Polluted Troposphere data management at the BADC
April 2003 to March 2004

Report to the Polluted Troposphere Steering Committee

Anne De Rudder and Wendy Garland, BADC
March 2004

1. Data management plan and data protocol

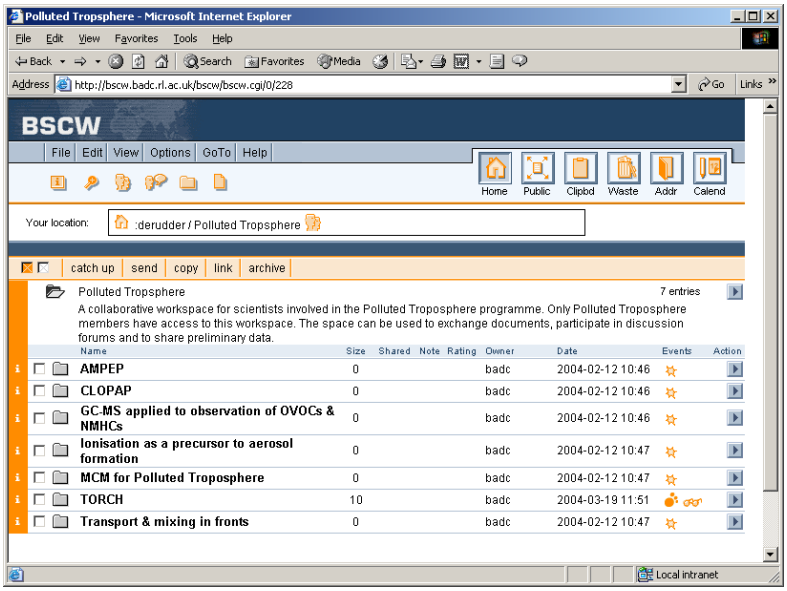
Issues such as the provision of metadata, data format, submission schedule, data accessibility, data publication, … have been addressed by the BADC. Options have been presented to the members of the Polluted Troposphere steering committee, who have discussed them. In agreement with the NERC data policy, a data management plan and a data protocol have been drafted by the BADC to reflect the steering committee's choices, and have been submitted to the Polluted Troposphere steering committee for discussion. The two drafts have been amended following these discussions, leading to the final versions attached to this report (Annexes I and II). The last amendments of the Data Management Plan, following the steering committee meeting of 12 February 2004, are the update of Sections 1 and 2; the insertion of a new Section 3 on the Polluted Troposphere web workspace; and the update of Sections 5.1 (web links added) and 5.2, 2nd paragraph (documentation on metadata).

2. Collection of information and communication with project investigators

Visits to the project principal investigators have been conducted by the BADC in the course of the summer to determine specific project data issues and inter-project relationships of interest to the Polluted Troposphere data management. A summary of the collected information is attached to this report (see Annex III).

BADC staff has attended Polluted Troposphere science workshops and conferences, initiating and developing contacts with all involved scientists. These contacts have been pursued at various occasions, including the development of some file naming standardisation and the support provided to TORCH data providers in formatting or submitting their data from the first campaign.

3. Workspace



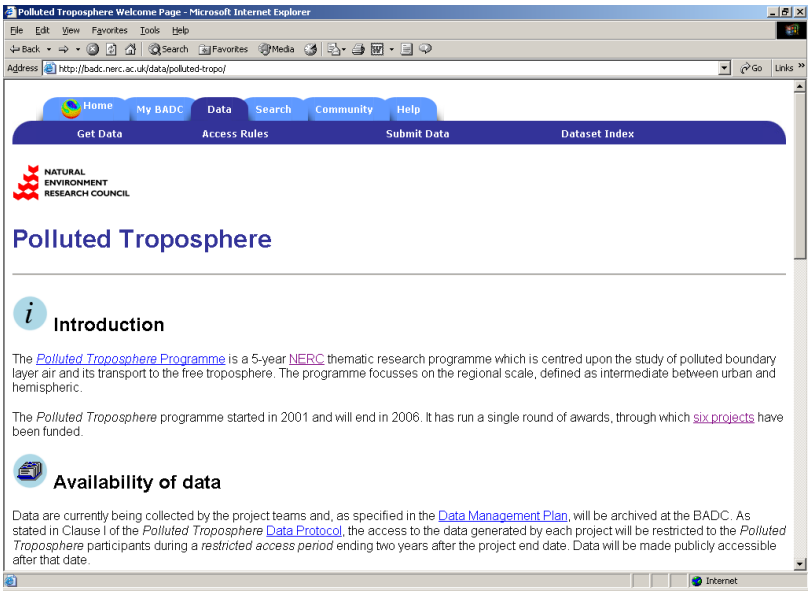
The Polluted Troposphere Workspace top level directories as they currently appear within the BSCW system. The workspace can be accessed from the BADC "Community" thumbnail ("Workspaces" section).

