, SO₂ and O₃, and subsequently the AQIH. This work fulfils the key EPA requirement for an air quality forecast system that requires minimal resources to operate on a routine basis. The fellow has also developed a manual version of the model that can be run for any given date/time. In collaboration with a second research project (2013-EH-FS-7) national-scale annual mean maps of background NO₂, PM₁₀, PM_{2.5}, SO₂ and O₃ have been produced as part of that project. An hourly/daily national-scale spatial model has also been developed.

This report provides a general overview of these major deliverables. It is not intended as a step-by-step guide on how to replicate the work but rather introduces the tangible outputs that have been produced as part of this research fellowship. Details are provided in a number of publications and three detailed reports, which were completed during the research fellowship. The publications are as follows:

- Donnelly, A., Naughton, O., Broderick, B. and Misstear, B., 2017. Short-term forecasting of nitrogen dioxide (NO₂) levels using a hybrid statistical and air mass history modelling approach. *Environmental Modelling and Assessment* 22: 231–241.
- Donnelly, A., Naughton, O., Misstear, B. and Broderick, B., 2016. Maximising the spatial representativeness of NO₂ monitoring data using a combination of local wind-based sectoral division and seasonal and diurnal correction factors. *Journal of Environmental Science and Health* 51: 1003–1011.
- Donnelly, A., Misstear, B. and Broderick, B., 2015. Real-time air quality forecasting using integrated parametric and non-parametric regression techniques. *Atmospheric Environment* 103: 53–65.
- Donnelly, A., Broderick, B. and Misstear, B., 2015. The effect of long-range air mass transport pathways on PM₁₀ and NO₂ concentrations at urban and rural background sites in Ireland: quantification using clustering techniques. *Journal of Environmental Science and Health* 50: 647–658.
- Donnelly, A., Naughton, O., Broderick, B. and Misstear, B., 2015. Air quality forecasting

using parametric and non parametric statistical modelling – prediction of the air quality index for health in Ireland. 34th international Technical Meeting on Air Pollution Modelling and its Application, Montpellier, 4–8 May.

- Naughton, O., Donnelly, A., Nolan, P., Pilla, F., Misstear, B.D. and Broderick, B., 2018. A land use regression model for explaining spatial variation in air pollution levels using a wind sector based approach. *Science of the Total Environment* 630: 1324–1334.

The reports are as follows:

- Donnelly, A., Misstear, B., Broderick, B. and Delaney, K., 2014. *Air Quality Modelling (2012-EH-FS-6) Interim Report: Review of Modelling Systems*. Environmental Protection Agency, Johnstown Castle, Ireland.
- Donnelly, A., Broderick, B. and Misstear, B., 2014. *Air Quality Modelling (2012-EH-FS-6) Interim Report: Validation of Point Wise Air Quality Forecasting Model*. Environmental Protection Agency, Johnstown Castle, Ireland.
- Donnelly, A., Broderick, B. and Misstear, B., 2015. *Air Quality Modelling (2012-EH-FS-6) Hybrid Model Validation Study*. Environmental Protection Agency, Johnstown Castle, Ireland.

Chapter 3, which details the point-wise model development, contains some reference to both the interim standard model validation study and the final hybrid model validation study but additional detail is contained in the reports referenced above.

2 Review of Modelling Systems

A model review was carried out to inform the development of an appropriate air quality forecasting model for Ireland. Air quality models have previously been developed for a range of different purposes, often with distinct advantages and limitations. The aim of this review was to provide an overview of different modelling approaches. The success of any model is dependent on the availability of the necessary input data. This review was an important first step in developing a modelling system for Ireland. Various modelling techniques were analysed, with consideration given to the resources and data available within Ireland at this time.

The range of individual modelling techniques discussed offers diverse and often unique advantages for a variety of purposes. An important aspect of modelling is determining which technique offers the best use of the resources and data available. The best model is not necessarily the most detailed or technically advanced and fundamental to the success of a given model is the availability at sufficient resolution of the necessary data to drive it. As this work was carried out in a relatively restricted time frame it was important to tackle the relevant priorities within the EPA and ensure that the most urgent deliverables were made available within the shortest time frame.

A priority within the EPA was to produce air quality forecasts based on the AQIH. The AQIH is based on point-wise measurements and, in order to extrapolate these measurements to the future, statistical regression and time series techniques were deemed the most suitable. The primary advantage of this approach was that it could be developed from first principles specific to the area of interest and completely removes the reliance on a third party to supply the model or apply licensing restrictions. Furthermore, a benefit of using such a method is the speed of computation. Forecasts are useful only if they can be computed and made available to the public relatively quickly. Such methods also tend to be highly

accurate with low bias, as they are developed site specifically, unlike large-scale deterministic models, which are often developed and tested in vastly differing domains. In particular, this method was capable of producing accurate point-wise forecasts without the need for a detailed emissions inventory. At the project outset, the emissions inventory was not of sufficient spatial resolution to make realistic point-wise forecasts in all air quality zones by deterministic means, and it would have been an inefficient use of resources to base the development of forecasts on what was currently available.

In order to provide detail on the spatial variation of concentration levels across the country, land use regression (LUR) was recommended in the model review as a suitable technique. This technique uses surrogate spatial indicators to explain the variation in concentration levels between monitoring points. Land cover data [Coordination of Information on the Environment (CORINE)], digital terrain model (DTM) output, road density information and population data are all factors that influence concentration levels and data that were broadly available.

A stepwise approach was chosen for model development as this crucially allowed deliverables prior to completion of the project. This minimised risks and allowed the production of preliminary air quality forecasts at the end of the first year of the project. The fluid, stepwise approach adopted meant that the work completed by the researcher working on an emissions inventory (2013-EH-FS-7) (who commenced at the end of year one) could be integrated efficiently into the current fellowship, making maximum use of resources. Details of each of the individual models developed are provided in Chapters 3, 4 and 5. The three primary models developed are as follows:

1. point-wise forecast model (Chapter 3);
2. spatial mapping of air pollution (annual mean) (Chapter 4);
3. temporal LUR model (Chapter 5).

3 Point-wise Forecasting of the Air Quality Index for Health

3.1 Standard Model

3.1.1 Overview

This section provides an introduction to the point-wise forecast model used to predict daily maximum NO₂, SO₂ and 8-hour O₃ and daily average PM₁₀ and PM_{2.5} at all of the sites used in the derivation of the AQIH. Necessary inputs are outlined and model outputs are illustrated. A full model validation report has been completed where details of model performance are examined.

The statistical forecast model provides point-wise predictions of daily maximum NO₂, SO₂ and 8-hour O₃ and daily average PM₁₀ and PM_{2.5} at all of the sites used in the derivation of the AQIH. The model has been developed based on:

- relationships that exist between air quality and meteorological parameters;
- long-term trends in air quality levels;
- diurnal and seasonal cyclical variations at individual site types;
- persistence of concentration levels from one day to the next;
- air mass history and its relationship with NO₂ and PM_{10/2.5} levels.

Aside from the actual predictions, the model provides useful information about concentration variations at each site in Ireland. This information is available for all pollutants and sites used in the AQIH. The data are available in tabular form for every site with values for the following parameters:

- concentrations for all wind speed and wind direction combinations in both seasons;
- concentrations for each hour of the day at weekends in winter, weekdays in winter, weekends in summer and weekdays in summer (diurnal variation);
- concentrations for each day of the year (seasonal variation);
- weekday variations in concentration levels;
- trends in concentrations across sites;

- relationships between other meteorological parameters and concentration levels;
- air mass history forecast for background sites;
- back trajectory cluster analysis results for NO₂ and PM_{10/2.5}.

The model is trained for each site individually and ideally will be based on > 1 year's data to enable long-term trends to be captured. Typically, the most recent 5 years of data have been used for model development at each site.

New sites can be added to the forecast model at any time provided there are sufficient monitoring data available on which to calibrate and train the model. Ideally, monitoring would take place for a minimum of a year before the model was trained. However, if necessary, the model can be trained using 3 months (a season) of data and correction factors applied to develop an interim model. After a year the model would then be recalibrated using the full data set. When a site is discontinued (or moved), the model can continue to make predictions at that site while data are being collected at the new site.

3.1.2 Variation in concentrations with meteorological parameters

The variation in concentration levels of all pollutants shows clear correlation with wind speed and wind direction. It is important that these factors are not considered in isolation as there is generally important interaction between both wind factors. Figure 3.1 shows a sample output (from Kilkitt) from the non-parametric model that is used to generate a wind speed/wind direction (WSWD) factor at each site (Donnelly *et al.*, 2010, 2011). This WSWD factor is used as an input for the forecast model and is calculated in operational mode using forecast meteorological data. This information can also be useful for source attribution or general analysis of air quality levels at certain sites.

Time series analysis is used to develop a diurnal and seasonal factor at each site, which is also used as

inputs to drive the forecast model. Concentrations vary between winter and summer months and between weekdays and weekends. An example is shown for Kilkitt in Figure 3.2. There is a clear difference between weekdays and weekends and between summer and winter months. Considering weekday concentrations it can be seen that there is a gradual increase in concentration levels throughout the day in the winter, and a peak is reached in the evening at approximately 5pm. This peak is later in summer months because of longer hours of daylight and subsequently better mixing conditions. The delayed peak and gradual increase observed at this site is suggestive of a reasonably distant source or sources affecting the site. Concentrations at weekends are lower but still display the delayed peak.

In the same manner as for the diurnal variations, seasonal variations are calculated for each site.

Figure 3.2 shows the results for Kilkitt. At all sites, lower concentrations are observed during summer months (as expected). Sites with very local, dominant sources might be expected to display less percentage variation across seasons.

3.1.3 Model fitting

The model is developed using the variables outlined in Table 3.1 as predictor variables. The general form of the model is:

$$C = b_0 + \sum_{i=1}^n b_i x_i + \sum_{j=1}^m d_j y_j + \varepsilon \quad (3.1)$$

where C is the response variable (pollutant concentration), b_0 is the regression constant, x_i is the meteorological predictor variable with coefficient b_i , y_j is the predictor variables output from the non-parametric and time series models with coefficients d_j and ε is the stochastic error associated with the

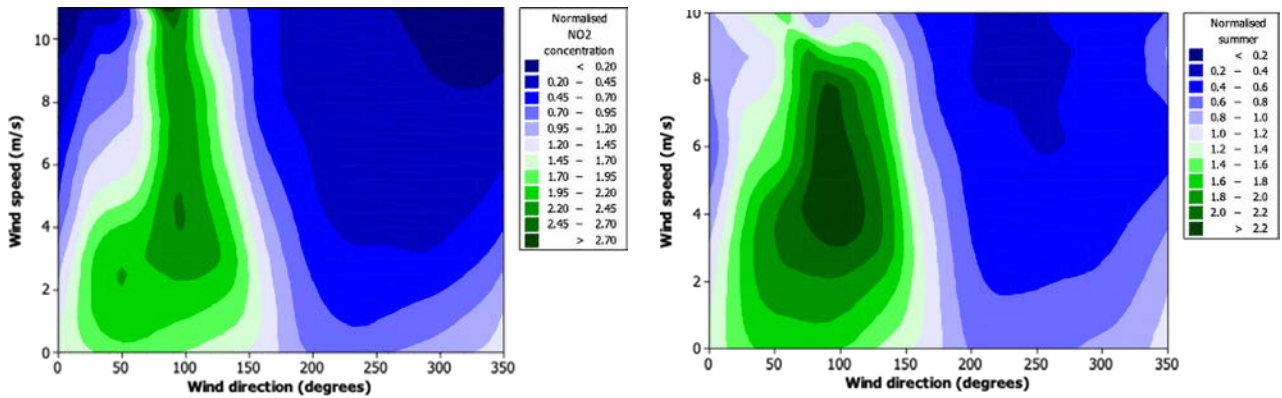


Figure 3.1. Variation of NO_2 concentrations at rural background site Kilkitt in winter (left) and summer (right) with wind speed and direction.

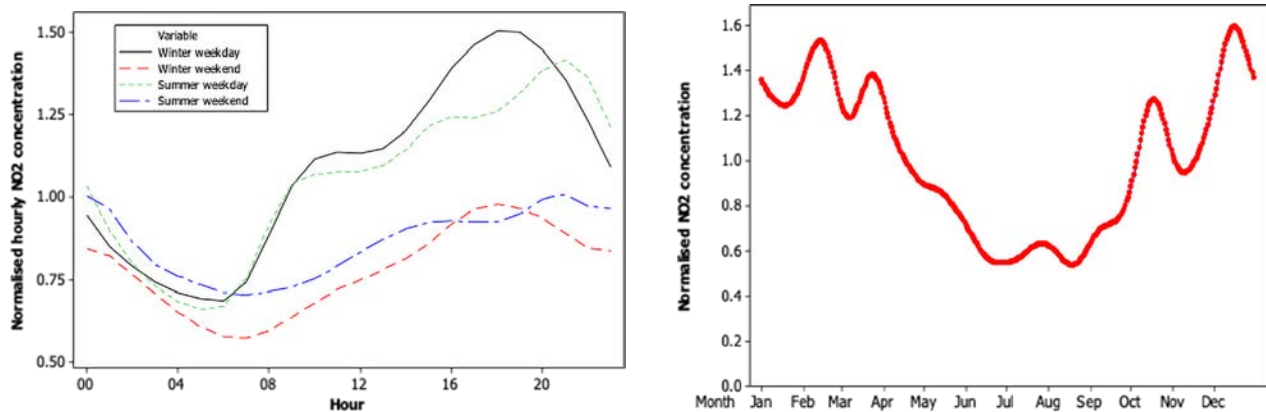


Figure 3.2. Diurnal (left) and seasonal (right) variation of NO_2 concentrations at rural background site Kilkitt.

Table 3.1. Predictor variables for standard point-wise forecast model

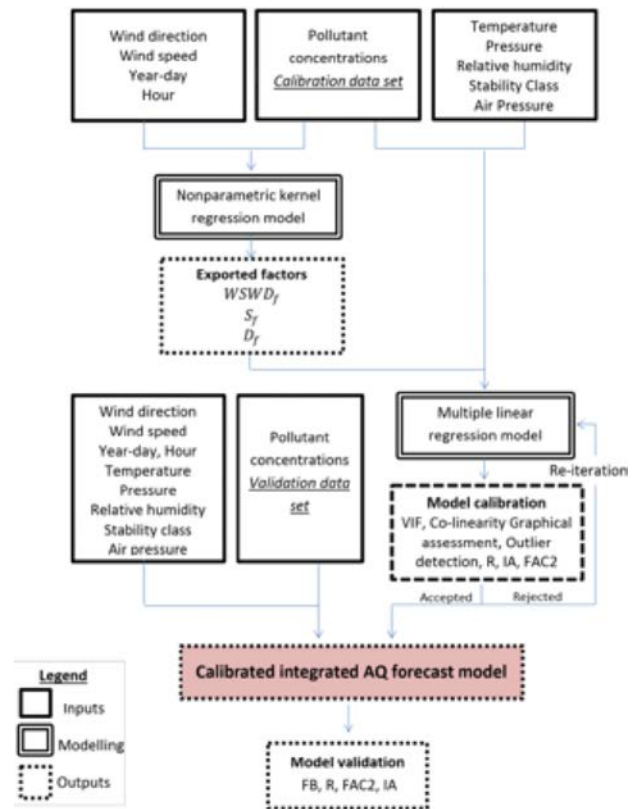
Variable category	Predictor variable	Description
Model (Y_i)	$WSWD_f$	WSWD
	S_f	Non-parametric seasonal factor
	D_f	Non-parametric diurnal factor
	TS_f	Time series forecast factor
Meteorological (X_i)	Temp	Hourly temperature
	SunHr	Sunshine hours
	RelHum	Relative humidity
	AtmPres	Atmospheric pressure
	StabilityCl	Stability class
	NO_2 h-24, NO_2 h-48	Daily average NO_2 concentration at 24-/48-hour lag
	NO_2 max-24, NO_2 max-48	Daily maximum NO_2 concentration at 24-/48-hour lag
	O_3 d-24, O_3 d-48	Daily average O_3 concentration at 24-/48-hour lag

regression. Technical modelling details, including the derivation of the model y_i factors by advanced non-parametric regression, are outlined in detail in Donnelly *et al.* (2015a).

Figure 3.3 outlines the general model development process. Measured pollutant concentrations together with wind speed, wind direction, day of the year and hourly information are fed into the non-parametric model. The $WSWD_f$, a seasonal factor and a diurnal factor are output from this model. These factors together with other meteorological data are fed into a multiple regression model as predictor variables, while measured pollutant concentration data are the response data. A first iteration model is then produced and this is assessed using a variety of techniques. Reiteration continues until the model is accepted. This model was then validated using a separate validation data set.

