SERVICES & FACILITIES ANNUAL REPORT - FY April 2010 to March 2011

SERVICE	FUNDING	AGREEMENT	ESTABLISHED as S&F	TERM
Molecular Spectroscopy Facility	Block	SLA	1997	5 years

TYPE OF SERVICE PROVIDED:

The Molecular Spectroscopy Facility (MSF) provides world-class central laboratories, scientific equipment, training, scientific/technical support, and high-quality data for the UK environmental science community in support of a wide range of interdisciplinary research across the spectrum of the NERC remit and strategic priorities. Infrared, visible, and ultraviolet spectroscopic data are increasingly important for studying the important chemical, physical, biological and geological processes occurring in the natural environment. The MSF provides essential inputs to many key NERC science areas, in particular Earth observation of the atmosphere and surface using optical remote sensing techniques, atmospheric chemistry and climate research.

Through the MSF, access to broadband high spectral resolution Fourier transform and fibre-optic spectrometers is provided to NERC researchers for measuring the absorption, emission and scattering properties of solid, liquid, gas/vapour and aerosol samples contained in a range of spectroscopic cells. High-quality spectroscopic data over the entire spectral range from wavelengths (wavenumbers) of 1 mm (10 cm^{-1}) in the far-infrared/terahertz range to 180 nm (55,000 cm^{-1}) in the far ultraviolet are generated at spectral resolving powers of up to 1 part in a million and time resolutions as high as 5 µs. Customised sample cells are available for specific temperature-dependent measurements over the range 77 to 470 K at optical path-lengths from less than 1 mm to over 1 km using multi-pass optical systems. For atmospheric chemistry studies, the chemical synthesis area and laser-designated laboratories permit a wide range of projects to be supported. Further details can be found at www.msf.rl.ac.uk.

ANNUAL TARGETS AND PROGRESS TOWARDS THEM

During 2010/11 the NERC MSF provided 211 days (baseline 174) of measurement time to support eleven different projects, eight of which were in support of NERC grants, and a further two were in support of the UKSA Centre for Earth Observation Instrumentation (CEOI, formally sponsored by the NERC and TSB).

The MSF continued to develop capability in response to user requirements, with further enhancements to the multi-pass aerosol cell, which was used to support three aerosol projects during the year. Work has also been undertaken to extend the long-wavelength limit of measurements to enable studies on water vapour absorption in support of the PREMIER candidate ESA Earth Explorer mission.

A new step-scan capability has been installed on the medium resolution spectrometer. This has been funded through a CEOI project to enable a study on the performance of a detector array as part of an investigation to determine suitability for future deployment with satellite-based spectrometers to monitor atmospheric composition and dynamics. Step scan is also enables a wide range of other measurements that require time resolution, for example the study of chemical reactions, a will be of interest to the wider community.

A new capability for high-resolution atmospheric spectroscopy has been developed, as part of preparation work for a RAL Spectroscopy Group project funded by the NERC Technology Proof of Concept scheme. The system allows users to make inter-comparison measurements between their field instruments and a state-of-the-art laboratory spectrometer for calibration-validation purposes. The first, CEOI-funded, project to use this facility is scheduled to make atmospheric measurements during 2011/12.

SCORES AT LAST REVIEW (each out of 5)			Date of Last Review:	March 2009
Need	**Uniqueness**	**Quality of Service**	**Quality of Science & Training**	**Average**
5	5	4.5	5	4.88

CAPACITY of HOST ENTITY FUNDED by S&F	Staff & Status	Next Review (March)	Contract Ends (31 March)
75%	Facility Scientist/Manager 80% FTE established RC band F Assistant Scientist 70% FTE established RC band E Facility Technician 100% FTE established RC band D Instrument Scientist 50% FTE established RC band D	2014	2015

FINANCIAL DETAILS: CURRENT FY						
Total Resource Allocation £k	**Unit Cost £k**			**Capital Expend £k**	**Income £k**	**Full Cash Cost £k**
	Unit 1 (Whole MSF)	Unit 2 (IFS 125/0HR)	Unit 3 (IFS 66v/S)			
366.00	4.20	1.5	0.75	0	0	401.65

FINANCIAL COMMITMENT (by year until end of current agreement) £k					
2010-11 366.00	**2011-12** 385.37	**2012-13** 365.05	**2013-2014** 365.05	**2014-2015** 365.05

STEERING COMMITTEE	Independent Members	Meetings per annum	Other S&F Overseen
MSF	4	2	None