An online Polluted Troposphere workspace, only accessible by registered Polluted Troposphere participants, has been created within the BSCW system to allow discussion and exchange of information or preliminary data. This workspace is not an alternative to data submission to the BADC but a tool to ease collaboration among the programme participants. All Polluted Troposphere scientists have been invited to the workspace in July 2003 and the scientists involved in the first TORCH campaign (Writtle, July 2003) have used the workspace as a quick way to exchange preliminary results for validation.

4. Archive and data file uploader

A password protected archive has been created for the programme, with a top directory for each project or for data useful to several projects (such as MCM schemes to be provided by M. Jenkin). A dozen of Polluted Troposphere participants have applied for access to the archive at the time of writing, mainly TORCH participants. The BADC web file uploader has been set up as to allow Polluted Troposphere data providers to transfer their data files directly from their home computers to the BADC incoming space, from where files are copied to the appropriate part of the archive. Documents and images can be submitted as well as numerical data.

5. Documentation



The Polluted Troposphere front page on the BADC web site, gateway to all other information and documentation.

http://badc.nerc.ac.uk/data/polluted-tropo/

A substantial amount of documentation has been provided online through the Polluted Troposphere front page on the BADC web server. It includes instructions to data providers on metadata, NetCDF and NASA Ames formats, file names, the registration/application procedure and how to upload data files. It also gives links to the Polluted Troposphere page at NERC, the Polluted Troposphere BSCW workspace, the text of the last issue of the Data Management Plan and the BADC file format checkers for both NetCDF and NASA Ames.

6. Data sets

Data from the first TORCH campaign held in July 2003 have been submitted to the BADC. They include ground based processed data from Aberystwyth, Leeds and York, and back trajectories calculated by John Methven.

7. Next year tasks

The following forthcoming events will drive the work that will be done at the BADC for Polluted Troposphere.

- TORCH campaign in May-June 2004 (involves TORCH, Giles Harrison's project, Dudley Shallcross' project and John Methven for the provision of trajectories).
- AMPEP and CLOPAP flight campaigns, currently scheduled in October-November 2004.
- Cross-project modelling activities.

Tasks will include the following.

- Communication with the project investigators to expand our thesaurus of file name elements (which are related to places, platforms, instruments, dates, universities).
- Support to data providers in formatting and submitting their data.
- Population of the archive.
- Update of the online documentation.
- Attendance at steering committee meetings and science workshops.

A progress report will be submitted to the steering committee towards the end of Financial Year 2004-2005.

Polluted Troposphere
NERC Thematic Programme

Data Management Plan

BADC

March 2004

Scope

The purpose of the Polluted Troposphere (PT) data management plan is to set up a coherent approach to data issues during the programme. Its objective is to ensure that

- Appropriate data support is provided to the scientists within the programme.
- PT data are made available to PT collaborators in a timely fashion.
- Distribution conditions and data usage do not infringe on the individuals' rights to publish their own work.
- Potentially scientifically valuable data are kept for the long-term.
- A high quality documented Polluted Troposphere data archive is created.
- Data and documents are eventually distributed to the scientific community.

The following sections tackle the issues to be addressed in terms of data management, namely the provision of a data management plan and a data protocol, the determination of the programme participants' needs, the setting up of the archive, the monitoring of data access, the data distribution, the publication of results based on Polluted Troposphere data and the support offered to data providers.

1. Data management plan and data protocol

The present document is the final version of a data management plan drafted by the BADC, submitted to the Polluted Troposphere Steering Committee for discussion, amended to reflect the outcomes of the discussions, and agreed by the steering committee. A Polluted Troposphere Data Protocol has also been issued. This last document is a list of clauses stating the conditions that rule various aspects of the Polluted Troposphere data submission, access and publication. All applicants to Polluted Troposphere data will be asked to abide by this protocol. The two documents can be freely consulted on the Polluted Troposphere web page at BADC (http://badc.nerc.ac.uk/data/polluted-tropo/).

2. Collection of information

Visits to the project principal investigators have been carried out by the BADC from May to September 2003 to determine their needs in terms of data support (provision of third-party data sets or other services). The enquiry has also addressed issues related to the data generated by the projects (nature, volume, flow, etc.). The collected information will provide the basis of a planned and coordinated data management.

3. A collaborative tool for the exchange of ideas and preliminary data

A Polluted Troposphere online workspace has been created on the BADC BSCW (Basic Support for Cooperative Work) server. The workspace is visible and accessible only by the Polluted Troposphere participants and is intended to ease the exchange of ideas, documents and preliminary data between the

members of the programme. It is not an alternative to data submission to the BADC but must rather be considered as a discussion forum, a workshop and a temporary repository for data in the validation phase, draft papers, reports, etc.

4. Third-party data

4.1 Third-party data external to the Polluted Troposphere programme

Third-party data required for the development of the projects and held at the BADC, such as ECMWF and Met Office data sets, will be made available to the participants, subject to current access conditions. If required, BADC will endeavour to retrieve data sets from other sources at no cost or will negotiate their acquisition at the best possible cost.

