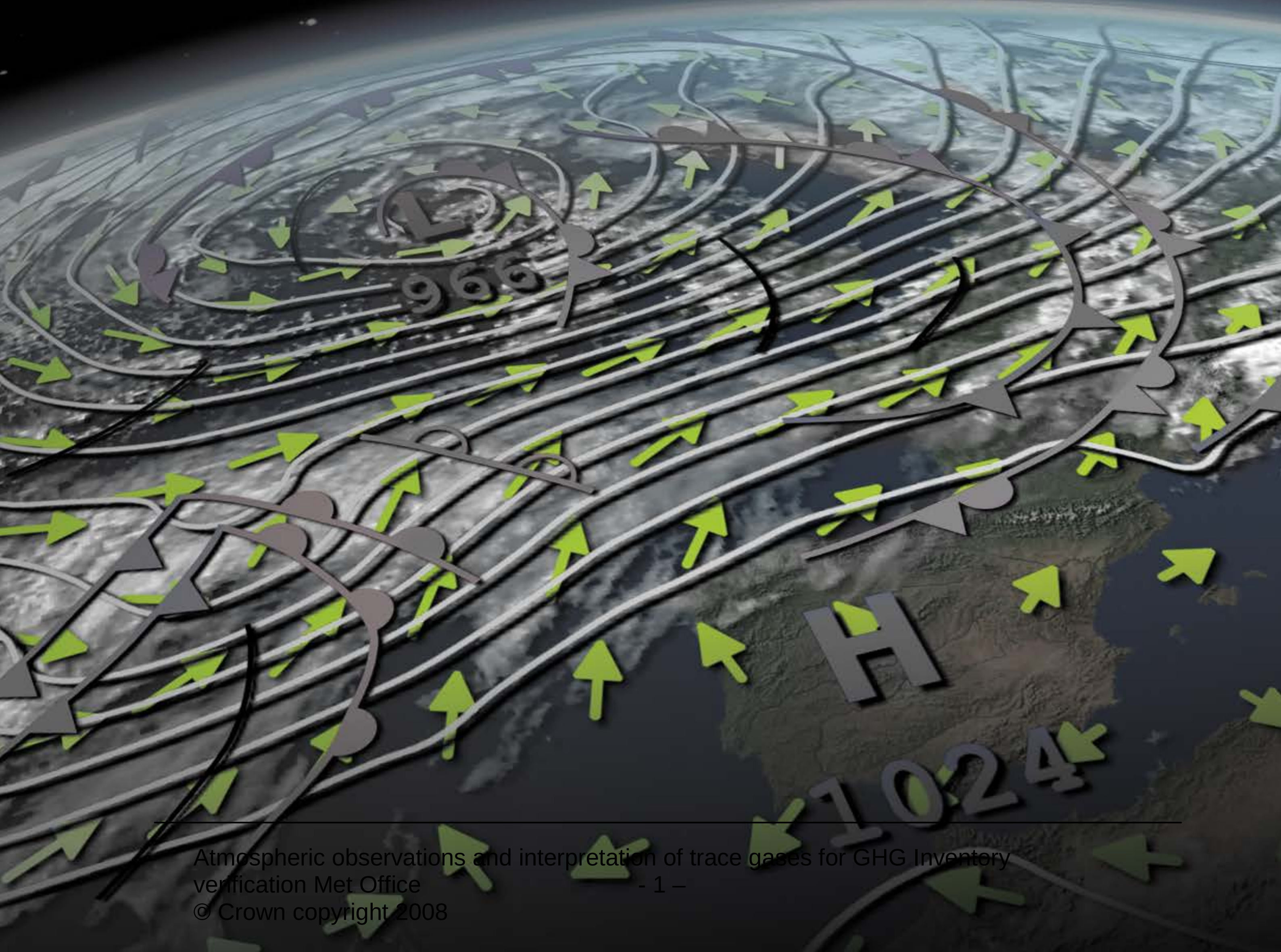
Met Office

Atmospheric observations and interpretation of trace gases, for GHG Inventory verification

Reference: 1028/06/2015

For: Department of Energy & Climate Change

Extract from TENDER Documents



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NOTE: This extract is taken from a Proposal submitted to DECC in response to an Invitation to Tender. As such the language used relates to a proposal, however it should be noted that Met Office have now been awarded this work by DECC.

Executive summary

This tender seeks three years of funding for the verification of the UK GHG inventory through, so called, 'top-down' inversion modelling.
The objectives of this LOT are numbered 3-7 in the ITT and are listed here:

3. To distinguish between those measurements that represent 'baseline' ambient gas concentrations and those that represent pollution events from the UK or elsewhere.
4. Modelling of UK emissions, split by gas, based on observed concentrations and their spatial distribution. This must include an analysis of uncertainty, along with a detailed description of the types and sources of uncertainty identified. Further consideration of the methods used to expand and improve the verification process should be considered.
5. To produce comparisons of resulting emissions estimates with UK GHG inventory emissions estimates, and investigate the reasons for differences.
6. Analysis of spatially disaggregated emission maps from the GHG Inventory in combination with modelled station data. This will likely use the geographical origin of emission events to identify likely sources and therefore identify drivers of discrepancies highlighted by the verification process.
7. To make atmospheric concentration observation data for the gases included publically available for the purpose of ongoing research, and to publish reports on the project's results and findings.

We propose to principally use a Lagrangian atmospheric transport model and inversion system to enable estimates of UK emissions to be calculated independent of the inventory process for all of the gases named in the ITT for all years 1990-current (where observations allow).
We will also utilise the output from two global models to investigate the provision of boundary conditions for the regional inversion modelling. The team has strong experience in the latest science of CO_2 inversion modelling, the latest science in the use of GHG satellite observations, cutting edge inversion modelling systems and uncertainty quantification, and the UNFCCC inventory process. The combination of these skills will enable the team to deliver a comprehensive response to DECC's verification requirements. Over the course of the contract we will:

- Calculate independent estimates of annual UK emissions of all of the gases specified in the tender using all observations within the UK DECC network independent of prior inventory estimates and with a comprehensive description of the uncertainty for each gas. For comparison, inversions will also be reported that use just MHD observations and also that use prior inventory estimates.

- Compare the inversion estimates and uncertainties with those reported by the UK to the UNFCCC, write a verification annex for inclusion to the UK submission to the UNFCCC and investigate differences between the inventory and the inversion estimates.
- Keep DECC informed of the latest science and developments in CO_2 inversions and the use of satellite observations in inversion modelling.
- Report on the global trends of emissions of the principal Kyoto basket of gases.
- Explore and implement improvements to the current inversion system.
- Where identified, further our understanding of why differences exist between the inversion estimates and the inventory and explore how the inversion results can be used to better inform the inventory process.

Contents

Met Office

Conflict of interest:

Conflict of interest declarations are contained in the declarations section at the end of this document. (REDACTED)
It is confirmed that there are no known conflicts of interest arising from this proposal of work.

Understanding requirement:

Specific aspects that will be considered: Knowledge of the reporting requirements to which the UK's GHG Inventory is subject; understanding of the key priorities of DECC in seeking to verify its inventory; and, consideration of the global context in which this data collection and analysis is useful.

Methodology:

PROPOSED MODELLING SYSTEMS

Met Office Unified Model

The NAME model utilizes the three dimensional meteorological information from the UK Met Office's Numerical Weather Prediction model, the Unified Model (UM). The UM is the operational weather forecast model and is also applied to climate change studies, so works at scales from hours to centuries. The UM is operationally run at global (17 km), regional (4 km) and high resolution (1.5 km) and is under constant review and improvement and is one of the world's leading forecast and climate models.