A 6-month validation study was carried out on the standard point-wise forecasting model and details from an associated report.

Table 3.2 shows key model performance statistics for each of the pollutants. In general, it was found that the model predicted mean concentration variations well for all pollutants indicated by high index of agreement (IA) values. On occasion it can miss peak events [highlighted by reduced correlation coefficient (r) values]. IA values are slightly lower for PM_{10} and $PM_{2.5}$ than for other pollutants, indicating poorer point-to-point agreement. This is also the case for the correlation coefficient (r), but as this measure is very sensitive to outliers this is most probably

**Figure 3.3. Methodology flowchart for standard point-wise model development.**

because of underprediction of peak events by the model. FAC2 is considered one of the most robust measures of air pollution model performance (Borrego *et al.*, 2011). FAC2 is the proportion of modelled values that lie within a factor of two of the measured value. It is recommended that an air quality model is considered acceptable if more than half of the model predictions lie within a factor of two of the observations

Table 3.2. Statistical parameters for each pollutant, September to March

Parameter	Ideal value	O ₃	NO ₂	PM ₁₀	PM _{2.5}	SO ₂
<i>r</i>	1	0.85	0.74	0.46	0.50	0.79
FAC2	1	1.00	0.71	0.90	0.79	0.54
IA	1	0.91	0.84	0.66	0.69	0.86

and faulty if not – this FAC2 criterion was chosen as it is a common metric in academic literature for assessing air quality model outputs (Derwent *et al.*, 2010). The modelled value is 100% for O₃, and values are adequately high for NO₂, PM₁₀ and PM_{2.5}, indicating no major false alarms. The value is poorer for SO₂ but this is thought to be because of the very low concentrations involved and a large number of measured zero values, making the test unreliable.

3.1.4 Discussion

This model benefits from simplicity of the input data and requires very low computational resources to run making it ideally suited to providing fast and reliable real-time air quality forecasts. The model validation study concluded that model performance for O₃ and SO₂ was of a suitably high standard. Mean NO₂ and PM₁₀/PM_{2.5} concentrations were also well predicted by the model. However, the underprediction of peak events for these pollutants warranted further investigation and led to an additional area of work being completed (air mass history modelling) and, ultimately, based on these results, the expansion of this point-wise model to produce an improved hybrid point-wise forecasting model.

3.2 Hybrid Point-wise Forecast Model

3.2.1 Analysis of air mass history and NO₂/PM_{10/2.5} concentrations at urban and rural sites

The hybrid single particle Lagrangian integrated trajectory (HYSPLIT) model was developed by the US National Oceanic and Atmospheric Administration's (NOAA) Air Resources Laboratory (ARL) and combines the Eulerian and Lagrangian approaches to track air mass movement (Draxler and Hess, 1998). Although the model is capable and frequently used to calculate concentrations of pollutants, it is applied

in this study to calculate back trajectories. With the HYSPLIT model, air mass paths from one region to another can be calculated and it can therefore be demonstrated whether or not the vector necessary for air pollutant transport is present (Anastassopoulos *et al.*, 2004). When the model is run in back trajectory mode, the movement of a parcel of air can be calculated backwards in time from the receptor where concentrations were measured, allowing the origin of the pollution to be identified. Based on the results of the validation study of the standard forecast model, an analysis of air mass history in relation to concentrations was carried out with the objective of determining if regional conditions could be contributing to peak NO₂ and PM events. The results are detailed in Donnelly *et al.* (2015b).

The specific aim of this work was to quantify the effects of various long-range transport pathways on NO₂ and PM₁₀ concentrations at various sites in Ireland and identify air mass movement corridors that may lead to incidences of poor air quality for application in forecasting. The origin of and the regions traversed by an air mass 96 hours prior to reaching a receptor was modelled and k-means clustering is applied to create air-mass groups.

Trajectory cluster analysis was employed to group trajectories based on their three-dimensional similarities and identify the primary meteorological pathways influencing the background site. This technique groups similar trajectories together, with the aim of minimising differences within clusters and maximising the differences between clusters. It allows for the inclusion of recirculated trajectories and trajectories with rapidly varying directionality. The hierarchical cluster method adopted in this study initially assumes that the number of clusters is equal to the total number of trajectories (N) and thus the spatial variance (SV) (the sum of the squared distances between end-points of the clusters component trajectories and the mean of that cluster) is zero. In the first iteration, each combination of trajectory

pairs is tested to compute the cluster SV. The total spatial variance (TSV) is then calculated by summing all of the clusters SVs. The two trajectories with the lowest SV are then combined into a single cluster, thus reducing the total number of clusters after the first iteration to $N-1$. Once paired, clusters remain together in subsequent iterations. In the second iteration, the clusters are either individual trajectories or the cluster of the initial pairing of trajectories. Again, every combination is assessed and the two clusters combined are those that result in the lowest increase in TSV. The iterations continue in this manner until the last two clusters are combined, resulting in all N trajectories in one cluster. In the first number of iterations the TSV increases greatly as the number of clusters combined increases. Thereafter, it tends to increase gradually up to a point when it increases sharply, indicating that the clusters being combined are not very similar. A plot of TSV against the number of clusters will clearly indicate this change and suggest where clustering should be stopped.

Significant differences in air pollution levels were found between air mass cluster types at urban and rural sites as shown in Table 3.3. It was found that easterly or recirculated air masses lead to higher NO_2 and PM_{10} levels, with average NO_2 levels varying between 124% and 239% of the seasonal mean and average PM_{10} levels varying between 103% and 199% of the seasonal mean at urban and rural sites. Easterly air masses are more frequent during winter months

leading to higher overall concentrations. The span in relative concentrations between air mass clusters is highest at the rural site, indicating that regional factors are controlling concentration levels. The methods used in this work were then applied to assist in modelling and forecasting air quality based on long-range transport pathways and forecast meteorology without the requirement for detailed emissions data over a large regional domain or the use of computationally demanding modelling techniques.

3.2.2 Data partitioning at AQIH sites

Building on these results, 48-hour air mass back trajectories were calculated for 2 full calendar years (2011 and 2012) with hourly end points located at two AQIH sites, Kilkitt and Claremorris monitoring stations, which were assumed to represent background conditions for NO_2 and PM, respectively.

Resulting trajectories were divided into seasonal groups to account for known variability in both synoptic scale variations and air pollution levels between the winter (January–March), spring (April–June), summer (July–September) and autumn (October–December) periods. The trajectory duration was chosen as 48 hours because too short a duration may miss the actual source of the emissions and important path crossings, whereas too long a run induces a large amount of uncertainty into the analysis and may produce misleading results. As an island with no

Table 3.3. Average NO_2 , NO_x/NO_2 ratio and PM_{10} expressed as a percentage of the seasonal mean at each site for the major clusters

Direction	Kilkitt			Glashaboy			Ballyfermot		
	NO_2	NO_x/NO_2	PM_{10}	NO_2	NO_x/NO_2	PM_{10}	NO_2	NO_x/NO_2	PM_{10}
Winter									
East	160	96	154	124	105	135	149	124	147
South-west	47	101	56	59	92	81	49	85	51
South-west/west	78	105	77	80	102	65	84	96	75
West	47	111	59	104	92	92	67	100	69
North	78	93	71	107	100	99	113	105	112
Summer									
East/recirculated	239	56	199	137	100	103	136	99	131
South-west fast	103	79	85	68	97	93	63	108	83
South-west slow	123	104	113	82	96	87			
West	36	141	84						
North-west	90	115	87	90	99	98	88	102	85
North	49	96	57	90	97	98	99	99	84

nearby land mass to the west and south-west and a significant nearby land mass to the east and south, the appropriate trajectory duration may differ in Ireland from that in land-locked countries. A simple analysis of air masses and clusters should reveal the appropriate trajectory duration for a given country. Clustering was carried out on each seasonal group individually and the optimum number of clusters was chosen in each case by visual inspection of the TSV plots.

Results of the cluster analysis are shown in Figure 3.4. Six clusters were defined from January to March. These include a slow-moving east/south-easterly cluster and a moderate-moving easterly cluster. These two clusters are associated with the highest NO₂ concentrations, (averaging 196% and 168% of the mean for this time period, respectively). From April to June only one easterly cluster is defined and NO₂ concentrations for these air masses average 161% of the mean for the time period. A similar result is observed between July and September when concentrations for the easterly cluster average 191%

of the mean for the period. The easterly cluster results in average concentrations of 196% between October and December. During this time period, Ireland is also frequently affected by slow-moving northerly air masses representative of cold winter weather conditions. The defined cluster is of much shorter length in this season than in other seasons and its slow-moving nature and its land track over parts of the UK result in an average NO₂ concentration of 153% of the mean for the time period.

Average concentrations for each cluster for NO₂, PM₁₀ and PM_{2.5} are displayed in Tables 3.4–3.6, respectively. After clustering, the variability in hourly NO₂ and daily PM between clusters was analysed and an analysis of variance (ANOVA) was applied to assess which cluster types led to increased concentrations. Data were partitioned into “high” background and “low” background groups at AQIH sites, with the shading in the tables illustrating the “high” background groups. In operation, if the air mass is forecast to come from a “high” cluster then the high background partition

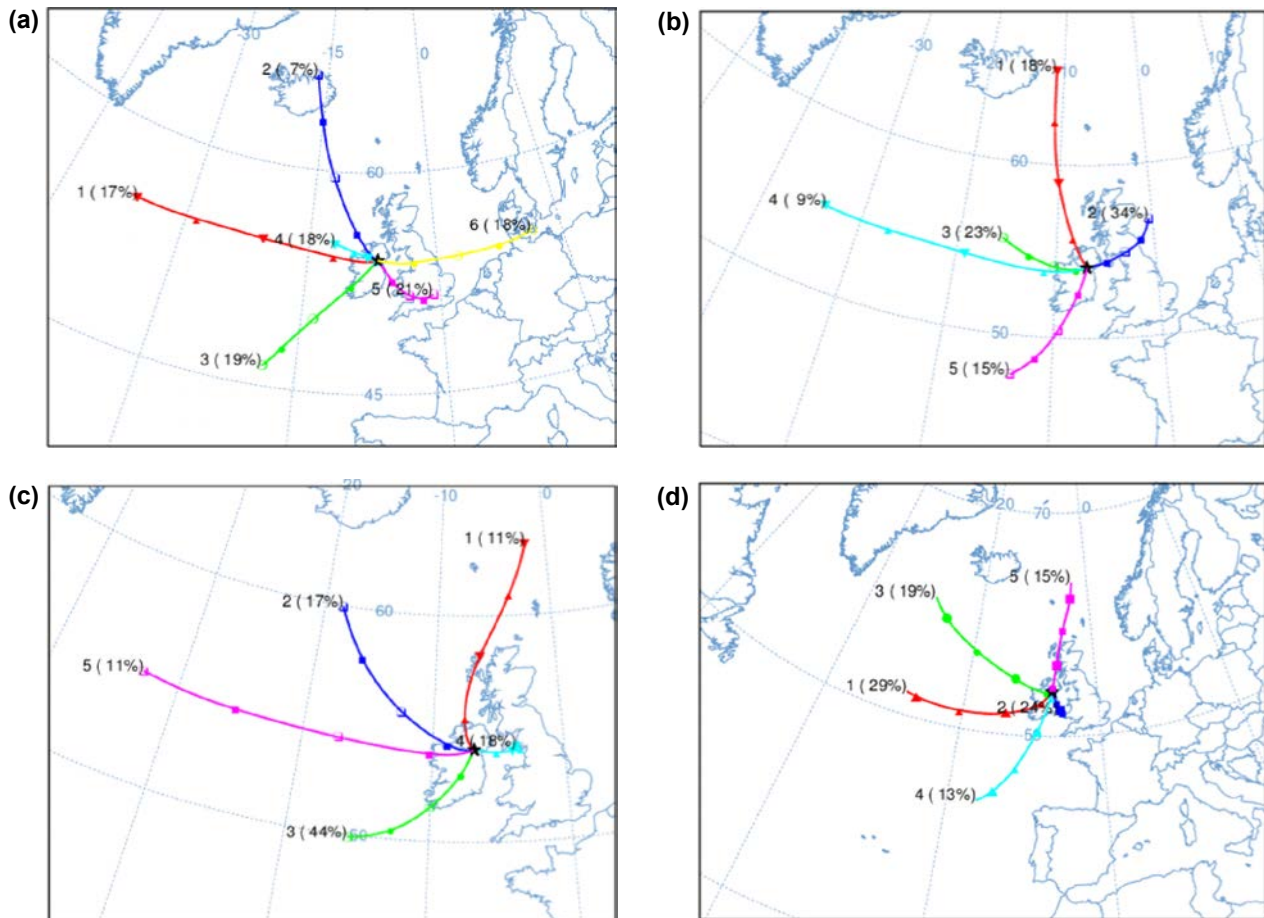


Figure 3.4. Cluster results from Kilcilt for 2012 and 2013 data: (a) January–March, (b) April–June, (c) July–September and (d) October–December.

Table 3.4. NO₂ concentrations for air mass clusters arriving at Kilkitt

January–March			April–June			July–September			October–December		
No.	Average NO ₂ (ppb)	% of mean	No.	Average NO ₂ (ppb)	% of mean	No.	Average NO ₂ (ppb)	% of mean	No.	Average NO ₂ (ppb)	% of mean
5	4.29	1.96	2	3.38	1.61	4	2.65	1.96	2	2.85	1.91
6	3.68	1.68	3	2.07	0.99	1	1.23	0.91	5	2.29	1.53
4	2.46	1.12	5	1.37	0.65	3	1.09	0.81	4	0.88	0.59
2	1.58	0.72	1	1.11	0.53	5	0.93	0.69	1	0.78	0.52
1	0.34	0.15	4	0.79	0.38	2	0.92	0.68	3	0.68	0.45
3	0.09	0.04	–	–	–	–	–	–	–	–	–

ppb, parts per billion.

Shading indicates the “high” cluster type.

Table 3.5. PM₁₀ concentrations for air mass clusters arriving at Claremorris

January–March			April–June			July–September			October–December		
No.	Average PM ₁₀ (µg/m ³)	% of mean	No.	Average PM ₁₀ (µg/m ³)	% of mean	No.	Average PM ₁₀ (µg/m ³)	% of mean	No.	Average PM ₁₀ (µg/m ³)	% of mean
5	25.42	137	2	12.69	119	5	12.73	134	5	12.64	112
6	21.20	114	4	9.91	93	4	12.35	130	1	11.47	101
4	14.24	77	3	9.87	92	2	8.29	87	4	11.46	101
1	13.70	74	5	9.83	92	1	8.17	86	2	10.86	96
2	11.84	64	1	9.69	91	3	8.10	85	3	10.47	93
3	8.15	44	–	–	–	–	–	–	–	–	–

Shading indicates the “high” cluster type.

Table 3.6. PM_{2.5} concentrations for air mass clusters arriving at Claremorris

January–March			April–June			July–September			October–December		
No.	Average PM _{2.5} (µg/m ³)	% of mean	No.	Average PM _{2.5} (µg/m ³)	% of mean	No.	Average PM _{2.5} (µg/m ³)	% of mean	No.	Average PM _{2.5} (µg/m ³)	% of mean
5	19.52	180	2	8.49	139	4	7.16	157	5	7.89	141
6	17.58	162	3	5.27	86	5	4.74	104	2	5.88	105
4	8.78	81	5	5.05	83	2	3.95	87	3	5.17	92
1	5.51	51	4	5.00	82	1	3.79	83	4	4.86	87
2	5.18	48	1	4.42	72	3	3.75	82	1	4.77	85
3	3.66	34	–	–	–	–	–	–	–	–	–

Shading indicates the “high” cluster type.

of the model is invoked (right arm of Figure 3.5). If the air mass is forecast to come from a “low” cluster then the standard form of the model is run (left arm of Figure 3.5).

3.2.3 Model fitting

Nitrogen dioxide

The premise of the hybrid model is that pollution contributions are split into local and regional effects and different models are then developed for the “high” and “low” air mass groups. Two unique local NO₂ forecast models were developed for each condition:

- Low cluster model: this model forecasts NO₂ concentrations at all AQIH sites in Ireland for “low” air mass groups.
- High cluster model: this model forecasts NO₂ concentrations at all AQIH sites in Ireland for “high” air mass groups. It comprises a “background” contribution and a “local” contribution. The forecast concentration at the local site on “high” days is thus the concentration computed by the “high” background model plus the concentration computed by the “high” local model.

