ATMOSPHERIC COMPOSITION:
LINKS TO CLIMATE AND POLLUTION

1 ABSTRACT

Atmospheric composition is driving climate change and governs air quality, which itself is linked to climate change. This Theme will investigate quantitatively the global distributions, sources and sinks of key atmospheric constituents and their links to climate and to air quality by exploiting, in innovative ways, new satellite observations in combination with state-of-the-art atmospheric models. A new, integrated approach will be pioneered to exploit optimally observations of different types from the new EPS-MetOp satellite in combination with Envisat, to derive tropospheric distributions of trace gases and aerosol, together with cloud and surface properties. The Theme has two broad scientific objectives: Firstly, to quantify *atmospheric distributions and surface emissions* of methane, shorter lived trace gases and aerosol and, secondly, to quantify *climate-composition* interactions. These objectives are co-aligned with those of NCAS and the Hadley Centre and will be addressed through co-operation. The first objective will be accomplished through critical comparison and assimilation of satellite data into *global chemical transport models.* The second objective will involve comparisons of multi-year time series (and variances) of satellite data with output from the UKCA *chemistry-climate model* sampled to simulate the characteristics of satellite observations. A further dimension of this Theme will be to undertake R&D in close co-operation with the Met Office and ECMWF, allowing NCEO to contribute to national and European initiatives, to establish new applications for satellite constituent data in *pollution monitoring*, *air quality forecasting* and *numerical weather prediction*. These co-operative activities will transfer NCEO scientific expertise and information (data, modelling tools) to the operational centres and thence to DEFRA. World-class expertise of participating groups at Cambridge, Edinburgh, Leeds, Leicester, Oxford, RAL, Reading and York (total **8 FTEs** and **7 PhD studentships**) will enable a cohesive, end-to-end programme to be undertaken.

2 BACKGROUND AND MOTIVATION FOR THE THEME

Changes in the abundances and distributions of trace gases and aerosols in the troposphere drive changes in climate and directly affect surface air pollution levels, and subsequently human health. The composition of the troposphere is determined by emissions of trace gases and aerosols, transport and exchange with the stratosphere and *in-situ* chemistry[1]. Atmospheric composition is linked to climate change through: (i) the primary radiative forcing of trace gases and aerosol; (ii) the indirect effects of aerosols on cloud radiative properties and (iii) through subsequent climate feedbacks involving clouds, water vapour and other trace gases. It is imperative that the processes which control composition, and thereby composition-climate interaction, be understood, so that this component of the Earth system can be represented accurately in climate model simulations and projections. However, there are major uncertainties in the magnitudes and distributions of sources and sinks, processes that produce secondary pollutants and transport these around the globe and climate feedbacks on atmospheric composition [IPCC, 2007].

The aim of this Theme in the first 5-year phase of NCEO is to study, through novel use of satellite data, some of the processes which control distributions of *short-lived (reactive) gases*, *methane* and *aerosol* and their links to climate and air pollution[2]. To accomplish this aim, difficulties inherent

[1] Direct emissions include both natural and anthropogenic sources at the surface and at elevation e.g. lightning and aircraft. Removal of primary gaseous pollutants is largely controlled by the oxidising capacity of the troposphere. This involves reaction with OH, in turn producing secondary pollutants such as ozone and also forming secondary aerosols.
[2] In the 2nd Phase, focus would be placed on processes in the upper troposphere / lower stratosphere, to exploit advances foreseen in cloud-resolving models and possibly also data from a dedicated, new-generation limb-sounding mission.

to sounding tropospheric composition from space will need to be overcome, for which it will be necessary to exploit satellite observations in new and innovative ways. So a major thread running throughout this Theme is the building of a world-class *national capability* for the retrieval and scientific exploitation of satellite observations of atmospheric composition, which will have two dimensions: (1) An integrated approach will be established to exploit complementary information from different types of sensor to determine tropospheric distributions of trace gases and aerosol jointly with cloud & surface properties for this and other NCEO Themes and for wider exploitation and (2) by developing modular tools for data assimilation, inverse modelling, and model sampling (observation operators) which will, again, benefit applications extending beyond this NCEO Theme.

The scientific aims of this Theme are aligned with NERC[3] and NCAS strategic goals, and will be pursued in parallel with international initiatives (IGBP/IGAC)[4], EU, national programmes in Europe, US and elsewhere). The Theme will also perform R&D contributing to national and European initiatives to establish *new (operational) applications* for satellite data on atmospheric composition: pollution monitoring, air quality forecasting and numerical weather prediction. Specific activities have been defined for NCEO in close co-operation with ECMWF and MetOffice, in the context of a pilot GMES Atmosphere Service (GEMS-II) to be developed in parallel[5]. This is intended to offer an improved capability to monitor adherence to the Convention on Long Range Transport of Air Pollution (CLRTAP) and EU directives on emission ceilings and air quality, for which DEFRA is responsible in the UK.

The aims of this Theme are achievable only through a programme which is *core-strategic* in its ambition, scope and duration[6] and centre on the exploitation of *satellite EO data*, for which NCEO offers the only route. Furthermore, the UK has established expertise for all stages of a cohesive, end-to-end programme:

- Characteristics of satellite sensors, data quality and error analysis
- Radiative transfer, instrument modelling, constituent retrieval and validation
- Development and application of assimilation schemes
- Assimilation of atmospheric data into CTMs and GCMs
- Development of chemistry & aerosol schemes for global and regional models
- Exploitation of data for scientific research and operational applications

Although the objectives of this Theme will be achieved through a focused programme which is largely self-contained, links to other NCEO Themes arise naturally through the weather, atmosphere/surface interfaces, volcanic eruptions, the carbon and hydrological cycles and Earth's radiation balance. The Theme will also draw on theoretical expertise in data assimilation and data handling infrastructure. So it will be mutually beneficial for this Theme to proceed in co-operation with others in the frame of NCEO (Annex 1).

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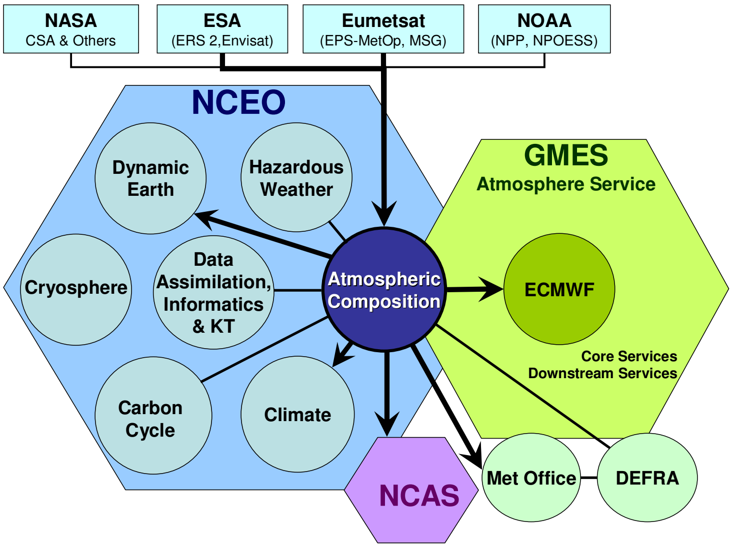
[3] NERC key challenges: *Climate* "Increase knowledge of chemical & biological feedback processes in the atmosphere, oceans and on land. This includes detailed understanding of how emissions from human activities are changing atmospheric composition."; *Earth System Science* "Increase knowledge of how atmospheric composition is controlled. Atmospheric chemistry plays a key role in climate change and air quality has major impacts on health and agriculture."

[4] IGBP/IGAC(2006): Theme 1 *Role of Atmospheric Chemistry in Amplifying/Damping Climate Change* Theme 2 *Effects of Emissions/Depositions, Transport and Chemical Transformations on Air Quality and Tropospheric Composition*

[5] GMES is part of GEOSS. The pilot Service will integrate measurements from surface & satellite observations to provide information at European, national and regional scales on pollutants, surface UV, ozone and other climate gases.