4.2 Polluted Troposphere third-party data and model results

Data and model results generated by PT groups in the course of the programme will be made available to all Polluted Troposphere groups through the BADC. Update of preliminary data should be announced as early as possible to collaborators from other Polluted Troposphere teams. Publication issues are dealt with in Section 6.

5. Polluted Troposphere archive

5.1 Archive location

The Polluted Troposphere archive is located at the BADC (http://badc.nerc.ac.uk/). All the documentation related to Polluted Troposphere data can be accessed from the BADC "Polluted Troposphere" front page at http://badc.nerc.ac.uk/data/polluted-tropo/ or by following various links from the BADC home page.

5.2 Archiving policy

In recognition that validated raw data (i.e. QA/QC'ed data prior to additional processing) potentially represent an invaluable source of information for the future, the programme participants are encouraged to archive them in a way that guarantees longevity and accessibility (for example by using the BADC archive), and to document them at the BADC. Processed (final) data will be archived at the BADC, as well as model output that will be requested by other PT groups. In addition, investigators are encouraged to submit model results which will have been the basis of theoretical studies or that illustrate the model capabilities. They are welcome to archive any relevant pieces of code.

5.3 Format

In order to ease future data use and unless this reveals inadequate to some particular cases (such as the widespread use of a specific format by a specialised community), NetCDF (and possibly NASA Ames if requested by some investigators) will be adopted for all the processed data generated by the programme. The reasons why the BADC encourages the use of NetCDF are its generalised use within the atmospheric community (which also holds for NASA Ames), the existence of a large library of software reading, writing and converting NetCDF files, and the fact that it will ease the datasets visibility through a number of devices currently under development (BADC Live Access Server, NERC metadata gateway, NERC data grid). Documentation on these two formats is available from the BADC (http://www.badc.rl.ac.uk/help/formats/), as well as links to downloadable free software packages to produce and read NetCDF files.

Note on the BADC Live Access Server (LAS).

This tool will allow users to select subsets of data sets and retrieve them or visualise them on their screen. It will also allow comparison and some manipulation of the data. Although a variety of formats will eventually be readable by the LAS, NetCDF files will first benefit from this new device.

5.4 Information on the data

Metadata (i.e. information on the data) are a crucial part of any data archive since they ensure the accessibility and readability of the data. It is therefore essential that metadata be submitted at the same time as the data sets to which they pertain. Metadata pertaining to all raw Polluted Troposphere data not archived at the BADC should also be supplied to the BADC.

To guarantee the PT data archive quality, full documentation on all validated raw and processed data, as well as on models and model results, must be provided to the BADC. The BADC has developed a set of metadata requirements which is available to PT participants via the BADC Web site (http://badc.nerc.ac.uk/help/metadata/) and is accessible via a link from the Polluted Troposphere front page. Metadata pertaining to NetCDF files should comply with the Climate Forecasting (CF) convention. Metadata inserted in NetCDF and NASA Ames files are fully documented online.

The provision of a complete and carefully written set of metadata by each investigator will ensure the swift integration of the Polluted Troposphere into the network system that will soon be under development at the BADC in the framework of the NERC Data Grid project. When operational, this system should provide searchable information about all NERC data that will have been integrated into the grid, and provide links to the NERC archives. For the future use of Polluted Troposphere results, it would be desirable that the Polluted data sets be visible through this gateway.

In addition to these minimal metadata, investigators are encouraged to archive at BADC all relevant information, including model and experiment descriptions, references, papers, reports, etc. Designated directories have been created in the PT archive for this purpose.

5.5 Data submission

If needed by other Polluted Troposphere groups, preliminary data should be made available to them as soon as possible, if possible via the BADC. Processed data and model results should be supplied to the BADC as soon as they are ready, and no later than the project end date. Individual project archives should be complete by the end date of the project.

The BADC provides an automatic Web based file uploader accessible by clicking on the *Submit Data* option in the BADC Web pages menu. The uploader has been set up to accept files from the Polluted Troposphere programme. Online assistance is provided. Alternatively, files can be submitted by *ftp*. Both ways are fully documented on the BADC Web site.

6. Data distribution

The access to all data submitted to the BADC will be restricted to the Polluted Troposphere participants during two years following the concerned project end date, after which they will be released into the public domain.

A password protected system has been set up at the BADC for the Polluted Troposphere participants. Whilst the data are restricted from the public domain and contingent on the adoption of a PT Data Protocol, it is suggested that participants would be prompted to agree with the Polluted Troposphere Data Protocol in order to access the PT archive (whether to submit, view or download data).

After release of the data to the public domain, anonymous users will be requested to contact the relevant data providers before using the data and to acknowledge the Polluted Troposphere programme and the

data suppliers in any publication using Polluted Troposphere data. Candidate users will be asked to indicate agreement to these terms prior to being given access to the data.

Distribution of the Polluted Troposphere data held at BADC will take place via the Web. During the validation period, entitled Polluted Troposphere participants who will have applied for access to the data will be allocated an account at BADC that will allow them to directly download the data from the archive. If the SC expresses the wish of it, this facility will be extended to external collaborators who will have been personally authorised to access the data by the project PI. A Polluted Troposphere Web front page has been set up at http://www.badc.rl.ac.uk/data/polluted-tropo/. This will be the gateway to all Polluted Troposphere data and metadata, and to all relevant information and links.

