

# Modelling air quality, climate change and volcanic ash



# Environmental Protection Agency

The Environmental Protection Agency (EPA) is a statutory body responsible for protecting the environment in Ireland. We regulate and police activities that might otherwise cause pollution. We ensure there is solid information on environmental trends so that necessary actions are taken. Our priorities are protecting the Irish environment and ensuring that development is sustainable.

The EPA is an independent public body established in July 1993 under the Environmental Protection Agency Act, 1992. Its sponsor in Government is the Department of the Environment, Community and Local Government.

## OUR RESPONSIBILITIES

### LICENSING

We license the following to ensure that their emissions do not endanger human health or harm the environment:

- waste facilities (e.g., landfills, incinerators, waste transfer stations);
- large scale industrial activities (e.g., pharmaceutical manufacturing, cement manufacturing, power plants);
- intensive agriculture;
- the contained use and controlled release of Genetically Modified Organisms (GMOs);
- large petrol storage facilities;
- waste water discharges;
- dumping at sea.

### NATIONAL ENVIRONMENTAL ENFORCEMENT

- Conducting over 1200 audits and inspections of EPA licensed facilities every year.
- Overseeing local authorities' environmental protection responsibilities in the areas of - air, noise, waste, waste-water and water quality.
- Working with local authorities and the Gardaí to stamp out illegal waste activity by co-ordinating a national enforcement network, targeting offenders, conducting investigations and overseeing remediation.
- Prosecuting those who flout environmental law and damage the environment as a result of their actions.

### MONITORING, ANALYSING AND REPORTING ON THE ENVIRONMENT

- Monitoring air quality and the quality of rivers, lakes, tidal waters and ground waters; measuring water levels and river flows.
- Independent reporting to inform decision making by national and local government.

### REGULATING IRELAND'S GREENHOUSE GAS EMISSIONS

- Quantifying Ireland's emissions of greenhouse gases in the context of our Kyoto commitments
- Implementing the Emissions Trading Directive, involving over 100 companies who are major generators of carbon dioxide in Ireland.

### ENVIRONMENTAL RESEARCH AND DEVELOPMENT

- Co-ordinating research on environmental issues (including air and water quality, climate change, biodiversity, environmental technologies).

### STRATEGIC ENVIRONMENTAL ASSESSMENT

- Assessing the impact of plans and programmes on the Irish environment (such as waste management and development plans).

### ENVIRONMENTAL PLANNING, EDUCATION AND GUIDANCE

- Providing guidance to the public and to industry on various environmental topics (including licence applications, waste prevention and environmental regulations).
- Generating greater environmental awareness (through environmental television programmes and primary and secondary schools' resource packs).

### PROACTIVE WASTE MANAGEMENT

- Promoting waste prevention and minimisation projects through the co-ordination of the National Waste Prevention Programme, including input into the implementation of Producer Responsibility Initiatives.
- Enforcing Regulations such as Waste Electrical and Electronic Equipment (WEEE) and Restriction of Hazardous Substances (RoHS) and substances that deplete the ozone layer.
- Developing a National Hazardous Waste Management Plan to prevent and manage hazardous waste.

### MANAGEMENT AND STRUCTURE OF THE EPA

The organisation is managed by a full time Board, consisting of a Director General and four Directors.

The work of the EPA is carried out across four offices:

- Office of Climate, Licensing and Resource Use
- Office of Environmental Enforcement
- Office of Environmental Assessment
- Office of Communications and Corporate Services

The EPA is assisted by an Advisory Committee of twelve members who meet several times a year to discuss issues of concern and offer advice to the Board.

**EPA CCRP Programme 2007-2013**

# **Modelling air quality, climate change and volcanic ash**

## **CCRP Report-09-FS-6-4**

*End of Project Report available for download on <http://erc.epa.ie/safer/reports>*

Prepared for the Environmental Protection Agency

by

National University of Ireland, Galway

**Authors:**

**Damien Martin, Saji Varghese and Colin O'Dowd**

**ENVIRONMENTAL PROTECTION AGENCY**

An Ghníomhaireacht um Chaomhnú Comhshaoil  
PO Box 3000, Johnstown Castle, Co. Wexford, Ireland

Telephone: +353 53 916 0600 Fax: +353 53 916 0699

Email: [info@epa.ie](mailto:info@epa.ie) Website: [www.epa.ie](http://www.epa.ie)

## **ACKNOWLEDGEMENTS**

This report is published as part of the Climate Change Research Programme 2007-2013. The programme is financed by the Irish Government under the National Development Plan 2007-2013. It is administered on behalf of the Department of the Environment, Heritage and Local Government by the Environmental Protection Agency, which has the statutory function of co-ordinating and promoting environmental research.

The authors gratefully acknowledge Alastair McKinstry and Jean-Christophe Desplat in the Irish Centre for High End Computing (ICHEC), Ray McGrath and Eoin Whelan in Met Éireann and the EPA technical officer, David Dodd, in assisting with this project.

## **DISCLAIMER**

Although every effort has been made to ensure the accuracy of the material contained in this publication, complete accuracy cannot be guaranteed. Neither the Environmental Protection Agency nor the author(s) accept any responsibility whatsoever for loss or damage occasioned or claimed to have been occasioned, in part or in full, as a consequence of any person acting, or refraining from acting, as a result of a matter contained in this publication. All or part of this publication may be reproduced without further permission, provided the source is acknowledged.

The EPA CCRP 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.

## **EPA STRIVE PROGRAMME 2007-2013**

Published by the Environmental Protection Agency, Ireland

PRINTED ON RECYCLED PAPER



ISBN: 978-1-84095-584-2

Price: Free

## Details of Project Partners

**Dr. Damien Martin**

School of Physics &  
Centre for Climate & Air Pollution Studies /  
Ryan Institute  
National University of Ireland Galway  
Galway  
Tel: +353-91-495468  
Fax: +353-91-494584  
E-mail: [Damien.martin@nuigalway.ie](mailto:Damien.martin@nuigalway.ie)

**Dr. Saji Varghese**

School of Physics &  
Centre for Climate & Air Pollution Studies /  
Ryan Institute  
National University of Ireland Galway  
Galway  
Tel: + 353-91-495068  
E-mail: [Saji.Vargese@nuigalway.ie](mailto:Saji.Vargese@nuigalway.ie)

**Professor Colin O'Dowd**

School of Physics &  
Centre for Climate & Air Pollution Studies /  
Ryan Institute  
National University of Ireland Galway  
Galway  
Tel: +353-91-493306  
Fax: +353-91-494584  
E-mail: [colin.odowd@nuigalway.ie](mailto:colin.odowd@nuigalway.ie)



## Table of Contents

<b>ACKNOWLEDGEMENTS .....</b>	<b>ii</b>
<b>DISCLAIMER.....</b>	<b>ii</b>
<b>Details of Project Partners .....</b>	<b>iii</b>
<b>Executive Summary .....</b>	<b>vii</b>
<b>1. Introduction.....</b>	<b>1</b>
<b>1.1 Air quality climate change interactions .....</b>	<b>1</b>
<b>1.2 Volcanic ash simulations.....</b>	<b>1</b>
<b>1.3 The use of the WRF-Chem (Weather Research and Forecasting – Chemistry)     Model for both air quality and volcanic ash simulations .....</b>	<b>2</b>
<b>2. Air quality climate change interactions .....</b>	<b>3</b>
<b>2.1 Model set up .....</b>	<b>3</b>
<b>2.2 Results .....</b>	<b>3</b>
<b>2.2.1 Coarse mode sea-salt concentrations .....</b>	<b>4</b>
<b>2.2.2 Accumulation mode sea-salt and organic enrichment .....</b>	<b>5</b>
<b>2.3.3 Isoprene and Isoprene SOA.....</b>	<b>6</b>
<b>2.2.4 Sulphate .....</b>	<b>12</b>
<b>3. Volcanic ash simulations using REMOTE .....</b>	<b>14</b>
<b>3.1 Background .....</b>	<b>14</b>
<b>3.1.1 Overview of Icelandic volcanic eruptions.....</b>	<b>14</b>
<b>3.1.2 Description of volcanic ash .....</b>	<b>15</b>
<b>3.1.3 Implications to the Irish economy .....</b>	<b>15</b>
<b>3.2 Modelling of volcanic ash using the REMOTE model.....</b>	<b>15</b>
<b>3.2.1 Overview of volcanic ash modelling.....</b>	<b>15</b>
<b>3.2.2 Description of REMOTE .....</b>	<b>16</b>
<b>3.2.3 Development of REMOTE to improve characterisation of volcanic ash .....</b>	<b>16</b>
<b>3.2.4 Emission rate data .....</b>	<b>17</b>

3.2.5 Model Sensitivity.....	17
3.2.6 Model validation and verification .....	22
3.2.7 Automation.....	23
<b>4. Air quality and volcanic ash forecasts .....</b>	<b>25</b>
4.1 The WRF-Chem model .....	25
4.2 Model set-up .....	25
4.3 Emissions and inventories .....	26
4.4 Boundary meteorological conditions and chemical conditions .....	27
4.5 Volcanic ash simulations .....	27
4.5.1 Method.....	27
4.5.2 Vertical emission distribution.....	27
4.5.3 Flux emission.....	27
4.5.4 Size distribution .....	28
4.6 Validation .....	28
4.7 Testing of operationally .....	32
<b>5. Conclusions.....</b>	<b>35</b>
<b>6. Recommendations .....</b>	<b>36</b>
<b>References.....</b>	<b>38</b>
<b>Acronyms .....</b>	<b>41</b>
<b>List of Figures.....</b>	<b>42</b>
<b>List of Tables .....</b>	<b>44</b>

## Executive Summary

- Future levels of air quality pollutants over a European domain, with particular emphasis on Ireland, have been simulated up to the year 2100.
- The individual effect of reducing anthropogenic emissions and changing meteorology on future speciated aerosol and aerosol precursors has been determined for a particular emission storyline.
- For PM10 sea-salt, there is no clear trend over the European domain from the year 2006 to 2100.
- Ambient sulphate concentration is set to reduce significantly over the European domain under the emission storyline presented here, with the overall reduction in sulphate over Irish domain being smaller due to the continued influence of biogenic sulphate.
- In response to the 2010 Icelandic volcanic eruptions, an automated system for the forecasting of volcanic ash was designed, developed, validated and automated. This system allows for ash forecasts to be produced and output disseminated within two hours.
- The sensitivity of the model to a range of volcanic input parameters was also determined in order to optimise model performance.
- A 20 year climatological assessment of the seasonal effect of Icelandic volcanic emissions has also been undertaken.
- Ireland's first air quality modelling forecasting platform was developed during the course of this project. 54 hour air quality and meteorological forecasts were run and model output was streamed to the web during an operational phase.
- The model output was validated against meteorological and aerosol measurements and has been shown to perform well, when compared to other state-of-the-art air quality models.
- It is recommended that this pilot demonstration is developed further, in order to facilitate permanent, fully-automated, real-time air quality forecasting.
- This model also has the capability to provide real-time volcanic forecasts and this capability should be incorporated into real-time forecasting capability.
- Investment in this forecasting platform would significantly enhance Ireland's air quality modelling capability.
- Continued work in developing the modelling platform is recommended, in order to incorporate radiological releases and other accidental releases.



# 1. Introduction

The recently published Fifth Assessment Report (AR5) of the IPCC (Intergovernmental Panel on Climate Change) has adopted four greenhouse gas concentration trajectories known as Representative Concentration Pathways (RCPs). In this work, one of these trajectories (RCP 6 - stabilisation pathway, in which radiative forcing is stabilised at approximately  $6 \text{ W m}^{-2}$  after 2100) has been used in order to determine changes in future air quality due to air quality climate change interactions.

Air quality modelling can be seen as a numerical tool used to describe the relationship between meteorology, emissions, atmospheric concentrations and other factors (Daly and Zannetti, 2007). Atmospheric measurements give us useful information on different aerosol or trace gas concentrations but it does not give us the full picture. The source of the pollutant and its trajectory are just as important as the instantaneous or integrated measurement at a single measurement location. In this research fellowship, three themes have been investigated. These can be described as follows:

- Air quality climate change interactions
- Volcanic ash simulations
- Air quality and volcanic ash forecasts.

## 1.1 Air quality climate change interactions

Mortality rates, particularly in urban areas, have been linked to levels of atmospheric particulates (Schwartz et al., 1996). The sources of this particulate matter are generated from incomplete combustion processes, industry, construction and natural sources and, in many cities, the principal source is road traffic emissions,

particularly from diesel vehicles. Typically,  $\text{PM}_{10}$  (Particulate Matter of 10 microns in diameter or smaller) will consist of inorganic elements, ions, trace metals, elemental carbon (EC), and organic compounds and water, all of which are in a variety of proportions depending upon their origin, chemical processes in the atmosphere, long-range transport effects and meteorological conditions (Müller, 1999). The researchers discuss the effects of changing meteorology within the European model domain on particulate matter levels in Europe, with particular reference to natural processes such as sea-salt formation, secondary organic aerosol (SOA) formation from biogenic terrestrial isoprene emissions, and assess the future contribution of these processes to ambient particulate levels under changing meteorological conditions due to climate change. Isoprene is an organic compound released into the atmosphere by plant activity, both land-based and oceanic. Depending on conditions, organic compounds such as these can act as condensation nuclei for the growth of particulate matter in the atmosphere.

## 1.2 Volcanic ash simulations

Iceland's Eyjafjallajökull volcano first erupted on 14<sup>th</sup> April 2010. Volcanic ash was emitted up to a height of 9 km. Prevailing weather conditions resulted in the transport of ash and other pollutants to central Europe, where it remained up to the 20<sup>th</sup> April 2010 (Ansmann et al., 2010; Flentje et al., 2010). A number of further incidences of ash incursion into European airspace occurred until the 20<sup>th</sup> May 2010. This caused havoc for European airlines, in terms of financial losses, and for passengers, in terms of disrupted travel.

The Volcanic Ash Advisory Centre (VAAC) in London issued advisories on areas contaminated by ash, based on model predictions from the UK Meteorological Office's NAME (Numerical Atmospheric-dispersion Modelling Environment) model. NAME is the operational dispersion model of the London Volcanic Ash Advisory Centre (VAAC). Volcanic ash is modelled in NAME using a representative size distribution and density for the ash particles. Ash is released at the volcano over a height range between the volcano's summit and the maximum observed height of the eruption plume. The eruption height is critical for estimating the mass of ash erupted under the current procedure. The level of confidence in this maximum height depends on the availability of observations of the plume. Based on these advisories, air space was closed by the relevant national aviation authorities. This resulted in the cancellation of a number of flights across Europe and caused widespread disruption. Once a threshold was specified by the engine manufacturers, the VAACs were required to move from a total avoidance forecast to a threshold forecast;  $0.2\text{mgm}^{-3}$  being the limit below which aircraft may fly without special attention, and  $2\text{mgm}^{-3}$  being the limit above which flights should be avoided. From 18<sup>th</sup> May 2010, the safe limit was revised upwards to  $4\text{mgm}^{-3}$ .

In this work, the researchers have applied a Regional Climate Model to forecast and study the dispersion of volcanic ash from the 2010 eruption of Eyjafjallajökull. Using prescribed ash emission rates and size distribution data for selected

events, the model sensitivity to eruption column height and vertical release distribution was studied. Validation of forecasts using available in-situ measurements was also undertaken. An automated system for the delivery of real-time volcanic ash forecasts was designed and developed.

### **1.3 The use of the WRF-Chem (Weather Research and Forecasting–Chemistry) Model for both air quality and volcanic ash simulations**

WRF-Chem is an online model which has been adapted for use in this research. The model was set up and simulations were undertaken using computational infrastructure from ICHEC (Irish Centre for High End Computing). Input ECMWF (European Centre for Medium-Range Weather Forecasts) meteorological data for forecasting was provided by Met Éireann. An operational period between 18<sup>th</sup> and 30<sup>th</sup> November 2013 was used to deliver daily 54 hour air quality and meteorological forecasts. This tested the computational infrastructure, model performance and post-processing software over this period and proved a viable system for providing air quality forecasts. In addition to previously published data on model performance with a European domain, the performance of the model for sea-salt within an Irish context for both a winter and summer month was undertaken for two different resolutions. As an island nation, sea-salt can be an important component of airborne particulate matter, in particular at coastal locations.

## 2. Air quality climate change interactions

### 2.1 Model set up

In this work, the researchers have deployed the online climate-chemistry/aerosol model REMOTE model (Regional Model with Tracer Extension) for the domain comprising Europe and North-East Atlantic (Figure 2.1) for horizontal resolutions of  $0.5^\circ$  (~50 km),  $81 \times 91$  grid points. Simulations were performed for the years 2006, 2030, 2050 and 2100. REMOTE is initialised at the first time-step using the down-scaled meteorological analysis data from coupled ECHAM5-HAM-MPIOM-HAMMOC model (Kloster et al., 2007), which are updated at the lateral boundaries every 6 h and used for nudging the model in the boundary zone of 8 grid cells. Trace species concentrations are initialised for each simulated month using the monthly mean output of the ECHAM5-HAM-MPIOM-HAMMOC model and the same data set is used at the lateral boundaries for the monthly simulation.

Representative Concentration Pathways (RCPs) are four greenhouse gas concentration trajectories adopted by the IPCC (Intergovernmental Panel on Climate Change) for its Fifth Assessment Report (AR5). The RCP pathway chosen for this study is a stabilisation pathway, in which radiative forcing is stabilised at approximately  $6 \text{ W m}^{-2}$  after 2100. In this stabilisation pathway, emissions are set to rise until mitigation takes effect (around 2050), after which time emissions decrease (Moss, et al., 2007). A more complete description of the model set up is given elsewhere (Coleman et al., 2013). Recent model developments relating to processes contributing to ambient particulate matter are briefly described.