[6] To provide the satellite data sets and observation operators needed for exploitation, an ambitious integrated approach is proposed, to be developed as a national capability. Science exploitation also requires development of generic tools for data assimilation and inverse modelling in order to advance (UK) state-of-the-art to the necessary level. Development of national capabilities for new operational applications for satellite composition data in pollution monitoring and air quality forecasting will require sustained development over a decade to reach maturity, as these are in their infancy cf NWP for which satellite data have been in use for several decades. These dimensions of the Theme move well beyond what could be achieved in an individual standard grant or consortium grant.

Relationships of this Theme to other NCEO Themes and to partners outside the NCEO are illustrated in Fig1. The Theme's internal structure is shown in Fig. 2. Scientific exploitation (ST-2 & 3) will be in collaboration with NCAS and Hadley Centre. Development of new applications (ST-4) will be in co-operation with MetOffice and ECMWF and also provide information for DEFRA.



Thin lines: Two-way information exchange
Thick lines: Data transfer & information exchange

Fig.1 Atmospheric Composition Theme in relation to other Themes and co-operative links outside NCEO

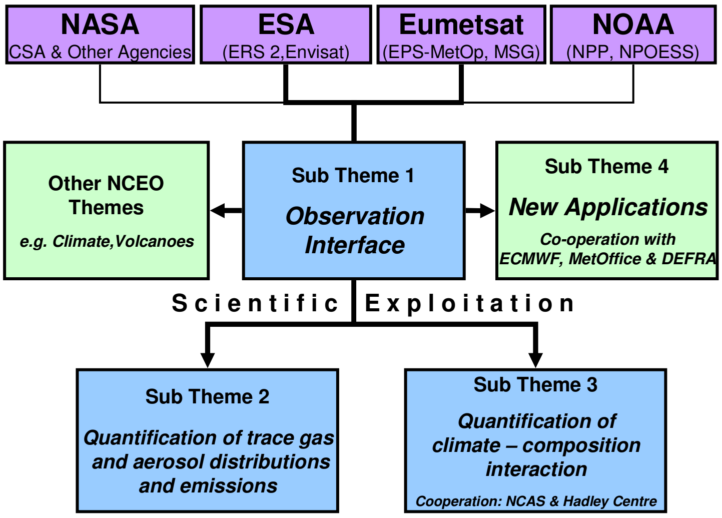


Fig. 2 Structure of Atmospheric Composition Theme

3 SPECIFIC OBJECTIVES

We will exploit the opportunity presented by the new MetOp mission, in combination with Envisat, SCISAT-1 and other observations, to investigate and quantify processes controlling atmospheric composition and links to climate and pollution and establish a national capability in this field.

a) Improve quantitative understanding of trace gas and aerosol distributions and emissions

- New satellite data on composition will be compared with (3-D) chemical-transport models to improve estimates of organic budgets and the oxidising capacity of the troposphere.
- Satellite data and models will be used to quantify the role of regional/intercontinental transport of primary pollutants and precursors in production of secondary trace gas and aerosol pollutants, complementing existing aircraft and ground-based data.
- *Biogenic*, *pyrogenic* and *anthropogenic* emission sources of methane, shorter-lived gases and aerosol will be determined on scales accessible to satellite observations.

b) Improve quantitative understanding of chemistry-climate coupling

- The UKCA chemistry-climate model will be compared with multi-year time series and variances of satellite data on atmospheric composition.
- The response of UKCA to changing climate (e.g. ENSO) will be verified by comparing with key satellite-observed trace gases and aerosols.

c) Establish a national capability in use of satellite data to sound atmospheric composition

- Develop and apply an integrated approach to tropospheric composition sounding, to produce the data required for exploitation in this Theme and more widely.

- Develop and apply observation operators, data assimilation and inverse modelling schemes needed to exploit satellite data in this Theme and more widely.
- Contribute to national and European initiatives to establish new applications for use of satellite composition data in pollution monitoring, air quality forecasting & NWP.
- Transfer to Met Office/Hadley Centre, DEFRA and ECMWF, data, tools and specialist knowledge in use of satellite observations and derived information.
- Enhance capability of UKCA for exploitation of satellite composition data.

The programme is divided into four sub themes (STs). **ST-1** develops new retrieval techniques and tools to interface observations with models. **ST-2** uses these new observations, and others, along with 3D chemistry-transport models (CTMs) to quantify distributions and emissions of trace gases and aerosols. **ST-3** uses satellite data to test the UK coupled chemistry-climate model (CCM). **ST-4** provides data and tools to test or assimilate into operational models for new applications: pollution monitoring, air quality forecasting and NWP.

3.1 Sub–theme 1: Observation Interface

3.1.1 Summary of the sub-theme

The purpose of ST-1 is to deliver unique data on atmospheric composition required for *scientific exploitation* (ST-2 & -3) and for *new applications* (ST-4), by consolidating the UK's world-class expertise in atmospheric retrievals into a *national capability* within NCEO[7]. The programme will focus on new opportunities to sound tropospheric composition presented by MetOp in combination with Envisat, along with SCISAT, which UK scientists, through involvement in international science teams and thirty-years experience, are well-positioned to exploit. These foci are selected to impact most effectively in ST-2 & -3 (emphasis on troposphere) and ST-4 (reliant on *operational* satellites) and to complement parallel national and international activities with different foci, such as the UTLS and stratospheric objectives to be served by HIRDLS and MLS limb-sounders on Aura.

An Integrated Approach to Tropospheric Composition Sounding

To advance understanding of processes which link atmospheric composition with climate and to establish a capability for pollution monitoring and air quality forecasting, demands satellite observations of trace gases and aerosol in the lowest stratosphere and troposphere. This is a formidable challenge because clouds and surface properties must be accounted for accurately, vertical and horizontal resolution will be vital and discrimination of the near-surface layer from overlying layers will be an objective. To meet this challenge, it will be necessary to exploit data from current and planned missions in new ways. Through developments in DARC and elsewhere, the NCEO is well-positioned to make significant advances during its first five years by developing an *integrated approach,* to use different types of measurement (uv–mm, spectrometer/radiometer, limb/nadir geometries, polar/geo orbits) synergistically to determine jointly the distributions of trace gases, aerosol, cloud and surface properties.

Opportunity for Innovation from EPS-MetOp

The first MetOp platform in the European Polar System (EPS) was launched on 19th Oct'06. In conjunction with satellites operating concurrently, MetOp offers a valuable new resource for this Theme to exploit. MetOp itself provides spectrometer and imager data which, if analysed in an integrated manner, offers improved observations of a range of tropospheric constituents. Envisat provides profiles from limb sounding and nadir-swir spectra which are complementary and close in time. The three EPS-MetOp satellites should operate continuously from 2006-20, so transfer to operational systems in subsequent phases of the NCEO would potentially benefit from R&D activities during its first 5-years.

[7] Knowledge of data and error characteristics of standard *operational* products from Eumetsat, ESA and CSA will also be transferred to ST-2, -3 & -4 in cases where these meet requirements, along with information on products from other missions to be exploited by those STs, such as NASA's Aura (HIRDLS, MLS, OMI & TES) and others in A-Train.

3.1.2 Work description and methodology

Internationally-recognized expertise of groups at RAL, Oxford, Leicester and York will be integrated to establish a national capability for atmospheric composition sounding and retrievals to conduct a programme in co-operation with colleagues in Europe, USA & Canada with whom close links exist.

3.1.2.1 Development of retrieval schemes

GOME-2 (uv/vis-nadir spectrometer): RAL's scheme to retrieve O_3 profiles from backscattered solar UV spectra has been applied extensively to ERS-2 GOME-1 data and is uniquely able to retrieve tropospheric information [Munro et al., 1998; Meier 2006] [8]. Adaptation of this scheme for GOME-2 will commence in 2007/8 within DARC. Advances on GOME-1[9] will be (i) improved geographical sampling and accuracy of O_3[10] distributions retrieved in the troposphere and (ii) potential to discriminate aerosol in the near-surface layer from the overlying atmosphere[11].