The model fitting procedure and technical details are described in Donnelly *et al.* (2017). The hybrid NO₂ model is developed using the same techniques as the standard model but, with the incorporation of the air mass history term, the modelled outputs now include:

- forecasts for background locations in Ireland for high cluster time periods;
- forecasts at non-background locations because of local sources only for high cluster time periods;
- forecasts at all locations for non-high cluster time periods.

Particulate matter_{10/2.5}

For PM_{10/2.5} the same approach was also used and the model results were tested. However, it was found that because of the difficulty in defining a “background” location the results were not as strong. An alternative approach was therefore adopted whereby the data were partitioned as described above using the background monitoring data from Claremorris. A unique “high” cluster model was developed for Claremorris for high pollution days. Operationally,

the results from this “high” forecast were compared with the results of the “basic” forecast at Rathmines and concentrations at other sites were multiplied by the difference to provide a better description of the regional influences on PM levels across Ireland.

Ozone/sulfur dioxide

Model fitting for both O₃ and SO₂ did not make use of partitioned data but rather total data sets. Analysis of air mass history in relation to concentrations indicated that the prediction of peak events would not be significantly improved through the inclusion of an air mass history term in the model for these pollutants.

3.2.4 Model operation

In the operational model the model completes a number of tasks in sequential order to produce final forecasts of individual pollutants and subsequently the AQIH. These tasks are as follows:

- download forecast meteorological data from the Met Éireann file transfer protocol (ftp) server;
- download real-time air quality data from all AQIH monitoring sites;
- download forecast hemispheric meteorological data from the NOAA server;
- run the HYSPLIT model in back trajectory mode for the next 48 hours;
- assess each forecast trajectory path and assign it to one of the predefined clusters;
- if a high cluster is identified then run the “high” model for NO₂, PM₁₀ and PM_{2.5}; run the standard model for O₃ and SO₂;
- if no high clusters are identified then run the standard model for all pollutants.

The model decision tree for NO₂ is illustrated in Figure 3.5. The model is written from first principles using Visual Basic code and presented using a Microsoft Excel Interface. Any model operational editing (such as adding a new site) must be carried out using Visual Basic code. Model coefficients for existing sites can be changed by adjusting the values in the model settings spreadsheet. However, this should be done with caution and only after a full calibration of response/predictor data. A standard operating procedure has been written as part of this research project to provide guidance for model updates and adjustments.

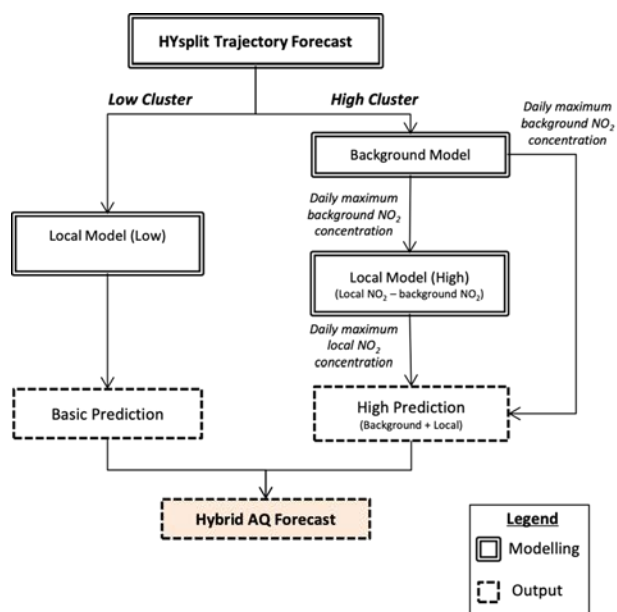


Figure 3.5. Hybrid model operational decision tree.

3.2.5 Validation study

A comprehensive hybrid model validation study has been completed. The statistical forecast model was run daily for the time period from January 2013 to December 2013 to provide 48-hour forecasts. This involved running the entire modelling system retrospectively in forecast mode. The model decision tree is shown in Figure 3.5. The HYSPLIT model was first run for every forecast day. Each trajectory was assessed and assigned to the relevant cluster. Based on this assignment either the standard or hybrid model was run for NO_2 , PM_{10} and $\text{PM}_{2.5}$. The standard model was run for O_3 and SO_2 . Twenty-four-hour, 48-hour and 3-day forecasts were produced by the model. These data were then compiled as time series for each of the pollutants. These time series were compared with observed time series data for the same time period. The observed data used in the comparison have been validated.

Descriptive modelled and measured statistics are shown in Table 3.7. The mean O_3 value measured across sites was $70.25 \mu\text{g}/\text{m}^3$. This was slightly underpredicted by the model ($64.46 \mu\text{g}/\text{m}^3$). Mean NO_2 values were slightly overpredicted by the model because the data distribution was shifted by incorporating the HYSPLIT term ($17.4 \mu\text{g}/\text{m}^3$ modelled compared with $13.5 \mu\text{g}/\text{m}^3$ measured). Mean SO_2 concentrations were accurately predicted with an overall prediction of the average within $1 \mu\text{g}/\text{m}^3$. The mean measured and modelled PM_{10} and $\text{PM}_{2.5}$

concentrations were very similar ($<2 \mu\text{g}/\text{m}^3$ of a difference for PM_{10} and $<5 \mu\text{g}/\text{m}^3$ for $\text{PM}_{2.5}$). Median values largely followed the same pattern as mean values and were accurately predicted by the model for all pollutants. There was some overprediction of the median SO_2 concentration, which arose from the Kilkitt data where the model consistently overestimated the concentration. However, in absolute terms, the magnitude was very small.

In addition to the median and mean values, the 90th 95th and 99.8th percentile values were assessed to examine the distribution of data. These percentile values also largely correspond to the number of exceedances per year, as defined by the EU limit values. For O_3 , the 90th and 95th percentiles were well mirrored by the modelled value. There was a small underprediction of the 99.8th percentile but this statistic is subject to a large degree of chance variation. The actual underprediction was $<7\%$ of the true value. NO_2 percentile values are slightly overpredicted by the model (meaning a conservative estimate of the data distribution) but as the NO_2 values being considered are individual hourly values they are subject to a large degree of inherent variation. Nevertheless, the model captures the overdistribution of data well. SO_2 predictions of percentile values by the model displayed good agreement with the 99.8th percentile. The distribution of daily average PM_{10} and $\text{PM}_{2.5}$ concentrations was well captured across sites with some slight overprediction at high percentile values.

Table 3.8 shows the statistical parameters for all modelled values. The r values were good for gaseous pollutants. PM_{10} and $\text{PM}_{2.5}$ had lower r values but this can be attributed to a small number of outliers in the data set. Ideally, the fractional bias (FB) should equal zero. A negative value indicates that there is some underprediction by the model. This was previously observed when using the standard model for NO_2 and $\text{PM}_{10/2.5}$. The hybrid model has a very slight positive bias for PM_{10} and SO_2 (0.09 and 0.14, respectively) and a slight negative bias for O_3 (-0.09). The negative bias in the O_3 results may be due to some oversmoothing in the model development at some sites. The positive bias is higher for $\text{PM}_{2.5}$, SO_2 and NO_2 , which reflects a slight overprediction of the mean value. The HYSPLIT add-on enables the model to forecast a greater number of high pollution events but it also results in a slight shifting of the overall

Table 3.7. Modelled versus measured descriptive statistics

Statistic	O ₃ (µg/m ³)			NO ₂ (µg/m ³)			SO ₂ (µg/m ³)			PM ₁₀ (µg/m ³)			PM _{2.5} (µg/m ³)		
	24-hour forecast	≥3-day forecast	Monitored	24-hour forecast	≥3-day forecast	Monitored	24-hour forecast	≥3-day forecast	Monitored	24-hour forecast	≥3-day forecast	Monitored	24-hour forecast	≥3-day forecast	Monitored
Mean	64.46	67.55	70.25	17.4	17.93	13.53	7.45	7.18	6.46	18.1	17.07	16.52	15.6	14.1	11.50
Median	64.43	69.50	69.90	13.9	14.27	10.3	5.82	4.81	4.52	14.4	14.55	14.43	8.2	8.98	8.2
90th percentile	86.70	88.30	93.87	35.9	36.7	30.7	13.94	16.61	11.97	32.9	30.3	28.1	37.2	33.64	23.8
95th percentile	91.90	90.33	99.40	43.5	42.71	35.9	19.78	21.93	19.57	39.1	36.59	34.45	50.9	42.56	33.3
98th percentile	98.63	90.51	105.21	51.5	52.08	44.0	25.76	26.36	28.4	46.2	43.6	42.84	63.1	56.47	44.98

Table 3.8. Statistical parameters for each pollutant

Parameter	Ideal value	NO ₂			PM ₁₀			PM _{2.5}			SO ₂			O ₃		
		24-hour forecast Hybrid	≥3-day forecast Hybrid	24-hour forecast Standard	≥3-day forecast Standard	24-hour forecast Hybrid	≥3-day forecast Hybrid	24-hour forecast Standard	≥3-day forecast Standard	24-hour forecast Hybrid	24-hour forecast Hybrid	≥3-day forecast Hybrid	24-hour forecast Hybrid	24-hour forecast Hybrid	≥3-day forecast Hybrid	≥3-day forecast Hybrid
FB	0	0.26	-0.278	0.09	0.02	-0.03	0.30	-0.05	-0.05	-0.2	0.14	0.13	-0.09	-0.11		
R	1	0.82	0.80	0.72	0.46	0.62	0.74	0.50	0.50	0.647	0.69	0.47	0.82	0.80		
FAC2	1	73.4	70	93	90	93	79	79	79	80	77	79	99.5	99.1		
IA	1	0.88	0.83	0.84	0.66	0.70	0.84	0.69	0.69	0.77	0.80	0.59	0.88	0.82		

distribution of data in a positive direction, although this is not considered a significant issue. It is important to note that pollutant concentration distributions tend to be log-normal and therefore the linear measures of the FB and correlation coefficient can be disproportionality influenced by infrequently occurring high pollutant events.

FAC2 exceeds 70% for NO_2 and is close to 100% for O_3 . It is 93% for PM_{10} and 80% for $\text{PM}_{2.5}$. It is lowest for SO_2 but this is because of the very large number of measured zero values that the model cannot be within a factor of 2 of without perfect prediction (i.e. this measure fails for such conditions).

The IA is a robust measure of the degree to which the measured value is accurately estimated by the model. It is similar to the correlation coefficient and also has an ideal value of 1, but unlike the correlation coefficient the IA measures the error of the modelled data rather than the direct correlation between variables and is not as sensitive to outliers. The IA is very high for all pollutants (≥ 0.8) and compares favourably with values obtained in other air quality modelling studies (Kumar and Jain, 2010; Voukantsis *et al.*, 2011; Zhang *et al.*, 2012; Beelen *et al.*, 2013).

Figures 3.6–3.10 show scatter plots of measured versus modelled concentrations (colour-coded by AQIH site) for NO_2 , PM_{10} , $\text{PM}_{2.5}$, O_3 and SO_2 . These plots together with time series plots and detailed validation statistics are discussed in detail in the model validation report. This is not repeated here for brevity but, in general, results were highly acceptable and comparable or better than results achieved by other forecast models. The hybrid model offered significant improvements over the standard model for prediction of NO_2 , PM_{10} and $\text{PM}_{2.5}$ peak events.

Figure 3.11 illustrates the improvement obtained by incorporating the air mass history term into the model at Rathmines. The red symbols show that the standard model had a tendency to underpredict at higher concentrations and could not account for concentrations over $45 \mu\text{g}/\text{m}^3$ at this site in general. The hybrid model, however, results in a much stronger linear relationship between measured and modelled values across the entire range of concentrations.

The model was found to perform better at urban sites than the rural site. There are a number of reasons for this. First, concentrations at the rural site are very

low, which means that the monitoring instrument is often not sufficiently precise to measure near-zero concentrations. As a result, these values are estimated to be equal to zero or the nearest $0.01 \mu\text{g}/\text{m}^3$, which leads to an unnatural distribution within the data. Therefore, although the modelled data follow the measured data reasonably closely, the statistical tests do not account for this lack in precision and indicate poorer results. Second, rural sites are less impacted by local anthropogenic activities, which tend to be repetitive and cyclical (e.g. rush-hour traffic). As emissions travel a greater distance prior to reaching the rural monitoring site, there is more opportunity for dispersion and transformation of pollutants. Although this results in lower NO_2 concentrations, it also leads to more variability in concentration levels (albeit at much lower total concentrations).

3.3 Discussion

Real-time air quality forecasting has become an area of much interest in recent years and various deterministic and statistical techniques have been used to produce functional forecasts. Numerous studies have used statistical techniques to develop air quality forecasts. Techniques adopted include multiple linear regression (Genc *et al.*, 2010; Vlachogianni *et al.*, 2011), autoregressive integrated moving average (ARIMA) modelling (Kumar and Jain, 2010; Zhang *et al.*, 2012), neural networks (Moustris *et al.*, 2010; Feng *et al.*, 2011; Voukantsis *et al.*, 2011), non-linear regression (Singh *et al.*, 2012; Donnelly *et al.*, 2015b), Kalman filtering (Hoi *et al.*, 2010) and various combinations of these (Zhang *et al.*, 2012; Voukantsis *et al.*, 2011). However, most of these methods suffer from the disadvantage that they cannot capture the contribution of distant weather-dependant sources and regional air mass movement. Although deterministic models can account for air parcel history, they are computationally intensive, require detailed emissions inventories over the modelled domain and have a high operational cost (Zhang *et al.*, 2012), which can make them unsuitable for real-time air quality forecasting in many situations. Furthermore, many applications of real-time air quality forecasting require predictions at only certain locations and, in such instances, the processing required by deterministic models to provide detailed spatial variations may be a misuse of resources. As noted by Zhang *et al.* (2012), statistical models often have a better capability for describing

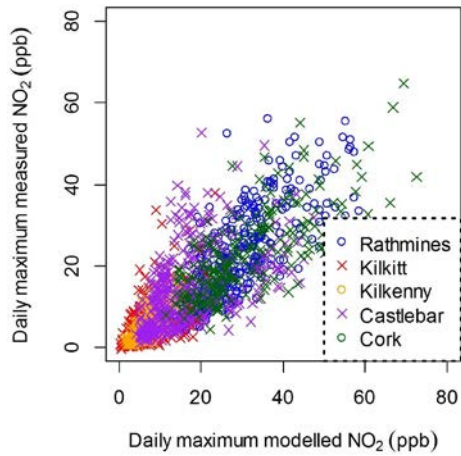


Figure 3.6. Measured versus modelled daily maximum NO₂ concentrations.

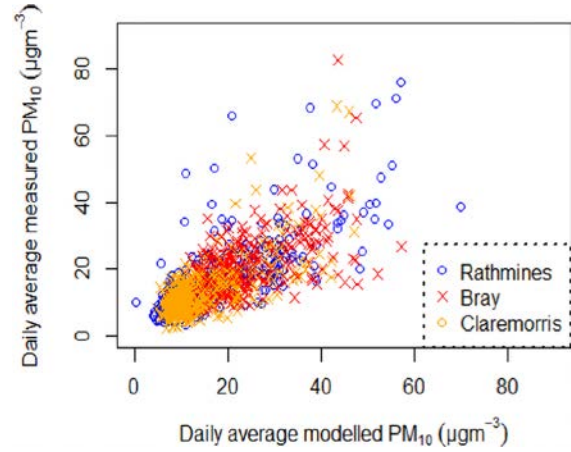


Figure 3.7. Modelled versus measured daily average PM₁₀ concentrations for 24-hour forecasts.

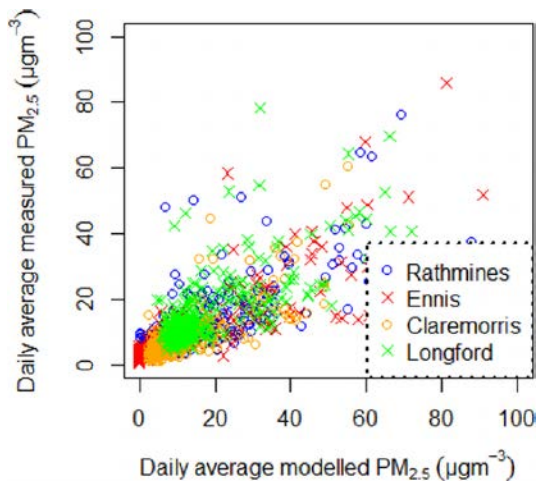


Figure 3.8. Modelled versus measured daily average PM_{2.5} concentrations for 24-hour forecasts.