Aerosol dynamics and thermodynamics are dealt with using the M7 aerosol dynamics module

(Stier, et al., 2005; Vignati et al., 2004). M7 simulates nucleation, coagulation and condensation for seven aerosol lognormal distribution modes, including soluble and insoluble aiten, accumulation and coarse modes and an additional soluble nucleation mode. Aerosol components considered in M7 include sulphate, black carbon, and organic carbon, sea-salt and mineral dust.

These components have either negligible or low solubility, or are treated as an internal mixture of insoluble and soluble compounds. Mixed particles are formed from insoluble particles by coagulation and condensation. Each mode can be described by three moments; aerosol number  $N$ , number median radius  $r$  and standard deviation  $\sigma$ . Standard deviations are prescribed in M7 (Vignati, et al., 2004) so that the median radius of each mode can be calculated from the corresponding aerosol number and aerosol mass, which are transported as tracers. These speciated model output modes are determined and the researchers focus on these as well as the contribution to regulatory values. Recent model developments include improved parameterisation of sea-salt; organic enrichment of sea-spray and the formation of SOA from isoprene give a high degree of confidence in the predictive ability of the model.

### 2.2 Results

In the simulations presented here, the primary domain comprises Europe and North East Atlantic with horizontal resolution of  $0.5^\circ$  (~50 km),  $81 \times 91$  grid points. The model domain covers an area from  $10^\circ$  W to  $30^\circ$  E at the southern boundary of about  $30^\circ$  N and from  $40^\circ$  W to  $60^\circ$  E in the north at about  $70^\circ$  N. Within the primary domain, three sub-domains have been selected for trend analysis. These can be defined

as a North-East Atlantic marine sub-domain representing background air entering into Europe but not influenced by local emissions, a continental central (mainland) European domain

expected to be predominantly influenced by local emissions, and finally a hybrid domain (specifically Ireland), expected to be influenced by both marine trends and local emissions.

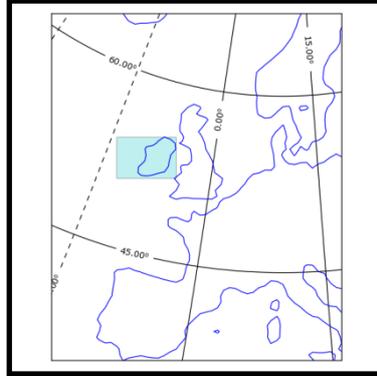


Figure 2.1. REMOTE primary domain with Irish sub-domain (highlighted in grey scale), in which regional analysis is performed

### 2.2.1 Coarse mode sea-salt concentrations

Changes in both coarse and accumulation mode sea-salt concentration, as well as submicron organic enrichment, are clearly dependent on a number of factors relating to changing meteorology. Given the dependence of both accumulation mode and coarse mode on wind speed, these projected changes will have an influence on the future sea-salt particulate levels. Previous studies centred on the north Atlantic domain indicate that annual mean wind speeds are set to reduce by the order of 1% under 4 of the SRES (IPCC Special Report on Emissions Scenarios) emission scenarios. These changes have a seasonal dimension with estimates, with

a clear reduction in Oceanic summertime wind speed (1-5%) and a corresponding increase in the wintertime mean wind speed (1-4%) (Nolan et al., 2011).

Shown in [Figure 2.2](#) are the monthly mean ocean coarse mode, sea-salt concentrations for the simulation years, normalised to the base year for both the model domain and the Irish domain. The future trend in concentrations clearly illustrates no defined trend, with 2100 full domain monthly means being no more  $\pm 20\%$  of the 2006 values. This suggests that the combined effect of changes in oceanic sea-salt flux and changes in wet deposition combine to give these changes in sea-salt.

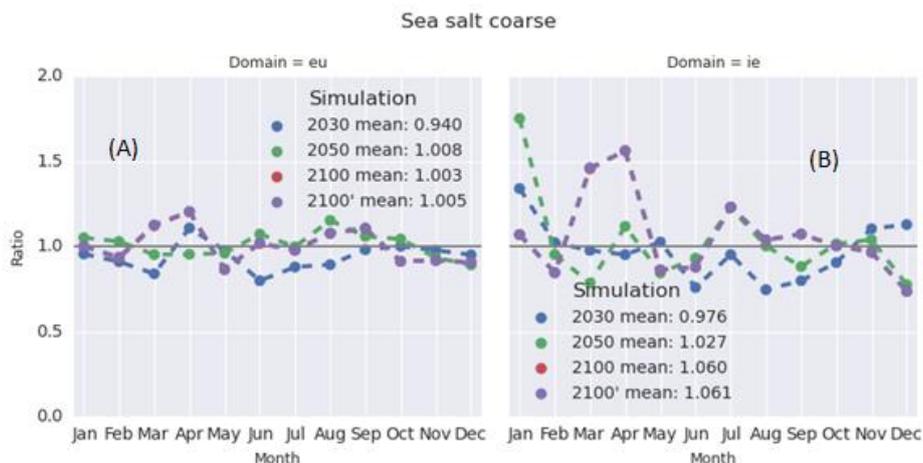


Figure 2.2. Monthly mean coarse mode, sea-salt concentrations normalised to 2006 values for both (A) the full model domain and (B) the Irish domain

### 2.2.2 Accumulation mode sea-salt and organic enrichment

Given the power-law dependency on wind speed of the accumulation mode, a number of production changes in meteorology may have an effect on the seasonal burden of sea-salt. Typically, the maximum organic enrichment (and associated depletion) of sea-salt occurs during the summer period, when oceanic chlorophyll-a is at its maximum. Under changing meteorology, associated changes in chlorophyll-a concentrations will clearly influence the composition of sea-spray. Historic levels of chlorophyll-a in the North-Eastern Atlantic suggest an annual increase somewhere in the region of  $0.071 \text{ mg m}^{-3} \text{ yr}^{-1}$  between 1889 and 2000 (Wernard et al., 2013). However, it has been speculated that there will be changes in the North-Eastern Atlantic chlorophyll concentrations by 2100 for a number of reasons, which include; increased sea-surface temperatures reduce local deep mixing and, hence, reduce the nutrient supply from waters at intermediate depths, and a steady shoaling of the Atlantic overturning cell tends to transport increasingly nutrient-depleted waters from the Southern Hemisphere towards

the north, leading to further diminishment of nutrient supply (Hofmann et al., 2011). Changing wind patterns and increasing chlorophyll-a levels will clearly have an effect on future air quality levels.

Shown in [Figures 2.3a](#) and [2.3b](#) is the mean accumulation mode organic carbon concentrations normalised to 2006 values, whilst [Figures 2.3c](#) and [2.4d](#) show the accumulation mode sea-salt concentrations normalised to 2006 values for both the whole model domain and the Irish domain respectively. It is apparent that there are changes in the future trend of the organic enrichment ratio, with significant seasonal changes over the simulation period over both the European domain and the Irish domain. The Irish domain shows the larger changes over the simulation period, although the trend is less pronounced. Recent work (Vaishya et al., 2013) has shown that sea-spray, light-scattering enhancement,  $f(\text{RH})$ , as a function of relative humidity (RH) is suppressed when enriched with organic matter. A new hygroscopic growth factor parameterisation reveals a dual hygroscopicity state, flipping from high hygroscopicity and high

f(RH) to low hygroscopicity and low f(RH) as the organic fraction mixing exceeds ~ 55% in sea-spray. Under elevated wind speeds, this affects the top-of-atmosphere direct radiative forcing ( $\Delta F$ ) by reducing the cooling contribution of sea-spray by ~ 5.5 times compared to pure sea-salt spray. These results suggest a positive feedback coupling between the marine biosphere, sea-

spray aerosol, and the direct radiative budget. Results suggest that the ratio of organic enrichment between the future years and the simulation period may change and thus, has the possibility of changing the magnitude of this positive feedback coupling. This change in the organic fraction of sea-spray has the capacity to influence future Irish climate.

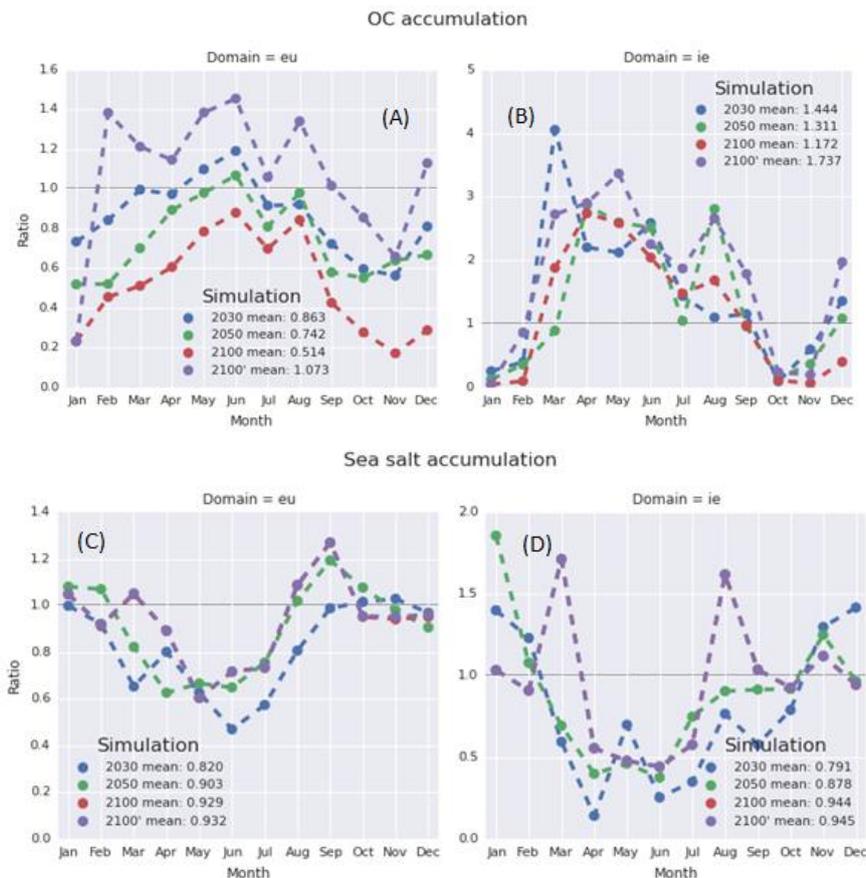


Figure 2.3. Monthly mean accumulation mode organic carbon concentrations normalised to 2006 values for both (A) the full model domain and (B) the Irish domain and Monthly mean accumulation mode sea-salt concentrations normalised to 2006 values for both (C) the full model domain and (D) the Irish domain (2100' – 2100 meteorology with 2006 emissions)

### 2.3.3 Isoprene and Isoprene SOA

Figure 2.4 presents the ground level isoprene concentrations for January and August 2006,

2030, 2050 and 2100, while Figure 2.5 shows the associated changes in monthly mean 2metre temperature for 2050 and 2100 relative to 2006.

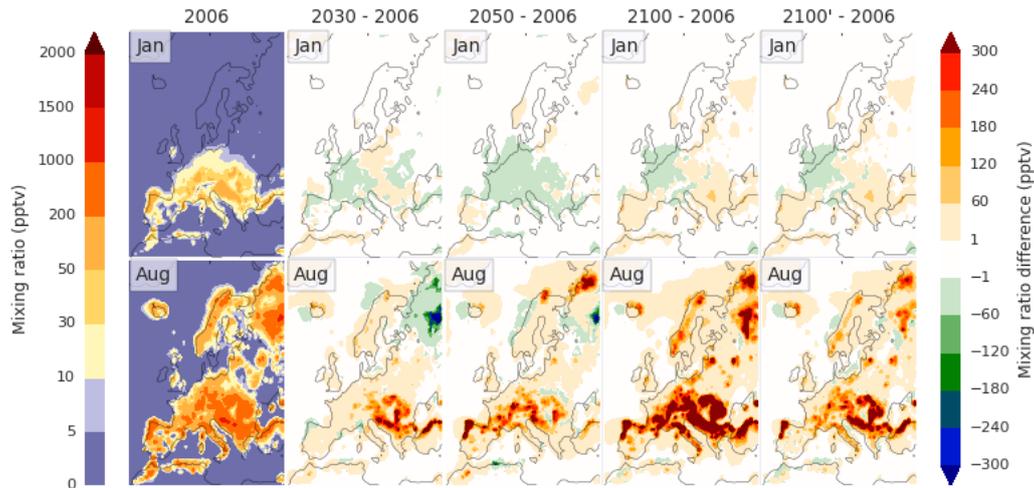


Figure 2.4. Monthly mean isoprene ground level mixing ratio (pptv) for January and August (2006, 2030, 2050, and 2100)

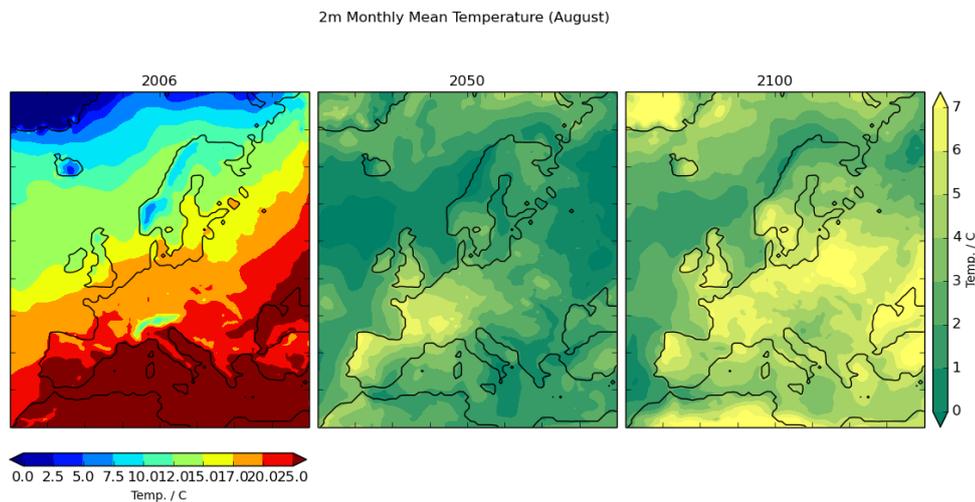


Figure 2.5. Changes in monthly mean 2metre temperature for 2050 and 2100 relative to 2006

It is apparent that there are large increases (> factor of 2 for August monthly mean) in isoprene concentrations for August across Europe, as would be expected with the large increase in predicted mean summertime temperatures. This clearly shows very large differences between the different simulated years under investigation in this study, with average August monthly mean values increasing by over a factor of 2 in the European domain between 2006 and 2100. There is still some doubt as to the overall contribution of isoprene to the total aerosol mass

(Kloster et al., 2007). It has been shown (Zhang et al., 2007) that the inclusion of isoprene SOA increases simulated surface concentrations in the U.S. of total organic mass by 65% and total PM<sub>2.5</sub> (Particulate Matter of 2.5 microns in diameter or smaller) mass concentrations by 25%. Given that future emission scenarios have suggested a reduction in anthropogenic precursors of particulate matter, and with biogenic isoprene emissions set to increase under increasing temperatures, it is important to understand the future levels of speciated aerosol

components and their precursors. [Figure 2.6](#) below presents the isoprene concentration for the different model sub-domains as well as the main domain. It clearly illustrates that the increase in ground level isoprene concentrations across the model domain are set to rise significantly by 2100. The trend over the European sub-domain is even clearer, with the

mean August value set to double by 2100. Over the Irish domain, the overall change in the 2100/2006 ratio is similar to the European domain. The increase in monthly mean ambient isoprene levels ([Figure 2.6a](#)) (~factor of 2) over the European domain can be attributed to changes in temperature associated with changing meteorology.

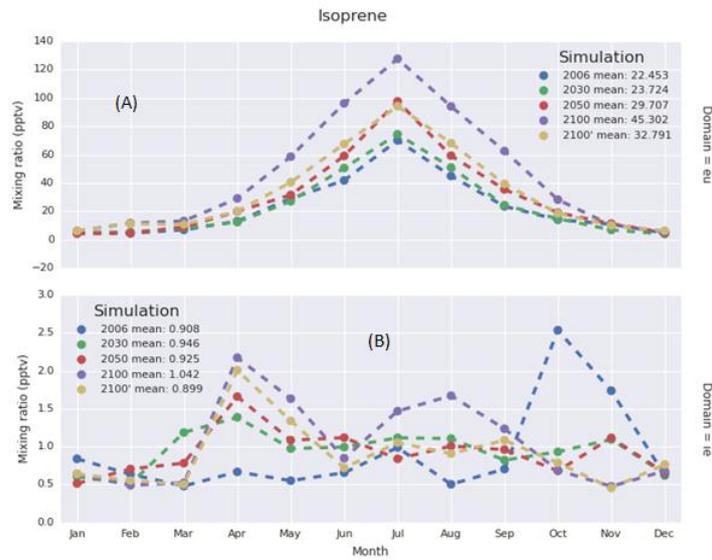


Figure 2.6. Ground level isoprene monthly mean concentrations for full model domain (A) and the Irish model sub-domain (B) (2100' – 2100 meteorology with 2006 emissions)

Future emissions of isoprene will clearly depend on other factors such as changes in land use and CO<sub>2</sub> inhibition. It has been shown that for a fixed vegetation distribution, isoprene emissions can be directly inhibited under elevated concentrations of CO<sub>2</sub> (Rosenstiel et al., 2003).