SCIA (swir-nadir spectrometer): Height-resolved aerosol information can be derived from strong O_2 and CO_2 absorption bands in the shortwave IR (SWIR), as required to retrieve CH_4 accurately from the SWIR, as well as for its inherent scientific value (both to be exploited in ST-2). RAL's simulation scheme for height-resolved retrieval of tropospheric trace gases jointly with aerosol from SWIR spectra, as used extensively in ESA studies, will be adapted to SCIA-nadir observations in the 1.6-2.35μm region to target CH_4 and aerosol. Co-located AATSR data (see below) will be used to constrain aerosol in the height-resolved SWIR retrieval, using a joint imager/O_2 A-band approach pioneered by RAL [Siddans, 2007]. Analysis of SCIA SWIR spectra will also benefit from methods developed by RAL to characterise the GOME-2 spectral response [Siddans, 2006].

IASI (ir-nadir spectrometer): A *physically-based* scheme[12] will be developed for trace gas retrieval from IASI, to focus on O_3, CH_4, HNO_3 and NO_2[13]. This will build on Oxford's extensive experience in retrieval of trace gases from IR-nadir spectra from NASA's TES [Bowman, 2006] and IR-limb spectra from MIPAS [Dudhia 2002, Raspolini 2006, Burgess 2004] and RAL's scheme to simulate IASI retrievals [Kerridge, 2005].

AVHRR/3 (vis/ir imager): The scheme to generate cloud, aerosol and surface properties from ATSR-2 images for use in (co-located) GOME-1 trace gas retrieval will be adapted to AVHRR/3 for use in (co-located) GOME-2 & IASI trace gas retrieval. This will benefit from improvements made within the NCEO to the (A)ATSR cloud & aerosol scheme (see below).

MIPAS (ir-limb spectrometer): Limb-emission complements the MetOp nadir-sounders through (i) *height-resolved* trace gas and aerosol distributions which span the mid-upper troposphere and/or stratosphere, and (ii) information on trace gases which are detectable only in this geometry.

Water vapour and ozone are ubiquitous in the IR, so a scheme to retrieve these jointly with cloud in the upper troposphere is a necessary foundation for a MIPAS scheme dedicated to NCEO objectives. Within DARC, RAL is developing such a pilot scheme for MIPAS observations in its new mode(s). This will also exploit a 2-D tomographic approach, afforded by the finer spacing of limb-profiles along-track in the new mode(s). In NCEO, the next step will be to focus on other required tropospheric trace gases (nb CH_4, HNO_3 and CO together with VOCs such as ethane, ethyne, PAN and acetone). In co-operation with European colleagues, Oxford and Leicester have pioneered

[8] This scheme has also now been demonstrated on a limited basis to function with Envisat SCIA data.
[9] Advances from GOME-1 are through: (a) 8-fold increase in no. of ground-pixels across-track; (b) calibration of spectral-response and more accurate radiometry and (c) spectrally-resolved polarisation measurements.
[10] Columns of NO_2, H_2CO, SO_2, BrO, whose spectra overlap the O_3 Huggins bands, are retrieved as by-products.
[11] Through use of spectrally-resolved, polarised measurements in the O_2 A-band in cloud-free scenes.
[12] Eumetsat will implement a *neural-net scheme* for IASI, ie will not incorporate radiative transfer on-line.
[13] To retrieve tropospheric trace gases with sufficient accuracy, it may prove necessary to retrieve jointly meteorological variables (eg humidity, atmospheric or surface temperature) or interfering trace gas absorbers. As baseline, ECMWF analyses will be used as *a priori* for met variables and O_3 and Eumetsat SAF products for other gases available.

early exploitation of MIPAS spectra, and are well-placed to undertake the necessary R&D [Remedios et al,2007; Greenhough et al, 2005].

Integration of Metop and Envisat data: Within DARC, initial steps have been taken towards an integrated approach to tropospheric composition sounding, and two further advances for tropospheric ozone are planned for 07/08. Firstly, by combining limb observations from the dedicated MIPAS UTLS scheme with nadir UV observations and, secondly, through re-processing the full GOME-1 mission with ATSR-2 cloud & aerosol explicitly incorporated. Within NCEO, this integrated approach will be extended to observations from MetOp sensors GOME-2, IASI and AVHRR/3, in conjunction with those from Envisat[14] MIPAS and SCIA(-nadir/SWIR). Significant advances in vertical resolution and accuracy can be foreseen for tropospheric O_3, NO_2, HNO_3 and CH_4 (possibly SO_2, CO)[15], as required for scientific advances in (ST-2), and for assimilation trials by ECMWF and evaluation of Met Office UMAQ and NAME models (ST-4).

Within DARC, Leeds and RAL developed a scheme to generate *tropospheric distributions of trace gases* from line-of-sight columns derived from uv/vis (GOME-1) nadir-spectra, specifying: *stratospheric distributions* from a CTM into which solar occultation (HALOE) profiles of chemically-linked gases are assimilated and *cloud and aerosol* from co-located imager (ATSR-2). In NCEO, this approach will be extended to additional tropospheric gases detectable by GOME-2 &/or IASI and to any for which the stratosphere/upper tropospheric profile is represented more accurately at MetOp locations through assimilation of SCISAT-1 or Aura profiles than from co-located MIPAS measurements.

ATSR (vis/ir imagers) cloud, aerosol and surface properties: The Oxford-RAL Aerosol and Cloud (ORAC) scheme developed for ATSR-2, AATSR and SEVIRI sets a precedent for successful collaboration between these two NCEO partners. The scheme is applied in the NERC GRAPE [Poulsen 2007, Thomas 2007] and ESA GlobAerosol [Carboni 2006] projects to deliver data on cloud from ATSR-2 and aerosol from both ATSR-2 and AATSR. Algorithm developments are required within NCEO to improve the quality of aerosol retrieval over land in particular. These include implementation of: (i) dual-view; (ii) IR channels for aerosol layer height and (iii) improved treatment of surface bi-directional reflectance distribution function (BRDF) for global processing of the joint ATSR-2/AATSR mission. This will deliver a self-consistent data set on aerosol, cloud[16] and surface properties (BRDF and temperature) for exploitation in ST-2 & 4 and possible use in the *Climate Theme.* This work will be coupled to that on SEVIRI, AVHRR/3, GOME-2 & SCIA and could benefit also from methods used in the *Climate Theme* to parameterise land-surface BRDF.

SEVIRI (Geostationary vis/ir imager) aerosol and surface properties:
Pilot schemes to retrieve aerosol and ozone from MSG-SEVIRI have been funded through ESA and Eumetsat contracts[17] [Siddans 2006], respectively. A major advance for aerosol retrieval accuracy, especially over land, will be to exploit the systematic variation in solar geometry, unique to *geostationary* observations, to characterise the angular dependence of surface BRDF and separate from aerosol properties. The distinctly different spatio-temporal variabilities of land surface BRDF and aerosol make this a separable problem[18]. The improved characterisation of BRDF will also apply to the particular solar geometries of AATSR (and ATSR-2) and AVHRR/3 in *sun-synchronous* polar orbit.

[14] MetOp and Envisat are in the same orbit, with daytime equator crossings ~9:30am and ~10am, respectively.
[15] Vertical resolution is gained by exploiting differing height sensitivities of nadir solar scatter and emission sensors and limb vs. nadir. Co-located aerosol and cloud improves tropospheric gas retrieval accuracy.
[16] Cloud products have yet to be generated for AATSR.
[17] The SEVIRI aerosol algorithm for GlobAEROSOL (adapted from ORAC) and a SEVIRI ozone algorithm have been developed by RAL. Reading is undertaking experiments to assimilate retrieved ozone data into the ECMWF IFS.
[18] Land-surface BRDF is variable on spatial scales below the smallest accessible to SEVIRI (~4km x 4km), whereas aerosol properties typically remain coherent up to larger scales. By contrast, temporal variation in surface BRDF is typically slow (e.g. seasonal) by comparison to the evolution and dispersion of aerosol plumes.