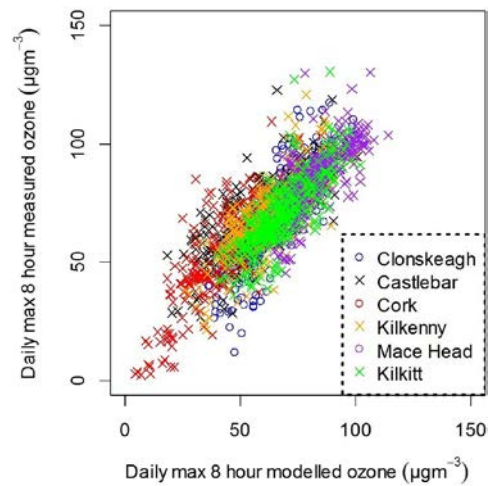


Figure 3.9. Modelled versus measured daily maximum 8-hourly O₃ concentrations for 24-hour forecasts.

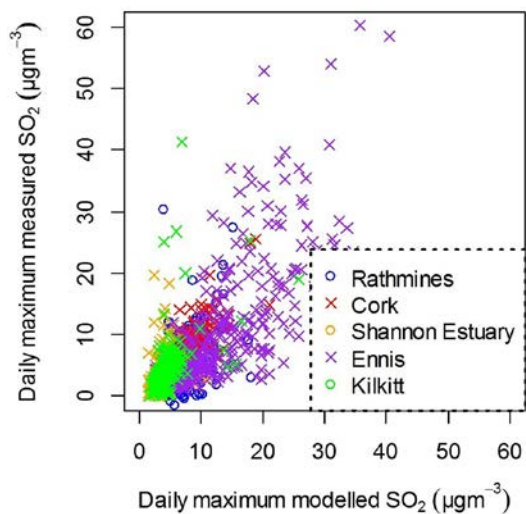


Figure 3.10. Modelled versus measured daily maximum hourly SO₂ concentrations for 24-hour forecasts.

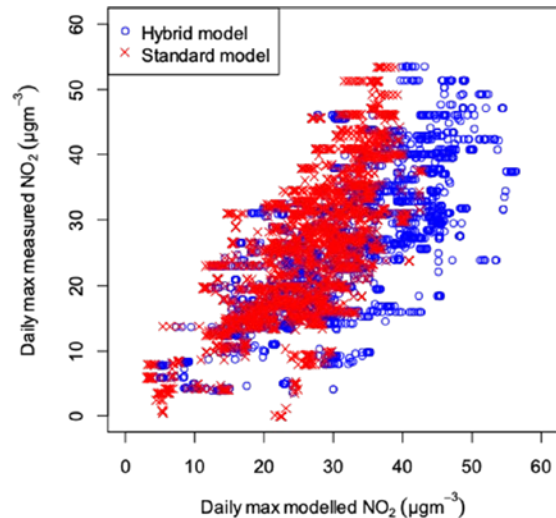


Figure 3.11. Observed NO₂ concentrations (rolling 24-hour maximums) at Rathmines showing improvement in the hybrid model over the standard model.

complex site-specific variations in concentrations than deterministic models, often with a higher accuracy than deterministic models.

The hybrid model developed as part of this research fellowship represents a novel way to forecast air quality routinely and accurately with minimal resource requirements. The hybrid model incorporates the advantages of the standard statistical model outlined in Donnelly *et al.* (2015a) and combines it with the (open-source) deterministic HYSPLIT model. This allows regional effects to be included in the forecasts without the need for a complex deterministic and computationally demanding air quality model to be used. Hybrid model advantages include:

- requires only simple input data;
- minimises model selection error by combining various statistical methods;
- low bias;
- ability to forecast cyclical and anthropogenic effects without the need for an emissions inventory;
- ability to describe complex site-specific variations while including the effects of regional weather patterns;
- speed of computation;
- ease of operation.

3.4 International Model Application

A key underlying assumption in this hybrid approach is that the transboundary contribution to air quality at the background site is representative of that at the forecasting site. The geographical location, prevailing climatic conditions and relatively low urbanisation characteristic of Ireland make this a reasonable assumption in the case presented here. However, when applying the method internationally it should be considered that some areas may be influenced by heavy urbanisation, industrialisation or more complex regional air mass transport and care should be taken in the selection of an appropriate background site to ensure representativeness. Multiple background sites may thus be required when applying the model across a national monitoring network, with parallel trajectory forecasts necessary to enable model selection and forecasting. Owing to the low computational resources of the statistical model and the ease with which trajectory forecasts can be produced, this

does not represent a substantial increase in resource requirements and so this approach remains a viable option for producing fast and reliable real time air quality forecasts in regulatory environments where resource availability is low.

3.5 Summary

- A fully operational air quality forecast model has been produced. The model runs in an automated manner to produce twice-daily 48-hour forecasts of NO₂, SO₂, O₃, PM₁₀ and PM_{2.5} at AQIH sites in Ireland.
- Incorporation of an air mass history parameter has resulted in a large improvement in the prediction of NO₂ and PM concentrations.
- The model is quite conservative in its PM₁₀ and PM_{2.5} predictions. There is a slight positive bias at all sites as a result of the methodology used to account for regional air mass movement and pollutant transport. PM is one of the most difficult pollutants to model because of its wide range of anthropogenic and natural sources. Therefore, a conservative estimate accompanied by some specialist interpretation is considered to be the best means of producing a forecast. When the AQIH is forecast to be poor, air mass history and other conditions relating to PM concentrations should be examined in conjunction with the value given by the air quality model to produce a final forecast.
- During the next model calibration/training, O₃ should be trained using hourly data. The use of 8-hour averages as the response variable has resulted in some oversmoothing of the data.
- SO₂ values are very low at most sites. There is some overprediction by the model at Kilkitt but the very low values involved make this a relatively insignificant issue.
- Statistical parameters for SO₂ are stronger than initial model training would have suggested.
- Air quality forecasts should be made using a combination of:
 - numerical output directly from the model;
 - assessment of forecast local meteorological conditions;
 - assessment of regional air mass movements as forecast by the HYSPLIT model, which is built into the operational air quality model;

- consideration of any other unusual events or conditions (e.g. volcanoes or Saharan dust episodes).
- The model should be recalibrated using up-to-date validated air quality and meteorological data on an annual basis. This process will ensure that air quality trends at individual sites are well captured and any new sources in an area are identified and included in the model.
- However, it should be noted that, if major changes in the emission source were to occur (such as a sudden increase in road traffic volume), the model would require recalibration.
- In the case where new air quality monitoring sites are used for the derivation of the AQIH, the model

can be used to continue to forecast at the old site until a full year of data are available at the new site. This will avoid any break in forecasts within any one air quality zone. Once at least a full year of data are available, the model should be recalibrated and updated to include this new site within the model architecture.

This model has been brought to full operation as part of this research project and has been set up to run in a completely automated manner to provide daily forecasts of the AQIH in each zone in Ireland. The model can also be operated manually (retrospectively or in forecast mode) for any date/time for which appropriate meteorological data are available.

4 Land Use Regression Modelling: Annual Mean Maps

4.1 Introduction

The application of land-use regression techniques provides the opportunity to produce high-resolution maps of background air pollution on a national scale. Linear regression methods have frequently been employed in air quality modelling in the past (Robeson and Steyn, 1990; Briggs *et al.*, 1997; Shi and Harrison, 1997). Konovalov *et al.* (2009) found that in applying model output statistics to the CHIMERE model using both linear regression and non-linear neural networking, there was no significant difference between the performance of PM₁₀ forecasts carried out by each method.

Stedman *et al.* (1997b) developed maps of NO_x and NO₂ concentrations across the UK using an approach that involved a number of methods, one being regression. First, concentrations from monitoring stations that were representative of concentrations over areas of >20 km were directly interpolated. Second, the impact of local NO_x emissions (<20 km from the monitoring sites) were estimated using a box modelling approach incorporating surrogate statistics. At the time of the study, emissions data for the UK were available at a resolution of 10 km by 10 km. As it was noted that NO_x and NO₂ concentrations vary at a much finer spatial scale than emissions from major roads, the percentages of urban and suburban land cover were used as surrogate statistics rather than the emissions data. This could be applicable to Ireland as emission data are not currently available at a 1-km resolution. The development and derivation of these maps is discussed in detail in a number of papers and reports (Stedman *et al.*, 1997a,b; Stedman, 1998; Abbott and Stedman, 1999; Abbott and Vincent, 1999; Stedman and Bush, 2000; Kent *et al.*, 2006; Stedman *et al.*, 2007). They have been developed from a combination of emission estimates from the UK National Atmospheric Emissions Inventory (NAEI) and measurements from the national air monitoring networks (Stedman and Bush, 2000). Variable degrees of agreement between measured and modelled values were found, with coefficients of determination (R^2 values) ranging from 0.33 to 0.78 for various pollutants (Stedman and Bush, 2000). It can be argued that

these maps are limited in their usefulness, particularly in the area of exposure analysis as they provide only an annual mean value and no indication of shorter term values. There is also a substantial risk of double counting the source in certain cases.

Beelen *et al.* (2009) developed maps for the EU for NO₂, PM₁₀ and O₃ at 1-km resolutions using ordinary kriging, universal kriging and LUR techniques. They cited the need for detailed input data together with the need for powerful computing facilities (for large areas and fine resolution) as a limitation in approaching air quality modelling through the use of dispersion models. They found that universal kriging performed the best of the three techniques, with R^2 values ranging from 0.45 to 0.7.

Vienneau *et al.* (2010) noted that LUR has the potential to produce maps of air pollution on national and European scales, in a relatively simple manner, suitable for informing policy and as a basis for risk management. In their study they developed LUR models for both Great Britain and the Netherlands for NO₂ and PM₁₀. They found that the performance of models based on common data was only slightly worse than that of models optimised with local data. However, they advise the need for caution in transferring models across different study areas.

The spatial modelling carried out under this research project builds on many of these previous studies but incorporates a novel means of accounting for variability in prevailing wind directions and orientation of land use types in relation to receptors.

4.2 Sector-based Land Use Regression

In contrast to previous LUR approaches, the approach adopted in this project did not use circular buffers. Rather, a sector-based technique was used whereby the land area affecting air quality at a given site is dependent on wind direction.

The basis of LUR mapping is a multiple linear regression that uses summaries of spatial variables in the vicinity of the monitoring point. In general, spatial

indicators are calculated within circular buffers of varying radii around the monitoring point and the most significant used as predictor variables in the regression equation. However, circular buffers effectively apply equal weights to emission sources around a receptor, irrespective of the prevailing meteorological conditions and the relative positions of receptor and source. This limitation may be minor when LUR is applied within a local region, but when used on a national scale, as required by this project, varying regional wind patterns may lead to poor model performance. Pollutant concentrations can show significant asymmetry depending on wind conditions, as demonstrated in Figure 4.1, where the variance in NO_2 concentrations with wind speed and direction can be seen at both urban (Figure 4.1a) and rural (Figure 4.1b) sites.

As regional prevailing wind conditions can vary substantially and thus impact the applicability of ordinary LUR techniques on a national scale, a novel LUR methodology was devised that incorporates wind effects using angular sectors or “wedges”. The 360° wind field is discretised into a set of eight wind sectors; average pollutant concentrations and predictor variables are then calculated for each sector and used in the LUR process. The use of continuous monitoring data from the national network (monitoring sites shown in Figure 4.2), rather than short-term

passive monitoring, allows the calculation of average concentrations within each wind sector. However, as prevailing wind directions vary geographically, seasonally and diurnally, a biased sectoral average may be obtained in some instances. For example, if a wind direction was more frequent during winter than summer months the raw sector average would be excessively high. Consequently, a non-parametric regression correction method has been applied to remove diurnal and seasonal bias from the data prior to sector averaging. There are four key steps involved in the wind sector land use regression (WS-LUR) model development and mapping process:

1. calculate annual average pollutant concentrations within each wind sector at each monitoring site using a combination of hourly meteorological inputs and continuous monitoring data;
2. generate predictor variables from geospatial data sets for each directional sector within a GIS environment;
3. select predictor variables for LUR equations using a supervised stepwise approach;
4. calculate key predictor variables on a national scale at a fine resolution and weight using interpolated local wind frequency.

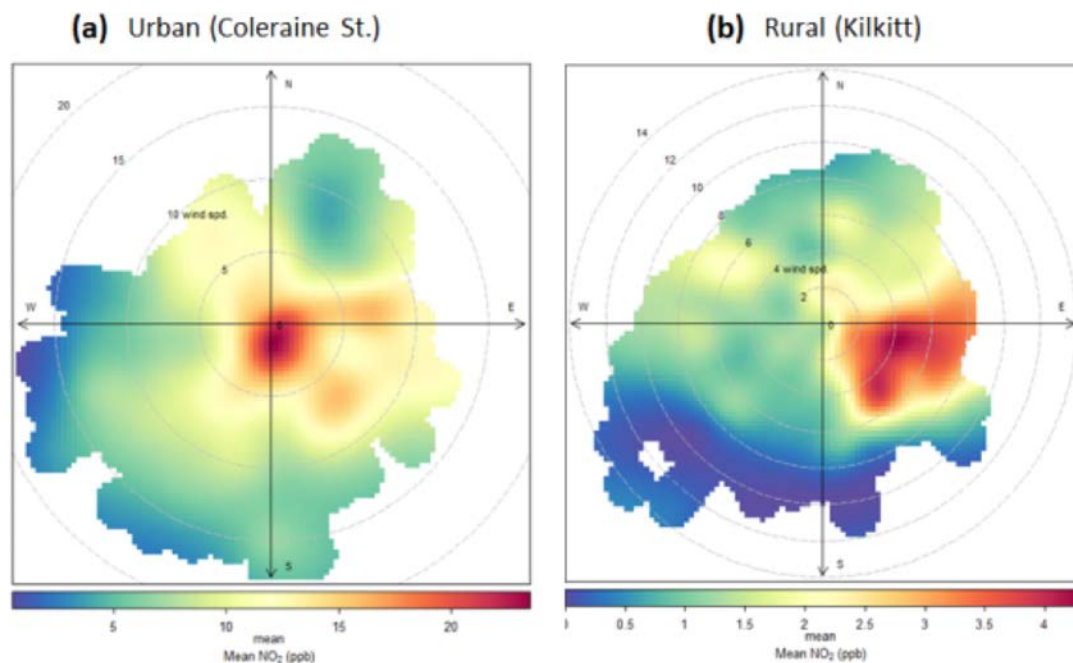


Figure 4.1. Polar plots of NO_2 concentration at (a) an urban site (Coleraine St) and (b) a rural background site (Kilkitt).

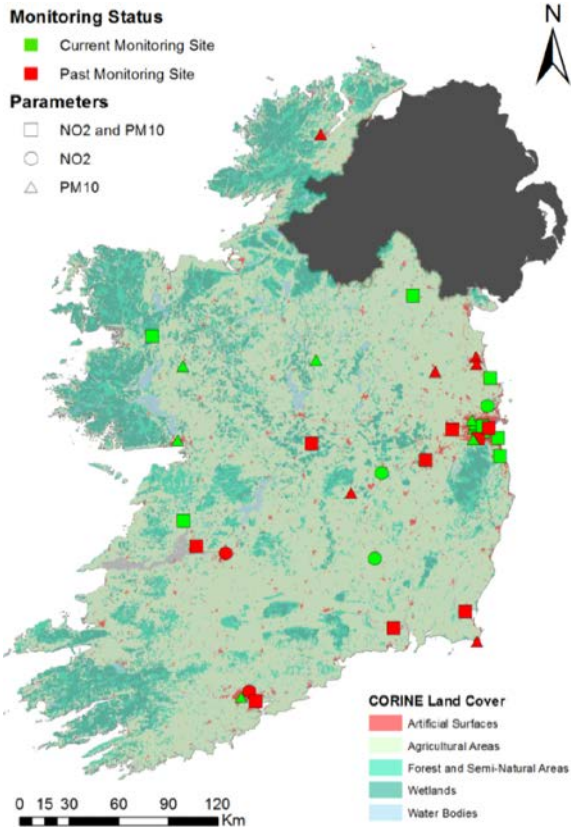


Figure 4.2. Monitoring site locations.

4.3 Correction Factors

A correction method was developed to improve the representativeness of the monitoring data used in the sector-based LUR and to account for uneven weighting of data from each season that may arise within different sectors. A brief overview of the correction method is provided here; a comprehensive explanation is provided in Donnelly *et al.* (2016).