7. Publication

Results coming out of the Polluted Troposphere research projects will be published in the usual way. During the data validation period, each investigator will have the right to refuse the use of his results in a publication or a presentation prior to the investigator's own publication of that work. If measurements or model results from other groups within the PT programme are used in a PT participant's publication during or after the programme, joint authorship must be offered. This will not necessarily have to be accepted, particularly in cases where due credit and acknowledgement can be given in other, possibly more appropriate, ways. References of publications will be communicated to the BADC so that they can be integrated into the PT documentation.

8. Liaison between BADC and programme participants

The BADC Polluted Troposphere homepage (http://www.badc.rl.ac.uk/data/polluted-tropo/) and its links will be the primary source of information regarding the PT archive. The Web pages will be updated as new pieces of information are available and new data files are submitted.

The BADC will keep in touch with the PIs and their collaborators during and after the programme development. In particular, information on the submission procedure, on the relevant WWW links, on the Data Management Plan and on the population of the PT archive will be sent to PIs via this mean.

9. Support to PT participants

In addition to the provision of third-party data, the BADC will endeavour to provide services that would be required by the project PIs. PT participants will benefit from the existing BADC services (file uploader, NASA Ames file checker, online trajectory calculator, quick plot facility) and from the future developments of access technology mentioned above (format converter, LAS, NDG).

Polluted Troposphere Data Protocol

The aims of the Data Protocol are

- to encourage rapid dissemination of scientific results from the Polluted Troposphere programme;
- to protect the rights of the individual scientists funded Polluted Troposphere;
- to have all the involved researchers treated equitably;
- to ensure the quality of the data in the Polluted Troposphere data archive.

These aims conflict at times, and it is hoped that the provisions of the protocol resolve these conflicts fairly. It is recognised that this cannot always be achieved to everyone's complete satisfaction; there are bound to be cases where individual interests clash with those of the Polluted Troposphere programme. Therefore, to try to meet these aims, all PIs involved in Polluted Troposphere, in accordance with and on behalf of their co-investigators, must agree to abide by the following conditions:

1. Data and model results of interest to Polluted Troposphere groups that will be produced during the programme will be made available to all Polluted Troposphere participants, and Polluted Troposphere participants only, during a *restricted access period* ending two years after the concerned project end date, after which data and model results will be released to the public domain. At a principal investigator's request, access may be extended to personally authorised collaborators.
2. The designated Polluted Troposphere data centre is the BADC.
3. When relevant, preliminary data must be made available to Polluted Troposphere collaborators as soon as possible. Any corrections or amendments to the preliminary data should be announced as soon as possible.
4. All validated processed data (i.e. data sets in their final form), as well as quality-checked raw data that will have been recognised of general interest to the community, will be archived at the BADC. Archival must take place no later than the end of the concerned project.
5. If an error in the data is signalled to the BADC after archival, the updated version provided by the originator of the data will be archived alongside the old version or will replace the old version, depending on the nature of the error and in agreement with the data provider. If the error is detected by a user, the originator of the data will be consulted and only changes provided by him/her will be archived, following the same procedure as above. Both errors and updates will be reported and documented in the metadata attached to the respective data files.
6. Results of model studies feeding other Polluted Troposphere projects will be submitted to the BADC.
7. Data submitted to the BADC must be in the data format agreed between Polluted Troposphere principal investigators and the BADC (namely NetCDF and NASA Ames).
8. All agreed metadata describing data, models and model results, regardless of their archival location, must be supplied to BADC. Format and metadata are documented at BADC.
9. It is each principal investigator's responsibility to ensure that the data used in publications are the best available at that time.
10. If measurements or model results from other Polluted Troposphere research groups are used in a publication by a Polluted Troposphere participant, joint authorship must be offered. This does not necessarily have to be accepted, particularly in cases where due credit and acknowledgement can be given in other, possibly more appropriate, ways.
11. Whilst the data are restricted from the public domain (see Clause 1), each principal investigator has the right to refuse to allow his/her work, whether measurement or calculation, to be used in a publication or presentation prior to the PI's own publication of that work.
12. Whilst the data are restricted from the public domain, no data should be transferred to a third party without the originator's consent.
13. In the event of dispute the final decision rests with the Polluted Troposphere Scientific Steering Committee.