NAME

NAME (Numerical Atmospheric dispersion Modelling Environment) is the UK Met Office's Lagrangian (parcel) atmospheric transport model [*Jones et al.,* 2007] and is a world leading system that is operationally employed by the UK government to respond to a very wide range of atmospheric dispersion applications including volcanic ash, dust, fire plumes, nuclear accidents and biological releases such as foot and mouth virus and midges carrying bluetongue disease [*Gloster et al.*, 2007; *Leadbetter et. al.*, 2011, *Ryall et al.*, 1998, *Witham and Manning*, 2007; *Leadbetter et al*, 2015]. It is actively developed and improved and is widely used across the UK research community. It principally uses the UM three-dimensional meteorological fields but also three-dimensional fields from other world leading meteorological datasets e.g. ECMWF (European Centre for Medium Range Weather Forecasting).

InTEM

The UK and European emission estimates would be made using a sophisticated inversion methodology referred to as InTEM (Inversion Technique for Emission Modelling) and described in detail in *Manning et. al.*, (2011) and previously in *Manning et al.* (2003), and briefly here with a focus on the developments since 2010. The methodology is flexible in that where observations (and uncertainties) are available from other additional monitoring stations they can be readily incorporated into the inversion system to better constrain the location of the source regions, thus improving the estimated emissions. This flexibility has been readily demonstrated in our work within the EU project, InGOS, and previously in NitroEurope and also in the NERC project, GAUGE. The Met Office is one of the five inversion modelling groups involved in InGOS. Figure 1 shows an example from GAUGE of the InTEM estimated emissions of UK CH_4 for 2014 incorporating 9 high-frequency stations distributed across the UK. The work within GAUGE, InGOS and previously in NitroEurope has clearly demonstrated the need for strongly inter-calibrated and inter-comparable measurements, biases in any of the systems leads to systematic errors in the inversion results. One of the key points is that all observations from across the network are regularly and systematically inter-compared with those from Mace Head to ensure an un-biased data set of observations.

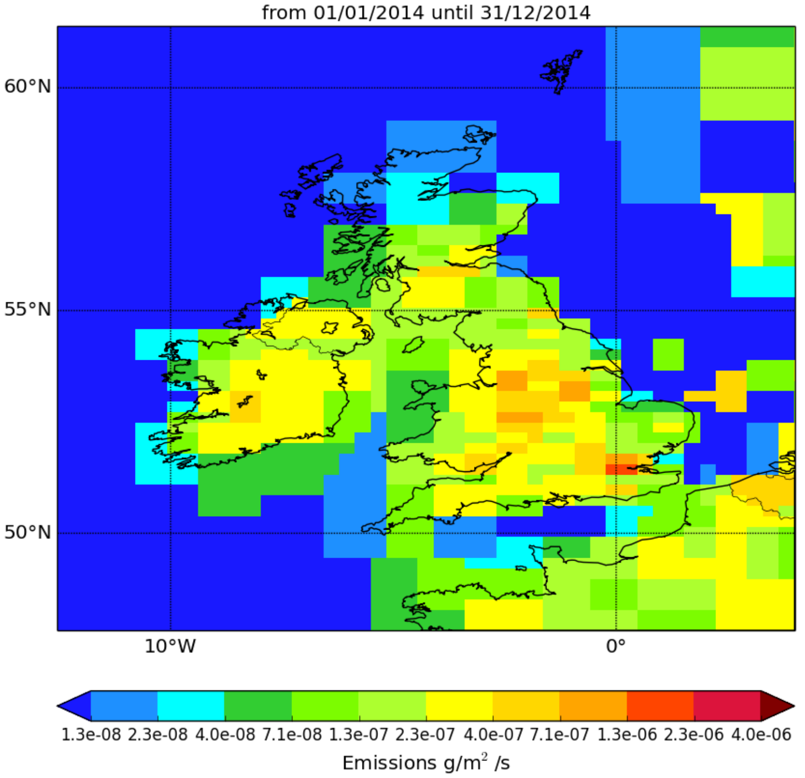


Figure 1: Estimated emissions of CH_4 using nine high-frequency stations for 2014 as part of the GAUGE project.

The observations will be averaged (where the frequency of observation is greater than 2 hours) over each two-hour period and the standard deviation of the observations over the two hours will be used as part of the observational uncertainty. These observed deviations above baseline are assumed to be caused by emissions on regional scales that have yet to be fully mixed on the hemisphere scale.
The observation time series, together with the NAME model output predicting the recent history and dilution of the air, will be used to estimate the emission distributions. The iterative best-fit technique, simulated annealing (Press *et al.,* 1992), will be used to derive these regional emission estimates based on a statistical skill score (cost function) comparing the observed and modelled time-series at each observation site. In this contract we propose to use two different but related cost function (CF1 and CF2) as described by equations 1 and 2 that have been used extensively in the current contract and a wide range of inverse modelling frameworks (e.g. *Bergamaschi et al.*, 2015, *Rigby et al.*, 2011).

CF1: $cost = (Me + fb - y)^T R^{-1} (Me + fb - y)$ Equation 1

CF2: $\text{cost} = (Me + fb - y)^T R^{-1} (Me + fb - y) + (e - e_p)^T B^{-1} (e - e_p)$ Equation 2

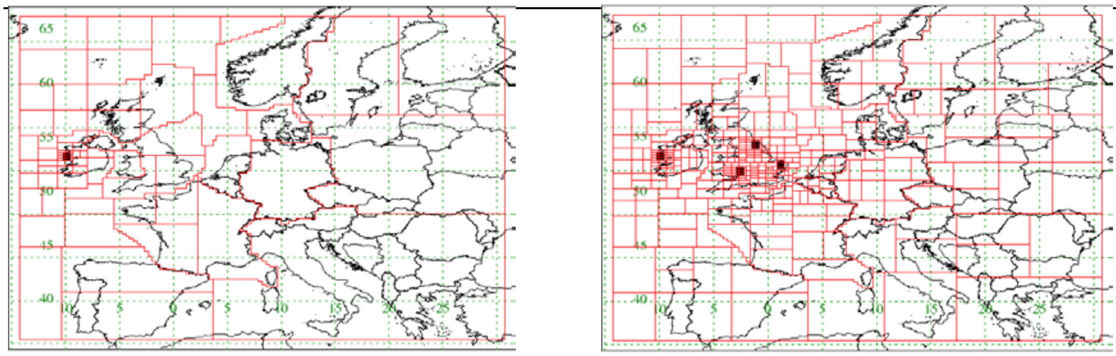
Where: M = Dilution matrix from NAME; e = Calculated emission estimate; b = Baseline time-series; f = 11 Direction-specific baseline adjustments; y = Observations; R = Model-observation uncertainty matrix; e_p = Prior emission estimate; B = Prior uncertainty matrix.

The technique starts from a set of randomly generated emission maps (or prior for CF2), it then searches for the emission map that leads to a modelled time series at all observation sites that most accurately mimics the observations. The use of *prior* emission estimates is possible within InTEM and will be used for CF2, however the use of such data *in any inversion system* has drawbacks, namely:

- The *prior* information usually originates from the inventory estimates that the inversion system is attempting to validate, hence making the inversion estimates dependent on the inventory rather than independent of it. At an extreme, where model or observational evidence is very sparse in time or space, the posterior estimate will tend to the prior values rather than an unknown.
- For the some of the gases listed (e.g. PFCs) in the tender there is only poor information on the geographical distribution of their emissions, i.e. the *prior* data have large and unquantified uncertainties.
- *Prior* information used within an inversion system limits its ability to highlight any significant deviations from the a priori distribution. This is because the *prior* solution restricts (dependent upon the prior uncertainty) the inversion solution from moving too far from the prior.

The aim of the inversion method is to estimate the spatial distribution of emissions across a defined geographical area. The emissions are assumed to be constant in time over the inversion time period. The model time-series are converted from air concentration [g m^{-3}] to mole fraction [ppb] using the modelled temperature and pressure at the observation point.