Continuous monitoring data were used to calculate eight defined wind sector means for each station. The division of a concentration time series at a point into eight sectors maximises the number of data points available for the LUR; however, it also reduces data points available for long-term mean value calculation. Diurnal and seasonal concentration variations may lead to a biased annual sector average estimate when calculated from sub-annual data sets. Concentrations tend to be higher in winter months than summer months (in Ireland) and, for example, if data within a sector comprised 20% from winter months and 80% from summer months, an unrealistically low value for the annual average would be obtained. Consequently, a short-term correction factor (S_i) was applied to remove bias from the concentration data prior to sector

averaging. Direct averaging of these data within each wind sector will not necessarily result in reasonable predictions of the long-run mean because of seasonal differences in wind direction frequencies and other external forcing factors, such as variation in sunshine hours and stability conditions. Long-term correction factors (L_i) have been developed to apply to the data post binning. Figure 4.3 illustrates the procedure for correcting raw data from a given monitoring site.

The removal of concentration fluctuations due to meteorological and seasonal factors allows the isolation of external forcing factors and thus improved quantification of spatial variability in concentration levels using spatial descriptors and subsequently a more robust LUR model. This is illustrated by an improvement in the correlation between pollutant concentrations and spatial emissions indicators, as shown in Figure 4.4 for NO_2 .

4.4 Predictor Data

Geospatial predictor variables (Table 4.1) were calculated within each sector from nationally available, spatially homogeneous data sets for all sites using the ArcGIS 10.0 software package (Esri, 2011). Eight circular buffers of variable radii were defined around each monitoring site, ranging from 25 m to 5 km, and were further subdivided into eight 45° wind direction sectors (e.g. north, north-east, east) (Figure 4.5a). Residential and commercial property variables were derived using geographical coordinates from GeoDirectory (Figure 4.5b). Traffic network and flow data were obtained from the National Traffic Model (NTM), part of the National Transport Model (NTpM) developed by the National Roads Authority (NRA) (Figure 4.5c). Road length variables were calculated within each sector for each road category, and the length of each major road link passing through the sector was multiplied by the link annual average daily traffic-flow (AADT) to give annual vehicle-kilometres (Vkm). Owing to the high correlation between the NO_2 concentration and traffic parameters across the range of buffer radii, a weighted Vkm ($\text{Vkm}_{\text{weighted}}$) parameter was developed. The weighting applied to each sector is related to the inverse of the distance of the sector from the monitoring point, with the closest sector (i.e. 25 m) carrying the highest weighting. The inverse-distance weighted Vkm factor was calculated as:

$$\text{Vkm}_{\text{invw}} = \frac{1}{r_0} \text{Vkm}_0 + \sum_{i=1}^N \frac{1}{r_i} (\text{Vkm}_i - \text{Vkm}_{i-1}) \quad (4.1)$$

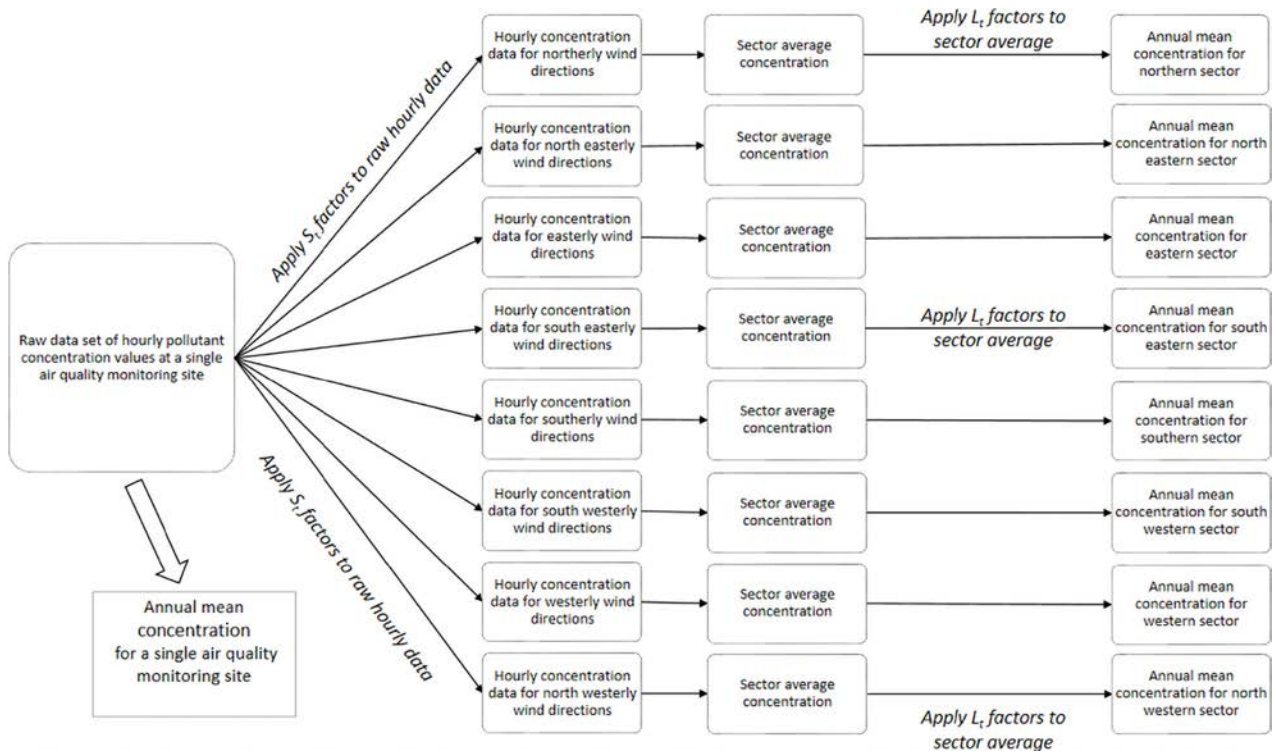
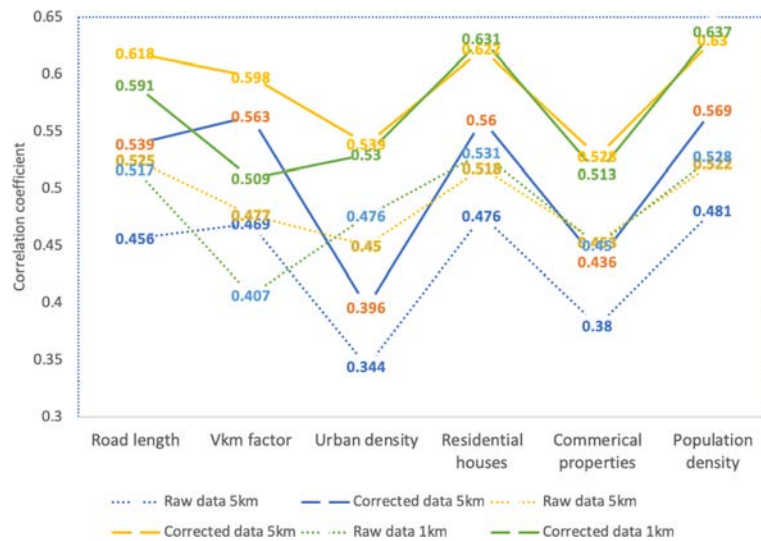


Figure 4.3. Application of correction factors flowchart.

Figure 4.4. Improvement in correlation with land use variables using raw (dotted lines) and corrected NO₂ data (solid lines).

where $i=0$ to $i=N$ represent each of the sectors considered, r is the distance from the monitoring point to the centre of a given sector and Vkm_i is the sum of the Vkm in a given sector i . In this case, eight sector sizes are considered: 25 m, 50 m, 100 m, 250 m, 500 m, 1 km, 2 km and 5 km.

Population and residential combustion data were derived from census data and spatially disaggregated on the basis of residential property locations, whereby

average household statistics were calculated within each census small area (SA) using the total number of occupied residential properties within the SA. In each instance, predictor variables were calculated by summing totals (e.g. total road length, total population) within each sector.

Land cover variables were derived from CORINE land cover data for 2006. Following the methods outlined in Vienneau *et al.* (2010) and Beelen *et al.* (2013) the 44

Table 4.1. Predictor variables with variable names, units and sector size

Category	Units	Sector size (m)	Subcategory	No. of Variables
Road length	km	25, 50, 100, 250, 500, 1000, 2000, 5000	All roads, national road, regional road, local road, major road	56
Proximity to road	km ⁻¹ , km ⁻²	N/A	Nearest road, nearest major road	8
Traffic flow	Vkm	25, 50, 100, 250, 500, 1000, 2000, 5000	N/A	8
Weighted traffic flow	Vkm	N/A	Inverse distance, Gaussian	2
Land cover	Hectares	25, 50, 100, 250, 500, 1000, 2000, 5000	High-density residential, low-density residential, industry, port, urban green, semi-natural and forested, natural, sea/ocean	64
Population density	Persons km ⁻²	25, 50, 100, 250, 500, 1000, 2000, 5000	N/A	8
Property density	No. properties	25, 50, 100, 250, 500, 1000, 2000, 5000	Residential, commercial	16
Residential heating	Properties per heating type	25, 50, 100, 250, 500, 1000, 2000, 5000	Solid, gas, electricity, oil	32
Household cars	Cars	25, 50, 100, 250, 500, 1000, 2000, 5000	N/A	8
Proximity to coast	km	N/A	N/A	1
Point source (PRTR)	kg	25, 50, 100, 250, 500, 1000, 2000, 5000	N/A	8
Elevation	m	N/A	N/A	1
Wind speed	m/s	N/A	N/A	1

N/A, not applicable; PRTR, Pollutant Release and Transfer Register.

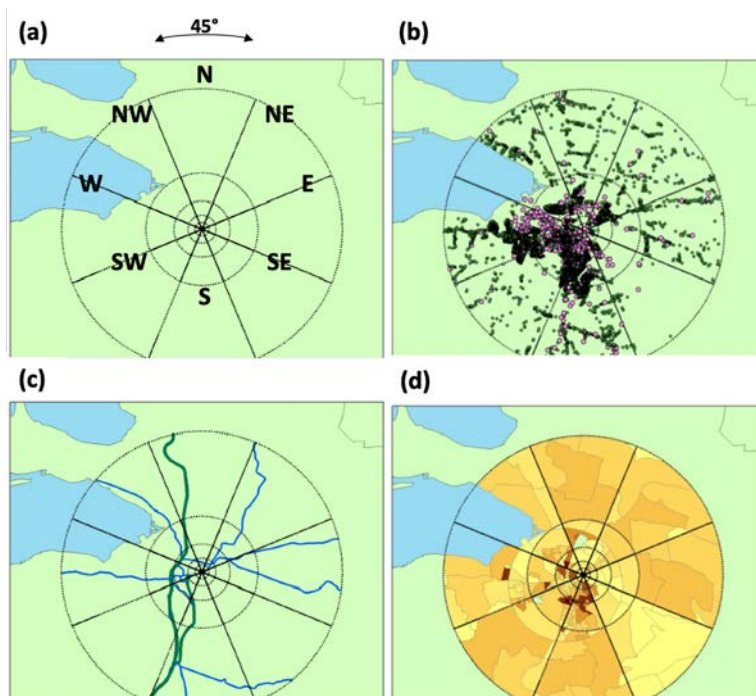


Figure 4.5. (a) Wind direction sectors, (b) residential and commercial properties, (c) major roads and (d) solid fuel combustion.

land cover classes in CORINE were regrouped into six areas (high-density residential, low-density residential, industry, port, urban green, and semi-natural and forested) as well as an additional land use class representing areas of sea and open ocean. Predictor variables were determined by calculating the area of each of these land use groups within each sector.

Large point source pollutant emissions were derived from the Pollutant Release and Transfer Register (PRTR), operated by the EPA. Point emission totals were assigned to each sector based on PRTR point locations and the annual emissions during the year (or years) for which monitoring data were available in the sector. The list of predictor variables and sector radii is provided in Table 4.1.

4.5 Model Fitting

Selection of the most appropriate explanatory variables within suitable sector sizes is important for defining final model performance. Variable selection was carried out using a supervised stepwise approach. Each predictor variable was assigned a plausible direction of effect and univariate regression analyses were carried out for all predictor variables. The model with the highest adjusted R^2 having an appropriate slope, as predefined by the direction of effect, was considered as the start model. Additional predictor variables were then added consecutively to the model and maintained if the following three conditions were met:

1. the R^2 value increases by at least 1%;
2. the direction of effect of the new variable is as a priori defined;
3. the direction of effect of previously included variables does not change.

The large number of predictor variables examined meant that many of them were correlated. The variance inflation factor (VIF) was used to assess how much the variance of an estimated regression coefficient increases if predictors are correlated; it is equal to 1 if no factors are correlated. Variables with a high VIF were removed from the model, ensuring that each variable removed is redundant in the explanation of concentration. The set of predictor variables giving the highest adjusted R^2 value, which conformed to

a priori defined directions of effect, was selected for inclusion in the final model. As a final step, variables with a p -value of > 0.05 were removed from the model.

Standard diagnostic tests for ordinary least-squares regression were carried out. These included assessing residuals for heteroscedasticity and normality. Residuals were also analysed for influential or controlling observations or outliers. In a small number of instances this led to removal of certain data points after detailed investigations of the baseline data. Iterations cease and the final model is defined when residual diagnostics prove satisfactory.

4.6 Modelled Versus Measured Values

A leave-one-out process was used to assess the annual mean maps. Scatter plots of measured versus modelled (leave-one-out) values are shown in Figure 4.6. Results were strongest for NO_2 . This is because of a combination of a well-represented monitoring network and the good description of NO_2 spatial variation by traffic-related spatial variables.

4.7 Results and Applications

The output from this modelling work is a set of annual mean maps for each of NO_2 , PM_{10} , $\text{PM}_{2.5}$, O_3 and SO_2 . These maps are shown in Figures 4.7–4.10. The NO_2 maps shows the dominant influence of traffic emissions on national (and urban) NO_2 concentrations. PM_{10} shows increases near coastal regions and also in regional towns because of the effects of solid-fuel burning. $\text{PM}_{2.5}$ increases near major roads because of fine particulate emissions. As expected, O_3 shows increases near coastal regions and decreases in heavy-traffic areas where there are elevated NO_x emissions. The SO_2 map was limited by the number of monitoring stations available within each air quality zone. However, the clear influence of the coal ban zones can be observed in the final map.

These annual mean maps can be used for a variety of purposes:

- direct analysis of air quality anywhere in Ireland;
- assistance in determining appropriate areas to locate future air quality monitors (minimise monitor placement bias);
- personal exposure studies.

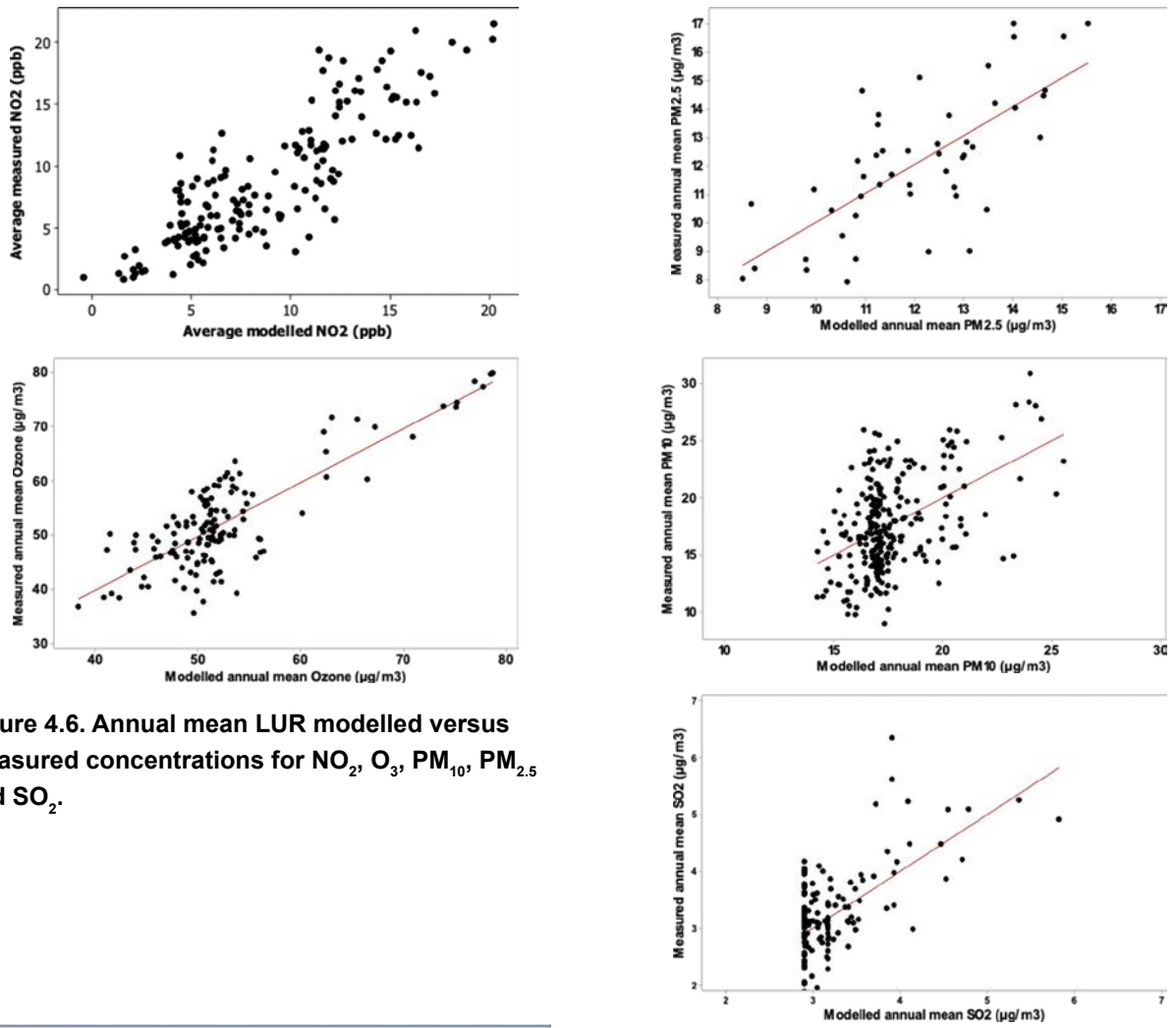


Figure 4.6. Annual mean LUR modelled versus measured concentrations for NO₂, O₃, PM₁₀, PM_{2.5} and SO₂.

