Polluted Troposphere
Visits to 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