In order for the best-fit algorithm to provide robust solutions for every area within the domain, each region needs to significantly contribute to the mole fraction at the observation network on a reasonable number of time periods. If the signal from an area is only rarely or poorly seen by the observations then its impact on the cost function is minimal and the inversion method has little skill at determining its emission. The contribution that different regions make to the observed mole fraction varies from region to region. Regions that are distant from the observation sites contribute relatively little to the observations, whereas those that are close can have a large impact. In order to balance the contribution from different regions, those that make a large contribution are split into progressively smaller areas (the smallest grid used in this work is defined as 25 km). The starting regions are defined by country boundaries or collections of countries in the case of the Benelux (Belgium, Luxembourg, The Netherlands) countries or countries further east and south of Germany. Figure 2a shows an example of the splitting that results when MHD-only data, 3-year inversion period, 2-hour maps, and 25 km resolution grids are used and Figure 2b shows an example grid when the proposed DECC network (MHD + TAC + RGL + Bilsdale [BSD]) is used (1-year inversion period, 2-hour maps and 25 km resolution). The splitting varies for each time period considered and between the different gases due to varying meteorology and the impact of missing observations respectively.



(a) (b)

Figure 2: Example of the distribution of the different sized regions used by the inversion method to estimate regional emissions (smallest grid ~25 km): (a) MHD-only, 2-hourly resolution, 3-year inversion period (b) proposed DECC network 2-hourly resolution, 1-year inversion period.

With the introduction of a network of stations it is necessary to define a baseline for each of the stations across the network. A baseline for each station cannot be estimated in the same way as for MHD because the other stations within the network do not receive air that is unaffected by UK (and regional) emissions. The MHD baseline cannot be used directly for each station as the different stations do not receive air from the same direction and height as Mace Head at the same time. For example, TAC may be observing air from the north at the same time as MHD is observing air from the south-west. The impact of air from the upper troposphere is also important and is variable across the network at different times. The mole fraction of a gas usually has a vertical and latitudinal gradient due to heterogeneous global emissions. It is therefore important to reflect these differing baselines within the inversion system. InTEM has a method that directly solves for adjustments to the MHD baseline depending on the direction and height the air entered the regional modelled domain, so as these contributions differ across the network each station has a unique baseline time-series.

The direction and height the air enters the regional modelled domain is recorded for each observation time-step (e.g. 2-hour) for each station when observations were made. This information is interrogated and the percentage contributions from 11 different directions and heights for each observation time-step for each station is determined. The 11 directions are: WSW, WNW, NNW, NNE, ENE, ESE, SSE, SSW (all below 6 km); From the south 6-9 km; From the North 6-9 km; Above 9 km. Figure 3 shows a schematic of the different directions used within InTEM. CF1 and CF2 have an extra term, namely *fb*, which describes the time-series of baseline influence at each observation station separately using these direction specific parameters. It is comprised of the 11 terms ($f_1 – f_{11}$) that are solved as part of the inversion process.

$$b_s(t) = fb = [f_1\, p_1(t) + f_2\, p_2(t) + f_3\, p_3(t) + f_4\, p_4(t) + f_5\, p_5(t) + f_6\, p_6(t) + f_7\, p_7(t) + f_8\, p_8(t) + f_9\, p_9(t) + f_{10}\, p_{10}(t) + f_{11}\, p_{11}(t)]\, b_{MHD}(t)$$

where, $p_1(t)$ is the percentage of air from direction 1 at time t for station s, etc., $b_{MHD}(t)$ is the baseline at MHD at time t in mole fraction and $b_s(t)$ is the calculated baseline at the station s.

The inversion process works by iteratively choosing different emission magnitudes and distributions and boundary condition fractions (*f*) with the aim of minimizing the mismatch between the observations and the modelled mole fractions. The relative skill of a derived emission distribution is tested by comparing the modelled and observed time-series by using one of two cost functions as shown in equations 1 and 2. The iteration process is repeated until any potential improvement in skill in the emission map is estimated to be negligible.

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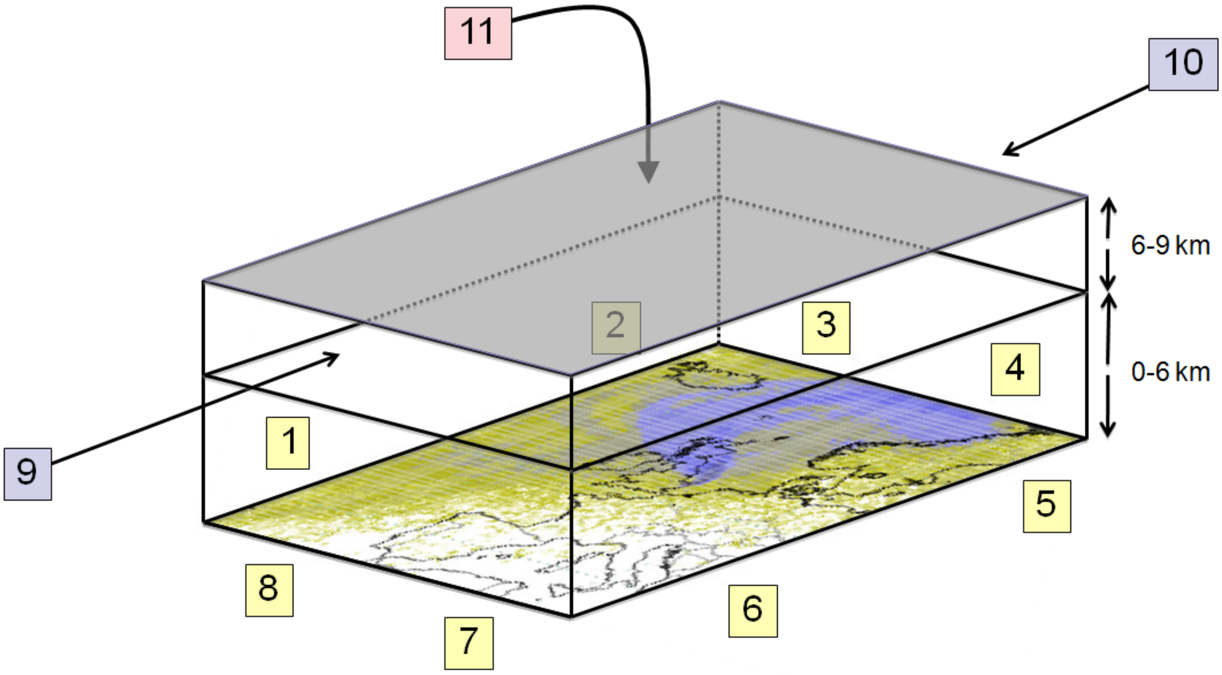


Figure 3: Schematic of the 11 different directions used within InTEM.

The uncertainties in the meteorology, dispersion and observations are captured in the inversion process as part of the matrix *R*. This matrix contains the time-varying overall uncertainty at each individual observation time (e.g. 2-hour|). The greater the magnitude of the uncertainty for a particular observation time the smaller the contribution this observation makes to the fitting process and vice versa. For CF2 the uncertainties in the prior emission estimates are required and are estimated in the main diagonal of matrix *B*. Again if the uncertainty of a particular region is large then its contribution to the fitting process is small. CF2 is identical to CF1 when the uncertainties in matrix *B* are infinite. The overall uncertainty of the inversion output is given by the matrix A, as defined in Equation 3.

$$A = (M^T R^{-1} M + B^{-1})^{-1} \qquad \text{Equation 3}$$

Global Models

The concentration of the air, as it enters the domain modelled by NAME, varies along its different boundaries both horizontally and vertically. The direction-specific baseline method described above is one technique that helps to account for these variations. Another possibility is through the use of global models, we have chosen two here that may provide an improvement to understanding the incoming air concentration.