These other factors have been shown to be considerable and have been estimated to cause greater reductions in isoprene levels than the increase associated with climate change (Squire

et al., 2014). These other contributing factors to future simulated isoprene mixing ratios will be the focus of future studies, as they are not included here. Clearly, increases in isoprene levels will have an effect on both ozone and isoprene SOA levels. This change in SOA levels will clearly have an effect on future levels of particulate matter. Shown in [Figure 2.7](#) are the monthly mean SOA values for both the model domain and the Irish sub-domain.

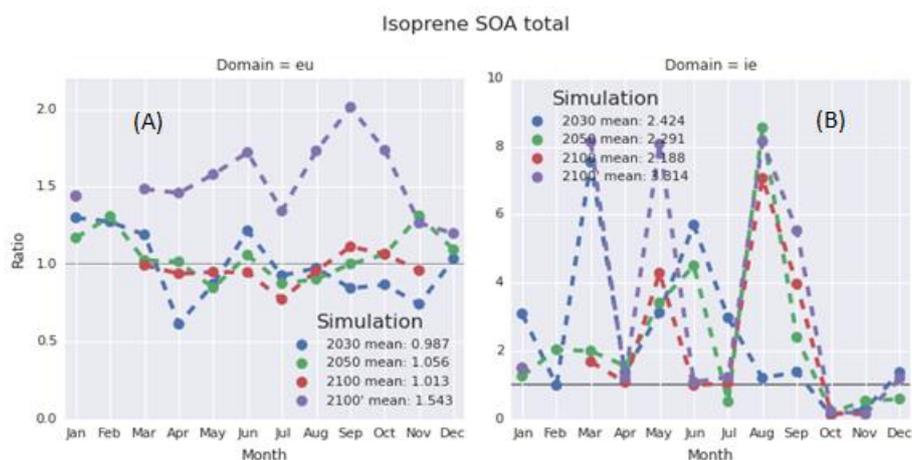
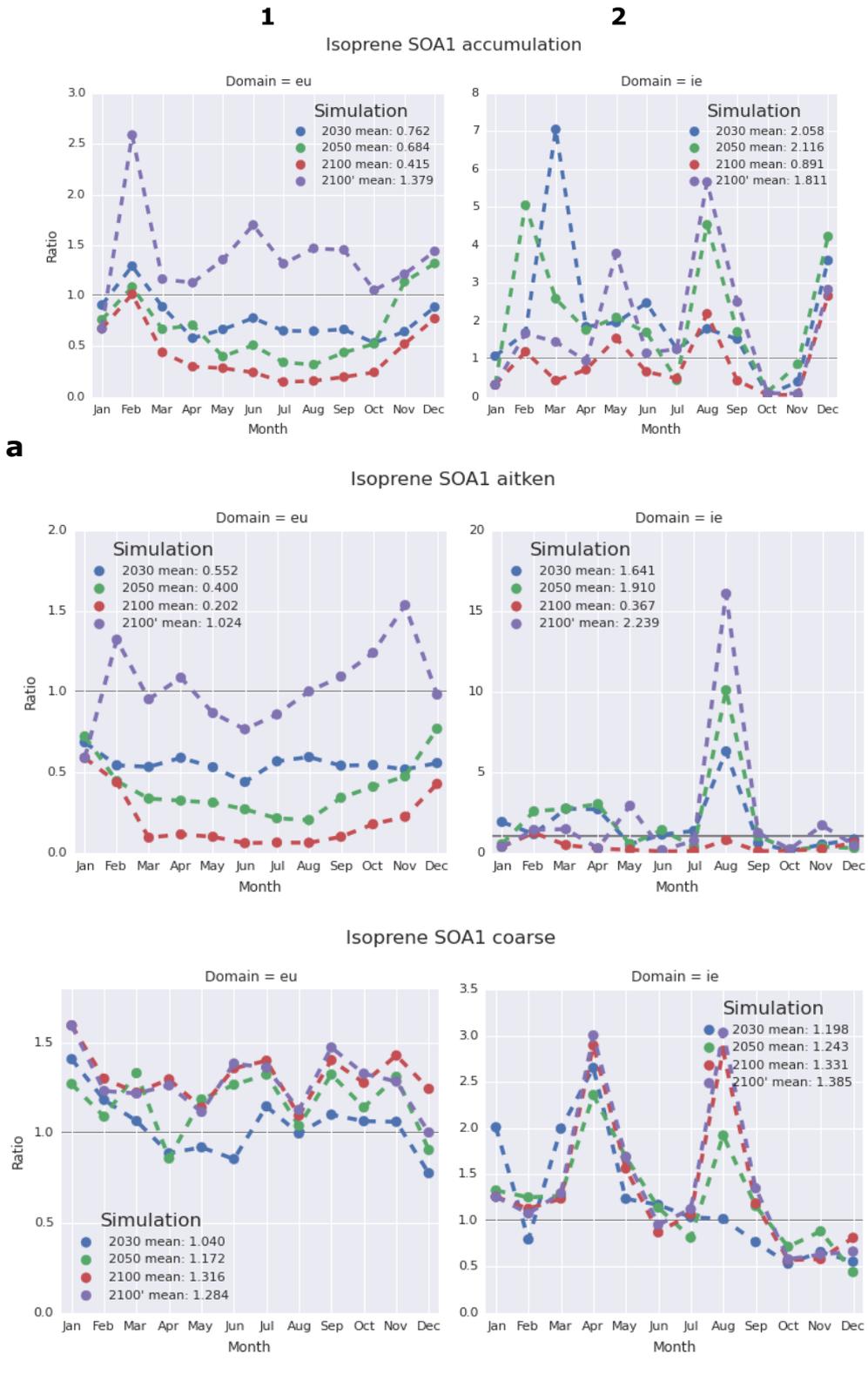


Figure 2.7. Ground level isoprene SOA monthly mean concentrations for full model domain (A) and the Irish sub-domains (B) relative to 2006 (2100' - 2100 meteorology with 2006 emissions)

Figure 2.7 illustrates that there is not an equivalent increase in magnitude over the European domain for isoprene SOA as there is for isoprene. Monthly mean isoprene concentrations over the European domain are set to rise by a factor of 2 during the summer months, when biogenic emission is at a maximum. Figure 2.8 shows the monthly mean isoprene derived SOA of both the high (a, b and c) and low yield (d, e and f) for the aitken, accumulation and coarse mode respectively. The SOA scheme involves oxidation of isoprene into high- and low-yield semi-volatile compounds. Gas-particle partitioning of these products is calculated according to Henry's Law equilibrium. Using this approach, partitioning is limited by the availability of pre-existing aerosols (some anthropogenic) that provide condensation surface area for the oxidation products. The yield

is therefore affected by the solubility of the compounds and available aerosol surface area, so in the case of less anthropogenic aerosols, there is a lower proportional yield of isoprene SOA due to less condensation surface for oxidation products. For both the low- and high-yield products, it is apparent that there is a clear reduction in the trend of both the aitken and the accumulation mode, whereas there is a clear increase in the coarse mode monthly mean. The change in size distribution can be attributed to reductions in future emissions of anthropogenic aerosols under the emission scenario prescribed here. This is illustrated in Figure 2.8, where the isoprene derived SOA for both the high- and low-volatility yield product for 2100 meteorology with 2006 emissions can be seen to exhibit a different relative size distribution for the different modes.



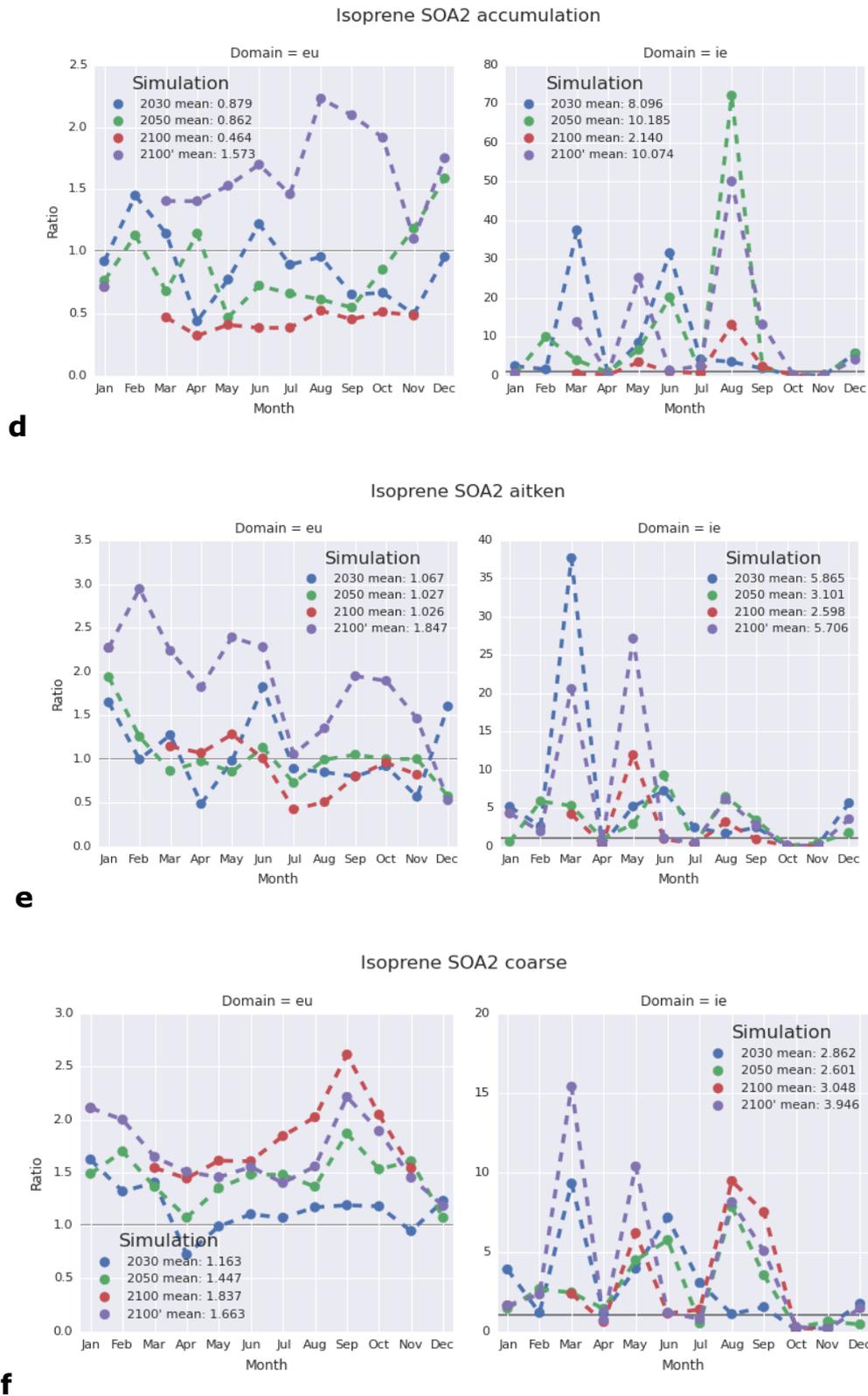


Figure 2.8. (a1-f2): Monthly mean aitken, accumulation and coarse mode mass (a,b,c for SOA1) and (d, e f for SOA2) for full model domain (1) and Irish domain (2) relative to 2006 values (2100' - is the year 2100 ran with 2006 emissions)

### 2.2.4 Sulphate

Gaseous  $\text{SO}_2$  becomes oxidised to form sulphuric acid, influential upon particle nucleation and growth. The monthly mean  $\text{SO}_2$  concentrations for 2006, 2030, 2050 and 2100 over both the model domain and the model sub-domain are shown in [Figure 2.9](#), as well as the values of mean  $\text{SO}_2$  concentrations simulated using 2006 climatology (including natural emissions) with 2030, 2050 and 2100 RCP6.0 anthropogenic emissions. [Figure 2.9](#) also shows

the monthly mean sulphate mass concentrations for the simulation years for both the whole model domain (a) and the Irish domain (b). [Figure 2.9 \(a-f\)](#) shows the total monthly mean model domain sulphate mass for aiten, accumulation and coarse mode sulphate. This clearly illustrates the large reduction in anthropogenic emissions under the scenario described here. For the Irish domain, the trend in reduction is less clear and these differences can be attributed to the contribution from marine DMS (dimethyl sulphide) production.

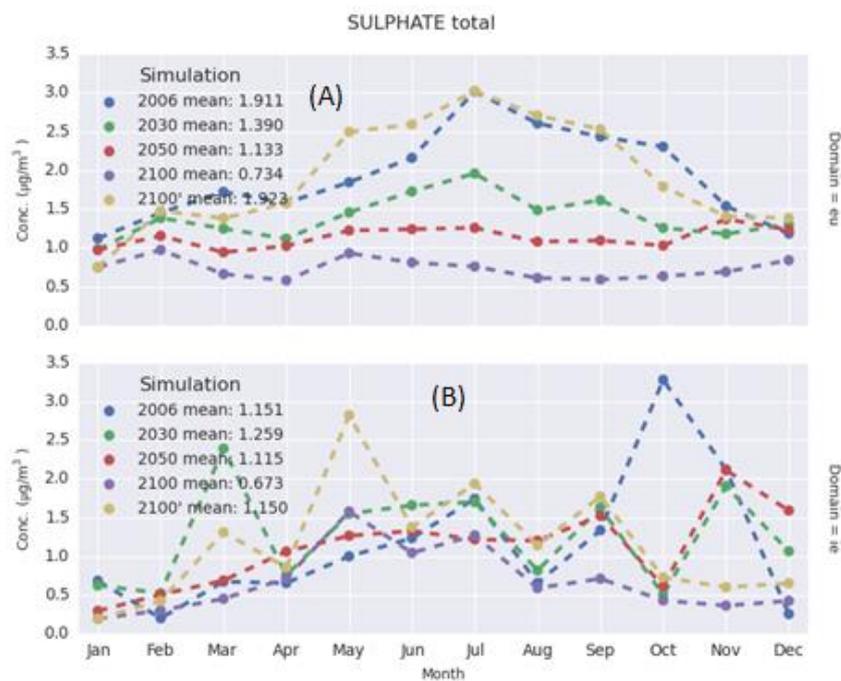


Figure 2.9. Total monthly mean sulphate concentrations for full model domain (A) and Irish domain (B) for the simulation years (2100' = 2100 meteorology with 2006 emissions)

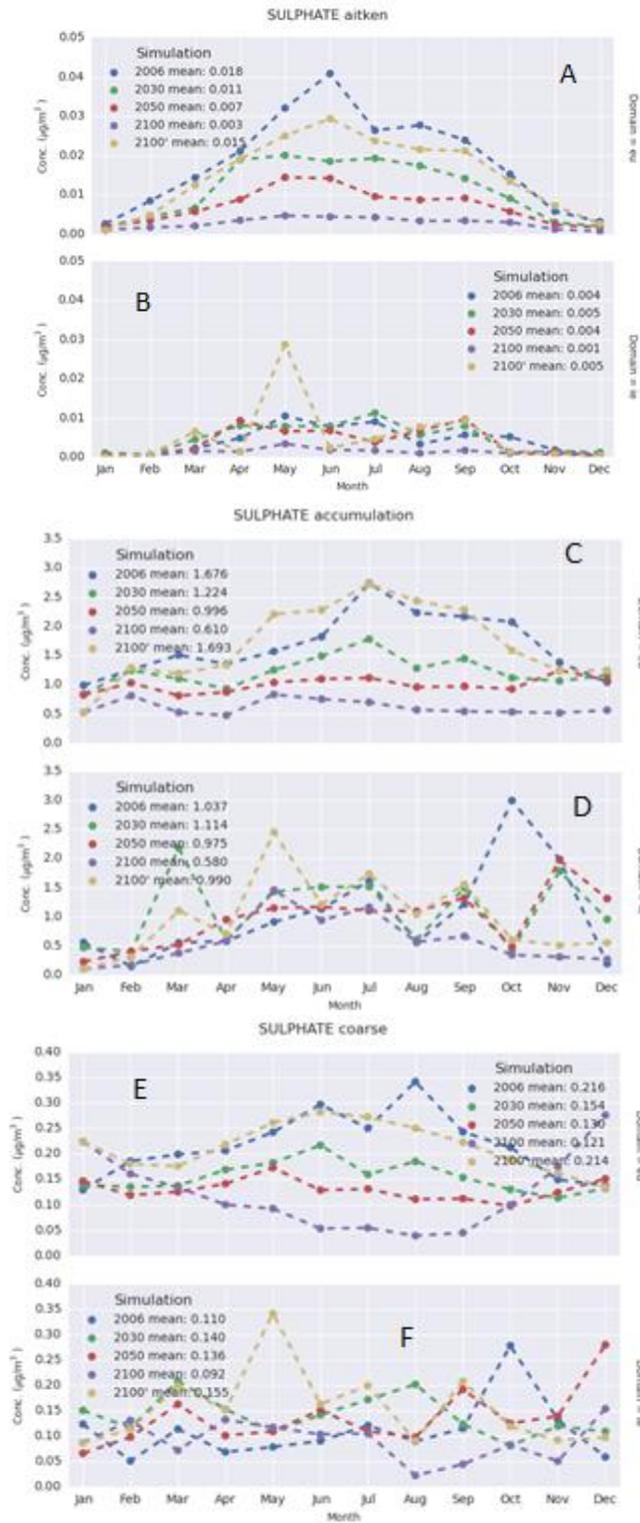


Figure 2.9. (a-f) Total monthly mean sulphate aitken, accumulation and coarse mode concentrations for full model domain (a,c,e) and Irish domain (b,d,f) (2100' - refers to 2100 meteorology with 2006 emissions).