ACE (ir solar occultation spectrometer): Attributes of the IR solar occultation technique [Bernath, 2005] are highly complementary to those of other sensors to be exploited in NCEO. ACE detects additional VOCs and offers higher precision on individual profiles of trace gases observable by MIPAS[19]. Although ACE sampling on a given day is restricted to only 15 longitudes at two specific latitudes, the multi-year data-set will accumulate profiles over the range 85°S-85°N. The suite of organic compounds offers new means to verify CTMs (ST-2) and *chemistry-climate interaction* in the UM/UKCA (ST-3), in particular, representation of interannual variations such as ENSO. NCEO will focus on VOCs whose spectral signatures have been detected by ACE (acetone, formaldehyde, peroxyacetylnitrate, methyl bromide and methyl cyanide)[20]. This will be led by Prof.P.Bernath, the ACE PI at U.York, and will exploit U.Leicester's experience in retrieval of organics from MIPAS.

Production and Validation of Satellite Data Required for Exploitation in NCEO

The rationale for data processing within NCEO is two-fold: firstly, the data are r*equired* for ST-2, -3 or -4 and, secondly, the product is *novel* (i.e. not available by other means) or of *demonstrably higher value* than operational products from Eumetsat, ESA, NASA. Building on R&D components outlined above, data will be processed, archived and disseminated via the *EO Informatics Theme*. For effective exploitation, validation is imperative to: characterise quality of a new product; monitor changes occurring over time; and demonstrate improvements from re-processing. Correlative data from sondes, aircraft and ground-based sensors will be used where available and *assimilation* will be used interpolate observations which are not co-located, by applying methods devised in DARC.

3.1.3 Deliverables

- Demonstrated and validated retrieval schemes
- Data-sets on trace gases & aerosol, with associated cloud & surface parameters, from individual sensors and from the integrated scheme, for exploitation in ST-2 & -4
- Multi-year data-sets for verification of chemistry-climate model (ST- 3), including:
  1. Profiles of VOCs, CO and CH_4 from ACE (2004 onwards)
  2. Profiles of HNO_3, CO and VOCs (in UT) from MIPAS (2002 onwards)
  3. Height-resolved O_3 from GOME-1/SCIA/GOME-2 (1995 onwards)
  4. Cloud, aerosol (& surface properties) from ATSR-2/AATSR (1995 onwards)
- Observation operators to allow products to be optimally exploited in ST-2, -3 or -4

3.1.4 Key dependencies on other programmes and organisations

Dependencies on Space Agencies for satellite data and sensor operation are as outlined in Sections 4 and 7, respectively. Auxiliary data on met parameters are required from ECMWF or MetOffice, and will be made available through the EO Informatics Theme. A current NERC EO mission support grant application would enable sea-surface temperature to be produced with cloud and aerosol in a self-consistent manner from (A)ATSR within NCEO.

3.2 Sub–theme 2: Quantification of Trace Gas / Aerosol Distributions and Emissions

3.2.1 Summary of the sub-theme

The overarching objective of ST-2 is to test *and* develop our understanding of processes which control the distributions of trace gases and aerosols that are important to climate and air quality[21] by

[19] Solar spectra measured with high photometric sensitivity and spectral resolution through the atmospheric limb are ratioed to the solar spectrum measured just above the atmosphere, requiring no changes to instrument optical configuration or to signal channel electronics. Calibration of ratioed spectra is inherently stable in the long-term.

[20] To supplement those for which schemes are already available operationally (CO, CH_4, HCN, OCS, C_2H_6, C_2H_2, F_2CO, CH_3Cl) or are under development (CH_3OH, ethyne, HC(O)OH (formic acid), ClFCO, Cl_2CO (phosgene)).

[21] Tropospheric ozone (O_3) is: a surface air pollutant, related to human respiratory illnesses and reduced yields for agricultural crops; a greenhouse gas (GHG) in the mid and upper troposphere with a radiative forcing similar to CH_4; and the major source of the hydroxyl radical (OH), the main sink for the GHG CH_4. Tropospheric O_3 is produced from the oxidation of CO, CH_4 and non-CH_4 volatile organic compounds (NMVOCs) in the presence of nitrogen oxides (NO_x

combining new satellite observations (ST-1) with state-of-the-art 3-D chemical-transport models (CTMs) and surface-level observations. Improved understanding and modelling of these processes would be transferred to the coupled climate-chemistry model (ST-3) used by NCAS/Hadley Centre. In a number of cases (e.g. VOCs observed from space for the first time and aerosol), significant advances are foreseen through a *1st step* to simply compare satellite distributions and variances with those of the CTM, sampled with the appropriate satellite observation operator (ST-1). Once satellite and CTM fields are demonstrated to be consistent within their estimated errors, a *2nd step* will be to move to assimilation, to allow consistency to be tested at the next level, e.g. for O_3 and several other reactive gases. Discrepancies between observed and analysed fields (biases and standard deviations) will reveal inadequacies for subsequent attention in either the CTM representation of relevant processes and/or the observations. Assimilation of tropospheric constituent data into a CTM is a major scientific challenge which will require a substantial R&D effort in preparation that will also draw on specialist theoretical expertise from the *DA Theme*. For the specific objectives to be addressed here, assimilation of constituents into a CTM (driven by analysed wind fields from a GCM into which met data have been assimilated) offers the most efficient and flexible approach to optimise science return in the first phase of the NCEO. The starting-point will be a Kalman filter (KF) scheme, as already interfaced to TOMCAT and demonstrated for assimilation of stratospheric data. ST-2 will benefit from international initiatives in this new field through interactions with colleagues in Europe and USA. It will also complement initiatives directed towards future *operational applications,* to which there are explicit links through ST-4 to ECMWF and MetOffice, which centre on GCMs for NWP.

Tropospheric distributions of certain constituents are affected significantly by spatio-temporal variability in surface sources in addition to chemical or transport processes occurring within the atmosphere. The most ambitious objective for ST-2 will be to attribute and estimate quantitatively biogenic, pyrogenic and anthropogenic emissions. In cases for which climatologies of surface emissions are found not to be sufficient, a *3rd step* will be to add surface emissions to the assimilation state-vector. For CH_4 in particular, atmospheric lifetime is sufficiently long that deviations from uniform mixing are typically only a few % in the troposphere and mostly located in proximity to source regions. If relevant atmospheric processes (dynamics and loss by reaction with OH) have been shown by other means to be represented adequately in the CTM and observational constraints are tight, data assimilation could, in principle, determine surface emissions (inverse modelling). A long-term goal would ultimately be to couple a biophysical model to the CTM and to replace surface emissions by model parameters in the assimilation state-vector, which would involve interaction with biophysical modelling experts in the *Climate and Carbon Themes.*

3.2.2 Work description and methodology

Two world-class global tropospheric 3-D CTMs with complementary attributes, TOMCAT and GEOS-Chem, will be used in ST-2 to exploit data provided through ST-1. The main distinctions, other than resolution[22], are that *TOMCAT* includes a detailed stratosphere and the GLOMAP aerosol scheme and is driven by *ECMWF* meteorology, whereas *GEOS-Chem* includes a more complete heterogeneous chemistry scheme in the troposphere and is driven by *GMAO* meteorology. Access to GEOS-Chem allows NCEO to benefit from extensive intellectual investment by US and European scientists in its development and the opportunity for continued co-operation[23]. CTM development within NCEO will, however, focus on TOMCAT and, specifically, on modules for use also in the UKCA chemistry-climate model (ST-3), so that deliverables from ST-2 will be directly applicable also to UKCA, as part of a UK model hierarchy and development of

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= $NO+NO_2$). Primary and secondary atmospheric aerosols (solid or aqueous phase particles) have significant implications for climate (direct and indirect effects), air pollution chemistry, and human health.