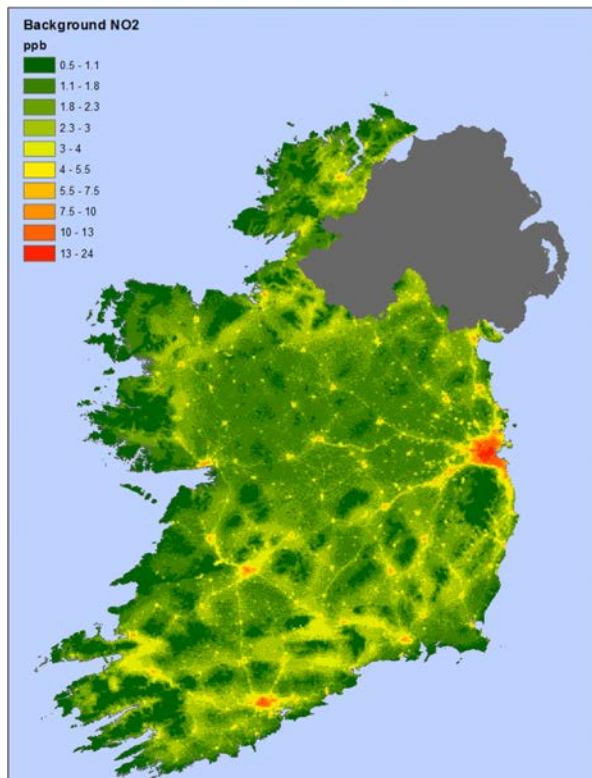


Figure 4.7. NO₂ map (national).

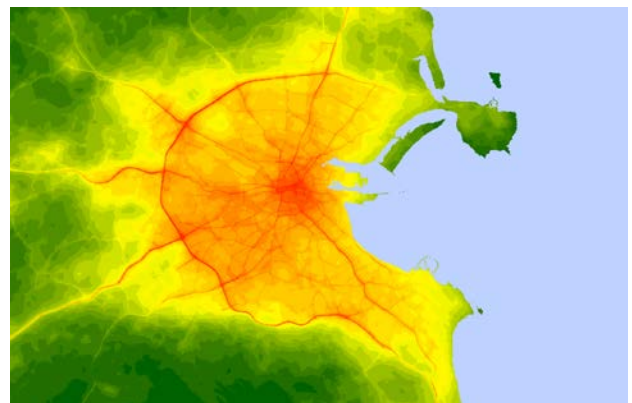


Figure 4.8. NO₂ map (Dublin).

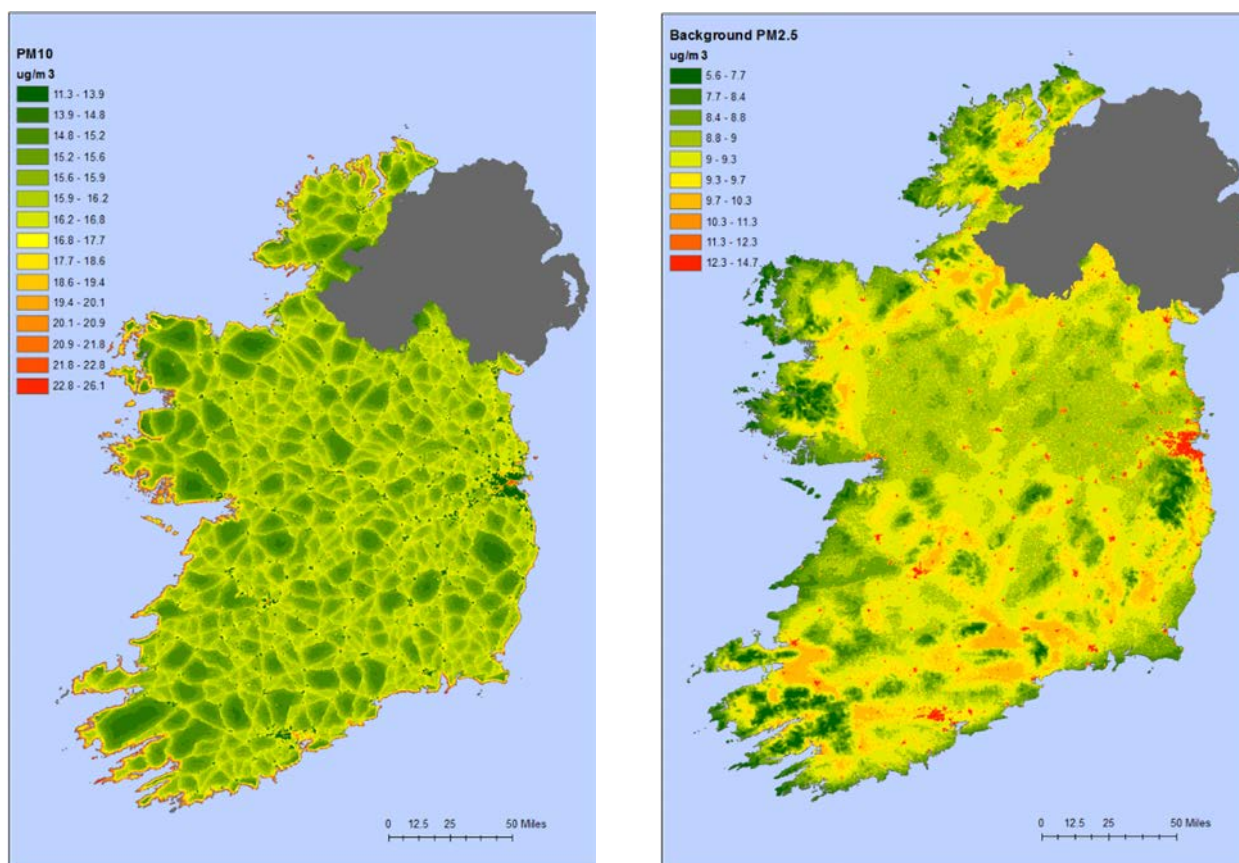


Figure 4.9. PM₁₀ (left) and PM_{2.5} (right) maps.

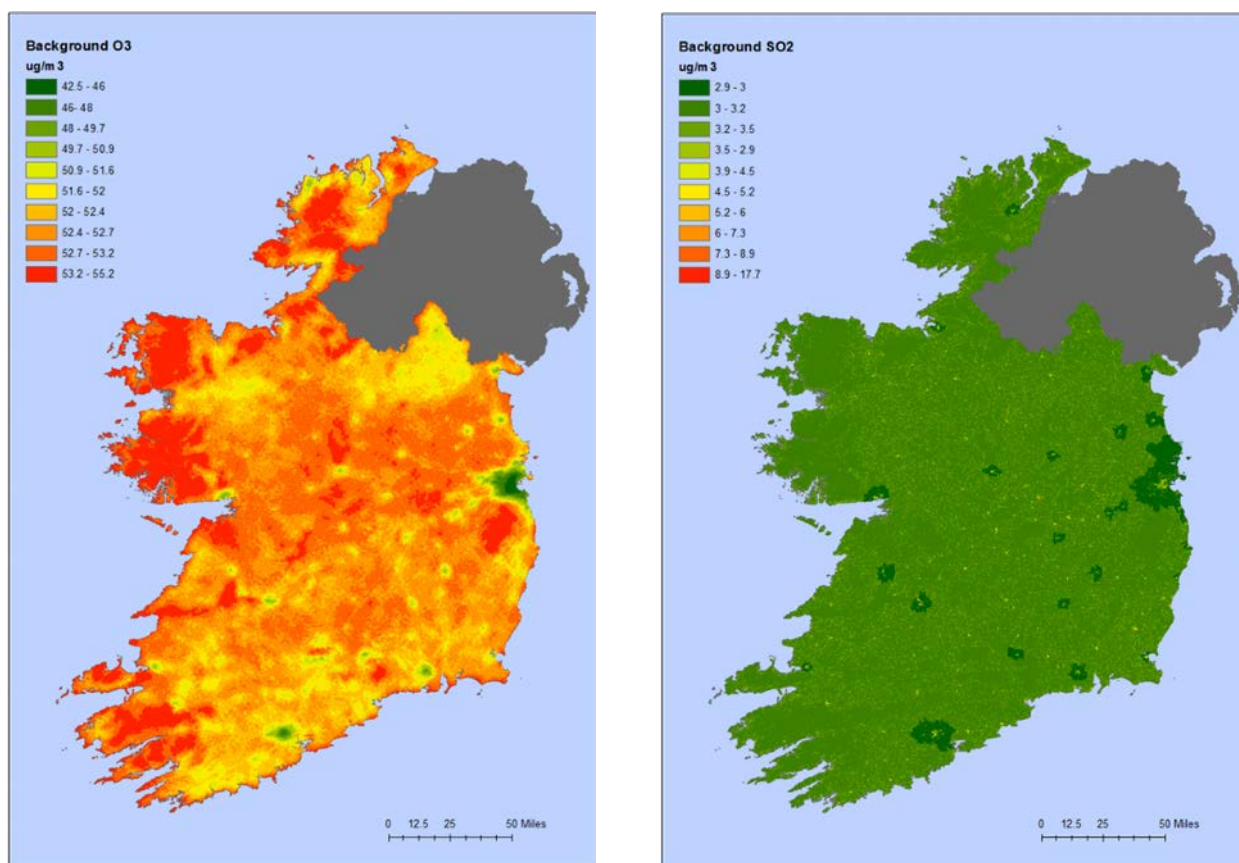


Figure 4.10. O₃ (left) and SO₂ (right) maps.

5 Hourly Land Use Regression Modelling

5.1 Overview of Methodology

Land use regression models generally aim to explain spatial variation in concentrations and do not include a temporal aspect. Some studies have, however, attempted to model both temporal and spatial variation using a LUR base. Mölter *et al.* (2010) modelled annual concentrations of PM₁₀ and NO₂ for Manchester between 1996 and 2008 using a LUR model from 2005. This model was temporally recalibrated and also made use of some temporal values of predictor variables and temporal trends. Dons *et al.* (2013) tested two methods of incorporating a temporal resolution into their model of BC in Flanders, Belgium. In the first approach they used 48 dummy variables for weekday and weekend hours (R^2 of 0.44) and in the second approach they developed independent hourly models (R^2 between 0.07 and 0.8). Chen *et al.* (2010) included a temporal aspect to their LUR model of NO₂ and PM₁₀ in Tianjin, China, by establishing four separate models, one for the heating season and one for the non-heating season for each of NO₂ and PM₁₀. R^2 values ranged between 0.49 for PM₁₀ in the non-heating season and 0.4 for NO₂ in the heating season.

Saraswat *et al.* (2013) developed spatio-temporal models for PM_{2.5} and BC in New Delhi using a combined spatial monitoring campaign and data from a fixed continuous monitoring site. LUR data were sampled one site at a time and, at each site, measurements were collected for 1–3 hours during each time period (separate models were developed for morning and afternoon hours). The pollutant concentration was assumed to be associated with a multiplicative combination of a background temporal component (fixed site) and the spatial components. They assumed that the temporal component was spatially invariant and the spatial components were temporally invariant. PM_{2.5} model fits of 85% and 73% were obtained for the morning and afternoon models, respectively. Su *et al.* (2008) developed a source area LUR for predicting hourly NO₂ concentrations in Vancouver from land use types and hourly wind speed, wind direction and cloud cover. They interpolated hourly meteorological data from 19 regulatory continuous monitoring stations for

116 passive samplers to create a source area LUR model. They compared these results with a source area LUR created from the 19 continuous monitoring stations and those from a regular LUR. Estimated concentrations for the hourly model were aggregated back to seasonal averages. They concluded that when variability in seasonal concentrations is present the source area LUR provides stronger results than the regular LUR.

In this research project, a novel model for forecasting spatially resolved hourly or daily concentrations was developed, which also tackles two of the main limitations of LUR. First, the issue of wind direction and area of influence when using circular buffer zones is addressed through the use of “sectors”, within which predictor variables are defined and calculated (as introduced in Chapter 4 for the annual mean LUR). In the operational model, the appropriate “sector” will vary with local wind direction. Second, the temporal resolution of the LUR is greatly improved through the inclusion of hourly meteorological data and seasonal factors as predictor variables.

Using the methods developed in this research project, hourly concentrations can be mapped on a national scale and forecasts of daily average and daily maximum concentrations can be made across the country with minimal computational requirements.

5.2 Model Development

5.2.1 General model fitting

The WS-LUR model uses the same spatial predictor variables (where significant) as presented in Chapter 4 and Table 4.1. In addition, the following temporally varying predictor variables are used:

- WSWD_{*i*} (WSWD factor, as introduced in Chapter 3);
- S_{*f*} (seasonal factor, as introduced in Chapter 3);
- weekday/weekend dummy variable;
- hourly temperature;
- hourly precipitation;
- hourly atmospheric pressure;
- hourly relative humidity;

- sunshine hours;
- hourly stability class.

The premise of the WS-LUR is that separate prediction equations are developed for different environmental conditions and/or time periods. A first step is to identify appropriate methods of partitioning the data so that robust models can be developed. The grouping allows a unique prediction of air quality to be made at any location in Ireland for any hour where the appropriate meteorological data are available. Model development proceeded following these steps:

1. generate an hourly data set of measured concentrations at air quality monitoring sites and associated hourly meteorological factors for 2 full calendar years (2011 and 2012);
2. assign a weekday/weekend dummy variable and S_t to each data point;
3. generate predictor variables from geospatial datasets for each directional sector within a GIS environment;
4. assign relevant spatial predictors to each hourly data point at each monitoring site;
5. divide the data set into pre-identified environmental groups;
6. select appropriate spatial and temporal predictor variables for each data set using a supervised stepwise approach;
7. merge the data sets to form a single model for all hours/seasons;
8. complete the mapping process by calculating key predictor variables on a national scale at a fine spatial resolution and hourly temporal resolution for the validation year (2012);
9. validate results by comparing to measured daily average and daily maximum concentrations for the same time period.

5.2.2 Nitrogen dioxide

Nitrogen dioxide exhibits strong seasonal and diurnal variations, the magnitude of which vary significantly on a national scale. Therefore, 48 separate regression equations were developed (one for each hour in each season) to feed into the WS-LUR model.