## 3. Volcanic ash simulations using REMOTE

### 3.1 Background

The model used in the previous section for air quality climate change interactions was adopted

for volcanic ash forecasts, in response to the eruption of the Eyjafjallajökull volcano in 2010 ([Figure 3.1](#)). An overview of the circumstances surrounding this is given below.

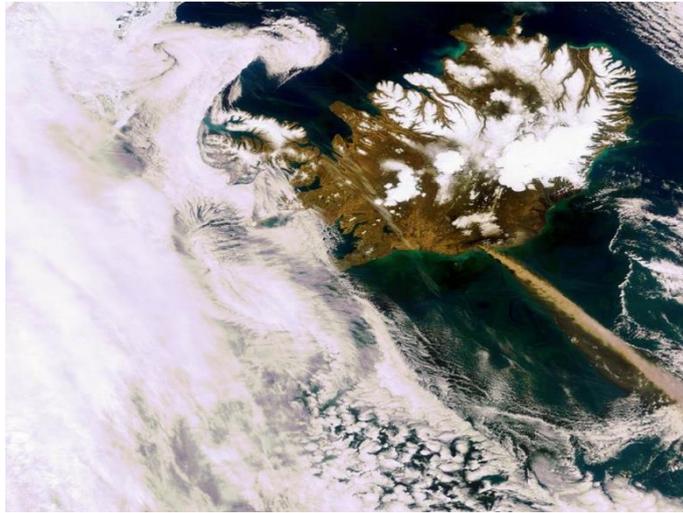


Figure 3.1. Satellite image of 2010 Eyjafjallajökull volcanic eruption (Source: Iceland Volcano, May 2010, ESA – Envisat – MERIS)

#### 3.1.1 Overview of Icelandic volcanic eruptions

Iceland's Eyjafjallajökull volcano first erupted on 14<sup>th</sup> April 2010. Volcanic ash was emitted up to a height of 9 km. Prevailing weather conditions resulted in the transport of ash and other pollutants to central Europe, where it remained up to the 20<sup>th</sup> April 2010 (Ansmann et al., 2010; Flentje et al., 2010). A number of further incidences of ash incursion into European airspace occurred until the 20<sup>th</sup> May 2010. This caused havoc for European airlines, in terms of financial losses, and for passengers, in terms of disrupted travel.

The Volcanic Ash Advisory Centre (VAAC) in London issued advisories on areas contaminated by ash, based on model predictions from the UK Meteorological Office's NAME (Numerical Atmospheric-dispersion Modelling Environment)

model. NAME is the operational dispersion model of the London Volcanic Ash Advisory Centre (VAAC). Volcanic ash is modelled in NAME using a representative size distribution and density for the ash particles. Ash is released at the volcano over a height range between the volcano's summit and the maximum observed height of the eruption plume. The eruption height is critical for estimating the mass of ash erupted under the current procedure. The level of confidence in this maximum height depends on the availability of observations of the plume. Based on these advisories, air space was closed by the relevant national aviation authority. This resulted in the cancellation of a number of flights across Europe and caused widespread disruption. Once a threshold was specified by the engine manufacturers, the VAACs were required

to move from a total avoidance forecast to a threshold forecast;  $0.2\text{mgm}^{-3}$  being the limit below which aircraft may fly without special attention, and  $2\text{mgm}^{-3}$  being the limit above which flights should be avoided. From 18<sup>th</sup> May 2010, the safe limit was revised upwards to  $4\text{mgm}^{-3}$ .

### ***3.1.2 Description of volcanic ash***

The term “volcanic ash” refers to a variable mixture of fine particles, including silica (>50% of ash composition), aluminium, calcium, and sodium. Silica is a very hard, abrasive substance and has a melting point ( $\sim 1100^\circ\text{C}$ ) significantly lower than that of the temperature commonly found within a jet engine ( $\sim 1400^\circ\text{C}$ ). Products that are ejected from volcanoes (known as “tephra”) can be greatly varied in size, from microscopic debris to rock boulders. Smaller tephra ( $< 2\text{mm}$ ) is defined as volcanic ash.

A variety of gases are also ejected during volcanic eruptions, including water vapour, sulphur dioxide, and chlorine, as well as hydrogen sulphide and oxides of nitrogen. After release, the sulphur dioxide population is affected by oxidation and hydration, creating sulphuric acid and rendering the ash/gas mixture as highly corrosive.

### ***3.1.3 Implications to the Irish economy***

There have been significant implications from the Eyjafjallajökull volcanic eruptions, resulting in the cancellation of roughly 100,000 flights affecting 8 million passengers. The European Commission estimated airline and travel agency losses from the grounding of air traffic at up to 2.5 billion euro (three billion dollars). There were a series of closure of Irish airports centred across three main events (15/04/10 - 20/04/10, 04/05/10 - 06/05/10, 16/05/10 - 17/05/10). One Irish airline (Ryanair) has estimated a loss in revenue of 50 million euro during this period due to 10,000

cancelled flights. In addition to this, there are additional associated losses with income derived from accommodation and other associated spend.

## **3.2 Modelling of volcanic ash using the REMOTE model**

### ***3.2.1 Overview of volcanic ash modelling***

While satellites can produce regular images of volcanic ash clouds as they undergo changes in the atmosphere, an effective predictive scheme is needed so that timely decisions can be made for airlines and any groups potentially affected by the presence of a volcanic plume. Computer models have been made to emulate and predict the movement, spread and dispersion of volcanic ash clouds, sometimes based on previous models such as those used for the study of radioactive debris. These models vary from simple 2D trajectory models to advanced 3D models of transport and dispersion.

Output from these models includes estimated average concentrations of ejected ash particles by size and location within the source volcano’s region of interest, doing so by incorporating such conditions as wind speed, particle aggregation, column height, and mean grain size. Data can typically be output graphically, commonly showing any regions with ash concentrations above a chosen level as overlaid onto a regional geographic map. Such information on the ash cloud can be forecast for a range of specific times in the future.

Several parameters are required for such a study, including the altitude reached by ash particles, distributions of particle concentrations with size and mass, wind forces, atmospheric turbulence, and the effects of precipitation. Typical input data includes eruption time and location, column height, and analysed and forecast meteorological fields.

### 3.2.2 Description of REMOTE

The work outlined in this section addresses the further development, validation and utilisation of a three-dimensional, online climate chemistry/aerosol model called REMOTE (Regional Model with Tracer Extension (Langmann, 2000)) in ash plume forecast / hindcast mode. This is a regional climate model that determines the physical, photochemical and aerosol state of the model atmosphere at every model time step, thus offering the possibility to consider trace species effects on climate. During the recent Eyjafjallajökull eruptions, an operational volcanic plume forecasting model was developed in order to provide Ireland with its own capability of assessment and prediction.

### 3.2.3 Development of REMOTE to improve characterisation of volcanic ash

For the climatological and risk assessment work outlined in this study, the domain has been expanded. The impetus to undertake this work is that, under particular meteorological conditions, volcanic ash advection can stray outside the western model boundary. Should meteorological conditions dictate that this ash is then re-entrained into the model domain, then this may result in an underestimation of the total column burden. The new enhanced domain will ensure that advection of volcanic ash out of the model domain is minimised. The standard domain contains 81 x 91 x 19 vertical grid boxes at 0.5° grid resolution (approx. 50 km<sup>2</sup>). The new model dimensions are 161 x 91 x 31 grid boxes ([Figure 3.2](#)).



Figure 3.2. REMOTE extended domain

In order to best understand the atmospheric transformations and processes that volcanic emissions are subject to, it is important to have a state-of-the-art chemical mechanism describing these reactions. As outlined previously, the current mechanism is determined by the RADM 2 (Regional Acid Deposition Mechanism - Version 2) chemical scheme (Stockwell et al., 1990), with 163 chemical reactions in the gas phase. The

RADM 2 mechanism will be updated to the most recently published scheme (RACM 2 Regional Atmospheric Chemistry Mechanism - Version 2), which includes rate constants and product yields from the most recent laboratory measurements and has been extensively tested against environmental chamber data. The relevant mechanistic differences between the two schemes are detailed below:

	<b>RADM 2</b>	<b>RACM 2</b>
Number of reactions	155	347
Number of photolysis reactions	21	34
Inorganic species	14	17
Inorganic intermediates	4	4
Stable organic species	26	56
Organic intermediates	16	40

This more explicit and up-to-date mechanism will afford the best opportunity to assess potential air quality impacts from volcanic emissions.

### 3.2.4 Emission rate data

Emission rate data used for simulations has been taken from the European Monitoring and Evaluation Programme (EMEP, 2011) estimations. These data are based on tephra estimates derived from preliminary thickness data obtained when measured on the 17<sup>th</sup> April 2010 at two locations 20 and 50 km east of the volcano. Size distribution measurements of these samples allow estimates of emission rates to be calculated. Whereas ash data in the EMEP study were collected independently of volcanic strength measurements, sources (Witham et al., 2007) have pointed to theoretical relationships between eruption height and volumetric flux (with the same trends as mass flux, assuming the common treatment of ash density as a constant value). Once the tephra volume is calculated, a mass flux can be derived using an assumed density. A ratio from previous volcanic emissions of  $m_{63}$  (fraction of particles less than 63 $\mu\text{m}$ ) to total mass emissions for different eruption types (Mastin et al., 2009) can be used to determine feasible release rates. Given that the EMEP release rates are based on both in-situ tephra and size distribution measurements they can be treated as a refinement of the Mastin relationship.

Other techniques have been deployed to determine ash emissions, including an inversion

scheme which couples a priori source information and the output of a Lagrangian dispersion model with satellite, which has then been used to estimate the volcanic ash source strength as a function of altitude and time (Stohl et al., 2011).

### 3.2.5 Model sensitivity

The input parameters may be evaluated using direct measurements, remote observations and previous studies of eruptions having similar features. Accurate eruption source information is crucial in initialising volcanic ash models and for reliable ash forecasting. It is also critical in validating model output. The largest uncertainties in ash dispersion modelling depend on the precise estimation of the status of the eruption during model initialisation. Key eruption parameters are:

- column height
- the total erupted mass
- grain-size distribution
- vertical distribution and
- density.

For all the sensitivity tests, the period 2<sup>nd</sup> to 8<sup>th</sup> May, 2010 was arbitrarily chosen. As seen during the Eyjafjallajökull volcano eruption, there was limited accurate information available on the source parameters, which are essential for model initialisation and parameterisation. Therefore, it was important to determine the sensitivity of models to such arbitrary prescription of certain input information. The uncertainties in the chosen

key parameters associated with the description of volcanic ash emissions and sensitivity studies will need to be evaluated through a range of sensitivity studies. A series of sensitivity tests were performed varying the eruption source parameters such as vertical distribution of mass flux and plume height.

Eruption heights from the reports of the Institute of Earth Sciences (IES) at the University of Iceland and the Icelandic Meteorological Office (IMO) include a range of sources, but mostly centre on observations of the IMO's weather radar (time ranges often not specified) and reports from aircraft pilots at specific times, which have often been different from the radar data. In the first sensitivity test, as shown in [Figure 3.3](#), vertical distribution of mass flux at each level was

made a constant, injection height was varied from 4.5 km to 5.4 km and 6.5 km, while keeping the total mass flux constant. The general distribution pattern appears to be quite similar for the range of injection heights considered. However, there is strong variability in the fine-scale structures, both in the temporal and vertical scale. For example, in Figure A, only one prominent feature is seen at around 7.5 km, while in Figure C, two such features are visible. Furthermore, the duration of higher concentration around 6<sup>th</sup> May 2010 is higher in A relative to C. To highlight the differences distinctly, difference plots are shown in [Figure 3.4](#). This illustrates the necessity to clearly define the injection height which is dictated by the vertical resolution within the model.

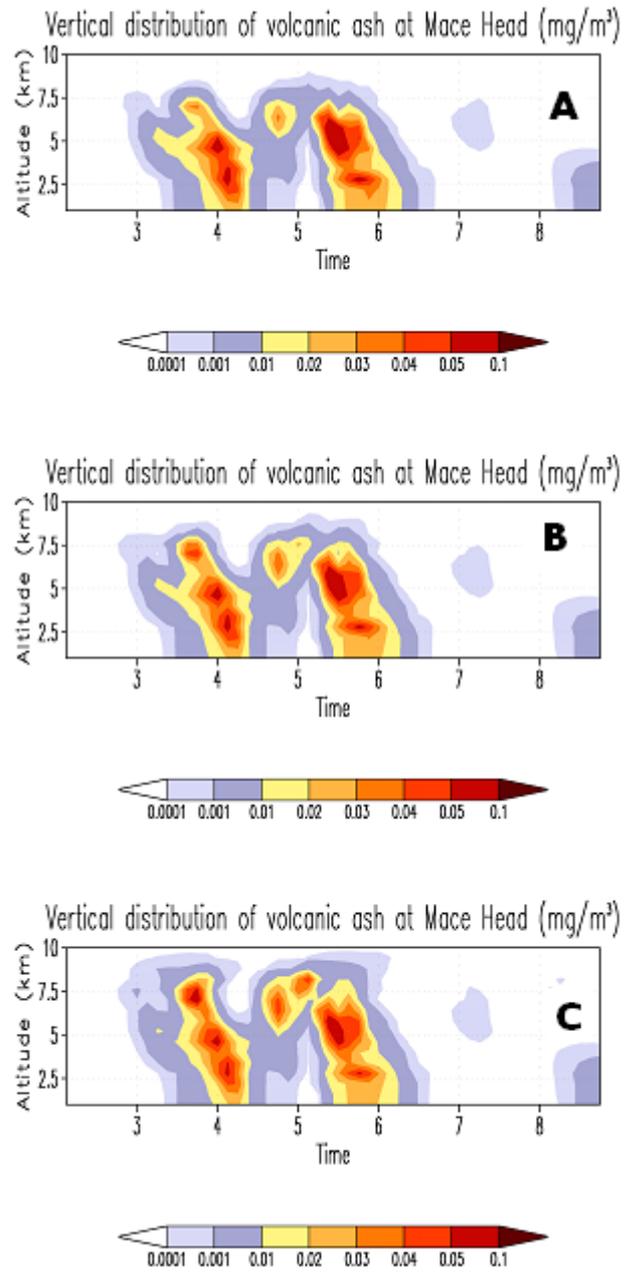


Figure 3.3. Changes in vertical distribution of volcanic ash by varying injection to 4.5 km (A) 5.4 km (B) and 6.5 km (C), whilst maintaining a constant mass flux

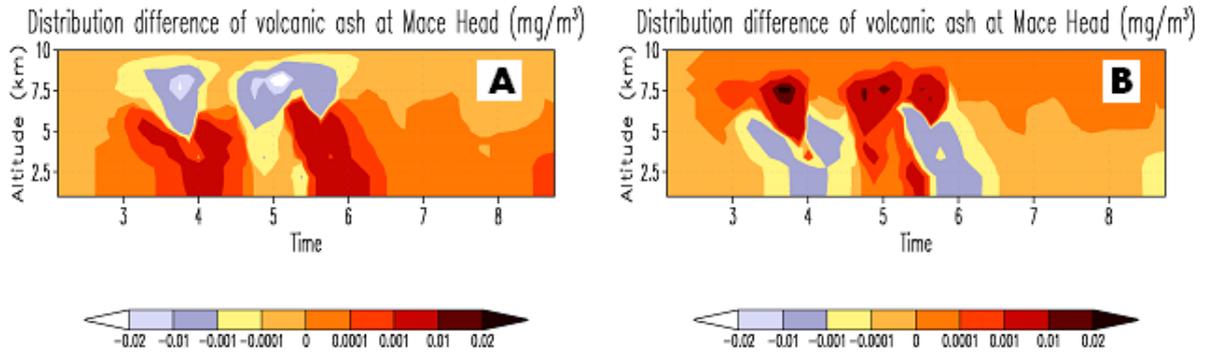


Figure 3.4. Difference plots for variable injection heights, whilst maintaining a constant mass flux. (A: 5.4 -6.5 km, B: 5.4 – 4.5 km)

The difference plots in Figure 3.4 show that volcanic ash tends to be suspended in the atmosphere for a longer time if released from a higher injection height, while higher deposition is noticed when released at lower heights, as can be seen around 4<sup>th</sup> and 6<sup>th</sup> May, 2010 at Mace Head.

A source of significant uncertainty in volcanic ash simulations is the best way to represent the vertical distribution of the ash. The REMOTE model allows a user-defined distribution of release points throughout the eruption column. Volcanoes have been observed to release a substantial fraction of their ash in the high-

altitude “umbrella region” of the eruptive column (where buoyancy between rising ash and the surrounding air is achieved) and it would seem realistic for ash to be modelled with greater emissions near the top of the column. Currently, the most advanced treatment of vertical release distributions is in the FALL3D model, which releases much of the ash in a Gaussian distribution over a daily constant height (Barcelona Supercomputing Centre, 2011). Subsequent analysis of the Icelandic eruption has indicated a large degree of variability in the vertical release distribution over short-time averages.

Significant difference is seen in the ash concentration of the two cases (Figures 3.5 and 3.6), where 50% of mass flux is released at the top level of the plume column and where 25%

each is released at the top two levels. The key differences are in the days from 4<sup>th</sup> – 6<sup>th</sup> May 2010.