Annex III

Visits to Polluted Troposphere project investigators: Summaries

Anne De Rudder, BADC
July 2003 – Updated October 2003 & February-March 2004

1. Visit schedule

23 May 2003	*Reading*	*G. Harrison*	*Ionisation as a precursor to aerosol formation*
4 Jun 2003	*Reading*	*S. Gray*	*Transport and mixing in fronts*
6 Jun 2003	*York*	*A. Lewis* *J. Hopkins*	*TORCH - Tropospheric Organic Chemistry Experiment*
9 Jun 2003	*Manchester*	*M. Gallagher*	*CLOPAP - Cloud Processing of Regional Air Pollution Advecting over Land and Sea* *AMPEP - Aircraft Measurement of Chemical Processing and Export Fluxes of Pollutants over the UK*
10 Jun 2003	*Bristol*	*D. Shallcross*	*Advanced GC-MS technology for observing OVOCs and NMHCs in the polluted troposphere*
24 Sep 2003	*Edinburgh*	*A. McDonald* *T. Dore* *E. Nemitz*	*AMPEP - Aircraft Measurement of Chemical Processing and Export Fluxes of Pollutants over the UK*

Additional information has also been collected from Polluted Troposphere participants at the occasion of science meetings, by e-mail and by telephone, and from the FAAM Operations Committee and FAAM web site.

2. Visit summaries

NER/T/S/2002/00145 - TORCH (http://www.env.leeds.ac.uk/~jim/torch/)

PI	Ally Lewis, York
Universities involved	York, Leeds, Leicester, UEA, UMIST, Wales at Aberystwyth, Essex, King's College, Imperial College
Visit	York, June 6, 2003. Ally Lewis and James Hopkins.
Team	Ally Lewis, PI (formerly at Leeds) York: Jim Hopkins, James Lee (formerly at Leeds), Chris Ennis, Nicola Carslaw, Lucy Carpenter, Jacqui Hamilton, Kathryn Emmerson, Nicola Watson Leeds: Lisa Whalley, Andrew Ricard (formerly at Leicester), Gavin Johnson, Dwayne Heard, Mike Pilling, Jim McQuaid, William Bloss, Jenny Stanton, pauls@chemistry.leeds.ac.uk (?), tomg@chem.leeds.ac.uk (?), trevori@chem.leeds.ac.uk (?) UEA: Brian Bandy, Dave Oram, Bill Sturges, Stuart Penkett, Claire Reeves, Graham Mills, Simon Clegg Leicester: Paul Monks, Zoe Fleming, Mark Jacob UMIST: Hugh Coe, Gordon McFiggans, Paul Williams, Michael Flynn, Mike Cubison, James Allan Imperial College: Mike Jenkin, Steven Utembe Wales at Aberystwyth: Geraint Vaughan, Emily Norton King's College: David Carslaw Essex: Guy Coulson
3rd party data required	ECMWF, Met Office
Field campaigns	• Summer 2003, Writtle • May-June 2004, Weybourne
Platforms	1. NERC Airborne Remote Sensing Facility (ARSF) Dornier 228 aircraft (see http://www.nerc.ac.uk/lois/plane.shtm): 3 to 4 flights 2. Ground-based: • Leeds FAGE container

- York GC container
- York portacabin
- UEA trailer
- UEA portacabin
- Leicester portacabin
- UMIST container

Instruments
- Onboard the aircraft: in situ measurement of O3 and CO in the boundary layer + meteorological variables (instruments run by Jim McQuaid)
- From the ground: see Section 3 below

Data produced
- Time series from the above list of instruments. Similar to NAMBLEX in content and size (for 1 campaign) except for halogenated species
- Images from Aberystwyth radar

Raw data will be archived at the BADC as they are produced. Processed data will be submitted right after the 2 campaigns.

Data flow / volume: 40 to 50 kb / hr during campaigns (N.B. NAMBLEX ≈ 200 Mb)

Data format: NASA Ames for instrumental data (time series)

Modelling
- MCM coupled with UMIST transport model to compute concentrations along trajectories (run by Mike Jenkin)
- MCM runs including radicals (Nicola Carslaw, York)
- UMIST model (Hugh Coe and Gordon McFiggans, UMIST) – no data to be archived
- Particle microphysics (Simon Clegg, UEA)

Project end date: ?

NER/T/S/2002/00147 - CLOPAP

PI: Tom Choularton, UMIST

Universities involved: UMIST, York, UEA

Visit: Manchester, June 9, 2003. Martin Gallagher.

Team: Tom Choularton, PI
UMIST: Martin Gallagher, Hugh Coe, Gordon McFiggans, James Allan, Rami Alfarra
York: Ally Lewis
UEA: Stuart Penkett

Goal: Monitor the processing of aerosol downward pollution plumes from London.

3rd party data required
- Back trajectories from the BADC
- Radiosonde data
- UK Met Office data
- Surface charts provided via FAAM

ECMWF forecasts

Field campaign: Flights should preferably take place in Spring (possibly joint AMPEP-CLOPAP flights). About 60 hours of flight.
N.B. Originally scheduled in Spring 2004, flights are currently rescheduled for October-November 2004, with one possible other window in June-July 2005.

Platform: FAAM BAe 146-300

Instruments: Aerosol mass spectrometer (AMS) and particle physics instruments.
Gas probes.