The GEOS-Chem global 3-D atmospheric chemistry transport model is driven by GEOS-5 analysed meteorology provided by the Global Modelling and Assimilation Office at NASA Goddard (*Rienecker et al.*, 2011). The meteorology has a native horizontal resolution of 0.25^o latitude by 0.3125^o longitude. However for computational reasons, typically, GEOS-Chem is run at a horizontal resolution of 1^o latitude by 1.33^o longitude, with 47 vertical levels at a temporal resolution of 30 mins. GEOS-Chem has been evaluated extensively for many different trace gases, including

CH_4, and aerosols using surface, aircraft, train-bourne and satellite data over many parts of the world [*Fraser et al.*, 2011, 2013, 2014]. More recently we have used it as part of the NERC-funded GAUGE project in which it is run in a nested mode at the native horizontal resolution centred on the UK. As part of the DECC work, lateral boundary conditions will be delivered for CH_4 mole fraction at a resolution of 0.5^o latitude by 0.666^o longitude that envelop the limited spatial domain of the NAME model at a temporal resolution of six hours between 2014 and 2015, inclusive. The CH_4 mole fraction fields will represent *a posteriori* values after fitting for global NOAA surface data.

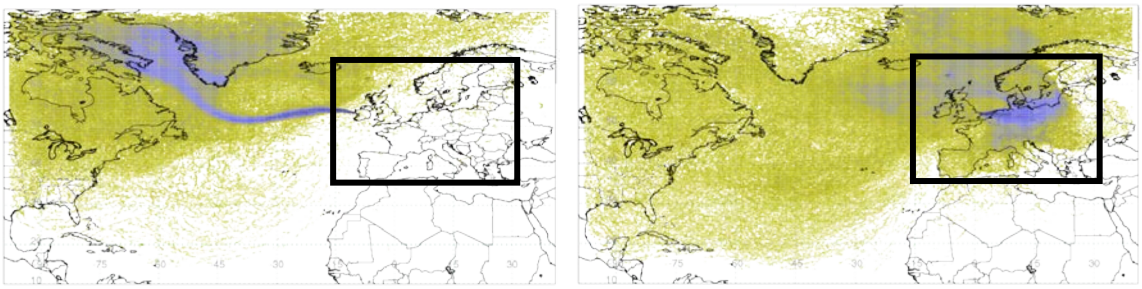
The Model for OZone And Related chemical Tracers (MOZART) is a state-of-the-art global chemical transport model developed by the National Centre for Atmospheric Research (*Emmons et al.*, 2010). The model has been used for simulating global distributions and performing global inverse model calculations of radiatively import trace gases such as SF_6 (*Rigby et al.*, 2010), CH_4 (*Rigby et al.*, 2012) and HFCs (*Lunt et al.*, 2015). In this project, a 10-year climatology of CH_4 and N_2O mole fractions will be calculated and used as a boundary condition for InTEM inverse model simulations. We will also continue to leverage on-going projects at the University of Bristol to provide boundary conditions for other trace species, as they become available (e.g. PFCs).

Global fluxes of long-lived atmospheric gases can be determined using simplified, computationally efficient, models of the atmosphere. Based around a 12-box model, an inverse modelling system for determining the emissions of most long-lived greenhouse gases and ozone depleting substances has been developed (*Rigby et al.*, 2014).

PROPOSED METHODOLOGY

Air history data set

NAME will be run backwards in time to estimate the recent (30-day) history of the air before it arrives at *each measurement height* at *each observation station* across the UK DECC network (currently; Mace Head [MHD], Tacolneston [TAC], Ridgehill [RGL], Angus [TTA]) for each 2-hour period 1990-current day (see Figure 4 for two examples). Global resolution UM data (improving from 40 to 17 km 2002 – 2015) and ECMWF ERA-Interim data (80 km) 1990 – 2002 will be used to drive NAME. The horizontal resolution of the data set will be 25 km and will estimate the surface (0-40m) impact of a large regional domain stretching from North America to Russia (-98^o to 40^o longitude) and North Africa to the Arctic circle (10^o to 79^o latitude). The 3-D locations and times when the model parcels leave the regional domain are also recorded and used later in the inversion process to inform the baseline estimation.



(a) (b)

Figure 4: Examples of 2-hour air history maps derived from NAME (a) for MHD, baseline period (b) for TAC, regionally polluted period. The air-history maps describe which surface areas (0-40m) in the previous 30-days impact the observation point within a particular 2-hour period. The black box indicates the geographical domain used for the inversion study.

The NAME model is three-dimensional therefore it is not just surface to surface transport that is modelled. The NAME parcels are released in a 20 m vertical line centred on the height of the observation. An air parcel can travel from the surface to a high altitude and then back to the surface but only those times when the air parcel is within the lowest 40 m above the ground will it be recorded in the 'air-history' maps. Parcels leaving the domain at all elevations will be recorded for baseline optimisation. The computational domain extends to more than 19 km vertically. For each 2-hour period thousands of inert model particles will be used to describe the dispersion. Running NAME backwards is very computationally efficient as every modelled parcel has a direct impact on the air histories produced.

Specific InTEM inversion setup

Through modelling the recent history of the atmosphere on a regional scale InTEM will be used to estimate the magnitude and distribution of emissions in the UK, Ireland and North West European (UK, Ireland, France, Germany, Denmark, the Netherlands, Belgium, Luxembourg, henceforth referred to as NWEU). Annual estimates in line with the reported inventory will be reported for all of the gases listed in the tender given the availability of measurement data supplied through LOTS 1 & 2 (CH_4, N_2O, HFC-134a, HFC-152a, HFC-125, HFC-143a, HFC-23, HFC-32, HFC-365mfc, HFC-227ea, HFC-43-10-mee, PFC-14, PFC-116, PFC-218, PFC-318, SF_6, NF_3). For CH_4 and N_2O, given their increased number of observations across the UK due to their relative importance, and because they have, potentially, emissions that vary seasonally, emissions will also be estimated monthly and 3-monthly. These inversions will be performed with use of cost function 2 (CF2, Equation 2) and the NAEI/EDGAR prior because of the reduced number of observations available in these shorter time periods. In each of the inversions the baseline will be solved for as part of the methodology as described above. Thus InTEM will estimate for each station a site-specific baseline time-series as each station receives air from different directions and quantities throughout the time-series.

InTEM will be applied in three configurations per gas:

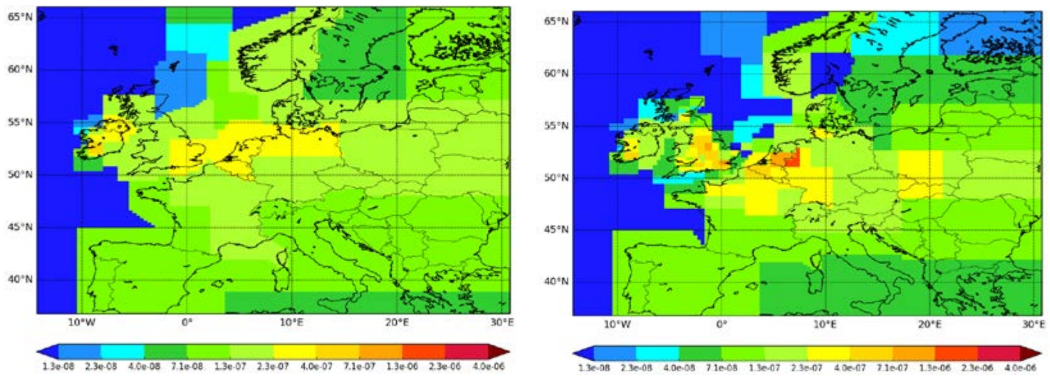
1. Using MHD only observations. Each inversion will use cost function 1 (CF1, Equation 1) and cover 3 years of data, and the time-window will move forward in monthly intervals. Uncertainties are estimated through the application of Bayesian uncertainty analysis. Annual emissions and uncertainties are estimated by calculating the median and 5^{th} – 95^{th} percentile of all inversions that contain each full calendar year. The data period assessed will be 1990 – current.