[22] TOMCAT has a typical horizontal resolution of 2.8^o x 2.8^o with 3 levels below 2km and a vertical resolution of ~1 km throughout the troposphere. GEOS-Chem is typically run at 2^ox2.5^o horizontal resolution, but has a nested capability allowing regional calculations at 1^ox1^o, and includes 20 layers in the troposphere; five are below 2km

[23] An option to use ECMWF meteorology in GEOS-Chem will be assessed. This would allow sensitivity to prescribed wind fields to be assessed, and aspects of ECMWF and GMAO model dynamics to be compared indirectly.

national capability. A longer-term aim is to improve national CTM capability by integrating modelling components from GEOS-Chem into TOMCAT. Surface-level and aircraft observations will be used for ongoing evaluation of the CTMs, drawing on U.Leicester expertise and links to NCAS, DEFRA/EA and international surface networks.

Step 1: We will initially conduct model simulations and comparisons for specific years, to focus on particular episodes (e.g., major burning years) and the annual cycle, and subsequently extend to interannual variability[24].

Step 2: A data assimilation (DA) scheme will be developed from a sub-optimal Kalman filter formulation already in use with TOMCAT [Chipperfield et al, 2002], moving initially to an Ensemble Kalman Filter. Major technical challenges will be confronted in extending this scheme to cope satisfactorily in the mid- and lower troposphere as well as the stratosphere and upper troposphere. Characterisation of observational errors, background error covariances and model errors, for example, will be more challenging, as will stabilisation issues caused by non-linearity associated with (fast) chemistry and interactions with clouds and the surface. This development in NCEO will benefit substantially from co-operation with colleagues in Europe and the US. As and when appropriate, satellite data will be introduced into the assimilation, to permit more critical evaluation of both the CTM and the observations, and for science applications[25].

Step 3: Improved estimation of surface emission fluxes through data assimilation (inverse modelling) would have future application in both climate and pollution monitoring, but is a very ambitious goal[26]. For trace gases with lifetimes of greater than a few weeks (e.g. CO and CH4), it has been shown that the problem can be simplified greatly through linearization by adopting a fixed sink distribution, pre-calculated using a detailed version of the chemistry. We will build on this, carefully assessing the timescales over which chemical systems can be linearized, with the ultimate goal to develop a fully-coupled global analysis of non-linear oxidant chemistry. For CH_4, we will also investigate parameter estimation using a surface flux model based on JULES [Gedney et al, 2004] coupled with GEOS-Chem, with the aim to contribute to understanding of underlying processes.

Short-lived trace gases. Use of satellite data to verify global CTMs is reaching a mature stage in Europe [van Noije, 2006], and the proposers have extensive experience of analysing data from all relevant sensor-types. In particular, the MetOp sensors, in combination with Envisat, will provide powerful, new, global, height-resolved data-sets on short-lived gases (ST-1) to test and assimilate into CTMs in ST-2: NO_2 for NO_x emissions; HCHO for VOC emissions; CO, NO_2 and HCHO for biomass burning and O_3, HNO_3, CO, and several VOCs for long-range transport. Data from ACE include a number of VOCs (ST-1) not previously observed from space in the mid/upper troposphere, which will test certain pathways of the CTM chemical schemes for the first time.

The sub-optimal Kalman filter approach to data assimilation will be used to quantify errors in the model and subsequently to also fit surface fluxes of NO_x and VOCs to the observed NO_2 and HCHO data, advancing on previous work by the proposers using *ad hoc* inversion methods. Additional constraints on emission estimates from correlations between gases emitted by the processes or more generally through chemical mass balance will be explored.

Emission estimates will be analysed in terms of their impact on modelled OH, and hence the oxidising capacity of the troposphere. The suite of organic species to be targeted provide, through simultaneous observations, a new ability to differentiate source emissions, utilise differing chemical

[24] Multi-year observational records for several trace gases will be available from certain sensors through ST-1.

[25] Assimilation of stratosphere/upper troposphere trace gas profiles from ACE will be relevant also to constraining retrievals of lower tropospheric concentrations in the integrated approach proposed in ST-1. This will build on use in DARC of a sub-optimal Kalman filter to assimilate profiles from HALOE into TOMCAT.

[26] Forward approaches such as KF require the *distribution* of emissions to be fixed *a priori*. Backward approaches such as 4D-VAR/adjoint, to which NCEO would aim to evolve, are flexible, allowing emissions to vary in space and time.

lifetimes of species to constrain evolution along transport pathways, link the NOx and VOC cycles, and test the sensitivity of the model to changes in ability to oxidise both anthropogenic greenhouse gases and primary pollutants.

Methane. Methane (CH_4) has biogenic, pyrogenic and anthropogenic sources. Its main sink is oxidation by OH, leading to a lifetime of ~8 years. The globally-integrated CH_4 trend is well-characterised by surface *in situ* measurements, but the strengths, regional distributions and variability of different sources are uncertain. CH_4 has recently come under scrutiny because of 1) unexpected, and largely unexplained, changes in the growth rate of its atmospheric burden measured by *in situ* data [Wang et al, 2004], 2) new observations of its atmospheric distribution and variability from satellite instruments, 3) a newly-identified aerobic source from terrestrial plants, and 4) a number of other potentially significant sources related to climate, in particular warming, at high latitudes and in the deep ocean. These four factors challenge our understanding of the budget of CH_4. The combination of MetOp and Envisat data (ST-1) will provide a powerful new global height-resolved data-set on tropospheric CH_4 for comparison with and assimilation into the CTMs; initially GEOS-Chem driven by start-of-the-art emission inventories. Complementary satellite data e.g., active fire intensities from AATSR-derived fire radiative power (*Carbon Cycle Theme*) will be used subsequently to assess the roles of different sources. Structure in model CH_4, driven by prescribed estimates, will be evaluated using surface, tall-tower and aircraft observations from NCAS, CarboEurope and NOAA ESRL. Estimating model parameters that describe surface flux variability is an elegant but non-trivial extension to this work. We will use a simple, falsifiable surface flux model based on JULES [Gedney et al, 2004] to ensure results can be easily interpreted.

Accurately estimating model error is critical for data assimilation. Errors in atmospheric transport, particularly convection, are significant. We will use the NMC method to quantify error in modelling CH_4, following Jones et al [2003] for CO[27], and will work in concert with the *Data Assimilation Theme* to explore new methods of accurately estimating model error. Source attribution for CH_4 can be improved by estimating simultaneously surface fluxes of another trace gas that is a marker for a particular process, e.g. CO for incomplete combustion[28] (based on Palmer et al [2006]).

International initiatives (e.g. EU FP6 HYMN) are developing inverse models to estimate surface fluxes of CH_4, including the use of SCIAMACHY *total-column* data [Bergamaschi et al, 2007]. The proposed NCEO initiative will benefit from co-operation with the HYMN consortium and intercomparison of flux estimates.

Aerosol.
Using data produced in ST-1, we will conduct a statistical analysis of aerosol loading, effective size and layer height, on regional and global scales for specific time periods (seasonal and interannual) and compare with TOMCAT/GLOMAP CTM. Representation of aerosol plumes from stochastic sources (e.g., volcanic emissions, desert dust plumes and biomass burning) whose properties (composition, size distribution and mixing and thus their optical properties) can evolve rapidly is a more stringent test of models[29]. We will investigate evolution from selected sources or episodes, using detailed microphysical aerosol modules within the CTM, tagging aerosols from specific sources. The retrieved and model results will be evaluated against *in-situ* and AeroNet photometer data. A more ambitious objective will be to then attribute specific sources and sinks to satellite-observed distributions of aerosol optical properties.

[27] Estimates of model error may be refined with advanced methods devised by the Data Assimilation Theme.
[28] Simultaneous inversion requires physically-justified error correlations as prior constraint. The EnKF provides a method to calculate the moments of the optimal solution without having to assume Gaussian error statistics, which are not valid when solving for correlated species. EnKF will be investigated for flux estimation.
[29] Optical properties of different aerosol types add nonlinearly, so specific emission scenarios will be developed to quantify the contributions of individual sources.