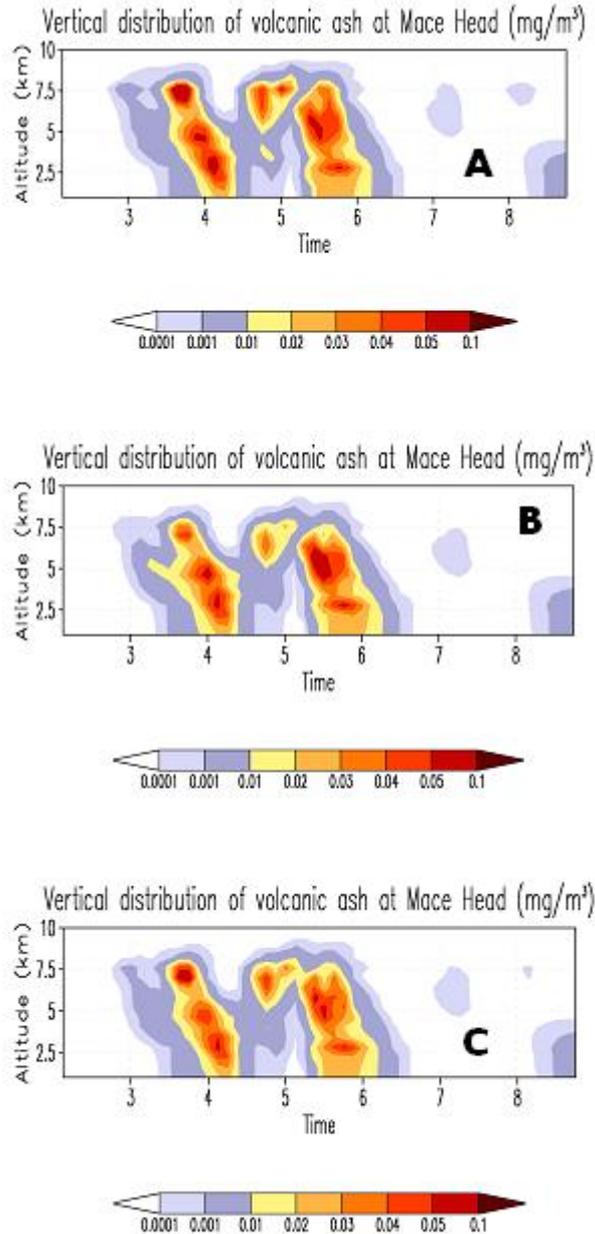


Figure 3.5. Changes in vertical distribution of volcanic ash by varying vertical release distribution, whilst maintaining a constant ash plume height (5.4 km)  
(A) 50% release at uppermost level  
(B) Equally distributed over the release height  
(C) 50% release in the two uppermost levels.

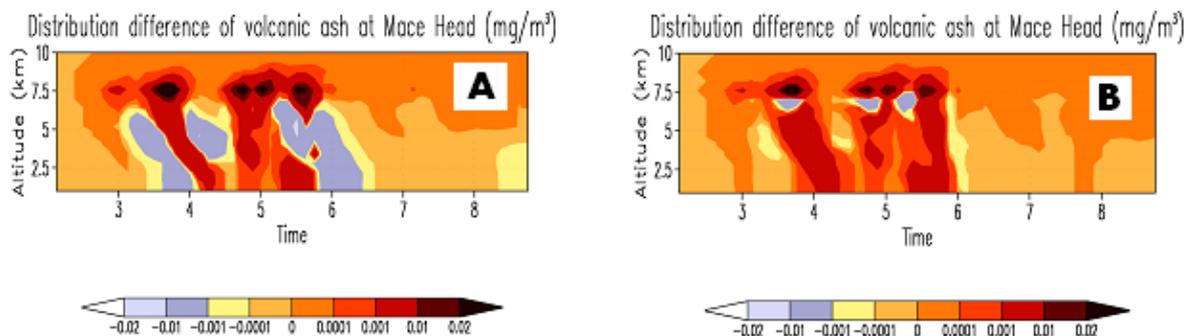


Figure 3.6. Difference plots for variable release distribution, whilst maintaining a constant mass flux and constant plume height  
 (A) 50% release at uppermost level - equally distributed over the release height  
 (B) 50% release at uppermost level - 50% release in the two uppermost levels.

These sensitivity studies illustrate the importance of the injection heights and the distribution of ash mass over these heights to the vertical and spatial dispersion of the ash cloud.

### 3.2.6 Model validation and verification

#### (i) Model evaluation and validation of *in-situ* plume physio-chemical characterisation data:

NUIG (National University of Ireland Galway) operates one of the most advanced aerosol monitoring supersites in Europe at Mace Head. The station provided important *in-situ* ash property data during the April and May volcanic events. For example, at Mace Head, the volcanic ash plume was encountered 33 times over a six-week period. Three to four of these events were

extremely strong ash events, lasting more than 12 hours in duration, and occurring in the cleanest of polar air masses. Thus, the characteristics of the plume could be quantified without contamination of other anthropogenic and/or dust sources. The plume characterisation available for model evaluation and verification include aerosol size distributions (number and mass), aerosol scattering and absorption properties, aerosol chemical composition from online mass spectrometry and off-line analytical techniques. [Figures 3.7](#) and [3.8](#) show a range of volcanic ash plume characterisation data measured during a volcanic ash event at Mace Head. These data are used to evaluate and verify model performance during these events.

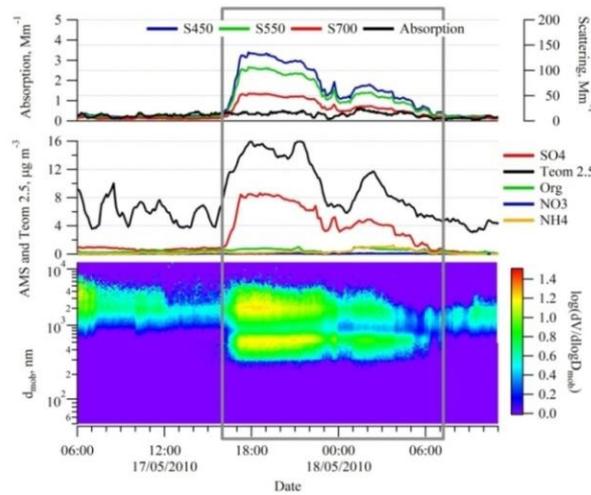


Figure 3.7. Example of the *Eyjafjallajökull* plume being intercepted at Mace Head 17<sup>th</sup>-18<sup>th</sup> May, 2010 for a 14 hour period. (Top) Aerosol absorption and scattering (450 nm, 550 nm and 700 nm wavelengths), (middle) PM<sub>2.5</sub>, sulphate (SO<sub>4</sub>), nitrate (NO<sub>3</sub>), ammonium (NH<sub>4</sub>) and organic (Org) aerosol mass, (bottom) bi-modal volumetric size distribution (modes at 750 nm and 450 nm).

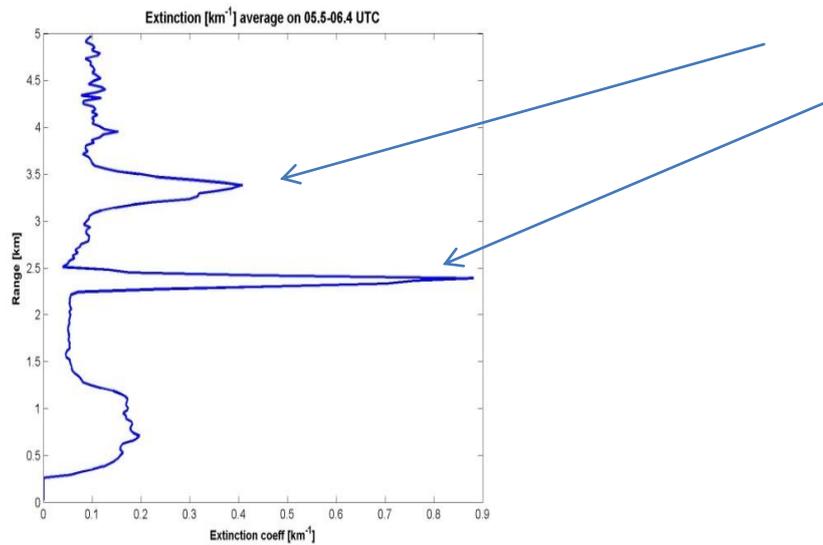


Figure 3.8. Vertical profile of ash plume extinction aloft at Mace Head prior to descending into the boundary layer. The peak at 2.4 km is a cloud layer, while the peak at 3.5 km is the ash cloud layer.

### 3.2.7 Automation

Meteorological boundary data for the model simulations have been obtained from the ECMWF ERA-Interim reanalysis database. The global European Centre for Medium-range Weather Forecasts (ECMWF) data are obtained on a 0.5°x0.5° regular latitude/longitude grid with

91 vertical levels. All the data fields are extracted and interpolated to the REMOTE regional model domain. Each step of the interpolation process has been checked and validated to ensure consistency with the original global data. [Figure 3.9](#) presents the general scheme for model automation.

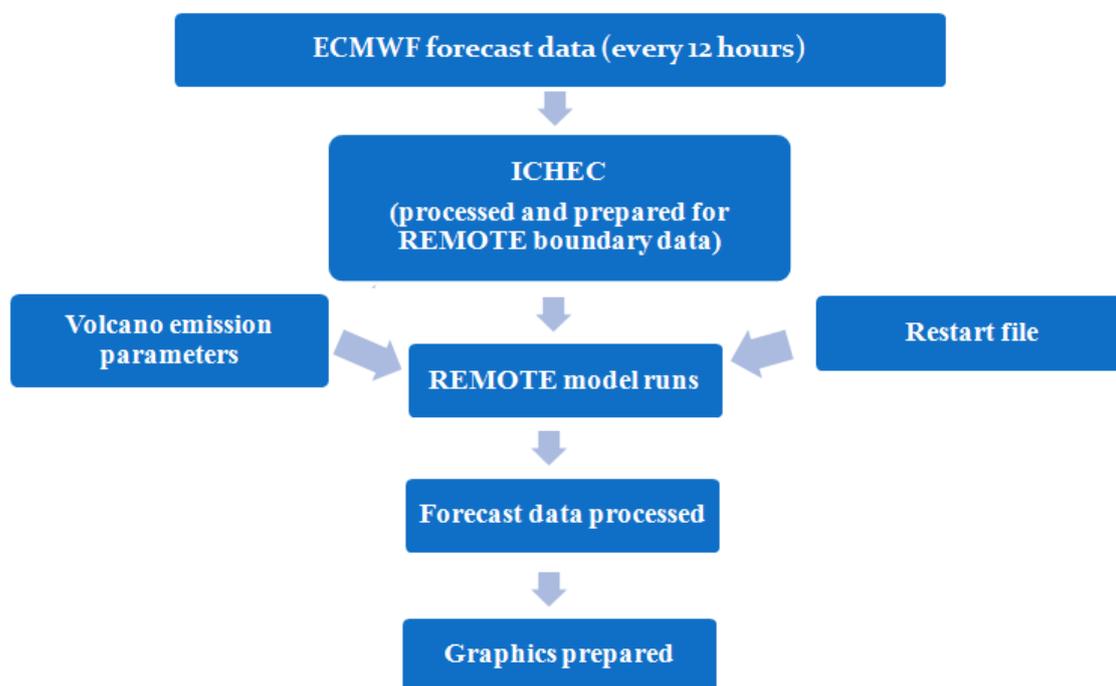


Figure 3.9. Flow system for REMOTE model automation

## 4. Air quality and volcanic ash forecasts

### 4.1 The WRF-Chem model

WRF-Chem is the Weather Research and Forecasting (WRF) model coupled with Chemistry (Grell et al., 2005). The model simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology. The model is used for investigation of regional-scale air quality, field programme analysis, and cloud-scale interactions between clouds and chemistry. The development of WRF-Chem is a collaborative effort among the community, whilst NOAA/ESRL (National Oceanic and Atmospheric Administration/Earth System Research Laboratory) scientists are the leaders of this project. The collaborative nature of this model means that development is rapid and on-going, with modules continuously being updated. Recent developments include improvements in cloud-aerosol interactions (Chapman et al., 2008), advances in emission pre-processors (Sakulyanontvittaya et al., 2008) and improvements in the treatment of secondary organic aerosol (Ahmadov et al., 2012).

Key features of the model are the following:

- fully compressible, non-hydrostatic
- vertical co-ordinate is based on normalised atmospheric pressure
- higher order advection schemes
- nesting of the domains
- can be run on a variety of platforms on single processor or with shared or distributed memory
- the software architecture makes it easy for the users to modify or develop the code

- can be run in a number of aerosol modes.

The predominant reason behind the adoption of this model has been that its performance against air quality (AQ) measurements across Europe has been comprehensively evaluated using available EMEP emission inventory (Tuccella et al., 2012). This provides a high degree of confidence that this model can perform well in an Irish context. Particular issues, such as the prevalence of sea-salt in Irish particulate matter and the ability of the model to replicate this, have been investigated.

### 4.2 Model set-up

For the purpose of this work package, a European domain based on a coarse grid that extends over Western Europe was used. The horizontal resolution is approximately 50 km and 29 vertical levels, which extend up to about 50hPa (about 20 km). The initial and boundary meteorological conditions by the European Centre for Medium-range Weather Forecast (ECMWF) analyse with a horizontal resolution of 0.5°. The chemical boundary conditions of trace gases consist of idealised, northern hemispheric, mid-latitude, clean environmental profiles based upon the results from the NOAA Aeronomy Lab Regional Oxidant Model (NALROM). The NALROM model simulates the chemistry with the lumped species which are separated into the individual model species of RADM2. The major processes and their parameterisations within the version of WRF-Chem are shown in [Table 4.1](#).

**Table 4.1. WRF-Chem model set-up**

Process	WRF-Chem
Microphysics	Lin
Long-wave radiation	RRTM
Short-wave radiation	Goddard
Surface layer	Monin-Obukhov
Land surface model	Noah LSM
Boundary layer scheme	MYNN Level 2.5 PBL
Cumulus parameterisation	Grell- Devcanyi
Photolysis scheme	Fast –J
Gas phase mechanism	RADM2
Aerosol model	MADE/SORGAM

### 4.3 Emissions and inventories

A number of options are available and for the demonstration period, the following emissions were used:

For SO<sub>2</sub> the researchers use EDGAR (Emissions Database for Global Atmospheric Research) global, annual dataset (for the default year 2005) at 0.1° resolution. This gives the high spatial resolution seen here. For other gaseous emissions, the researchers use 0.5° resolution emissions based on EMEP, while for BC (Black carbon) and OC (Organic Carbon), GOCART (Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport Model) emissions (1 x1°) are used. This isn't the optimal set up but it is what the researchers used for this prototype demonstration.

A pre-processor script was deployed for EMEP emissions and BC and OC emissions that applies a daily temporal species profile, speciates VOCs (Volatile Organic Compounds) according to model chemical mechanism speciation, and considers height dependence of point sources. The BC and OC emissions are total annual data emissions provided by the

Laboratoire d'aerologie ([www.aero.obs-mip.fr](http://www.aero.obs-mip.fr)) and are treated the same way as EMEP data.

The conversion factor used to convert the emissions of OC to OM (Organic Matter) is 1.6. SO<sub>2</sub> emissions will be split into 95% as SO<sub>2</sub> and 5% as particulate sulphate, the latter is distributed for 20% into nuclei mode and for 80% into the accumulation mode. PM<sub>2.5</sub> emissions are assigned to unspciated primary PM<sub>2.5</sub> model species, and also distribute for 20% into nuclei mode and for 80% into accumulation mode. Coarse PM emissions are assigned to PM<sub>10</sub> model species.

Anthropogenic emissions are taken from the EMEP data base ([www.ceip.at/emission-data-webdab/emissions-used-in-emep-models](http://www.ceip.at/emission-data-webdab/emissions-used-in-emep-models)), which provide a total of 2,007 annual emissions of nitrogen oxides (NO<sub>x</sub>), carbon monoxide (CO), sulphur oxides (SO<sub>x</sub>), ammonia (NH<sub>3</sub>), Non-Methane Volatile Organic Compounds (NMVOC), and particulate matter (PM<sub>2.5</sub> and coarse PM) over Europe with a resolution of 50 km for 11 source types (SNAP sectors) (Vestreng, 2003).

Total amount of NMVOC emissions is disaggregated into several species using UK

speciation profiles (Passant, 2002). Aggregation of NMVOC species into RADM2 model species is done in two steps, following the procedure proposed by Middleton et al. (1990). The NMVOC obtained from Passant speciation are first lumped on a mole-to-mole basis into 32 chemical groups according to their expected impact on oxidants and acid formation, and then aggregated into RADM2 model species, applying the reactivity weighting factor principle.

#### **4.4 Boundary meteorological conditions and chemical conditions**

There are a number of different options that can be utilised in order to generate boundary chemical conditions. The chemical boundary conditions of trace gases used here consist of idealised, northern hemispheric, mid-latitude, clean environmental profiles based upon the results from the NOAA Aeronomy Lab Regional Oxidant Model (NALROM).

#### **4.5 Volcanic ash simulations**

As well as air quality assessment, WRF-Chem offers the opportunity to study the dispersion of volcanic ash. There are a number of reasons why this model is preferred over REMOTE for volcanic ash simulations. These can be summarised as follows:

- more flexibility in the description of the size distribution (not constrained to a log normal distribution as in REMOTE)
- opportunity to run in a different number of modes depending on requirements
- more sophisticated treatment of in-cloud SO<sub>2</sub> oxidation
- fully parallelised (a forecast can be run on a number of processors simultaneously allowing for producing the forecast in a timely fashion).