5.2.3 Particulate matter_{10/2.5}

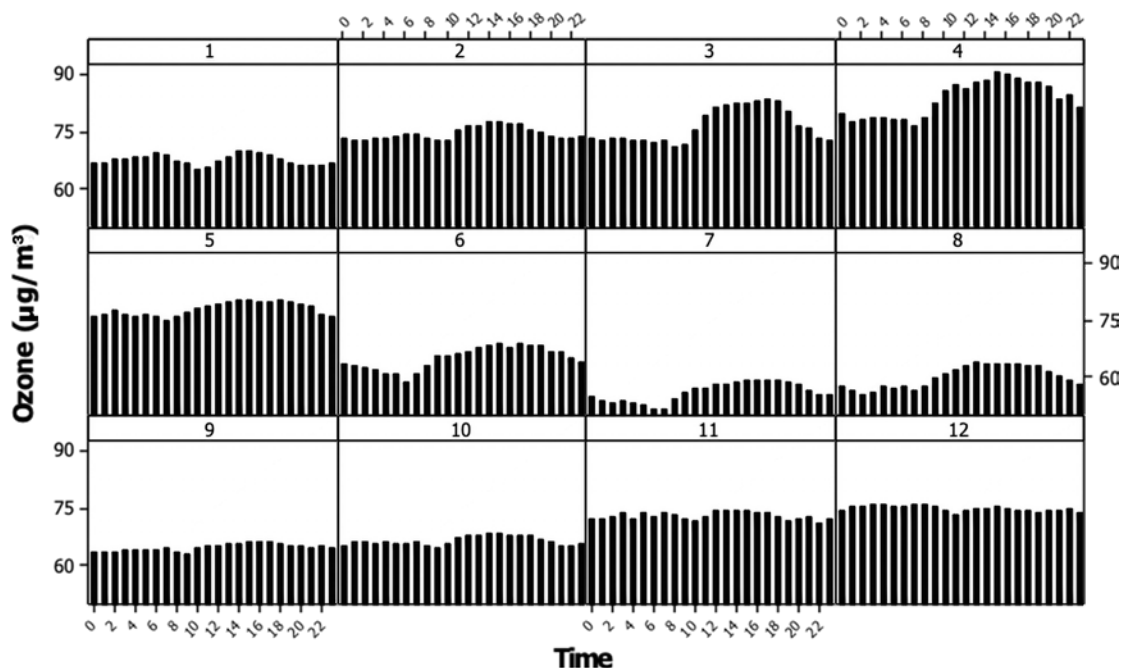
Particulate matter_{10/2.5} concentrations exhibit non-linear changes in concentration with wind speed and temperature. Therefore, this method divides the training data into four separate temperature classes and four temperature wind speed classes. A separate regression equation is trained for each of these, giving a total of 16 regression equations. In operational mode, the appropriate regression equation can be chosen based on the daily average wind speed and temperature that is forecast on a given day. The classes were chosen based on the first quartile, median and third quartile of the total temperature and wind speed data sets. The bands are shown in Table 5.1.

5.2.4 Ozone

In developing the WS-LUR for O₃ the data were separated into three (spatially distinct) groups: a coastal group, a rural/suburban group and a group comprising the Dublin and Cork air quality zones. The data were first grouped seasonally based on similarities between monthly values. They were then grouped for regression based on diurnal variations within each of the identified seasons and the three spatial location types. Figure 5.1 shows the diurnal variations at the coastal sites of Valentina and Mace Head split by month.

Table 5.1. Variable classes for PM₁₀ and PM_{2.5}

Variable class	Temperature (°C)	Wind speed (m/s)
1	<6.35	<2.87
2	<9.76	<4.18
3	<13.15	<5.81
4	≥13.15	≥5.81



Panel variable: Month

Figure 5.1. Diurnal variation in O_3 at Mace Head and Valentia by month.

5.3 Results

The model was fitted for NO_2 , O_3 and PM_{10} as discussed above. Hourly (or daily) modelled values were compared with monitored data for each of the pollutants. Standard statistical measures were used to assess model performance. The results are shown in Table 5.2. Scatter plots of measured versus modelled values are shown in Figures 5.2–5.4. Results confirmed that the WS-LUR model is a useful and efficient means of forecasting air quality on a national scale in Ireland. There is a fair degree of scatter in the PM_{10} plot and the detailed analysis of PM carried out

suggested that future spatio-temporal modelling of PM might be carried out using an interpolation method on the hybrid point-wise forecasts in conjunction with the annual mean LUR maps.

Figure 5.5 shows a sample output of the Dublin region for two different times of the day on 10 August 2014. A clear difference can be observed between the midday and evening concentrations. This is the effect of rush-hour traffic emissions. Clear definition can be observed around the road network, in particular the M50 and arterial routes, highlighting the large contribution of traffic emission to overall NO_2 concentrations.

Table 5.2. Statistical performance measures for the WS-LUR model

Measure	NO_2 (daily average)	NO_2 (daily maximum)	O_3 (daily average 8-hour value)	O_3 (daily maximum 8-hour value)	PM_{10} (daily average)
FAC2	95.69%	93.20%	98%	98%	94%
r	0.84	0.77	0.664	0.665	0.60
Mean fractional bias	–1%	–1%			–5%
IA	0.91	0.86	0.787	0.794	0.73

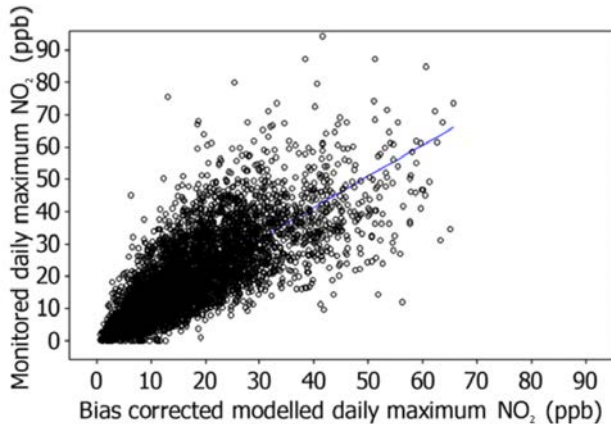


Figure 5.2. WS-LUR modelled versus measured NO₂ data.

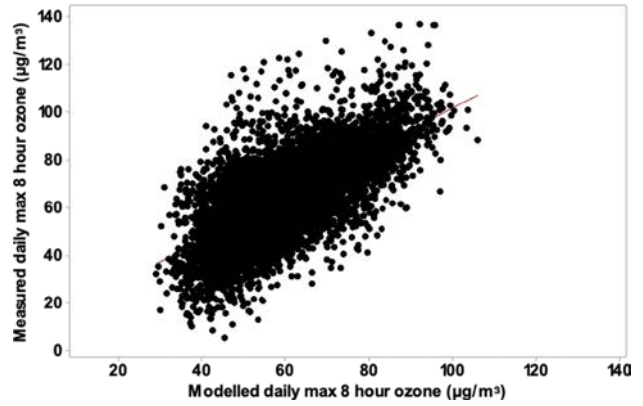


Figure 5.3. WS-LUR modelled versus measured O₃ data.

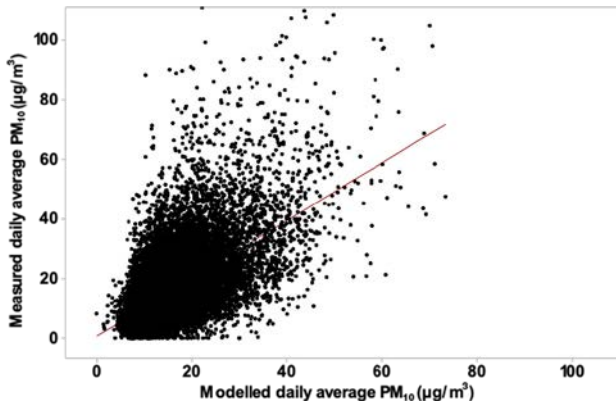


Figure 5.4. WS-LUR modelled versus measured PM₁₀ data.

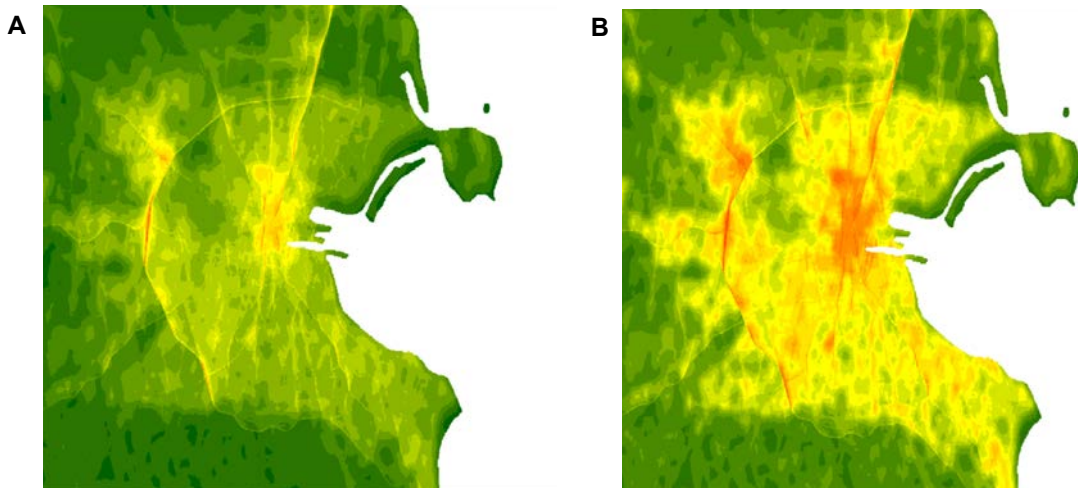
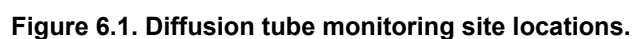


Figure 5.5. Sample output from the WS-LUR model for NO₂ in the region of Dublin on 10 August 2014 at (a) 1 pm and (b) 7 pm.

An urban monitoring campaign was carried out to provide additional information on the spatial variation of concentrations across urban and rural areas. This task was a joint work package between the air quality modelling fellow and the emissions inventory fellow (2013-EH-FS-7). The objective of the work is to develop linkages between air pollution levels at a fine spatial scale in Dublin and other spatial parameters. Seventy NO_2/SO_2 diffusion tubes and 59 O_3 diffusion tubes were deployed at pre-specified locations around Dublin. The sites were chosen using the annual mean maps detailed in Chapter 4. It was necessary that the locations cover primary land use classes as well as the full range of concentrations over the Dublin region. Guidelines laid out in the ESCAPE study manual (European Study of Cohorts for Air Pollution Effects, 2008) were also followed in choosing

The diffusion tubes were all deployed within 24 hours of each other and the Global Positioning System (GPS) coordinates and time of deployment were recorded. They were each left out for a period of 2 weeks between 10 and 24 June 2015. The time of collection of each tube was recorded and any missing or damaged tubes were noted. The tubes were placed in sealed plastic bags and returned to the laboratory for analysis along with a number of blank tubes for corrective purposes. Final concentrations of NO_2 , SO_2 and O_3 at each location are provided as a data set output from this project.



The diffusion tube survey results provide a valuable resource regarding spatial variation in concentration levels in the Dublin region. A second round of sampling will be carried out as part of an Emission Inventory fellowship (2013-EH-FS-7) to capture additional information on the seasonal variation in concentration levels. Thereafter, finely resolved spatial data provided will be used together with the results from the monitoring campaign to carry out geo-statistical modelling of the Dublin area as part of the Emission Inventory fellowship. A

model framework has been developed as part of the current fellowship, on which urban modelling will be based. This modelling will be carried out using the in-house statistical model developed as part of this fellowship and the short-term average values obtained will be converted to annual mean concentrations based on seasonal factors developed during the first 2 years of the fellowship. The methodology will be documented and a framework will be developed for model building and meteorological forecast integration.

7 Conclusions

A suite of air quality models has been developed as part of this research project to achieve key EPA objectives. The models provide the following information and operational capability:

- automated twice-daily 48-hour point-wise forecasts of NO_2 , SO_2 , $\text{PM}_{10/2.5}$, O_3 and the AQIH;
- automated twice-daily forecasts of the origin of air reaching Ireland (using HYSPLIT);
- annual mean maps of NO_2 , SO_2 , $\text{PM}_{10/2.5}$ and O_3 ;
- national-scale spatial model to predict hourly NO_2 , 8-hourly average O_3 and daily average PM_{10} .

Air quality model development has necessarily been a stepwise process making maximum use of available resources. A statistical approach to provide point-wise forecasts was adopted, which used historical monitoring data to train the model in the absence of a detailed emissions inventory. Inclusion of regional transport emissions improved model efficiency. Air mass history modelling was carried out and a HYSPLIT add-on was developed for the model. A validation study was carried out by comparing 12 months of modelled data with monitored data from the same period. Some general conclusions from this study were:

- Model validation statistics show good correlation between measured and modelled values and indicate a level of performance equal to or better than that generally expected from air quality models.
- Overall, IA values of 0.88, 0.84, 0.84, 0.80 and 0.88 were achieved for NO_2 , PM_{10} , $\text{PM}_{2.5}$, SO_2 and O_3 , respectively.
- Overall, r values of 0.82, 0.72, 0.74, 0.69 and 0.82 were achieved for NO_2 , PM_{10} , $\text{PM}_{2.5}$, SO_2 and O_3 , respectively.
- Overall, FAC2 values of 73%, 93%, 79%, 77% and 100% were achieved for NO_2 , PM_{10} , $\text{PM}_{2.5}$, SO_2 and O_3 , respectively.
- Incorporation of an air mass history parameter resulted in a large improvement in the prediction of NO_2 and PM concentrations.
- The model is quite conservative in its PM_{10} and $\text{PM}_{2.5}$ predictions. There is a slight positive bias

at all sites as a result of the methodology used to account for regional air mass movement and pollutant transport. PM is one of the most difficult pollutants to model because of its wide range of anthropogenic and natural sources. Therefore, a conservative estimate accompanied by some specialist interpretation is considered to be the best means of producing a forecast. When the AQIH is forecast to be poor, air mass history and other conditions relating to PM concentrations should be examined in conjunction with the value given by the AQ model to produce a final forecast.

- During the next model calibration/training, O_3 should be trained using hourly data. The use of 8-hour averages as the response variable has resulted in some oversmoothing of the data.

The stepwise approach adopted in model development allowed outputs before completion of the final study and achieved a key EPA objective of producing forecasts of the AQIH 24 and 48 hours in advance.

Mid-way through the original research fellowship the EPA funded an additional fellowship concerned with development of an emissions inventory for Ireland. This research was closely linked with the air quality modelling fellowship and influenced the direction of the work. Air quality modelling results were required to feed into the emissions inventory development to ensure that the most appropriate surrogate data are used, whereas the emissions inventory work provided spatial data sets for the development of the national annual mean maps.

Using air quality data from the national ambient air quality monitoring network and spatial predictor data a LUR technique was used to model air quality on a national scale. A novel technique was employed whereby the air quality data were split into eight wind-dependent sectors and corrected for short-term fluctuations. Spatial predictor variables were also defined using the same sector-based approach. This had the effect of maximising the number of data points available for the regression while also improving the description of spatial emissions/air quality relationships. The outputs from this modelling work

were annual mean maps of NO_2 , PM_{10} , $\text{PM}_{2.5}$, SO_2 and O_3 for 2012 (base year). A temporal aspect was introduced to the above model by including short-term meteorological predictor variables and seasonal and diurnal factors in addition to spatial variables. The resulting model has the ability to forecast hourly NO_2 , 8-hourly average O_3 and daily average PM_{10} at any location in Ireland.

This work highlighted some bias in the monitoring network, particularly in the case of O_3 and $\text{PM}_{10/2.5}$. A significant coastal influence was observed on PM_{10} but a lack of sufficient monitoring data meant that this could not be fully quantified. However, an approximation was developed and this is an area recommended for further work. Validation of the model using a “leave-one-out” procedure showed that the model performs excellently for NO_2 and is of a suitably high standard for $\text{PM}_{10/2.5}$, SO_2 and O_3 to be used for studies of spatial variation in concentrations across Ireland. Insufficient detail in background concentration data is frequently cited as the reason for poor results in local and urban modelling studies. The national-scale model outputs from this project have high relevance as inputs (background concentrations) for more detailed urban modelling studies.

A detailed study was carried out into incidences of high PM_{10} and $\text{PM}_{2.5}$ across Ireland. The following events (together) are likely to lead to high PM and should be associated with a PM alert system:

- low wind speed ($< 3 \text{ m/s}$);
- low temperature ($< 6^\circ\text{C}$);
- high pressure ($> 1020 \text{ mbar}$);
- shallow boundary layer ($< 500 \text{ m}$);
- stable conditions;
- low/no precipitation.

This fellowship has produced a number of key tangible outputs, as detailed in Chapter 8. The suite of models developed should form the building blocks for future modelling work, which is necessarily an iterative process. Although a direct output from this work has been a fully automated air quality forecast model, it should be noted that user knowledge and interpretation of model outputs are important in all air quality modelling work and the importance of developing a knowledge base in this area should not be underestimated. It is recommended that air quality forecasts should be made using a combination of:

- numerical output directly from the model;
- assessment of forecast local meteorological conditions;
- assessment of regional air mass movements, as forecast by the HYSPLIT model, which is built into the operational air quality model;
- consideration of any other unusual events or conditions (e.g. volcanoes or Saharan dust episodes);
- expert judgement.