Surface-level particulate matter (PM) is important to air quality and human health. Correlation with aerosol optical depth (AOD) has been used to estimate PM over urban areas [Liu et al., 2004]. A weakness of this approach is that substantial AOD variation can occur above the boundary layer, e.g., due to plume dispersion. Aerosol layer altitude (from ST-1) will be used to remedy this deficiency. An altitude threshold will be derived to screen out AOD values dominated by aerosol above the boundary layer, using aerosol fields from the CTM to test this procedure. The UK surface PM network is sparse and focussed on PM10 (diameter <10 μm) (in accordance with EU directives). Environmental agencies elsewhere are also using PM2.5 (diameter <2.5 μm) as an air quality indicator. We will evaluate our approach against the UK PM10 network and, if satisfactory, will also derive PM2.5 distributions. The impacts of natural sources and inter-continental transport on PM10 and PM2.5 levels derived over the UK will be quantified with the CTM, and the effects of local (urban) pollution on larger scale patterns of retrieved aerosol optical properties (and hence global aerosol radiative effects on climate) will be assessed.

3.2.3 Deliverables

- Tools for assimilation of satellite data on tropospheric composition into a CTM and for estimation of surface emissions.
- Improved quantitative estimates of long-range pollutant transport and impact on domestic pollutant levels
- An improved quantitative understanding of the contribution of anthropogenic and natural sources to atmospheric CH_4 variability.
- Detailed investigation of the evolution of aerosol plumes from their sources to sinks with a focus on the underlying microphysical and chemical processes.
- Improved method to estimate PM surface concentration from satellite data..
- Improved source attribution of global and regional aerosol distributions to their anthropogenic and natural sources.

3.2.4 Key dependencies on other programmes and organisations

- NCAS and DEFRA: Ground-based and aircraft-based measurements.
- NERC APPRAISE: Development of aerosol models.

3.3 Sub–theme 3: Quantification of Climate-Composition Interactions

3.3.1 Summary of the Sub-Theme

The purpose of ST-3 is to use satellite data to test and improve climate models, thereby forming a link between NCEO and NCAS/Met Office. NCAS controls the NERC-funded development of chemistry-climate models (CCMs). The importance of testing such models has been recognised by, for example, a recent WCRP/IGBP initiative. The NCEO work will complement NCAS modelling and use of surface observations by focussing on provision of satellite data, development of tools to sample the CCM and participation in the analysis of model/data comparisons. This will ensure the exploitation of satellite data by NCAS and help align the work programmes of the two Centres.

Our understanding of how the Earth's climate will evolve in the future is based on predictions of complex models. A key component to such climate models is the treatment of atmospheric chemistry and aerosols [e.g. see IPCC 2007]. Changes in atmospheric composition are known to affect climate. Cooling by direct and indirect aerosol effects regionally and globally masks global warming by greenhouse gases. Past depletion of stratospheric ozone has offset some of the surface temperature rise due to GHG increases. Changes in climate will also affect composition. For example, under warmer conditions biogenic emissions from vegetation are expected to increase. These changes are all highly coupled, meaning that for confident predictions of the future climate we need to test coupled chemistry climate models against observations.

Past work on coupled CCMs in the UK has been largely based on adding chemistry into versions of the Met Office Unified Model (UM). Versions of the UM have been used for both stratospheric and tropospheric studies. Recent work within NCAS and the Met Office has been focussed on developing a new 'whole atmosphere' chemistry and aerosol schemes to include in the latest version of the UM (i.e. the same 'new dynamics' model used for NWP). This model, called UKCA, will be a main tool for UK climate scientists and will also be coupled to other components of Earth System Models used in NCEO.

Satellite observations are well-suited for testing global models; they provide global observations on a resolution comparable to the model grid over a multi-annual timescale. However, the task of comparing such data with models is not straightforward. There is both the technical issue of developing algorithms so that the model data are sampled/averaged in the same way as the observations (i.e. an 'observation operator') and the scientific issue of how to compare observations under specific meteorological conditions with a climatological model. Moreover, it is important to test the model under a wide range of conditions (i.e. test the variability and not just the mean behaviour) to encompass possible future changes in climate. A *nudged* version of UKCA, where the model is forced to evolve in line with analyses, is being developed by NCAS. This will allow direct comparison of certain model processes with observations. However, it is also important to test the *free-running* model used for climate prediction.

3.3.2 Work description and methodology

NCEO work will provide data through ST-1 for comparing with UKCA and code[30] to allow sampling of the model runs (ST-4). This will focus on comparison of UKCA O_3, NO_x and other short-lived species, organic species and aerosols. Firstly, the nudged UKCA will be run to simulate the recent past. Comparison of this with the satellite data, for the same time period, will test the model chemical scheme. Then, the free running version of UKCA will be run. NCEO will investigate new ways of sampling the data for comparing with the climate model. These will include probability distribution functions in order to test the modelled variability as well as mean state. Recent preliminary work [Pyle et al., 2007] suggests that changes in probability distribution functions might be used to detect changes driven by chemistry/climate interactions.

Extremes of the present day climate variability can be used as a surrogate for the possible mean climates of the future. Therefore, a useful test of UKCA will be to see how well it captures the chemical-meteorological interactions under these events. We will examine the atmospheric behaviour, using satellite data and UKCA, under different climate modes, focussing on ENSO and the NAO. The UKCA model will be run (by NCAS / Met Office) for a series of decadal transient experiments for the recent past. Prescribed SSTs will ensure that the model captures El Nino events. Work with an earlier CCM [Zeng and Pyle, 2005] has shown that there is a strong correlation between ozone in the free troposphere (especially the UT) and the phase of ENSO, modulated both by changes in tropical convection as well as stratosphere-to-troposphere exchange in middle latitudes. We will use UKCA and satellite data to explore this relationship further. Satellite-derived emission datasets will be used to reproduce the observed anomalous wildfire emissions associated with El Nino (in collaboration with the *Climate Theme*), which caused severe air quality issues and regional climate perturbations.

Then, detailed comparisons of the aerosol/chemical species will be made for the tropical regions during ENSO events. Observations of short-lived organic species and CO (ACE, MIPAS) in the UT will be used to investigate differences in the pattern of convection. NO_2 and HNO_3 will be used to test UKCA's parameterisation of lightning, exploiting the co-located limb, nadir and cloud

[30] For critical comparison with satellite, 3D model output must be sampled in accordance with the sensor retrievals of real atmospheric profiles. Observation operators to perform this function for the relevant sensors (ACE, MIPAS & GOME-1/SCIA/GOME-2) will be provided for this purpose to the Met Office and NCAS.

observations integrated in ST-1. O_3 profiles (GOME, MIPAS) will be used to investigate differences in strat-trop exchange.

3.3.3 Deliverables

- Provision of datasets and tools to NCAS and Hadley Centre for testing UKCA model.
- New methodologies for comparing satellite data with CCMs.
- Comparison of UKCA model with satellite time series and variances on tropospheric composition including O_3, NO_2, and CO and aerosol optical properties.
- Specific case studies of behaviour of UKCA under extremes of current climate: (e.g. El Nino) as surrogate for conditions of climate change.

3.3.4 Key dependencies on other programmes and organisations

- Co-operation with Met Office Hadley Centre and NCAS

3.4 Sub –theme 4: New Applications

3.4.1 Summary of the sub-theme

The purpose of this sub-theme is to co-operate closely with partners outside NCEO in specific R&D activities to develop new applications for satellite composition data beyond the science research domain: pollution monitoring, air quality forecasting and NWP. These activities have been selected to exploit established expertise in particular niches and will leverage large investments at European level (Eumetsat/EU/GMES) and national level (MetOffice/DEFRA). It is also anticipated that NCEO could in course become a nationally-funded partner of the future ECMWF GEMS-II project and participate in further development of its chemical data assimilation system.

3.4.2 Work description and methodology

3.4.2.1 Provision of data sets and observation operators and model verification

Generation of specific new data-sets for assimilation trials or for re-analyses is covered in ST-1. NCEO scientists will co-operate closely with their counterparts in the relevant agencies in ST-4, firstly, to define detailed requirements and, secondly, to ensure timely and efficient transfer and implementation of data and/or code, together with auxiliary information. This will be accomplished in part through visits / placements of NCEO-funded staff and/or CASE studentships. Specific activities which it is planned to undertake are outlined below.