APPLICATIONS: DISTRIBUTION OF GRADES (current FY — 2010/11)								
	α5	α4	α3	α2	α1	β	R*/Pilot	Reject
NERC Grant projects*	1	3	0	0	0	0	3	0
Other academic	1	1	0	0	0	0	4	0
Students	0	0	0	0	0	0	0	0
Pilot	0	0	0	0	0	0	0	0
TOTAL	2	4	0	0	0	0	7	0
APPLICATIONS: DISTRIBUTION OF GRADES (per annum average previous 3 financial years —2007/2008, 2008/2009 & 2009/2010)								
	α5	α4	α3	α2	α1	β	R*/Pilot	Reject
NERC Grant projects*	1	2.33	0.33	0	0	0	0	0
Other Academic	0	1	0	0	0	0	0.67	0
Students	0	0.33	0	0	0	0	0	0
Pilot	0	0	0	0	0	0	1	0
TOTAL	1	3.67	0.33	0	0	0	1.67	0

PROJECTS COMPLETED (current FY – 2010/11)							
	α5	α4	α3	α2	α1	β	R*/Pilot
NERC Grant projects*	0	3	0	0	0	0	1
Other Academic	1	2	0	0	0	0	1
Students	0	0	0	0	0	0	0
Pilot	0	0	0	0	0	0	0

Project Funding Type (current FY – 2010/11) (select one category for each project)											
Grand Total	Infrastructure					PAYG				
	Supplement to NERC Grant *	PhD Students		NERC C/S	Other	NERC Grant*	PhD Students		NERC C/S	Other
		NERC	Other				NERC	Other		
12	7	0	0	0	5	0	0	0	0	0
Project Funding Type (per annum average previous 3 financial years - 2007/2008, 2008/2009 & 2009/2010)										
Grand Total	Infrastructure					PAYG				
	Supplement to NERC Grant *	PhD Students		NERC C/S	Other	NERC Grant*	PhD Student		NERC C/S	Other
		NERC	Other				NERC	Other		
7.67	4.67	0	0.67	0	2.33	0	0	0	0	0

User type (current FY – 2010/11) (include each person named on application form)				
Academic	NERC Centre/Survey	NERC Fellows	PhD Students	Commercial
16	0	0	2	3
User type (per annum average previous 3 financial years - 2007/2008, 2008/2009 & 2009/2010)				
Academic	NERC Centre/Survey	NERC Fellows	PhD Students	Commercial
15	0	0.67	5.33	2.67

OUTPUT & PERFORMANCE MEASURES (current year)										
Publications (by science area & type) (calendar year 2010)										
SBA	ES	MS	AS	TFS	EO	Polar	Grand Total	Refereed	Non-Ref/ Conf Proc	PhD Theses
0	0	0	5.5	0	1.5	0	**7**	5	2	0

Distribution of Projects (by science areas) (FY 2010/11)							
Grand Total	SBA	ES	MS	AS	TFS	EO	Polar
8	0	0	0	4.5	0	3.5	0

OUTPUT & PERFORMANCE MEASURES (per annum average previous 3 years)										
Publications (by science area & type) (Calendar years 2007, 2008 &2009)										
SBA	ES	MS	AS	TFS	EO	Polar	Grand Total	Refereed	Non-Ref/ Conf Proc	PhD Theses
0	0	0	4	0	2.67	0	**6.67**	3.33	1.67	1.67

Distribution of Projects (by science areas) (FY 2007/2008, 2008/2009 & 2009/2010)							
Grand Total	SBA	ES	MS	AS	TFS	EO	Polar
6.67	0	0	0	**4.61**	0.44	1.61	**0**

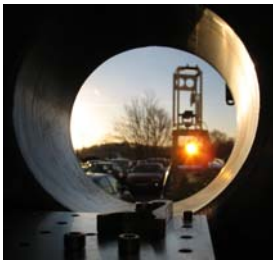
Distribution of Projects by NERC strategic priority (current FY 2010/11)							
Grand Total	Climate System	Biodiversity	Earth System Science	Sustainable Use of Natural Resources	Natural Hazards	Environment, Pollution & Human Health	Technologies
12	5	0	1.38	0	1	1.33	3

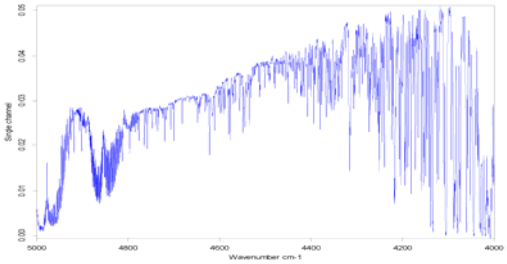
*Combined Responsive Mode and Directed Programme grants

OVERVIEW & ACTIVITIES IN FINANCIAL YEAR (2010/11):

Atmospheric spectroscopy

The MSF now has the capability to make high spectral resolution atmospheric solar occultation measurements using the IFS 120HR spectrometer. There is also the facility to run a second instrument alongside the FTS for inter-comparison purposes. The Centre for Earth Observation Instrumentation funded "Follow-On Study of the 2d Thermal Infrared Detector Array System and Signal Processing Unit" will make use of the solar tracking system and the IFS 66v/S spectrometer to investigate the performance of the TIDAS-SPU during atmospheric measurements.