Data produced: Core cloud microphysics and meteorological data from FAAM
- Total liquid water from the Johnson Williams probe
- Ice water
- Meteorological parameters

FAAM non-core data:
- Time series of droplet diameter from the airborne UMIST ADA-100 droplet analyser
- Particle size distribution, particle concentration as a function of time.
- Gif images of ~10μ particles and crystal aspect ratios from the CPI (if ice is present in cloud) + some online analysis of the images in binary format (raw data produced in .roi files by IDL processing software). Measurement frequency: 40 Hz.
- Min/max particle size ratio as a function of time.

	• Gas measurements from Ally Lewis and Stuart Penkett
Data volume/flow	Droplet size: 2 to 10 Mbytes/hour, depending on clouds. Particle images: 2 Mbytes/second.
Modelling	Microphysical modelling by Gordon McFiggans, James Allan, Hugh Coe, Rami Alfarra
Time schedule	N.B. FAAM core data must be made available as shortly as possible after production (requirement of FAAM data protocol).
Project end date	?

NER/T/S/2002/00149 - Transport and mixing in fronts

PI	Suzanne Gray, Reading
University involved	Reading
Visit	Reading, June 4, 2003. Suzanne Gray.
Team	Dr S. Gray, PI Dr Anna Agusti-Panareda, Reading – swr99aa@met.rdg.ac.uk
3rd party data required	• Data from the European Export of Precursors of Ozone by Long-Range Transport (EXPORT) campaign of August 2000 (joint UK/German/French airborne experiments) • Dynamics and Chemistry of Frontal Zones (DCFZ) data generated under the UTLS Ozone programme • Mesosphere-Stratosphere-Troposphere (MST) radar data from Aberystwyth • Possibly data from other Polluted Troposphere projects if fronts occur during field campaigns
Modelling	Model used: Mesoscale Unified Model (UM) with a finer resolution and new dynamics. The code will be run at Manchester by Met Office groups of the Joint Centre for Mesoscale Meteorology (JCMM) at Reading.
Data to be submitted	None – Unless required by other projects (?)
Project end date	?

NER/T/S/2002/00150 – Ionisation as a precursor to aerosol formation

PI	Giles Harrison, Reading
Institutions involved	Reading, Leeds, RAL
Visit	Reading, May 23, 2003. Giles Harrison
Team	Dr G. Harrison, PI Mr A.G. Lomas, Reading - a.g.lomas@rdg.ac.uk Dr K. Carslaw, Leeds - carslaw@env.leeds.ac.uk Dr K.L. Aplin, RAL - k.l.aplin@rl.ac.uk
3rd party data required	(No BADC intervention needed) • Cosmic rays data sets freely available from the Web, for example cosmic rays over the US and Central Europe from the Infrared Processing and Analysis Center (IPAC) *Spider* website • Real-time gridded lightning data from NASA, available from the Global Hydrology Resource Center (GHRC) website
Field campaign	One of the TORCH campaigns, i.e. Summer 2003 or 2004 (to be decided by Leeds partners)
Extra-campaign obs.	Measurements made locally (on Reading campus)
Instruments	4 surface programmable ion detectors (low-fast mobility) — saw prototype

Data produced	• In-house measurements of cosmic rays
	• Simultaneous weather data from Reading
	• In situ measurements of ion concentrations (time series) at a frequency of 1 measurement every 5 minutes
	  o Level 0: instrument count
	  o Level 1: ion concentrations
	  o Level 2: processed 2-D concentrations as a function of time and mobility

Data volume	200 kb/day → between 30 and 100 Mb for ion concentrations

Data archive structure	One directory per processing level
Modelling	Some modelling of tropospheric ions may be involved
Wishes	Polluted Troposphere CAST forum
Time schedule	• Beginning of June 2003: instrument calibration and testing • September 2003 (perhaps): first measurements • End of measurements: Easter-Summer 2005
Project end date	?

NER/T/S/2002/00151 - Advanced GC-MS technology for observing OVOCs and NMHCs in the polluted troposphere

PI	Dudley Shallcross, Bristol
University involved	Bristol
Visit	Bristol, June 10, 2003. Dudley Shallcross.
Team	Dudley Shallcross, PI; Prof. Peter G. Simmonds; Dickon Young
3rd party data required	TORCH data
Field campaign	Simultaneous to 2nd TORCH campaign (May-June 2004)
Data produced	Ground based time series of • CH3CHO & other aldehydes • CH3COCH3 & other ketones • CH3OH & other alcohols N.B. A detailed list provided by Dickon Young is included under Section 4. Quality controlled raw data (calibrated + submitted to a few tests): 10 min (1 air sample every 10 min) Processed data: mixing ratios integrated over 1 hr time intervals. ↔ Hourly data covering about 5 weeks. Computed mixing ratios of the same species (see "modelling" section below).
Modelling	Cambridge trajectory model + box chemical model (not the MCM) will be used to compute mixing ratios of the observed species, along forward trajectories.
Wishes	CAST forum could be visible (but not accessible) by public.
Time schedule	• Raw data: ~ 8 weeks after campaign • Validated processed data: ~ 3 months after campaign
Project end date	?