GOME-2: An early example will be height-resolved ozone data spanning the troposphere and stratosphere from GOME-2. If assimilation trials demonstrate sufficient benefit for Met Office and/or ECMWF to consider GOME-2 ozone from the NCEO scheme for operational assimilation, an observation operator could be provided to run within the MetOffice/ECMWF operational system[31]. A fast uv forward model will also be provided to ECMWF, to be initially used for radiance monitoring, and as precursor to possible future radiance assimilation.

MIPAS new observing modes: In addition to assimilating MIPAS ozone profile data operationally, ECMWF also performed assimilation trials with MIPAS radiance data acquired in its original observing mode. Radiance assimilation trials for the new modes will require new coefficients for the fast radiative transfer model (RTMIPAS) and impact assessment of observations in the new modes.

SEVIRI: The current (ORAC) aerosol scheme for MSG-SEVIRI is being transferred to the Met. Office as a tool to aid forecasters. Research in ST-1 to improve aerosol data quality and in ST-2 to link to PM concentration, is directed towards *quantitative* use in future.

[31] An alternative option, to acquire data, process in NCEO and then make available within near-real time constraints of operational users, could also be explored, although this would require additional resources.

3.4.2.2 Evaluation and trial assimilation of new satellite data sets and methodologies

Scientists in DARC have undertaken a number of successful projects to evaluate new types of satellite data and their assimilation into the MetOffice or ECMWF (NWP) systems. Notable examples include temperature, ozone and humidity profiles from the MIPAS and MLS limb-sounders and ozone columns from GOME-1 [e.g. Geer et al, 2006; Struthers et al 2002]. One of the theoretical advances made in DARC has been to recast the constituent profile assimilation problem so as to use more optimally the information contained in the original radiances; by eliminating off-diagonals in the observation error covariance matrix (which cannot be accommodated in conventional profile assimilation) and by removing observation bias which might result from use of *prior* information in the retrieval. Initial experiments have been performed in the MetOffice system, applying the new approach in practice to assess possible benefits for MIPAS and GOME-1 over conventional ozone profile assimilation [Migliorini et al, 2004].

It is proposed in NCEO to build on experience and collaborations formed in DARC to evaluate new satellite data sets of potential relevance to future operational applications for pollution monitoring and AQ forecasting, provided in ST-1. Early examples will be SEVIRI ozone data and MIPAS new observing modes. The information-based assimilation approach will also be assessed extensively.

3.4.2.3 Verification of Met Office models for pollution and air quality applications

Lagrangian models are employed to monitor pollution events, forecast air quality, assess future scenarios on pollution levels and estimate integrated national annual emission inventories for DEFRA. The NAME model can handle scales from urban up to global. Such models use measurements from the national network of surface (i.e. street-level) sensors (NETCEN) for verification. Satellites offer complementary observations of gaseous and particulate pollutants which are (a) *above surface level* and (b) not restricted to fixed locations, to verify different aspects of model performance. Subject to cloud, satellite observations are geographically and temporally homogeneous, sampling the whole country at a horizontal resolution of ~10's km and capturing the annual cycle and interannual variability. The UMAQ *Eulerian* model is in parallel development for regional AQ forecasting. The intention is to fully integrate this with the operational NWP system and to utilise global constituent fields from the ECMWF system, in addition to surface observations. Analysed and forecast fields from UMAQ as its development evolves, would be amenable to (off-line) verification against satellite observations independent to those assimilated by ECMWF. For quantitative comparisons of either NAME or UMAQ against satellite data, observation operators would be applied to the model fields, to integrate in the vertical and to sample and average as per the satellite sensor. This is a preparatory step towards assessing the potential benefit of assimilating directly into *regional air-quality models* rather than using satellite data indirectly to constrain initial/boundary conditions via *global model* assimilation.

3.4.3 Deliverables

- Transfer of new data sets and/or observation operators to Met Office & ECMWF
- Assessment of assimilation of new data sets in ECMWF IFS system
- Assessment with satellite data of Met Office models used for pollution applications

3.4.4 Key dependencies on other programmes and organisations

- ECMWF: EU FPVII GEMS (II) Project / GMES Pilot Atmosphere Service.
- Met Office: Output from UMAQ & NAME models to be made available

4 OBSERVATIONAL DATA REQUIREMENTS

Access to required satellite data-sets has already been formally approved by the Space Agencies, e.g. through relevant ERS, Envisat and EPS-MetOp Research Announcements of Opportunity:

1. **Eumetsat MetOp:** GOME-2, IASI and AVHRR/3 L1 and L2 products.

2. **Eumetsat MSG:** SEVIRI L1 and L2 products.
3. **ESA ERS-2:** GOME-1 and ATSR-2. L1 and L2 products for full global mission.
4. **ESA Envisat:** MIPAS, SCIA-nadir and AATSR. L1 and L2 products.
5. **CSA SCISAT-1:** ACE. L1 and L2 products for full mission.

Data from NASA's Aura and SSM/I are publically available. Data from surface sites are available either publically (aeronet) or via links to NCAS, DEFRA, EA and local authorities. Access to ancillary met analyses (ECMWF & MetOffice) and satellite data will be via EO Informatics Theme.

5 RESOURCE REQUIREMENTS AND JUSTIFICATION

The programme proposed in Sect 0 for the first 5-year phase of NCEO is scientifically and technically ambitious. Resources are requested here, firstly, for *essential core-strategic elements* of the programme to build national capability, i.e. to develop the specialist expertise, methodologies and S/W tools to produce and exploit satellite data and develop new applications and, secondly, to perform *high-priority research studies* which exploit the data. Opportunities will be explored to secure additional funding to consolidate and expand both dimensions of the programme, in the first case through NCEO New Opportunities Fund[32], NERC Partnership Research Grants, ESA, Eumetsat and DEFRA and, in the second case, through NERC standard grants and EU FPVII[33].

RAL: 1.0 FTE for Theme coordination and for a dedicated "data-processing scientist" to: design and implement the large-scale system, liaise between scientists developing retrieval schemes & computer support staff, intelligently monitor data quality (contributing to validation) and interface to users; **1.67 FTE** in **ST-1** for retrieval development: GOME-2/SCIA trace-gases & height-resolved aerosol; AVHRR/3 cloud/aerosol; MIPAS UT H_2O/O_3/cloud; integrated scheme for Metop & Envisat, & SEVIRI aerosol; **0.12 FTE** in **ST-4** for interaction with Met Office & ECMWF on datasets from ST-1 (initially GOME-2, MSG), adaptation to their needs and transfer of observation operators.
Univ. Cambridge: 0.45 FTE in **ST-3** for UKCA modelling and science exploitation.
Univ. Edinburgh: 1.21 FTE in **ST-2** CTM, data assimilation/inverse modelling; primary focus CH_4
Univ. Leeds: 1.0 FTE in **ST-2** for CTM, data assimilation/inverse modelling with primary focus on short-lived trace gases and **0.25 FTE** in **ST-3** for coupling UKCA with observation operators.
Univ. Leicester: 0.67 FTE in **ST-1** for developing retrieval of organics from MIPAS and ACE, and for provision of specialist expertise in molecular spectroscopy and surface-level measurements.
Univ. Oxford: 1.2 FTE in **ST-1** for: applying retrieval schemes to MIPAS, nb new observing modes, adapting new schemes to IASI, maintenance of the RFM, cloud/aerosol scheme for AATSR and transfer of schemes or data for use in the integrated scheme. **0.2 FTE** in **ST-2** for aerosol studies.
Univ. Reading: 0.5 FTE in **ST-4** for evaluation of new satellite data sets with ECMWF IFS.
Univ. York: 0.04 FTE in **ST-1** for specialist expertise in utilisation of ACE data and supervision of algorithm development for several new organic species, to be carried out through studentships.

Computing:
University groups have requested dedicated PCs for in-house development. RAL will initially use an existing cluster for development. To contribute to expansion of processing power and data-storage for large-scale processing, £30k is allocated[34]. HPCx/Hector time for modelling will be provided through the NCEO top slice and NCAS. Computer time at ECMWF will be requested from the allocation for Special Projects and from the UK national allocation.