2. Using the full UK DECC network observations. Each inversion will use CF1 and cover 1 year of data and the time-window will move forward in monthly intervals. Uncertainties are estimated through the application of Bayesian uncertainty analysis. Annual emissions and uncertainties are estimated by calculating the median and 5^{th} – 95^{th} percentile of all inversions that contain at least 6-months of each calendar year. The data period assessed will be 2012 – current (the period covered by the UK DECC network).

3. Using the full UK DECC network observations. Each inversion will use CF2 and cover each year 2012 - current. Each inversion will use a prior emission estimate with appropriate uncertainties derived from a combination of NAEI and EDGAR data as available. Uncertainties are estimated through the application of Bayesian uncertainty analysis. For CH_4 and N_2O, these inversions will also be performed at 3-month and 1-month intervals to estimate the seasonal variations in emissions.

The inversion domain is chosen to be a smaller subset of the full domain used for the air history maps. It covers 14˚ W – 31˚ E longitude and 36˚ N – 66˚ N latitude and is shown as the black box in Figure 4. The smaller domain covers all of Europe and extends a reasonable distance into the Atlantic. The inversion domain needs to be smaller to ensure re-circulating air masses are fully represented but also because emission sources very distant from Mace Head have little discernible impact on the concentration at the station, i.e. the signal would be too weak to be seen.

For each time period solved for, the whole inversion process will be repeated multiple times to understand the spread in the emission solutions given different random starting points. Solutions will be calculated for 3- and 1-year periods covering the full dataset of available observations. Figure 5 shows example output from InTEM, in this case the estimated distribution of emissions of CH_4 for two different periods using (a) MHD-only data, 1990-1992 and (b) UK DECC Network of observations, 2014.



(a) (b)

Figure 5: InTEM estimated emissions of CH_4 emission (g m^{-2} s^{-1}) for (a) 2012 – 2014, using MHD-only observations, and (b) 2014, using the current DECC Network.

Monthly and annual estimates of emissions per gas per geographical region (UK, Irish, NWEU) will be reported by calculating the median of all of the solutions that contain that month or year within the solved-for time period. An uncertainty range will be estimated for each month or year for each gas and geographical region by calculating the 5^{th} and 95^{th} percentile of the corresponding uncertainties. The inversion results will be compared to available inventories. Figure 6 shows an example of the time-series of emission output for the UK that will be generated per gas observed.

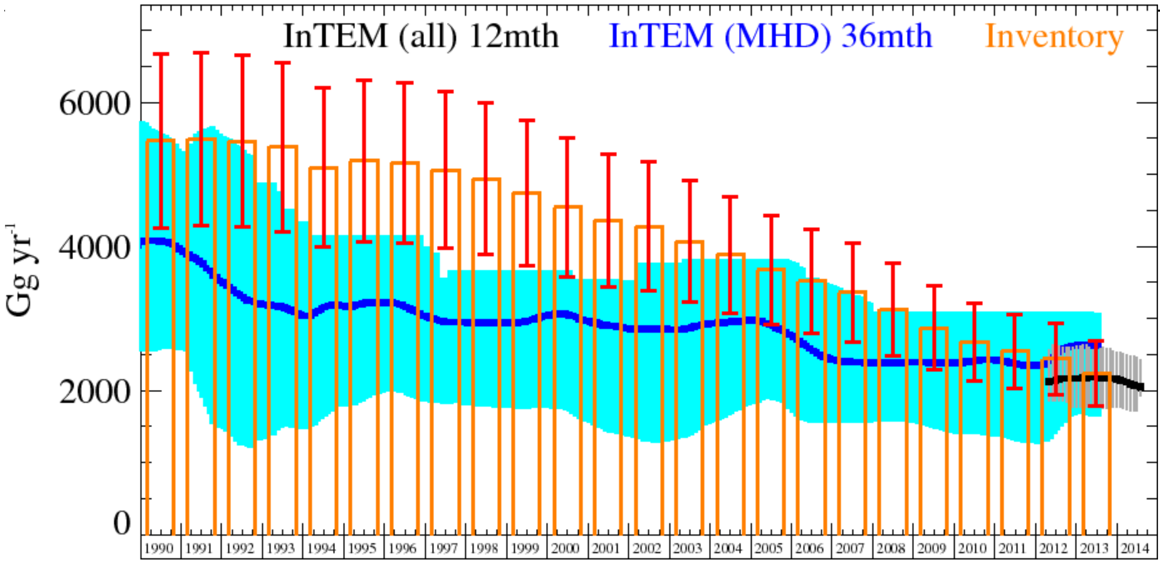


Figure 6: CH_4 emission estimates for UK (Giga gram per year). Orange columns are the UK UNFCCC submissions with uncertainty (red). The blue solid line is the inversion median value for MHD-only inversions and associated uncertainty (light blue shading). The black solid line is the inversion median value for inversion using the full UK DECC network and associated uncertainty (grey shading).

Baselines and Boundary Conditions

Baseline mole fractions are defined as those that have not been influenced by significant emissions within the regional domain shown in Figure 4 en-route to Mace Head, i.e. those that are well mixed and are representative of the mid-latitude northern hemisphere background concentrations. The analysis considers the long-term trend of the monthly and annual baseline mole fractions, their rate of growth and their seasonal cycle.

A two-hour period will be classed as ‘baseline’ if it meets certain criteria assessed using the NAME air history output:

- Local emissions do not significantly contribute.
- Populated regions do not significantly contribute.
- The air enters the domain from predominately the north west direction (chosen because southerly and south-westerly trajectories can be depleted in trace gas concentrations or influenced by the east coast of the USA).

As an example, Figure 7 shows a three-month extract of the CH_4 observations measured at Mace Head. The observations have been colour coded to indicate whether, using the above classification, the air mass they were sampled from was considered baseline. For the baseline analysis all non-baseline observations are removed.

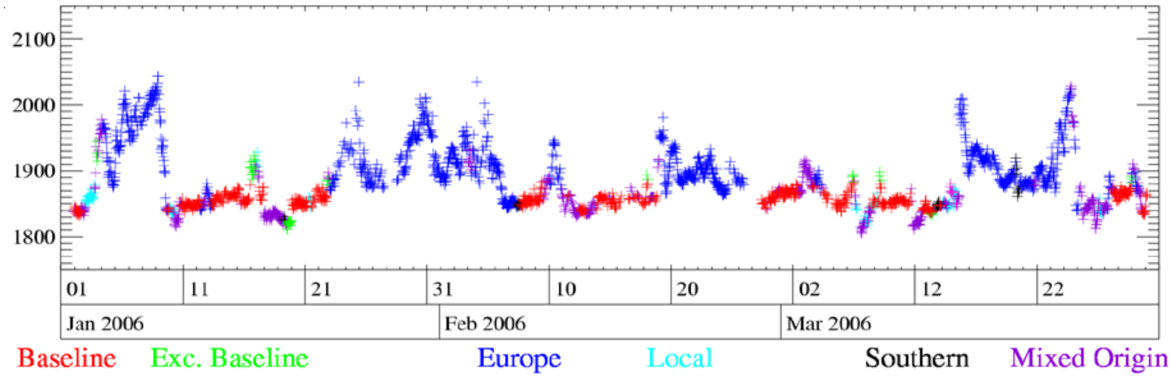


Figure 7: Example three-month time-series of Mace Head CH_4 observations (ppb) showing the impact of the baseline and non-baseline classification. The baseline observations are shown in red.