NER/T/S/2002/00152 - AMPEP

PI	David Fowler, CEH Edinburgh
Institutions involved	CEH Edinburgh, UMIST, possibly Leeds, Met Office
Visits	• Manchester, June 9, 2003. Martin Gallagher. • Edinburgh, September 24, 2003. Alan McDonald, Tony Dore, Eiko Nemitz.
Team	David Fowler, PI CEH: Alan McDonald (gas measurement + modelling), Tony Dore (modelling), Mrs Jillian Binnie (VOCs, particulates), Debbie Polson UMIST: Martin Gallagher, Hugh Coe (aerosol data), Rami Alfarra (interpretation of spectra), James Allan (AMS measurements + data acquisition software)
Goal	Fly round the UK and establish fluxes from the difference between West and East values of measured parameters.
3rd party data required	UM wind fields (to constrain NAME model – see "Modelling" section below)
Field campaign	Flights should preferably take place in Spring (possibly joint AMPEP-CLOPAP flights). About 100 hr of flight (18 flights of ~ 5 hours each). N.B. Originally scheduled in Spring 2004, flights are currently rescheduled for October-November 2004. Possible other windows are March-April 2005, June-July 2005 and September-October 2005.
Platform	FAAM BAe 146-300
Instruments	UMIST AMS Gas analysers operated by CEH

	Tunable diode laser (CEH) Aerosol filters (CEH) Particle counters
Data produced	UMIST AMS data: spectra of sulfate, nitrate, ammonium, total volatile organics as a function of size. Raw data are generated in binary format (analysis tool freely available on web). Raw data resolution: 5 sec (not kept). Data are integrated over 1 min time intervals. Total aerosol (time series): averages over 60 sec (the instrument records at 1 Hz) Images may be provided (contour plots as a function of diameter versus time). CEH Gas data: CO (10 Hz measurements), O3, NOx, SO2 (1 measurement every 10 sec to 1 min); sample bags of CH4 & N2O analysed by tunable diode laser; CO2, possibly Hg (every 2.5 min). N.B. NO & NO2 are FAAM core data. Other gas data are non-core. Data from aerosol filters (every ½ hour): heavy metals & ions. Core FAAM data from particle counters: CN & CNN at 1 Hz. Videos. Leeds (?) VOCs
Data volume / flow	UMIST 1 min spectra: up to 100 Mbytes / 6 hours (between 50 & 100 Mb / 6hrs) CEH: 100 measured variables at 1 Hz ↔ 8 Mbytes/flight. Model data from FRAME and NAME (see below): 250 Mbytes / run (18 runs, 2 models).
Data validation	UMIST AMS measurements checked against total aerosol concentration. In situ mass calibration.
Modelling	• FRAME – see http://www.frame.ceh.ac.uk/description.htm - CEH transport model run at CEH Edinburgh. Driven by observed emissions from the UK. Includes dry deposition. Horizontal resolution: 5 km x 5 km. Horizontal coverage: over the UK (172 x 244 km). Vertical resolution: 33 layers. Vertical coverage: from 0 to 2.5 km altitude. Chemical compounds included: 3 or 4 gases: SO2, NOx (NO + NO2), HNO3, perhaps NH3 (no PAN); 3 aerosol species in dry & liquid phases: sulfates, nitrates, ammonium. The model output at each time-step is ~ 250 Mbytes large. Annual averages will be derived. For each of the 18 flights, 3-D fields (annual averages) will be produced for the 6 or 7 species. • NAME - see http://www.met-office.gov.uk/research/nwp/publications/nwp_gazette/3rd96/name2.html - Met Office Nuclear Accident dispersion model run at Met Office by CEH student (or perhaps run at CEH if model is made public). Semi-Lagrangian transport model + chemistry. Forced by winds from the UM. Calculated species: same as in FRAME. The size of the output is not known but is likely to be similar to the one of the output from FRAME. In addition, inverse modelling experiments could be attempted with both models, consisting in deriving the UK emissions from the measured concentrations.
Time schedule	UMIST 1 min AMS spectra will be available at the time of production. A sample NetCDF file will first be sent to BADC by UMIST for checking. CEH model data will be available 3 months before final report. N.B. FAAM core data must be made available as shortly as possible after production (requirement of FAAM data protocol).
Project end date	?

3. Ground based instruments in use during the TORCH campaigns (NER/T/S/2002/00145), with their operators

List updated & supplemented with info from James Lee on instruments used during the 1st field campaign — a subset of the following list.