[32] Bid for scientific preparation for PREMIER or TRAQ would be made, if selected for ESA Explorer Phase A study.
[33] The precedent from DARC (atmospheric component) is that equivalent funding will be secured from other sources.
[34] Options would also be assessed to transfer mature, validated schemes to ESRIN's GRID for large-scale processing.

Studentships: The following 7 studentships will be funded directly[35].

- Edinburgh: Exploitation of Aura MLS data
- Leeds: CASE with Met Office/ Hadley Centre (ST-3)
- Leicester: (1) CASE with EA Surface obs in ST-2; (2) Organics from MIPAS/ACE (ST-1)
- Reading: Data assimilation linking new observations to ECMWF (ST-4).
- York: Two for retrieval of organics from ACE data in ST-1 and utilisation in ST-2, 3 and 4.

Partnerships have been agreed with **NCAS** (ST-3), **MetOffice/Hadley Centre** (ST-3 & 4) and **ECMWF** (ST-4), to be undertaken through NCEO staff and (CASE) studentships in co-operation with partners' contributions: *Met Office* will trial assimilation of GOME-2 ozone, assess improved MSG aerosol and provide access to NAME/UMAQ model data for comparisons with observations; *ECMWF* will trial assimilation of GOME-2 ozone and provide access to their system for assimilation trials and evaluation of new satellite data sets by NCEO.

6 KNOWLEDGE TRANSFER

Data will be disseminated to other scientists and end users through *EO Informatics*. Specialist knowledge of remote-sensing, retrieval and error characterisation gained through ST-1 and on atmospheric composition and assimilation acquired through ST-2 & ST-3 will be made available to the partners and to DEFRA (through NCEO's dedicated KT resource). The Theme will contribute to NCEO workshops and spring/summer schools and to public understanding of science, through initiatives at the National Space Centre at Leicester, RAL and other NERC/BNSC channels.

7 RISK ASSESSMENT

This Theme requires data from several satellite missions. However, all are already in orbit and the proposed programme is robust against early failure of relevant sensors, for reasons as follows. The 1st **MetOp** currently in orbit would be replaced by the 2nd or 3rd platform in event of failure. **Envisat** has fuel until 2010 (possibly 2013) and the relevant sensors are operating satisfactorily at present. One year's overlap of MIPAS and SCIA(-nadir/swir) with a fully-commissioned MetOp, for co-located observations around an annual cycle (ST-2), will have been accomplished before the April 2008 start of NCEO[36]. The existing MIPAS data set is sufficient to characterise atmospheric variances for ST-3. SCIA(-nadir/uv-vis) is required to establish continuity from GOME-1 on ERS-2 ('95–'03) to GOME-2 on MetOp ('06-) for STs 3 & 4, for which SCIA/GOME-2 overlap <1 year would be acceptable. AATSR applications are: (a) to deliver cloud & aerosol information co-located with SCIA-nadir (STs 2, 3 & 4) and (b) to deliver a self-consistent data set on cloud, aerosol and surface parameters in conjunction with ATSR-2 (1995-2003). For (a) early failure of AATSR could be partly mitigated through use of information internal to SCIA-nadir. For (b) the impact would be low because the combined ATSR-2/AATSR data-set is already >11 years duration, spanning several ENSO cycles. For **ERS-2** (GOME-1 and ATSR-2), data sets for the *global missions* ('95-'03) exist; so there is no risk. Finally, the Theme will use a multi-year time-series of atmospheric profile data from ACE on **SCISAT**. ACE has functioned well since launch in 2003 and operation is funded to Mar'09. Although overlap with Envisat and MetOp until Apr'08 would be preferred for ST-2, the existing 4-year data set would suffice for ST-2 and -3.

The proposed programme is complex and will depend upon cohesion within the team. However, the partners have good track records through successful collaborations in DARC, ORAC development and other NERC, ESA, Eumetsat and EU projects.

[35] Additional studentships will be requested to extend scientific exploitation: firstly, through the NCEO central budget to entrain other University groups and, secondly, through University quota awards including CASE, e.g. with RAL on use of CTM to constrain tropospheric trace-gas retrievals & with Met-Office for assessment of models (NAME/UMAQ).

[36] In event of MIPAS failure before April'08, recourse could be made through assimilation to use of alternative limb-sounder data (i.e. Aura and SCISAT) which are not co-located with MetOp. In event of failure of SCIA, the CH_4 analysis in ST-2 would exploit only IASI and MIPAS data

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APPENDIX 1. Connections with Other Themes

Data Assimilation, Treatment of Uncertainty and Observation Impact

Exploitation of satellite data within the *AC Theme* will involve assimilation of data into chemical transport models. Co-operation with Met Office and ECMWF to develop new applications for composition data (pollution monitoring, air quality forecasting and NWP) will be directed towards assimilation into systems based on global and possibly also regional NWP models. The advances in data assimilation theory/mathematics (4D-Var) required to support objectives of the *AC Theme* will be undertaken in part by specialists in the *Data Assimilation Theme*.

Synergistic Use of EO for High-Resolution Predictions of Hazardous Weather, Floods and Water Resources

The abundances and distributions of gaseous and particulate pollutants are controlled by meteorology (i.e. winds, temperature, humidity and precipitation). Evolution of national capability for pollution monitoring and air quality forecasting at regional scale is therefore closely linked to parallel mesoscale model developments in NCAS (and MetOffice) and will benefit from developments in high-resolution data assimilation within the *Hazardous Weather and Hydrological Cycle Theme,* which are directed primarily towards prediction of severe storms and flooding events. Experience from assimilation of (high-resolution) aerosol and ozone data from MSG SEVIRI within the *AC Theme* will also be relevant to the *Hazardous Weather Theme*.

EO for Climate Diagnosis and Prediction

Satellite data-sets of sufficient quality and decadal duration can now contribute viably to the verification of climate models, and the principal atmospheric components (cloud, aerosol and water vapour) and surface properties (temperature, emissivity and reflectivity) are central to radiation balance and other components of the *Climate Theme*. Quantification of processes which control the distribution and physico-chemical properties of aerosol is an objective of the *AC Theme* (ST-2). The self-consistent dataset on cloud, aerosol and surface properties from ATSR-2/AATSR (1995-present) produced from the new integrated scheme will be made available to the *Climate Theme*[37]. The *AC Theme* could benefit from improved representation of terrestrial, aquatic and marine surface interfaces by specialists in the *Climate Theme* to model biogenic emissions.

Monitoring, Diagnosis, Re-analysis and Prediction of the Global Carbon Cycle

The *AC theme* will use chemical transport models to study atmospheric distributions and emissions of trace gases and aerosol. The Carbon Cycle Theme will utilize these to model CO_2 transport in deriving surface emissions. These tools can later be applied to CO_2. The *Carbon Cycle theme* will determine fire parameters from imager data (e.g. AATSR) which will also be of use to specify pyrogenic emissions in the AC Theme. A biophysical model (JULES) for methane surface emissions will be developed in the *Carbon Cycle Theme* which could then be imported also into the AC Theme to be coupled to CTMs. Undertaking both Themes within NCEO will allow efficient knowledge transfer in either direction and more rapid progress to be made in exploiting new satellite data sets.

Dynamic Earth & Geo-hazards

The *Dynamic Earth Theme* will exploit satellite data on volcanic eruptions from all relevant sensors, and generate data customized for this application. However, several atmospheric constituents associated with volcanic eruptions are associated also with (biogenic, pyrogenic or anthropogenic) emission sources to be quantified in the *AC Theme*, for which data is to be produced through an advanced, integrated scheme and made available also to the *Dynamic Earth Theme*.

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[37] Humidity profiling is central to NWP, so analysed and forecast humidity fields are primary outputs from operational systems (ECMWF, MetOffice, Eumetsat NWP SAF), and these systems will exploit information from the new IASI on EPS-MetOp. To use IASI data within the AC Theme to sound other trace gases, it will be essential to handle water vapour accurately, and this is also the case for data from limb-sounders (e.g. MIPAS). Information relevant to the Climate Theme would also be made available.