##### ***4.5.1 Method***

In order to determine eruption source parameters during volcanic eruption events, the researchers use an emission pre-processing tool (Freitas et al., 2011) following the database developed by Mastin et al. (2009). This database provides a set of parameters to model volcanic ash cloud transport and dispersion during eruptions. This contains information on 1,535 volcanoes around the world comprising location (latitude, longitude and height) as well as the corresponding historical parameters of plume height, mass eruption rate, volume rate, duration of eruption and the mass fraction of erupted debris finer than about 63 µm.

##### ***4.5.2 Vertical emission distribution***

The emissions pre-processing tool provides the location of the volcano in the nearest model grid box and the emission parameters (i.e. mass eruption rate, plume height and time duration), if no other observations are given. This information is used within WRF-Chem to determine the vertical distribution of the erupted mass. Large volcanic plumes are typically “umbrella”-shaped (Sparks, 1997). The researchers use this umbrella shape observation – which may be modified by users – and assume that 75% of the erupted mass is detained in the umbrella cloud and 25% beneath, with a linear distribution from the umbrella to the vent. The base of the umbrella cloud is roughly located at 73% of the plume height.

##### ***4.5.3 Flux emission***

The total erupted mass is calculated using the corresponding erupted volume times the ash mass density, which is defined as 2,600 kg/m<sup>3</sup>. Then the total ash mass is distributed between 10 bins of aerosol particles, with diameter size range starting from 2 mm down to less than 3.9

$\mu\text{m}$ , using the corresponding percentage of mass derived from analysis of historic eruptions.

#### 4.5.4 Size distribution

For each bin, the aerodynamic radius, needed by the settling velocity calculation, is defined as half of the arithmetic mean between the limits of the diameters of each bin size:

- (1) The four finest ash species as invariant tracers that are being transported deposited and settled only.
- (2) A further option allows the selection of 10 ash variables, which also includes coarse ash species for estimates of ash fall.
- (3) The third option distinguishes only two different ash species by including the ash within the WRF-Chem particulate variables; this last option enables the

user to take advantage of all aerosol feedback processes implemented within WRF-Chem.

#### 4.6 Validation

The model was run over Europe for one month with ECMWF meteorological input data respectively. The model was run on a Lambert conformal grid with six hour time-steps. For air quality research, the model performance on wind direction, speed, and precipitation are the three most important parameters, so the validation should start with them. Output data from the model run was compared with observations over Ireland for the monthly averaged cumulative precipitation ([Figure 4.1](#)). Results show high agreement between the model and the observations; however the resolution is too low (50 km) to capture the sub-regional situations.

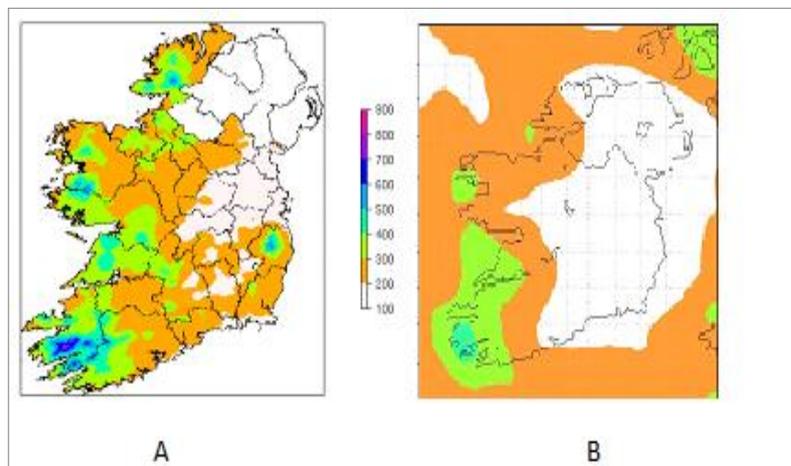


Figure 4.1. Observed monthly precipitation (A) 1 km x 1 km (Met Éireann) and modelled precipitation (B) 50 km x 50 km (WRF) for November 2009

[Figure 4.2](#) shows the comparison between the measured and modelled wind direction. A high correlation was found ( $R > 0.8$ ). It can also be

seen in [Figure 4.2](#) that north-western winds dominate throughout November.

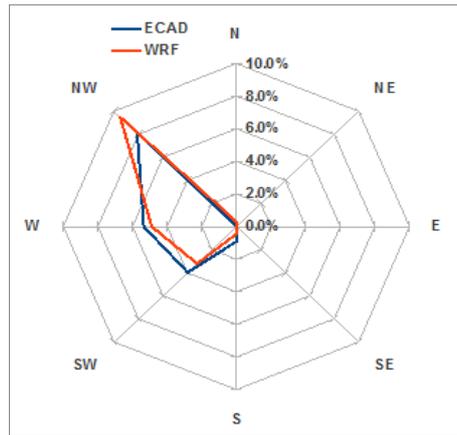


Figure 4.2. Observed monthly measured (ECAD) and modelled (WRF) wind direction for November 2009

Results for the ECWMF run on 10m temperature and wind speed are shown in [Figure 4.3](#). The model was run on the 25<sup>th</sup> of July in 2009 with interim reanalysis data. Despite the low

resolution, the model was successful in reproducing the temperature and wind patterns, as in the atmosphere over Europe and the north-east Atlantic.

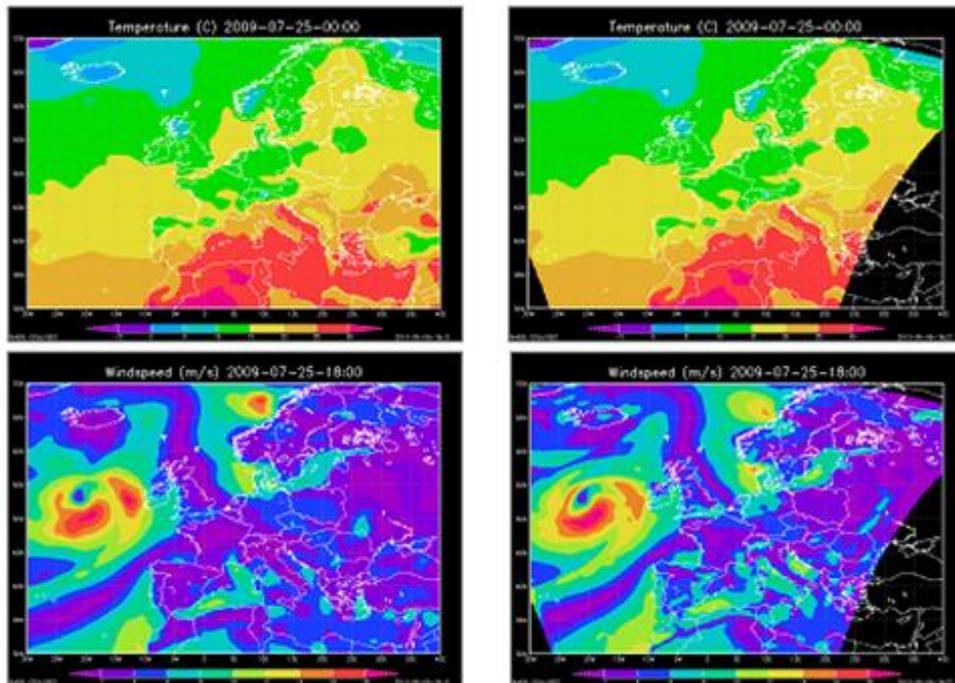


Figure 4.3. Observed (left) (ECMWF) and modelled (right) (WRF) temperature (top) and windspeed (bottom) over Europe on the 25<sup>th</sup> of July in 2009

From an Irish context, it is very important to understand the performance of this model WRF-Chem which was run over a European domain with two horizontal resolution (50 x 50 km, 25 x

25 km) and 29 vertical levels. A summer (July) and winter (December) month were run (12 days spin up time in each case) with ECMWF interim meteorological input data. The model was run on

a lambert conformal grid with one hour time-step using the GOCART (Chin et al., 2009) aerosol scheme. GOCART uses a sectional scheme for sea-salt with four bin sizes ( $\mu\text{m}$ ) (0.1-0.5, 0.5-1.5,

1.5-5, 5-10), and sea-salt fluxes are calculated as a function of wind speed (Gong et al., 2003). Results are shown in [Figures 4.4, 4.5, 4.6](#) and [4.7](#).

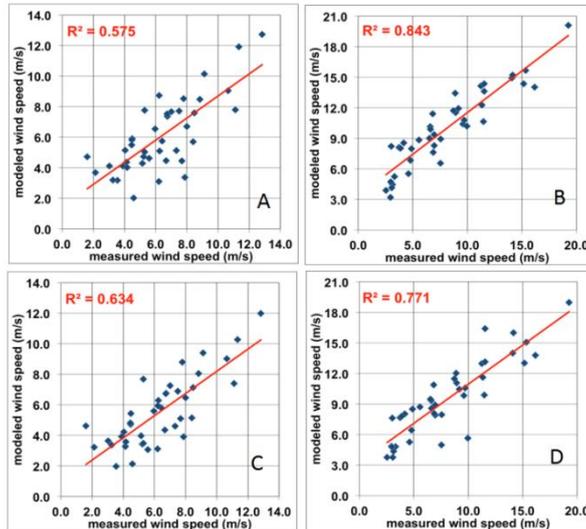


Figure 4.4. Measured and modelled wind speed (m/s) for Summer (July) (a) and Winter (December) (b) at 50 km resolution, and Summer (July) (c) and Winter (December) (d) at 25 km resolution at Mace Head

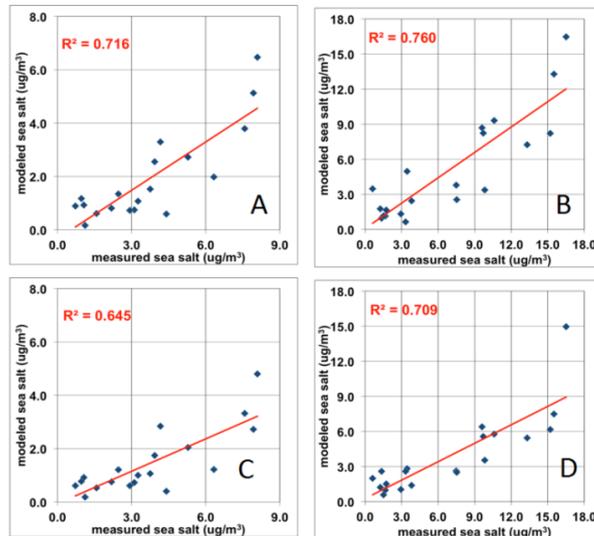


Figure 4.5. Measured and modelled  $\text{PM}_{10}$  sea-salt ( $\mu\text{g}/\text{m}^3$ ) for Summer (July) (a) and Winter (December) (b) at 50 km resolution, and Summer (July) (c) and Winter (December) (d) at 25 km resolution at Mace Head

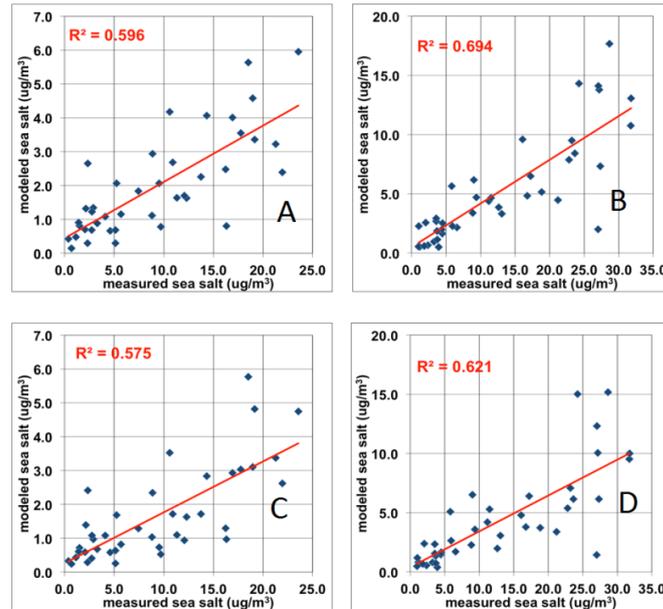


Figure 4.6. Measured and modelled total sea-salt ( $\mu\text{g}/\text{m}^3$ ) for Summer (July) (a) and Winter (December) (b) at 50 km resolution, and Summer (July) (c) and Winter (December) (d) at 25 km resolution for Carnsore Point

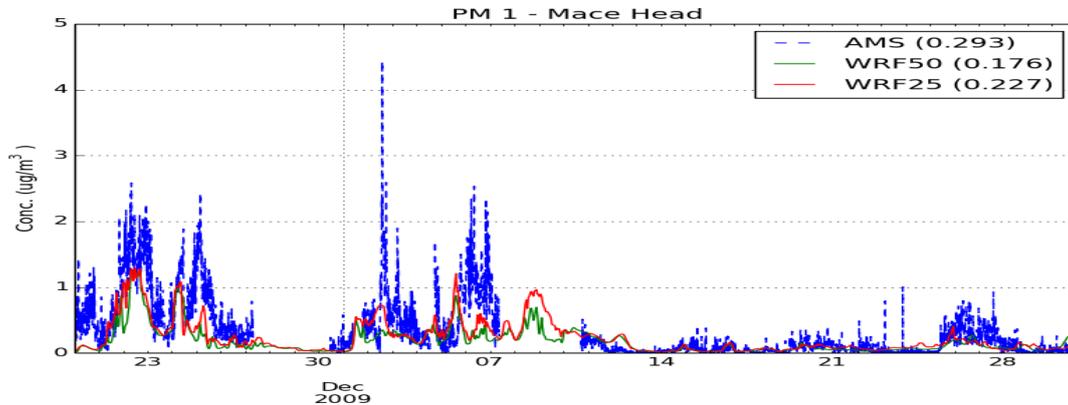


Figure 4.7. Time series of modelled (50 km and 25 km resolution) and measured sub-micron sea-salt measurements ( $\mu\text{g}/\text{m}^3$ ) for Mace Head

A provisional assessment of WRF-Chem’s ability to model sea-salt aerosol at two Irish coastal locations was undertaken at two different model resolutions. Results show a good correlation with measurements, which is in line with other state-of-the-art model performance. For total sea-salt aerosol,  $\text{PM}_{10}$  and  $\text{PM}_1$  (Particulate Matter of 1 Micron in diameter or smaller), there is a definite model under-estimation (resolution dependent)

which is more likely to be associated with sea-salt flux parameterisation, given the good agreement with wind speed. A more complete description of the model performance at Mace Head is shown in [Table 4.2](#).

**Table 4.2. Statistical evaluation of model performance for wind speed (m/s) and PM<sub>10</sub> sea-salt (µg/m<sup>3</sup>) at Mace Head**

		WIND			PM10		
		BIAS	RMS	R <sup>2</sup>	BIAS	RMS	R <sup>2</sup>
Summer	25km	-0.282	1.710	0.575	-1.806	2.208	0.716
	50km	-0.800	1.722	0.634	-2.282	2.755	0.645
Winter	25km	1.879	2.507	0.843	-1.817	3.151	0.760
	50km	1.396	2.441	0.771	-2.991	4.269	0.709

#### 4.7 Testing of operationally

As part of this work, the feasibility of operationally deploying the model for daily air quality forecasts was tested. The computational requirements of this model dictate running on multiple processors in order to deliver timely forecasts. The computational resources required to deliver these forecasts is routinely delivered by ICHEC (Irish Centre for High End Computing) as part of normal project access. This non-operational mode involves being part of a queuing system. ICHEC agreed to give a two-week operational period from 18<sup>th</sup> November 2013, where the normal queuing system was circumvented. The first few days of this period was used for internal testing and model initialisation, after which a series of daily 54 hour meteorological and air quality forecasts were delivered.

During the operational phase, forecasts of relevant meteorological parameters (wind speed and direction, precipitation, specific humidity and 2M temperature) were available from the Mace Head website:

[http://www.macehead.org/index.php?option=com\\_content&view=category&id=99:met-forecasts&Itemid=91&layout=default](http://www.macehead.org/index.php?option=com_content&view=category&id=99:met-forecasts&Itemid=91&layout=default)

whilst relevant air quality parameters were available from

[http://www.macehead.org/index.php?option=com\\_content&view=category&id=100:air-quality-forecasts&Itemid=91&layout=default](http://www.macehead.org/index.php?option=com_content&view=category&id=100:air-quality-forecasts&Itemid=91&layout=default)

Automated python scripts were developed in order to produce graphics for upload to the Mace Head website. Examples of uploaded graphics for meteorological and air quality parameters are shown in [Figures 4.8](#) and [4.9](#). The 2d animated forecasts for ozone over both the European and Irish domain is shown, as well as the time series at a number of Irish locations (Dublin, Galway and Mace Head), in the context of both WHO (World Health Organisation) guidelines and CAFE (Clean Air For Europe) Directive limits. This has clearly demonstrated that this product has the capability to be used by the relevant authorities for providing timely and reliable air quality forecasts.