8 Recommendations for Future Work

Recommendations for future work concerning model maintenance and development are as follows:

- The point-wise model should be recalibrated using up-to-date validated air quality and meteorological data on an annual basis. This process will ensure that air quality trends at individual sites are well captured and any new sources in an area are identified and included in the model.
- When new air quality monitoring sites are used for the derivation of the AQIH, the model can continue to be used for forecasts at the old site until a full year of data are available at the new site. This will avoid any break in forecasts within any one air quality zone. Once at least a full year of data are available, the model should be recalibrated and updated to include this new site within the model architecture.
- The national annual mean maps and temporal LUR models should be recalibrated every 2 years (or when new and significant spatial data become available).
- Recalibration of the national annual mean maps and temporal LUR models should also be carried out in the case of significant changes in spatial characteristics within a given zone or region.

The work carried out as part of this fellowship highlighted a number of areas that require, or would benefit from, further research. These are as follows:

- Further work is required to ensure that the national ambient air quality monitoring network has sufficient spatial coverage across the range of pollutant concentrations. Outputs from the current fellowship can be used to assist in determining spatial coverage. Using the national-scale maps, the total area within each AQ zone is calculated. The concentrations within each zone, as indicated by the model, are plotted as cumulative distribution plots. This is shown by the four curves in Figure 8.1. The concentrations at each of the AQ monitoring sites in the national network are then overlaid as points on these curves. Ideally, the monitoring sites should cover the full range of concentrations shown by the distributions for

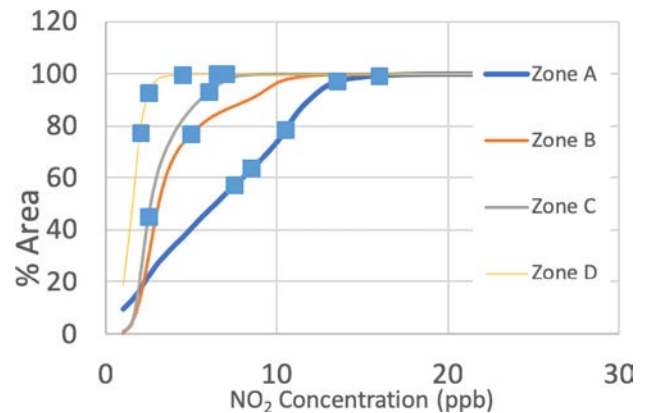


Figure 8.1. Cumulative distribution curves with concentrations at each monitoring site superimposed.

each zone. These distribution curves show a clear lack of monitoring stations at the upper levels of the curve (trafficked sites in the case of NO₂) in zones B and C. As the national-scale model has been developed using the current AQ monitoring network, an iterative process would be necessary whereby a new model is developed after the AQ review and the process repeated.

- PM₁₀ was found to display significant coastal influence. Bias in monitor placement in the national ambient network meant that an approximation had to be used in the present fellowship to quantify this. A research study should be carried out that quantifies PM_{10/2.5} concentrations at set distances from the coast (up to 10 km) during onshore, offshore and variable winds during different meteorological conditions and seasons. PM_{10/2.5} coastal fall-off curves should be developed for different meteorological classes.
- PM₁₀ and PM_{2.5} were found to display significant temporal variation due to both natural and anthropogenic effects. Further research is required to link source apportionment work with forecasting work. Quantifiable outputs from source apportionment could potentially be applied within a forecast environment to provide improved predictions of PM on a national scale.
- O₃ was found to be significantly higher in coastal regions but the small number of coastal sites

made this difficult to quantify. O₃ monitoring should be carried out in coastal regions using either passive or active techniques to improve the quantification of high O₃ events.

- The hybrid point-wise model developed as part of this fellowship was found to produce excellent 48-hour forecasts of the AQIH at pre-specified locations. A novel new area of work is the interpolation of these forecasts on a national scale. The number of monitoring sites is too limited to perform a direct interpolation; however, the integration of the hybrid point-wise model with the spatial model provides an innovative methodology for producing fast, resource-efficient

forecasts on a national scale at hourly resolution. Point-wise forecasts would first be developed for every monitoring site in Ireland. The technique would involve background stripping the point-wise forecasts in real time by subtracting the background concentration as provided by the annual mean maps from the concentration forecast at each location. These local forecasts are then interpolated using appropriate techniques. The background concentration can then be added back on nationally to provide real-time national-scale forecast maps. This model would be based in a GIS environment and could be fully automated.

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Abbreviations

AQIH	Air Quality Index for Health
BC	Black carbon
CAFE	Clean Air for Europe
CORINE	Coordination of Information on the Environment
EPA	Environmental Protection Agency
FB	Fractional basis
GIS	Geographic information system
HYSPLIT	Hybrid single particle Lagrangian integrated trajectory
IA	Index of agreement
LUR	Land use regression
MACC	Monitoring Atmospheric Composition and Climate
NO₂	Nitrogen dioxide
NO_x	Nitrogen oxides
NOAA	National Oceanic and Atmospheric Administration
O₃	Ozone
PAH	Polycyclic aromatic hydrocarbon
PM	Particulate matter
PRTR	Pollutant Release and Transfer Register
SA	Small area
SO₂	Sulfur dioxide
SV	Spatial variance
TSV	Total spatial variance
VIF	Variance inflation factor
Vkm	Vehicle-kilometres
WHO	World Health Organization
WS-LUR	Wind sector land use regression
WSWD	Wind speed/wind direction

AN GHNÍOMHAIREACHT UM CHAOMHNÚ COMHSHAOIL
Tá an Gníomhaireacht um Chaomhnú Comhshaoil (GCC) freagrach as an gcomhshaoil a chaomhnú agus a fheabhsú mar shócmhainn luachmhar do mhuintir na hÉireann. Táimid tiomanta do dhaoine agus don chomhshaoil a chosaint ó éifeachtaí díobhálacha na radaíochta agus an truaillithe.

Is féidir obair na Gníomhaireachta a roinnt ina trí phríomhréimse:

Rialú: Déanaimid córais éifeachtacha rialaithe agus comhlionta comhshaoil a chur i bhfeidhm chun torthaí maithe comhshaoil a sholáthar agus chun díriú orthu siúd nach gcloíonn leis na córais sin.

Eolas: Soláthraimid sonraí, faisnéis agus measúnú comhshaoil atá ar ardchaighdeán, spriocdhírthe agus tráthúil chun bonn eolais a chur faoin gcinnteoireacht ar gach leibhéal.

Tacaíocht: Bimid ag saothrú i gcomhar le grúpaí eile chun tacú le comhshaoil atá glan, táirgiúil agus cosanta go maith, agus le hiompar a chuirfidh le comhshaoil inbhuanaithe.

Ár bhFreagrachtaí

Ceadúnú

Déanaimid na gníomhaíochtaí seo a leanas a rialú ionas nach ndéanann siad dochar do shláinte an phobail ná don chomhshaoil:

- saoráidí dramhaíola (*m.sh. láithreáin líonta talún, loisceoirí, stáisiúin aistrithe dramhaíola*);
- gníomhaíochtaí tionsclaíocha ar scála mór (*m.sh. déantúsaíocht cógaisíochta, déantúsaíocht stroighne, stáisiúin chumhachta*);
- an diantalmhaíocht (*m.sh. muca, éanlaith*);
- úsáid shrianta agus scaoileadh rialaithe Orgánach Géinmhodhnaithe (*OGM*);
- foinsí radaíochta ianúcháin (*m.sh. trealamh x-gha agus radaiteiripe, foinsí tionsclaíocha*);
- áiseanna móra stórála peitril;
- scardadh dramhuisce;
- gníomhaíochtaí dumpála ar farraige.

Forfheidhmiú Náisiúnta i leith Cúrsaí Comhshaoil

- Clár náisiúnta iniúchtaí agus cigireachtaí a dhéanamh gach bliain ar shaoráidí a bhfuil ceadúnas ón nGníomhaireacht acu.
- Maoirseacht a dhéanamh ar fhreagrachtaí cosanta comhshaoil na n-údarás áitiúil.
- Caighdeán an uisce óil, arna sholáthar ag soláthraithe uisce phoiblí, a mhaoirsiú.
- Obair le húdaráis áitiúla agus le gníomhaireachtaí eile chun dul i ngleic le coireanna comhshaoil trí chomhordú a dhéanamh ar líonra forfheidhmiúcháin náisiúnta, trí dhíriú ar chiontóirí, agus trí mhaoirsiú a dhéanamh ar leasúchán.
- Cur i bhfeidhm rialachán ar nós na Rialachán um Dhramhthrealamh Leictreach agus Leictreonach (DTLL), um Shrian ar Shubstaintí Guaiseacha agus na Rialachán um rialú ar shubstaintí a ídionn an ciseal ózóin.
- An dlí a chur orthu siúd a bhriseann dlí an chomhshaoil agus a dhéanann dochar don chomhshaoil.

Bainistíocht Uisce

- Monatóireacht agus tuairisciú a dhéanamh ar cháilíocht aibhneacha, lochanna, uisce idirchriosacha agus cósta na hÉireann, agus screamhuisc; leibhéil uisce agus sruthanna aibhneacha a thomhas.
- Comhordú náisiúnta agus maoirsiú a dhéanamh ar an gCreat-Treoir Uisce.
- Monatóireacht agus tuairisciú a dhéanamh ar Cháilíocht an Uisce Snámha.

Monatóireacht, Anailís agus Tuairisciú ar an gComhshaoil

- Monatóireacht a dhéanamh ar cháilíocht an aeir agus Treoir an AE maidir le hAer Glan don Eoraip (CAFÉ) a chur chun feidhme.
- Tuairisciú neamhspleách le cabhrú le cinnteoireacht an rialtais náisiúnta agus na n-údarás áitiúil (*m.sh. tuairisciú tréimhsiúil ar staid Chomhshaoil na hÉireann agus Tuarascálacha ar Tháscairí*).

Rialú Astaíochtaí na nGás Ceaptha Teasa in Éirinn

- Fardail agus réamh-mheastacháin na hÉireann maidir le gáis cheaptha teasa a ullmhú.
- An Treoir maidir le Trádáil Astaíochtaí a chur chun feidhme i gcomhair breis agus 100 de na táirgeoirí dé-ocsaíde carbóin is mó in Éirinn.

Taighde agus Forbairt Comhshaoil

- Taighde comhshaoil a chistiú chun brúnna a shainathint, bonn eolais a chur faoi bheartais, agus réitigh a sholáthar i réimsí na haeráide, an uisce agus na hinbhuanaitheachta.

Measúnacht Straitéiseach Timpeallachta

- Measúnacht a dhéanamh ar thionchar pleananna agus clár beartaithe ar an gcomhshaoil in Éirinn (*m.sh. mórfhleananna forbartha*).

Cosaint Raideolaíoch

- Monatóireacht a dhéanamh ar leibhéil radaíochta, measúnacht a dhéanamh ar nochtadh mhuintir na hÉireann don radaíocht ianúcháin.
- Cabhrú le pleananna náisiúnta a fhorbairt le haghaidh éigeandálaí ag eascairt as taismí núicléacha.
- Monatóireacht a dhéanamh ar fhorbairtí thar lear a bhaineann le saoráidí núicléacha agus leis an tsábháilteacht raideolaíochta.
- Sainseirbhísí cosanta ar an radaíocht a sholáthar, nó maoirsiú a dhéanamh ar sholáthar na seirbhísí sin.

Treoir, Faisnéis Inrochtana agus Oideachas

- Comhairle agus treoir a chur ar fáil d’earnáil na tionsclaíochta agus don phobal maidir le hábhair a bhaineann le caomhnú an chomhshaoil agus leis an gcosaint raideolaíoch.
- Faisnéis thráthúil ar an gcomhshaoil ar a bhfuil fáil éasca a chur ar fáil chun rannpháirtíocht an phobail a spreagadh sa chinnnteoireacht i ndáil leis an gcomhshaoil (*m.sh. Timpeall an Tí, léarscáileanna radóin*).
- Comhairle a chur ar fáil don Rialtas maidir le hábhair a bhaineann leis an tsábháilteacht raideolaíoch agus le cúrsaí práinnfhreagartha.
- Plean Náisiúnta Bainistíochta Dramhaíola Guaisí a fhorbairt chun dramhaíl ghuaiseach a chos agus a bhainistiú.

Múscailt Feasachta agus Athrú Iompraíochta

- Feasacht chomhshaoil níos fearr a ghiniúint agus dul i bhfeidhm ar athrú iompraíochta dearfach trí thacú le gnóthais, le pobail agus le teaghlaigh a bheith níos éifeachtúla ar acmhainní.
- Tástáil le haghaidh radóin a chur chun cinn i dtithe agus in ionaid oibre, agus gníomhartha leasúcháin a spreagadh nuair is gá.

Bainistíocht agus struchtúr na Gníomhaireachta um Chaomhnú Comhshaoil

Tá an ghníomhaíocht á bainistiú ag Bord lánaimseartha, ar a bhfuil Ard-Stiúrthóir agus cúigear Stiúrthóirí. Déantar an obair ar fud cúig cinn d’Oifigí:

- An Oifig um Inmharthanacht Comhshaoil
- An Oifig Forfheidhmithe i leith cúrsaí Comhshaoil
- An Oifig um Fianaise is Measúnú
- Oifig um Chosaint Radaíochta agus Monatóireachta Comhshaoil
- An Oifig Cumarsáide agus Seirbhísí Corparáideacha

Tá Coiste Comhairleach ag an nGníomhaireacht le cabhrú léi. Tá dáréag comhaltaí air agus tagann siad le chéile go rialta le plé a dhéanamh ar ábhair inní agus le comhairle a chur ar an mBord.

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Air Quality Modelling for Ireland



Authors: Aoife Donnelly, Bruce Misstear
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Identifying Pressures

Air pollution is the primary environmental cause of premature death in the European Union (EU) and the most problematic pollutants across Europe have consistently been oxides of nitrogen [e.g. nitrogen dioxide (NO₂)], particulate matter (PM₁₀, PM_{2.5}) and ozone (O₃). Although measurements form an important aspect of air quality assessment, on their own they are unlikely to be sufficient to provide an accurate spatial and temporal description of the pollutant concentrations for exposure assessment. Moreover, they cannot provide information regarding future air quality. Thus, air quality models are an important aspect of air quality management, allowing identification of the concentration gradient and peak location in real-time, forecast and hindcast scenarios.

Informing Policy

Annex XVI of EU Directive 2008/50/EC requires Member States to “ensure that up to date information on ambient concentrations of the pollutants covered” by the Directive are “made available to the public”. This information must include actual or predicted exceedances of alert and information thresholds and a forecast for the following day, of which a model is an integral part. As a result, air quality models are increasingly required for public information, air quality management and research purposes. The primary objectives of this research fellowship were to develop a calibrated air quality forecast model for Ireland capable of predicting the Air Quality Index for Health (AQIH) in each of the air quality zones in Ireland and to model the spatial variation in concentrations on a national scale.

Developing Solutions

This research aimed to determine and quantify current and future air quality so that its impacts can be mitigated through effective solutions. A priority within the Environmental Protection Agency was to produce air quality forecasts based on the AQIH measurements. In order to extrapolate these measurements to the future, statistical modelling was deemed the most suitable. The advantages of this approach were that it could be developed from first principles, it was specific to the area of interest, it avoided any reliance on a third party to supply the model or apply licensing restrictions and it allowed for efficient computation of forecasts. This method was capable of producing accurate point-wise forecasts without the need for a detailed emissions inventory. At the project outset, the emissions inventory was not of sufficient spatial resolution to make realistic point-wise forecasts in all air quality zones by deterministic means and it would have been an inefficient use of resources to base the development of forecasts on what was currently available. This research project has produced a forecast model for predicting NO₂, PM₁₀, PM_{2.5}, O₃ and sulfur dioxide (SO₂), 48 hours in advance, at key monitoring locations across Ireland. The model was validated and the results are available in a separate model validation report.

In conjunction with a second research project (2013-EH-FS-7), a set of annual mean maps within a geographic information system (GIS) environment was created and validated for each of NO₂, PM₁₀, PM_{2.5}, O₃ and SO₂. These provide a highly relevant source of information regarding spatial variation in concentration levels on a national scale that can be used not only for exposure studies and general air quality assessment, but also as a tool to correlate emission sources and surrogates with air quality.

The stepwise approach chosen for model development allowed deliverables prior to completion of the project while minimising associated risks. The models developed as part of this fellowship form solid building blocks on which future air quality modelling studies in Ireland can be based.