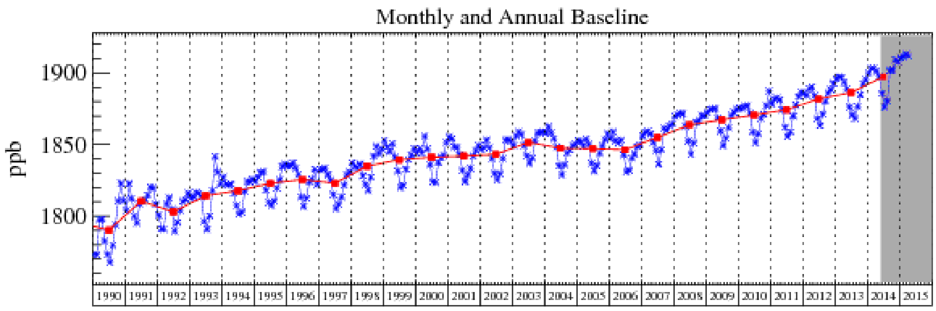
The points defined as baseline using the above methodology still have a certain level of noise e.g. from unexpected emissions (forest fires in Canada or shipping); or incorrectly modelled meteorology or transport. To capture such events, the baseline data are statistically filtered to isolate and remove these outliers that are actually non-baseline observations. The observations removed through applying this statistical filter are shown in green in Figure 7.

For each hour in the time-series the baseline points are locally (within a time window) smoothed, the result is an estimate of the baseline concentration for each hour for each gas covering the entire dataset. These hourly values are averaged into monthly and annual estimates and will be presented each quarter to DECC (e.g. Figure 8a)

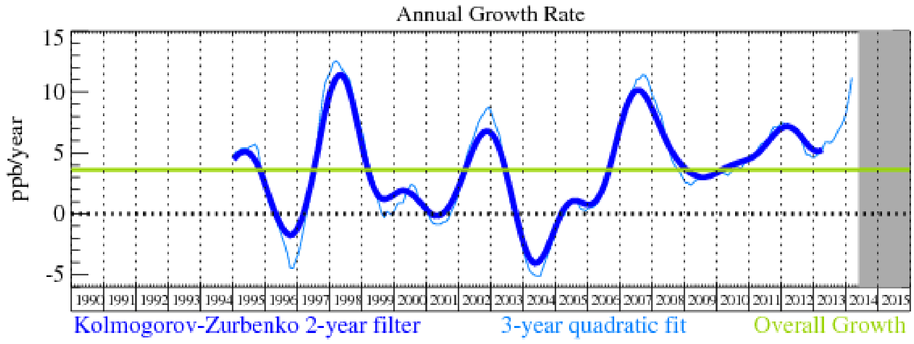
Monthly growth rates are estimated for each gas so that changes in the underlying trends can be identified and investigated. The hourly baseline data are de-seasonalised (two methods) before a local annual growth rate is defined for each hour. These hourly values are then averaged for each month (year) to estimate the annual growth rate per month (year) and reported (e.g. Figure 8b).

The seasonal cycle is estimated by subtracting the baseline mole fraction from the underlying trend value (as discussed in the previous paragraph). An estimate of the monthly seasonal cycle will also be reported to DECC (e.g. Figure 8c) each 6-months.

Any unexpected variations would be highlighted to DECC and where appropriate investigated with the use of the global models.



(a)



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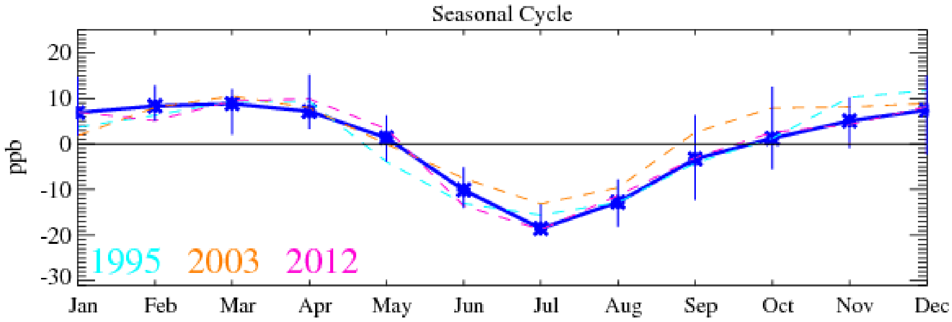

(c)

Figure 8: Example baseline analysis plot for methane (CH_4). (a) monthly (blue) and annual (red) mid-latitude Northern Hemisphere baseline mole fractions. (b) Monthly (seasonal cycle removed) baseline growth rate (blue – 2 methods) and overall growth rate (green). (c) Average seasonal cycle with year to year variability (uncertainty bars), the first (light blue), middle (orange) and last (pink) year of data are also shown. Grey shaded area indicates currently un-ratified data.

In addition to these Northern Hemisphere trends, the global 12-box model will be used to report, every 18 months, the global trends and fluxes of the gases measured under the AGAGE network.

Uncertainty

The Bayesian framework will be used to assess the uncertainties in the inversion system. This framework has a rigorous mathematical method for estimating the uncertainty reduction due to increased knowledge, in this case more observations. The errors are assumed Gaussian, this is a limitation, but one that is very widely used. A key point is that it is assumed the uncertainties in the prior, the observations and the model transport are well characterised and known. Quantifying these three areas of uncertainty is extremely challenging and is an area of on-going research directly (but not financially) linked to this proposal e.g. *Ganesan et al.*, 2015 and the research work undertaken by Dr Rigby and his team.

Observational Uncertainty

The observation uncertainty is derived from a combination of repeatability uncertainty and aggregation uncertainty. The former is from the instrument and is the variability observed when the same tank of air is repeatedly measured. The latter is from the variability, standard deviation, in the observations when they are aggregated up to the observation-model time-step (2 hours). The CH_4 observations are measured at 1-2 Hz at the tower stations (although there are regular data gaps as different heights are sampled) and 40 minute intervals at MHD.

$\sigma_{precision}$ → Uncertainty due to repeatability of observation

$\sigma_{2h\ time\ period}$ → Uncertainty when observations aggregated to 2-hours

Transport Model Uncertainty

The model transport uncertainties are very difficult to quantify, but are assumed to be related to the strength of the impact of very local emissions (high impact implies weak winds and low boundary layers and thus times when local un-modelled effects are strong) and the ability to estimate a good baseline mole fraction. The baseline is an estimate of the concentration of the gas in the air as it enters the inversion domain. The uncertainty of each model-observation time-step is increased on a linear scale as the contribution from the 9 grid boxes surrounding the observation site increases as determined from the NAME air history data. The 3-month rolling standard deviation of the points classed as baseline is used to quantify the baseline uncertainty (see Figure 9).