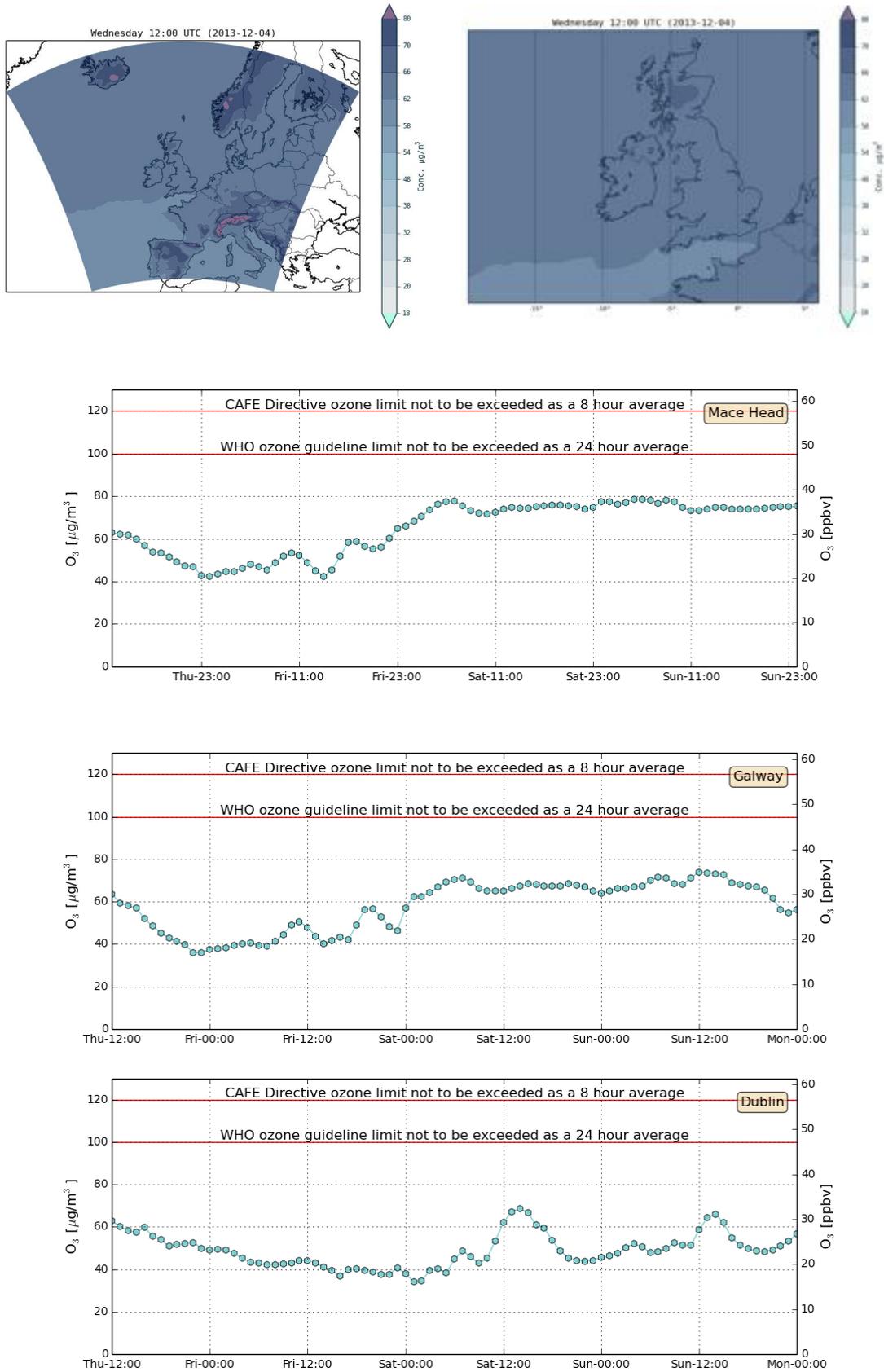


Figure 4.8. Screen shot of air quality forecast for ozone on the NUIG Mace Head webpage

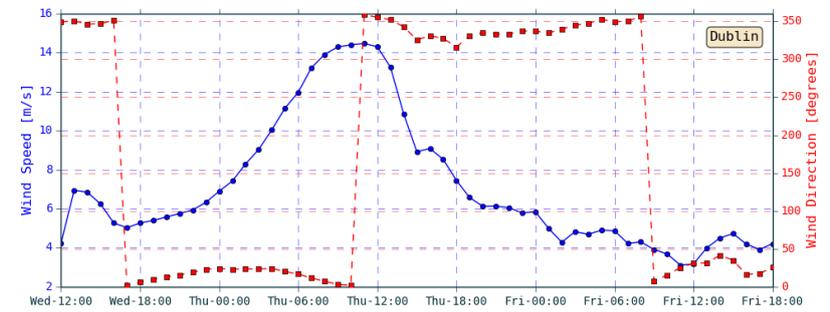
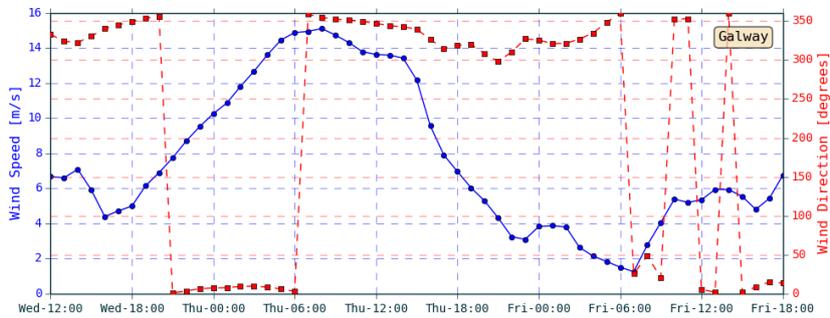
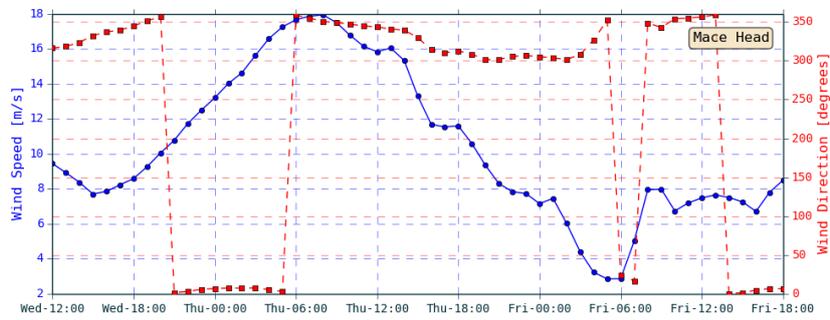
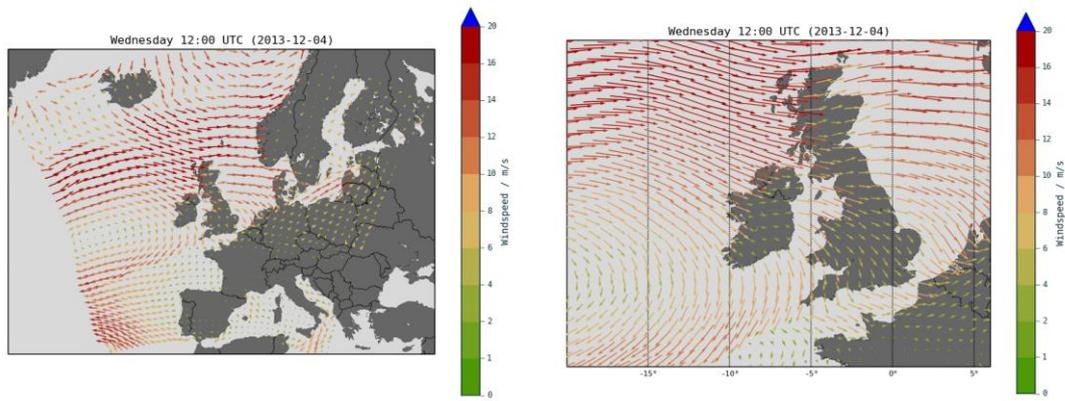


Figure 4.9. Screen shot of meteorological forecast (wind speed and direction) on the NUIG Mace Head webpage

## **5. Conclusions**

### **5.1 Air quality climate change interactions**

This research has investigated future levels of speciated components of ambient particulate matter under changing meteorology associated with an RCP emission storyline. In particular, the researchers look at future levels of ambient coarse and accumulation sea-salt, isoprene, isoprene SOA and sulphate under this changing meteorology. For coarse mode sea-salt, there is no clear trend in future levels under changing meteorology, with monthly mean value changing by no more than  $\pm 20\%$ . For accumulation mode sea-salt and the organic enrichment thereof, there is a clear increase in the trend of the level of organic enrichment under changes in meteorology and associated changes in chlorophyll-a.

Under this changing meteorology, it is apparent that there will be large changes over the European domain in ambient isoprene levels, which will also be reflected in changes in isoprene SOA levels which, in turn, will clearly have an effect on particulate matter loading. The data presented here suggest that future changes in meteorology with prescribed future anthropogenic aerosol emissions have an influence on SOA yields and size distributions. Monthly mean model domain total sulphate concentrations are seen to significantly decrease under prescribed emission scenarios, whilst the reductions over the Irish domain are offset by increasing sulphate levels associated with oceanic DMS emissions.

### **5.2 Volcanic ash simulations**

A forecasting system capable of near real-time volcanic ash forecasts over the European domain was developed during the course of this

project. The sensitivity of the model deployed to eruption parameters was investigated in order to optimise the model performance. A second model was deployed for volcanic ash simulations in order to improve simulations, by utilising a more complete description of volcanic ash size distribution and ash vertical distribution which improves the quality of forecasting.

### **5.3 Air quality and volcanic ash forecasts**

The operability of an air quality model within an Irish context, for delivery of near real-time air quality forecasting capability, has been demonstrated during this project. The system developed during this project, in conjunction with collaboration between ICHEC and Met Éireann, has proved itself capable of delivering near real-time air quality and meteorological forecasts within the Irish domain, and the infrastructure has shown itself to be robust and reliable during the test of operability. Validation of the model in relation to  $PM_{10}$  and submicron sea-salt at a number of Irish stations show good agreement with measurements. This validation, along with other published data on WRF-Chem performance over Europe (Tuccella et al., 2012), gives us a high degree of confidence in model capability. These data suggest that this model can be deployed successfully for operational forecasting and that further improvements can be made in order to further improve forecast accuracy. The model has also been adopted successfully to simulate volcanic ash emissions.

## **6. Recommendations**

### **6.1 Air quality climate change interactions**

- Understand further the effect of climate change on air quality by including a range of emission scenarios.
- Run simulations over larger time periods in order to better understand meteorological variability and its climatological effect on simulation results.
- Assess the direct and indirect effect of reducing anthropogenic aerosols on regional air quality.

### **6.2 Volcanic ash simulations**

- Develop further the capability of the volcanic ash forecasting system.
- Validate the model further using comparison with other European models harmonised across a number of historical European eruptions.
- Assess the effect of ash loss process (wet deposition, dry deposition and sedimentation) on the quality of volcanic ash forecasts.

### **6.3 Air quality and volcanic ash forecasts**

- It is recommended that this pilot demonstration is developed further, in order to facilitate permanent, fully automated, real-time air quality forecasting. This model also has the capability to provide real-time volcanic forecasts and this capability should be incorporated into real-time forecasting capability. Investment in this forecasting platform would significantly enhance Ireland's air quality modelling capability.

- Undertake a detailed comparison of the WRF-Chem model with the ongoing EPA-funded air quality modelling fellowship, which is based on statistical forecasting, and how these results can be interpreted in terms of performance relative to Air Quality Index for Health across the differing scales of these tangential approaches.
- Assess the possibility of assimilation of data from Ireland's monitoring network, in order to improve the quality and accuracy of forecasts.
- Increase the resolution of Irish emission inventory in order to maximise resolution of air quality forecasts. This would also require a development of the IT infrastructure network, in order to facilitate the timely production of high resolution air quality forecasts.
- Undergo a comprehensive on-going evaluation and validation with a large suite of available observations. This may include changes to inherent model processes, particularly important to air quality within an Irish context, i.e. sea-salt and organic carbon.
- Develop the model platform in order to incorporate radiological releases and other accidental releases.
- Develop other platforms for forecast dissemination, e.g. phone apps.
- Advance from the semi-automated operations process to a fully-automated process.
- Test different boundary layer parameterisations, chemical mechanisms, emission inventories and radiative feedback schemes, in order to optimise the model skill and scores in

the North-East Atlantic – Western Europe domain.

- Implement a new sea-spray source function with organic enrichment included.
- Test three aerosol models for optimal use in given domain.
- Optimise configuration on ICHEC to balance resources and timeliness. This would involve some scalability testing, as well as testing at higher horizontal and vertical resolutions.

## References

- Ahmadov, R., McKeen, S. A., Robinson, A. L., Bahreini, R., Middlebrook, A. M., de Gouw, J. A., Meagher, J., Hsie, E.-Y., Edgerton, E., Shaw, S., Trainer, M., 2012. A volatility basis set model for summertime secondary organic aerosols over the eastern U.S. in 2006, *J. Geophys. Res.*, doi: 10.1029/2011JD016831.
- Ansmann, A., Tesche, M., Gross, S., Freudenthaler, V., Seifert, P., Hiebsch, A., Schmidt, J., Wandinger, U., Mattis, I., Müller, D., Wiegner, M., 2010. The 16 April 2010 major volcanic ash plume over central Europe: EARLINET lidar and AERONET photometer observations at Leipzig and Munich, Germany, *Geophys. Res. Lett.*, 37, L13810, doi: 10.1029/2010GL043809, 12952.
- Barcelona Supercomputing Centre, 2011. 'Eyjafalla ash cloud modelling'. Webpage. <http://www.bsc.es/projects/earthscience/nube2010/>, Accessed February 20<sup>th</sup>, 2011.
- Chapman, E.G., Gustafson, Jr, W. I., Easter, R. C., Barnard, J. C., Ghan, S. J., Pekour, M. S., Fast, J. D., 2008. Coupling aerosols-cloud-radiative processes in the WRF-chem model: Investigating the radiative impact of large point sources, *Atmos. Chem. Phys.*, 9, 945-964.
- Chin, M., Diehl, T., Dubovik, O., Eck, T. F., Holben, B. N., Sinyuk, A., Streets, D. G., 2009. Light absorption by pollution, dust, and biomass burning aerosols: a global model study and evaluation with AERONET measurements, *Ann. Geophys.*, 27, 3439–3464, doi: 10.5194/angeo-27-3439-2009.
- Coleman, L., Martin, D., Varghese, S., 2013. Assessment of changing meteorology and emissions on air quality using a regional climate model: Impact on Ozone, *Atmospheric Environment*, 69, 198-210.
- Daly, A., Zannetti, P., 2007. Air Pollution Modelling – An Overview. Chapter 2 of AMBIENT AIR POLLUTION (Zannetti, P., Al-Ajmi, D. and Al-Rashed, S., Editors). Published by The Arab School for Science and Technology (ASST) and The EnviroComp Institute.
- EMEP, 2011. 'Eyjafjallajökull eruption'. Webpage. [https://wiki.met.no/emep/emep\\_volcano\\_plume#model\\_simulation/](https://wiki.met.no/emep/emep_volcano_plume#model_simulation/), Accessed February 20<sup>th</sup>, 2011.
- Flentje, H., Claude, H., Elste, T., Gilge, S., Köhler, U., Plass-Dülmer, C., Steinbrecht, W., Thomas, W., Werner, A. and Fricke, W., 2010. The Eyjafjallajökull eruption in April 2010 – detection of volcanic plume using in-situ measurements, ozone sondes and lidar-ceilometer profiles, *Atmos. Chem. Phys.*, 10, 10085–10092, doi:10.5194/acp-10-10085-2010.
- Freitas, S. R., Longo, K. M., Alonso, M. F., Pirre, M., Marecal, V., Grell, G., Stockler, R., Mello, R. F., Sanchez G., 2011. PREP-CHEM-SRC – 1.0: a preprocessor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models, *Geosci. Model Dev.*, 4, 419–433, doi: 10.5194/gmd-4-419-2011.
- Gong, S.L., 2003. A parameterization of sea-salt aerosol source function for sub- and super-micron particles, *Global Biogeochem. Cycles*, 17, 1097, doi: 10.1029/2003GB002079, 4.
- Grell, G. A., Peckham, S. E., McKeen, S., Schmitz, R., Frost, G., Skamarock, W. C., Eder, B., 2005. Fully coupled "online" chemistry within the WRF model, *Atmos. Environ.* 39, 6957–6975, doi: 10.1016/j.atmosenv.2005.04.027.
- Hofmann M., Worm B., Rahmstorf S., Schellnhube H.J., 2011. Declining ocean chlorophyll under unabated anthropogenic CO<sub>2</sub> emissions. *Environ. Res. Lett.* 6 (2011) 034035 (8pp) doi: 10.1088/1748-9326/6/3/034035.
- Kloster, S., Six, K.D., Feichter, J., Maier-Reimer, E., Roeckner, E., Wetzell, P., Stier, P., Esch, M., 2007. Response of dimethylsulfide (DMS) in the ocean and atmosphere to global warming. *J. Geophys. Res.* 112 (Seq. no. G03005).
- Langmann, B., 2000. "Numerical modelling of regional scale transport and photochemistry directly together with meteorological processes. *Atmospheric Environment* 34, 3585–3598.