York
- NMHCs C2-C8 (J. Hopkins)
- Small O-VOCs (J. Hopkins)
- Dual column GC – fid (J. Hopkins)
- Aerolaser CO analyser (J. Hopkins)
- Met sensor (AWS) (J. Hopkins)
- 2-D GC fid C6-C14 (J. Hamilton)
- Canisters for GCxGC-TOF (J. Hamilton)
- PTR-TOF mass spectrometer (C. Ennis)

Leeds
- OH lifetime sensor (G. Johnson)
- OH/HO2 FAGE (J. Lee)
- TEI O3 analyser (J. Lee / G. Johnson)
- J(O1D) filter radiometer (J. Lee / G. Johnson)
- Water vapour (G. Johnson)
- TEI NOx analyser (J.Lee)
- Met. Sensor (AWS) (J. Lee)
- PAN GC (L. Whalley)

UEA
- PAN GC (G. Mills / B. Bandy)
- Peroxides sensor (G. Mills / B. Bandy)
- Formaldehyde sensor (G. Mills / B. Bandy)
- TEI O3 analyser (B. Bandy)
- TEI NOx analyser (B. Bandy)
- Aerolaser CO analyser (B. Bandy)
- SO2 analyser (B. Bandy)
- PTR mass spectrometer (D. Oram)
- GC mass spectrometer (D. Oram)

Leicester
- HO2/RO2 PERCA (P. Monks)
- Filter radiometers for J(NO2) & J(O1D) (A. Ricard)
- Spectral radiometers for CH3CHO, CH3COCH3, J(HCHO), J(HONO), J(NO2), J(O1D) (A. Ricard)
- Relative humidity sensor (A. Ricard)
- Thermometer (A. Ricard)
- Ozone sensor (?)

UMIST
- TDL HNO3 (P. Williams, M. Flynn, J. Allan)
- TDL NH3 (P. Williams, M. Flynn, J. Allan)
- SMPS (3-500 nm) (P. Williams, M. Flynn, J. Allan)
- OPC (0.1-300 μm) (P. Williams, M. Flynn, J. Allan)
- CN counter (P. Williams, M. Flynn, J. Allan)
- Total/ultrafine particle 3010 (P. Williams, M. Flynn, J. Allan)
- Aerosol Mass Spectrometer (AMS) (P. Williams, M. Flynn, J. Allan)
- Impactors filters (P. Williams, M. Flynn, J. Allan)
- Hygroscopic Tandem Differential Mobility Analyser (HTDMA) (P. Williams, M. Flynn, J. Allan)
- Automatic Weather Station (AWS) (P. Williams, M. Flynn, J. Allan)
- Sonics (P. Williams, M. Flynn, J. Allan)
- Aerosol mass spectrometer (particle size & composition analysers) (H. Coe & G. McFiggans)

Aberystwyth
- Wind profiler (E. Norton)
- Ozone profiler (E. Norton)

4. Compounds measured by Project NER/T/S/2002/00151 (Bristol)

Compound	Formula	Mol. Wt.	b.p./K	b.p./C	CAS registry	IUPAC Name
methanol	CH_4O	32.04	337.8	64.8	67-56-1	methanol
ethanol	C_2H_6O	46.07	351.5	78.5	64-17-5	ethanol
1-propanol	C_3H_8O	60.1	370.3	97.3	71-23-8	propan-1-ol
1-butanol	$C_4H_{10}O$	74.12	390.6	117.6	71-36-3	butan-1-ol
1-pentanol	$C_5H_{12}O$	88.15	411	138	71-41-0	pentan-1-ol
methyl butenol	$C_5H_{10}O$	86.13	372	99	115-18-4	2-methylbut-3-en-2-ol
acetone	C_3H_6O	58.08	329.3	56.3	67-64-1	acetone
2-butanone	C_4H_8O	72.11	353	80	78-93-3	butan-2-one
2-pentanone	$C_5H_{10}O$	86.13	375	102	107-87-9	pentan-2-one
isoprene	C_5H_8	68.12	307	34	78-79-5	isoprene
acrolein	C_3H_4O	56.06	330	57	107-02-8	acrylaldehyde
methacrolein	C_4H_6O	70.09	342	69	78-85-3	2-methylacrylaldehyde
methyl vinyl ketone	C_4H_6O	70.09	355	82	78-94-4	but-3-en-2-one
3-methyl furan	C_5H_6O	82.1	338.5	65.5	930-27-8	3-methyl furan
formaldehyde	CH_2O	30.03	254	-19	50-00-0	formaldehyde
acetaldehyde	C_2H_4O	44.05	293.9	20.9	75-07-0	acetaldehyde
propanal	C_3H_6O	58.08	322.4	49.4	123-38-6	propionaldehyde
butanal	C_4H_8O	72.11	348	75	123-72-8	butyraldehyde
pentanal	$C_5H_{10}O$	86.13	376	103	110-62-3	pentanal
hexanal	$C_6H_{12}O$	100.16	402	129	66-25-1	hexanal
methane	CH_4	16.04	111	-162	74-82-8	methane
ethane	C_2H_6	30.07	184.6	-88.4	74-84-0	ethane
propane	C_3H_8	44.1	231.1	-41.9	74-98-6	propane
butane	C_4H_{10}	58.12	273	0	106-97-8	butane
pentane	C_5H_{12}	72.15	309	36	109-66-0	pentane
hexane	C_6H_{14}	86.18	341.9	68.9	110-54-3	hexane
1,3-butadiene	C_4H_6	54.09	268.6	-4.4	106-99-0	buta-1,3-diene
benzene	C_6H_6	78.11	353.3	80.3	71-43-2	benzene
toluene	C_7H_8	92.14	383.8	110.8	108-88-3	toluene