$\sigma_{baseline}$ → Uncertainty of MHD baseline

σ_{local} → Uncertainty increases as local influence increases

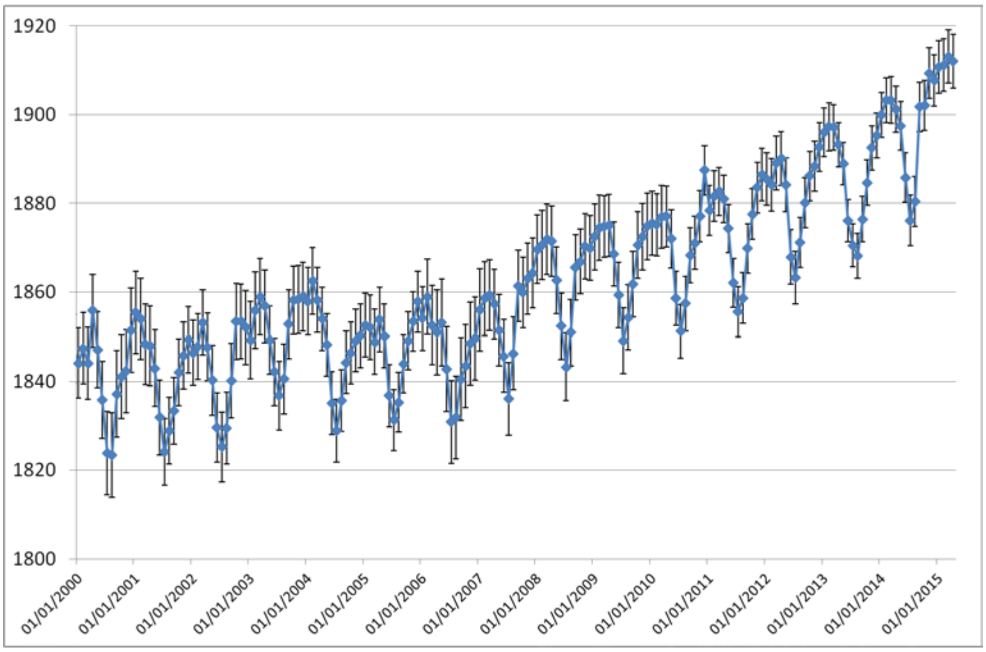

Figure 9: CH_4 monthly baseline mole fraction (ppb) as estimated from Mace Head observations 2000 – 2015. Baseline uncertainty at 1σ is shown.

Model-Observation Uncertainty

The overall model-observation uncertainties are combined together assuming uncorrelated errors and used to define the uncertainty matrix *R*. It is usually the case that the model uncertainty is much greater than observation uncertainty. The values in R vary from gas to gas and from one model-observation time-step (2-hour) to the next depending on the four time-varying different contributing factors, so there is no single number per gas. As a result, the uncertainty per annual UK estimate from InTEM varies from gas to gas but usually falls within 50-100% in the absence of any prior uncertainty estimates.

$$R = (\sigma_{precision})^2 + (\sigma_{2h\ time\ period})^2 + (\sigma_{baseline})^2 + (\sigma_{local})^2$$

Prior Uncertainty

For CF2 it is necessary to define uncertainties of the prior emissions for use in the matrix *B*. Some of the inventory sources, such as the NAEI, provide a countrywide annual estimate of the total uncertainty of the UK, e.g. for CH_4 for 2013 it was 24%, others such as EDGAR do not routinely provide such information and certainty not per source sector category. We propose to set the prior uncertainty to match that of the NAEI where available for the UK and apply that across Europe, following our work in the InGOS project.

CO_2 and Satellite observations

A section on current science activities associated with regional CO_2 flux estimation and the associated use of satellite data will form part of the annual report. Dr Palmer, who leads the NERC-funded GAUGE project, is a science team member of the NASA Orbiting Carbon Observatory (OCO-2) and the Japanese Greenhouse gases Observing SATellite (GOSAT), science director of the NERC National Centre for Earth Observation, and a regular contributor to the annual International Workshop on Greenhouse Gas Measurements from Space (IWGGMS) workshop. He is well placed to provide insights into new the scientific methods and findings, related to CO_2 inversions and to advise on the current status of existing and upcoming satellite observations of CO_2.

Proposed new developments

Link with boundary conditions from global models

Develop use of time-varying boundary conditions from 3-D global chemistry transport models and compare to MHD baseline method. The 3-D global models are able to estimate the variability of the atmospheric trace gases at the boundaries of the NAME domain. These could be linked to where the NAME particles leave the domain and used to estimate a baseline at each station in the network. This method would initially be compared to the baseline method for MHD.

Investigate the uncertainty due to resolution of meteorology

One of the key uncertainties in inversion modelling is the model transport uncertainty. The ability of the transport model to represent accurately the dispersion of the gas in the atmosphere from emission to measurement is challenging to quantify. Currently we use the variability of the baseline observations and the quantity of the local impact to estimate this quantity. We propose here to investigate the use of regional 4 km UM 3-D meteorology (from 2013 to current) to drive NAME. Air histories for each station will be generated and applied within InTEM to understand the impact of changing the driving meteorology.

Solve per emission sector rather than geographical distribution

Currently InTEM is applied to the problem of estimating both the emission magnitude and emission distribution but with the limitation of providing little understanding of the emissions per source sector category. If, through the use of NAEI and EDGAR, the source distribution and relative magnitude is assumed known, the emission factors per source category can be estimated.

Adaptive grid

Develop InTEM to adapt the inversion grid within the inversion process based on the relative emission estimates. This will allow regions of high emission estimate to be focussed on and so better describe the release of gases with significant emission point sources. Such a methodology may be particularly effective for estimating the emissions of gases such as the PFCs with specific industrial use.

Use the different inlet heights to assess uncertainty

It is hypothesised that the transport model will better describe the flow and dispersion of the atmosphere when the atmosphere is well mixed. The degree of agreement between the observations at different heights within the same hour and the also the degree of agreement of the modelled time-series at different heights will provide valuable insight into the modelling uncertainty at each time. This information will be used to investigate whether this potential methodology can be used within the inversion methodology.

Improved inversion methodology within InTEM

Through close collaboration with Dr Rigby at the University of Bristol we will make use of the cutting edge inversion modelling research undertaken by his group. His group have pioneered the use of Hierarchical Bayesian and Monte Carlo Markov Chain methods (*Ganesan et al,*. 2014) for emission estimation and continue this work through NERC grants to better quantify transport uncertainty through the use of statistical emulation of the NAME model.

Skills and expertise:

Technical ability

Dr Manning will be the Principal Investigator and co-ordinator of the contract. He has been at the forefront of regional GHG inversion modelling for 15 years and has developed the inversion system InTEM (Inversion Technique for Emission Modelling). He has worked closely with the University of Bristol during this period to provide ‘top-down’ verification estimates of UK GHG emissions for the UK government under contracts (EPG 1/1/142, CPEG 27, GA0201, GA01103). He is leading the Met Office involvement in the inversion modelling studies within the EU project InGOS, and previously in the EU projects NitroEurope and EuroHydros. As a manager in the Met Office atmospheric dispersion group he played a lead role in the development of the atmospheric transport model NAME (Numerical Atmospheric dispersion Modelling Environment) and its application to various emergency response situations e.g. volcanic ash released from Eyjafjallajökull in 2010 and the Buncefield oil fire in 2005.

Dr Arnold has been a Senior Scientist at the Met Office Hadley Centre since October 2014. Prior to this he was an Assistant Project Scientist at the University of California, San Diego (UCSD), where he conducted research on new methods to measure greenhouse and stratospheric ozone depleting gases, and calculating global emissions estimates. Dr Arnold was responsible for enabling measurement of nitrogen trifluoride around the globe and within the DECC network. Using an inverse modelling approach, he highlighted the huge inaccuracy in 'bottom-up' estimates of this ‘new’ greenhouse gas. HFC-43-10mee was another Kyoto Protocol gas that was lacking atmospheric observations and ‘top-down’ emissions estimates until his recent work. At the Met Office Tim has primarily been responsible for delivering outputs for the InGOS project for estimating greenhouse gas emissions across Europe and has quickly become an expert in the use and development of NAME and InTEM.