- Mastin, L., Guffanti, M., Servranckx, R., Webley, P., Barsotti, S., Dean, K., Durant, A., Ewert, J., Neri, A. and Rose, W., 2009. A multi-disciplinary effort to assign realistic source parameters to models of volcanic ash-cloud transport and dispersion during eruptions, *J. Volcanol. Geoth. Res.*, 186, 10–21.
- Middleton, P., Stockwell W.R., Carter W.P.L., 1990. Aggregation and Analysis of Volatile Organic Compound Emissions for Regional Modeling, *Atmos. Environ.*, 24A, 1107-1133.
- Moss, R.H., Baribaker, M., Brinkman, S., Calvom, E., Carter, T., Edmonds, J., Elgizouli, I., Emori, S., Erda, L., Hibbard, K., Jones, R.L., Kainuma, M., Kellerher, J., Lamarque, J.F., Manning, M., Matthews, B., Meehl, J., Meyer, L., Mitchell, J., Nakicenovic, N., O'Neill, B., Pichs, R., Riahi, K., Rose, S., Runci, P., Stouffer, R., van Vuuren, D., Weyant, J., Wilbanks, T., van Ypersele, J.P., Zurek, M., 2007. Towards new scenarios for analysis of emissions, climate change, impacts, and response strategies, IPCC expert meeting report, 19–21 September, 2007, Noordwijkerhout, The Netherlands, 166 pp. (<http://www.aimes.ucar.edu/docs/IPCC.meetingreport.final.pdf>)
- Müller, K., 1999. A three year study of aerosol in northwest Saxony (Germany). *Atmospheric Environment* 33, 1679–1685.
- Nolan, P., Lynch P., Sweeney C., 2011. Simulating Climate Change and its Effects on the Wind Energy Resource of Ireland. *Wind Energy* 15, 593-608.
- Passant, N., 2002. Speciation of UK emissions of NMVOC, AEAT/ENV/0545, AEA Technology, London.
- Rosenstiel, T., Potosnak, M., Griffin, K., et al., 2003. Increased CO<sub>2</sub> uncouples growth from isoprene emission in an agriforest ecosystem, *Nature*, vol. 421, 256–259.
- Sakulyanontvittaya, T., Duhl, T., Wiedinmyer, C., Helmig, D., Matsunaga, S., Potosnak, M., Milford, J., Guenther, A., 2008. Monoterpene and Sesquiterpene Emission Estimates for the United States. *Environmental Science & Technology*, 42 (5), 1623–1629.
- Schwartz, J., Dockery, D.W., Neas, L.M., 1996. Is daily mortality associated specifically with fine particles? *Journal of the Air and Waste Management Association* 46, 927–939.
- Sparks, R. S. J., Bursik, M. I., Carey, S. N., Gilbert, J. S., Glaze, L. S., Sigurdsson, H., and Woods, A. W.: Volcanic Plumes, John Wiley & Sons, Inc., England, 574 pp., 1997. 5544, 5549.
- Squire, O. J., Archibald, A. T., Beerling, D. J., et al., 2014. Influence of future climate and cropland expansion on isoprene emissions and tropospheric ozone, *Atmospheric Chemistry and Physics*, Vol. 14, pp 1011-1024.
- Stier, P., Feichter, J., Kinne, S., Kloster, S., Vignati, E., Wilson, J., Ganzeveld, L., Tegen, I., Werner, M., Balkanski, Y., Schulz, M., Boucher, O., Minikin, A., Petzold, A., 2005. The aerosol-climate model ECHAM5-HAM. *Atmos. Chem. Phys.* 5, 1125 – 1156.
- Stockwell, W. R., Middleton, P., Chang, J. S., Tang, X., 1990. The second generation regional acid deposition model: chemical mechanism for regional air quality modelling. *J. Geophys. Res.*, 95, 16 343–16 367.
- Stohl, A., Prata, A. J., Eckhardt, S., Clarisse, L., Durant, A., Henne, S., Kristiansen, N. I., Minikin, A., Schumann, U., Seibert, P., Stebel, K., Thomas, H. E., Thorsteinsson, T., Tørseth, K., and Weinzierl, B., 2011. Determination of time- and height-resolved volcanic ash emissions for quantitative ash dispersion modeling: the 2010 Eyjafjallajökull eruption, *Atmos. Chem. Phys. Discuss.*, 11, 5541–5588, doi:10.5194/acpd-11-5541-2011.
- Tuccella, P., Curci, G., Visconti, G., Bessagnet, B., Menut, L., Park, R., 2012. Modeling of gas and aerosol with WRF/Chem over Europe: Evaluation and sensitivity study, *J. Geophys. Res.*, 117, D03303, doi: 10.1029/2011JD016302.
- Vaishya, A., Ovadnevaite, J., Bialek, J., Jennings, S. G., Ceburnis, D., O'Dowd, C. D., 2013. “Bistable effect of organic enrichment on sea spray radiative properties,” *Geophysical Research Letters*, Vol. 40, no. 24, pp 6395–6398.

Vestreng, V., (2003), Review and revision: Emission data reported to CLRTAP, EMEP/MSC-W Note 1/2003, 134 pp., Norw. Meteorol. Inst.,Oslo.  
[Available at [http://emep.int/publ/reports/2003/mscw\\_note\\_1\\_2003.pdf](http://emep.int/publ/reports/2003/mscw_note_1_2003.pdf).]

Vignati, E., Wilson, J., Stier, P., 2004. M7: An efficient size-resolved aerosol micro-physics module for large-scale aerosol transport models. *Journal of Geophysical Research* 109.

Wernand, M.R., van der Woerd H.J., Gieskes W.W.C.: 2013. Trends in Ocean Colour and Chlorophyll Concentration from 1889 to 2000, Worldwide. PLoS ONE, **8**, e63766.

Witham, C. S., Hort, M. C., Potts, R., Servranckx, R., Husson, P., and Bonnardot, F.: Comparison of VAAC atmospheric dispersion models using the 1 November 2004 Grimsvötn eruption, Meteor, Appl., 14, 27–38, 2007, 5544- 5561.

Zhang, Y., Huang, J.P., Henze, D.K., et al., 2007. Role of isoprene in secondary organic aerosol formation on a regional scale, *Journal of Geophysical Research-Atmospheres*, Vol. 112, Article ID D20207.

## **Acronyms**

AQ	Air Quality
AR5	Fifth Assessment Report
BC	Black Carbon
CAFE	Clean Air For Europe
CO	Carbon Monoxide
CO <sub>2</sub>	Carbon Dioxide
DMS	DiMethyl Sulphide
EC	Elemental Carbon
ECMWF	European Centre for Medium-Range Weather Forecasts
EDGAR	Emissions Database for Global Atmospheric Research
EMEP	European Monitoring and Evaluation Programme
EPA	Environmental Protection Agency
GOCART	Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport Model
ICHEC	Irish Centre for High End Computing
IES	Institute of Earth Sciences
IMO	Icelandic Meteorological Office
IPCC	Intergovernmental Panel on Climate Change
NALROM	NOAA Aeronomy Lab Regional Oxidant Model
NAME	Numerical Atmospheric-dispersion Modelling Environment
NH <sub>3</sub>	Ammonia
NH <sub>4</sub>	Ammonium
NMVOC	Non-Methane Volatile Organic Compounds
NO <sub>3</sub>	Nitrate
NO <sub>x</sub>	Nitrogen Oxides
NOAA/ESRL	National Oceanic and Atmospheric Administration / Earth System Research Laboratory
NUIG	National University of Ireland Galway
OC	Organic Carbon
OM	Organic Matter
Org	Organic
PM	Particulate Matter
PM <sub>1</sub>	Particulate Matter of 1 Micron in diameter or smaller
PM <sub>2.5</sub>	Particulate Matter of 2.5 Microns in diameter or smaller
PM <sub>10</sub>	Particulate Matter of 10 Microns in diameter or smaller
Pptv	Parts per Trillion by volume
RADM 2	Regional Acid Deposition Mechanism - Version 2
RACM 2	Regional Atmospheric Chemistry Mechanism - Version 2
RCP	Representative Concentration Pathways
REMOTEX	Regional Model with Tracer Extension
RH	Relative Humidity
SOA	Secondary Organic Aerosol
SO <sub>2</sub>	Sulphur Dioxide
SO <sub>4</sub>	Sulphate
SO <sub>x</sub>	Sulphur Oxides
SRES	Special Report on Emissions Scenarios
VAAC	Volcanic Ash Advisory Centre
VOCs	Volatile Organic Compounds
WRF-Chem	Weather Research and Forecasting – Chemistry
WHO	World Health Organisation

## List of Figures

Figure 2.1. REMOTE primary domain with Irish sub-domain (highlighted in grey scale), in which regional analysis is performed

Figure 2.2. Monthly mean coarse mode sea-salt concentrations normalised to 2006 values for both (A) the full model domain and (B) the Irish domain

Figure 2.3. Monthly mean accumulation mode organic carbon concentrations normalised to 2006 values for both (A) the full model domain and (B) the Irish domain and Monthly mean accumulation mode sea-salt concentrations normalised to 2006 values for both (C) the full model domain and (D) the Irish domain (2100' – 2100 meteorology with 2006 emissions)

Figure 2.4. Monthly mean isoprene ground level mixing ratio (pptv) for January and August (2006, 2030, 2050, and 2100)

Figure 2.5. Changes in monthly mean 2metre temperature for 2050 and 2100 relative to 2006

Figure 2.6. Ground level isoprene monthly mean concentrations for full model domain (A) and the Irish model sub-domain (B) (2100' – 2100 meteorology with 2006 emissions)

Figure 2.7. Ground level isoprene SOA monthly mean concentrations for full model domain (A) and the Irish sub-domains (B) relative to 2006 (2100' – 2100 meteorology with 2006 emissions)

Figure 2.8. (a1-f2): Monthly mean aitken, accumulation and coarse mode mass (a,b,c for SOA1) and (d, e f for SOA2) for full model domain (1) and Irish domain (2) relative to 2006 values (2100' - is the year 2100 ran with 2006 emissions)

Figure 2.9. Total monthly mean sulphate concentrations for full model domain (A) and Irish domain (B) for the simulation years (2100' = 2100 meteorology with 2006 emissions)

Figure 2.9. (a-f) Total monthly mean sulphate aitken, accumulation and coarse mode concentrations for full model domain (a,c,e) and Irish domain (b,d,f) (2100' refers to 2100 meteorology with 2006 emissions)

Figure 3.1. Satellite image of 2010 Eyjafjallajökull volcanic eruption (Source: Iceland Volcano, May 2010, ESA – Envisat – MERIS)

Figure 3.2. REMOTE extended domain

Figure 3.3. Changes in vertical distribution of volcanic ash by varying injection to 4.5 km (A) 5.4 km (B) and 6.5 km (C), whilst maintaining a constant mass flux

Figure 3.4. Difference plots for variable injection heights, whilst maintaining a constant mass flux. (A: 5.4 - 6.5 km, B: 5.4 – 4.5 km)

Figure 3.5. Changes in vertical distribution of volcanic ash by varying vertical release distribution, whilst maintaining a constant ash plume height (5.4 km)

- (A) 50% release at uppermost level
- (B) Equally distributed over the release height
- (C) 50% release in the two uppermost levels.

Figure 3.6. Difference plots for variable release distribution whilst maintaining a constant mass flux and constant plume height

- (A) 50% release at uppermost level - equally distributed over the release height
- (B) 50% release at uppermost level - 50% release in the two uppermost levels.

Figure 3.7. Example of the *Eyjafjallajökull* plume being intercepted at Mace Head 17<sup>th</sup>-18<sup>th</sup> May, 2010 for a 14 hour period. (Top) Aerosol absorption and scattering (450 nm, 550 nm and 700 nm wavelengths), (middle) PM<sub>2.5</sub>, SO<sub>4</sub>, Organic, NO<sub>3</sub>, and NH<sub>4</sub> aerosol mass, (bottom) bi-modal volumetric size distribution (modes at 750 nm and 450 nm).

Figure 3.8. Vertical profile of ash plume extinction aloft at Mace Head prior to descending into the boundary layer. The peak at 2.4 km is a cloud layer, while the peak at 3.5 km is the ash cloud layer.

Figure 3.9. Flow system for REMOTE model automation

Figure 4.1. Observed monthly precipitation (A) 1 km x 1 km (Met Éireann) and modelled precipitation (B) 50 km x 50 km (WRF) for November 2009

Figure 4.2. Observed monthly measured (ECAD) and modelled (WRF) wind direction for November 2009

Figure 4.3. Observed (left) (ECMWF) and modelled (right) (WRF) temperature (top) and windspeed (bottom) over Europe on the 25<sup>th</sup> of July in 2009

Figure 4.4. Measured and modelled wind speed (m/s) for Summer (July) (a) and Winter (December) (b) at 50 km resolution, and Summer (July) (c) and Winter (December) (d) at 25 km resolution at Mace Head

Figure 4.5. Measured and modelled PM<sub>10</sub> sea-salt ( $\mu\text{g}/\text{m}^3$ ) for Summer (July) (a) and Winter (December) (b) at 50 km resolution, and Summer (July) (c) and Winter (December) (d) at 25 km resolution at Mace Head

Figure 4.6. Measured and modelled total sea-salt ( $\mu\text{g}/\text{m}^3$ ) for Summer (July) (a) and Winter (December) (b) at 50 km resolution, and Summer (July) (c) and Winter (December) (d) at 25 km resolution for Carnsore Point

Figure 4.7. Time series of modelled (50 km and 25 km resolution) and measured sub-micron sea-salt measurements ( $\mu\text{g}/\text{m}^3$ ) for Mace Head

Figure 4.8. Screen shot of air quality forecast for ozone on the NUIG Mace Head webpage

Figure 4.9. Screen shot of meteorological forecast (wind speed and direction) on the NUIG Mace Head webpage

## **List of Tables**

Table 4.1. WRF-Chem model set-up

Table 4.2 Statistical evaluation of model performance for wind speed (m/s) and PM<sub>10</sub> sea-salt ( $\mu\text{g}/\text{m}^3$ ) at Mace Head

# Environmental Protection Agency

The Environmental Protection Agency (EPA) is a statutory body responsible for protecting the environment in Ireland. We regulate and police activities that might otherwise cause pollution. We ensure there is solid information on environmental trends so that necessary actions are taken. Our priorities are protecting the Irish environment and ensuring that development is sustainable.

The EPA is an independent public body established in July 1993 under the Environmental Protection Agency Act, 1992. Its sponsor in Government is the Department of the Environment, Community and Local Government.

## OUR RESPONSIBILITIES

### LICENSING

We license the following to ensure that their emissions do not endanger human health or harm the environment:

- waste facilities (e.g., landfills, incinerators, waste transfer stations);
- large scale industrial activities (e.g., pharmaceutical manufacturing, cement manufacturing, power plants);
- intensive agriculture;
- the contained use and controlled release of Genetically Modified Organisms (GMOs);
- large petrol storage facilities;
- waste water discharges;
- dumping at sea.

### NATIONAL ENVIRONMENTAL ENFORCEMENT

- Conducting over 1200 audits and inspections of EPA licensed facilities every year.
- Overseeing local authorities' environmental protection responsibilities in the areas of - air, noise, waste, waste-water and water quality.
- Working with local authorities and the Gardaí to stamp out illegal waste activity by co-ordinating a national enforcement network, targeting offenders, conducting investigations and overseeing remediation.
- Prosecuting those who flout environmental law and damage the environment as a result of their actions.

### MONITORING, ANALYSING AND REPORTING ON THE ENVIRONMENT

- Monitoring air quality and the quality of rivers, lakes, tidal waters and ground waters; measuring water levels and river flows.
- Independent reporting to inform decision making by national and local government.

### REGULATING IRELAND'S GREENHOUSE GAS EMISSIONS

- Quantifying Ireland's emissions of greenhouse gases in the context of our Kyoto commitments
- Implementing the Emissions Trading Directive, involving over 100 companies who are major generators of carbon dioxide in Ireland.

### ENVIRONMENTAL RESEARCH AND DEVELOPMENT

- Co-ordinating research on environmental issues (including air and water quality, climate change, biodiversity, environmental technologies).

### STRATEGIC ENVIRONMENTAL ASSESSMENT

- Assessing the impact of plans and programmes on the Irish environment (such as waste management and development plans).

### ENVIRONMENTAL PLANNING, EDUCATION AND GUIDANCE

- Providing guidance to the public and to industry on various environmental topics (including licence applications, waste prevention and environmental regulations).
- Generating greater environmental awareness (through environmental television programmes and primary and secondary schools' resource packs).

### PROACTIVE WASTE MANAGEMENT

- Promoting waste prevention and minimisation projects through the co-ordination of the National Waste Prevention Programme, including input into the implementation of Producer Responsibility Initiatives.
- Enforcing Regulations such as Waste Electrical and Electronic Equipment (WEEE) and Restriction of Hazardous Substances (RoHS) and substances that deplete the ozone layer.
- Developing a National Hazardous Waste Management Plan to prevent and manage hazardous waste.

### MANAGEMENT AND STRUCTURE OF THE EPA

The organisation is managed by a full time Board, consisting of a Director General and four Directors.

The work of the EPA is carried out across four offices:

- Office of Climate, Licensing and Resource Use
- Office of Environmental Enforcement
- Office of Environmental Assessment
- Office of Communications and Corporate Services

The EPA is assisted by an Advisory Committee of twelve members who meet several times a year to discuss issues of concern and offer advice to the Board.

# EPA Research Report 147

## Modelling air quality, climate change and volcanic ash



### Identifying Pressures

This research identifies environmental pressures by assessing future changes in pollutant composition associated with climate change emission scenarios. It also has the possibility to identify potentially dangerous/troublesome levels of volcanic ash associated with volcanic eruptions. Environmental pressures associated with changing levels of air quality pollutants are also identified.

### Informing Policy

This research informs policy and decision making by:

- Quantifying future changes in Irish air quality associated with climate change emissions scenarios
- Providing air quality forecasts over the Irish domain and its relationship with air quality guidelines.
- Allowing timely forecasts of volcanic ash dispersion in the instance of an eruption event and their context within the regulatory guidelines.

### Developing Solutions

This research has developed a forecasting platform which has the capability within an Ireland context to inform the public and relevant authorities of future levels of air quality pollutants and volcanic ash dispersion. This tool can be used to assess the response of changes in emissions and Irish Air Quality as well as be used to minimise the effect of future volcanic ash events on the aviation industry.