Dr Matt Rigby is a Natural Environment Research Council (NERC) Advanced Research Fellow at the University of Bristol. He has written 29 publications, including 10 as first author, in subjects ranging from regional emissions of in synthetic greenhouse gases to global trends in atmospheric methane. Dr Rigby is Principal Investigator of two major grants from NERC: “Are national HFC emissions reports suitable for global policy negotiation?” which aims to quantify national emissions of hydrofluorocarbons and develop new “inverse” modelling methods, and; “Abrupt seasonal fluxes of methane from northern lakes and ponds”. He is Co-Investigator and work-package leader of the Greenhouse gAs Uk and Global Emissions consortium (GAUGE). Dr Rigby currently supervises two PhD students and three PDRAs, and co-supervises two further PhD studentships. He enjoys particularly close collaborations with tens of scientists around the world, in particular those working under the Advanced Global Atmospheric Gases Experiment (AGAGE), for which he leads much of the modelling effort. He is particularly recognised for his expertise in "inverse" modelling of trace gases in which atmospheric observations are used to constrain fluxes. He has developed novel frameworks for understanding atmospheric trace gas transport processes and has pioneered the use of hierarchical Bayesian methods for rigorously quantifying uncertainties in such systems.

Dr Palmer is a Professor at the University of Edinburgh, a Royal Society Wolfson Research Merit Award holder and is a lead researcher in the field of global CO_2 modelling and the incorporation of satellite data into inversion models. He has published over 100 papers in many aspects of collecting and interpreting measurements of atmospheric chemistry and greenhouse gases. Of relevance to this proposal, Dr Palmer currently leads the NERC-funded GAUGE project and is a science team member of the NASA Orbiting Carbon Observatory (OCO-2) and the Japanese Greenhouse gases Observing SATellite (GOSAT). He is also the science director of the NERC National Centre for Earth Observation. His current group comprises five postdoctoral researchers and five PhD students.

Aether has expertise spanning 20 years of GHG and Air Pollution emissions estimation, reporting, analysis and verification. Aether provide knowledgeable experts covering all sectors of the inventory (Energy, Industrial Processes (including F-Gases), Agriculture, LULUCF and waste). With two experienced lead UNFCCC reviewers and trained review experts in Industrial Processes, Agriculture, LULUCF and Waste, Aether has significant experience of the UNFCCC reporting and verification process and has strong links to the UNFCCC and IPCC activities. Aether experts have also contributed to the writing of guidelines for compilation (2006 IPCC) and reporting and verification (UNFCCC) of GHG inventories. At a European level Aether provide expertise and advice to the European Environment Agency on the Effort Sharing Decision review process. Aether provide expertise for the review and analysis of member state GHG estimates, development and design of EU reporting processes (e.g. Monitoring Mechanism Regulation). Aether are also engaged with a number of Measuring, Reporting and Verification (MRV) activities including support to the European Commission in progressing MRV in the climate negotiations including the development of independent verification techniques. Aether also provide support to the DECC international team during negotiations for matters relating to GHG estimates and MRV and supported the recent successful defence of the UK's mitigation policies during its Multilateral Assessment at SBI in Bonn 5th June.

Past Performance

We propose to continue to use and develop the UM - NAME – InTEM modelling system to estimate emissions across the UK, Ireland and North West Europe (NWEU). The Unified Model (UM) is the UK Met Office's world leading 3-D meteorological model that is used every day for forecasting across the globe and is continually in a cycle of improvement. NAME is the UK Met Office's sophisticated 3-D atmospheric dispersion model that is under on-going use and development and has been since its inception in the late 1980s following the Chernobyl nuclear disaster. NAME primarily uses the UM 3-D meteorological fields to drive its dispersion and transport algorithms. The UM-NAME partnership has been used extensively in both emergency response mode and also for policy work as described later in the relevant sections.

InTEM has been used and improved continually over the past 15 years to estimate regional emissions of long-lived trace gases from observations. The current version (v16) is being used to deliver the DECC contract GA01103 and is described in brief in the relevant sections. InTEM is also used by the Met Office to estimate the magnitude and height of the emission of volcanic ash from satellite observations during emergency response situations as part of the Met Office's role as a World Volcanic Ash Advisory Centre (VAAC) that provides forecasts of ash for the civil aviation authorities. The capability of InTEM has enabled the Met Office to participate in several EU consortia projects; InGOS (Integrated non-CO_2 Greenhouse gas Observing System), NitroEurope and EuroHydros. InGOS is focussed on estimating emissions of CH_4, N_2O and HFCs across Europe, NitroEurope was a precursor to InGOS and worked at estimating European emissions of CH_4 and N_2O, and EuroHydros investigated the European emissions and sinks of hydrogen. The UM-NAME-InTEM modelling system is also a key model in the NERC GAUGE project for the estimation of the three principal GHGs (CO_2, CH_4 and N_2O).

Through the UK government work, the results and outputs of InTEM GHG inversion modelling have been presented at numerous EU and UK government meetings for example NISC (National Inventory Steering Committee), JPI (EU Joint Partnership Initiative), EU workshops on inverse modelling hosted by the EEA (European Environment Agency) and JRC (Joint Research Centre). The emission estimates for the UK have been routinely included in the UK submission to the UNFCCC for the past decade as part of the UK's commitment to the IPCC good practice guidelines, one of only three countries to do so. The InTEM model and results have been presented at international science meetings (EGU and AGU) and published in peer-reviewed literature (*Bergamaschi et al.*, 2015, *Manning et al*., 2003 and *Manning et al.*, 2011).

In the current contract (DECC GA01103) there has been a focus on the UK emissions of HFC-134a, as there is a clear difference between the InTEM UK emission estimates and the UK inventory. In particular, we investigated the different emission factors and activity data used within the UK inventory of this gas. We have highlighted several areas of potential improvement and DECC have subsequently followed up on this work as part of the inventory improvement plan.

Addressing Challenges and Risks:

Risks

Resource: It is inevitable that with any project there will be a resource risk. The individuals identified in the CV's have all committed to this project. If there is a requirement to replace an individual for whatever reason, the project team would seek to identify an individual from within the partner's organisations before undertaking any external advertisement of a position. Any change of personnel will be discussed and agreed with DECC.

Completion of tasks: The project management team will be monitoring the progress of the project closely. If there is a possibility that a milestone or deliverable will not be achieved, then remedial action will be discussed and agreed with DECC at the earliest opportunity.

Core Funding: [REDACTED]

Management and Delivery:

Dr Manning will manage Lot 3 and be responsible for drafting the reports. He will work closely with the project manager of Lot1 and Lot2, Dr Palmer, Dr Rigby, Mr Goodwin and Dr. Young for the delivery of 6-monthly updates and annual reports (in addition to the methodology report and contribution to the risk register to be delivered in December 2015). The timing of the delivered reports are detailed in the invoicing schedule below. The reports will undergo quality assurance by Dr Young before submission to DECC.

The annual reports will take no longer than four weeks to produce and the 6-monthly updates no longer than two weeks. For each, a plan will be produced outlining the content of, and who is responsible for, each section and a delivery time schedule.

The project team will hold tele-conferences as and when necessary but at least 6-monthly to discuss the latest work and upcoming requirements. A brief record of the outcomes of each will be maintained.

Quality Assurance and Quality Control Processes, Risks and Challenges

Dr Young will be responsible for the quality assurance of the annual and 6-month reports.
The UM, NAME and InTEM are maintained under Met Office version control procedures and are fully backed up. These procedures include the maintenance of a file that details all changes to InTEM recording when and why each change was made.
As the current provider for this contract the risks and challenges are well known and understood. The risks and their likelihood are:

- Loss of key staff (very low). The Met Office have two trained members of staff involved in this project.
- Loss of IT (very low). The Met Office has a very robust system in place to protect against the loss of data, systems or software.

The most important challenge is maintaining a very strong collaboration not only within this Lot but across all three Lots. Past performance, most notably the EU and NERC collaborative projects, have demonstrated that the team proposed here are all team players and have a great deal of experience working with a wide range of different people.

The following Sections have been REDACTED:

- Cost
- Annex A: Declarations
- Annex B: Curriculum Vitae
- Annex C: Met Office Letter
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