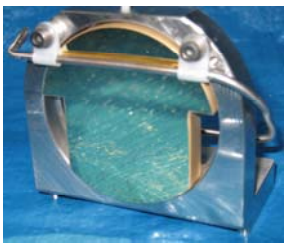


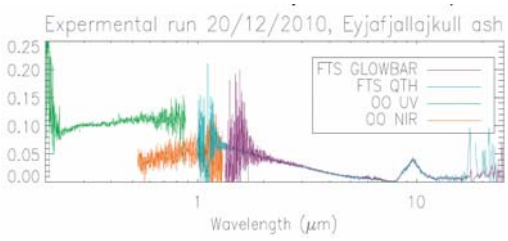


Above: (Left) A view from inside the laboratory of the automatic solar tracker that directs radiation into the spectrometer. (Right) An example solar occultation spectrum recorded with the IFS 120HR spectrometer showing atmospheric absorption lines between 4000 and 5000 cm^{-1}.

Multi-pass aerosol cell

During 2010/11 the second optical channel was installed, initially using the miniature spectrometers coupled via optical fibres. In combination with the FTS, three spectral regions can be measured simultaneously. The first particle dispersion test measurements, using volcanic dust, showed that aerosol contamination of the windows and White cell mirrors was a problem. Purge gas nozzles directed across the window and mirror surfaces were installed. The transfer optics used with the FTS were also modified to improve optical alignment and increase the maximum number of passes through the cell.





Above: (Left) Multi-pass mirror fitted with purge nozzles which produce a gas curtain to protect the reflective surface from contamination. (Right) Eyjafjallajökull ash extinction coefficients measured using the multi-pass aerosol cell. The plot compares IR measurements made with the FTS and the Ocean Optics miniature spectrometers operating in the near-IR, visible and ultraviolet spectral regions (OO NIR and OO UV). The mismatch between the orange and green data is due to non-uniform contamination of the cell windows. This will be avoided in future measurements by the use of the new purge gas system.

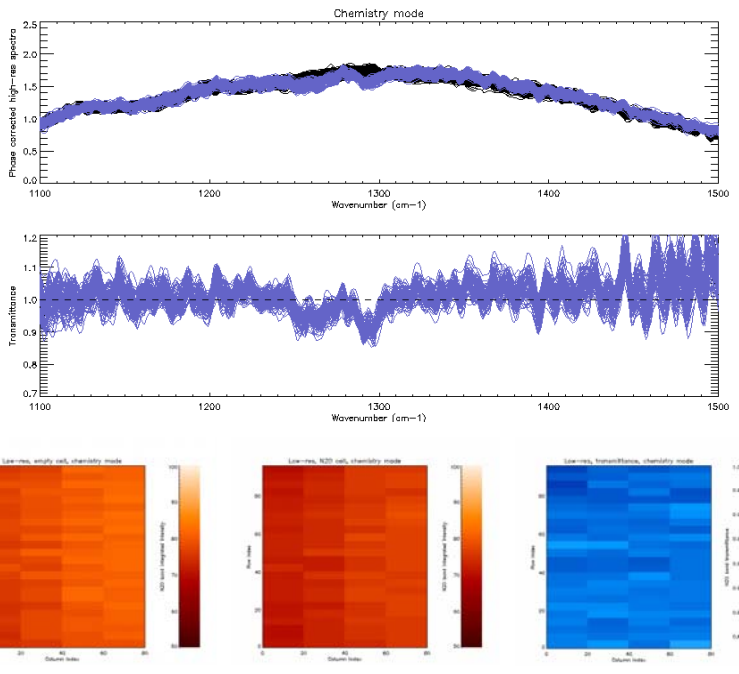
Step scan capability

The step-scan technique allows the monitoring of the temporal progress of very fast reproducible events. Example applications include high speed gas-phase kinetics, study of radical intermediates, photolysis experiments and time resolved emission spectroscopy. The technique also allows the scan speed to be significantly reduced compared to the standard spectrometer settings, and it was for this reason that the system was obtained with funding from the Centre for Earth Observation Instrumentation, as part of their Thermal Infrared Detector Array System and Signal Processing Unit project. Example data from that project are given below in the *Science Highlights* section. Following the end of that project the system will be available to other MSF users.

SCIENCE HIGHLIGHTS:

Technology for future atmospheric composition satellite missions

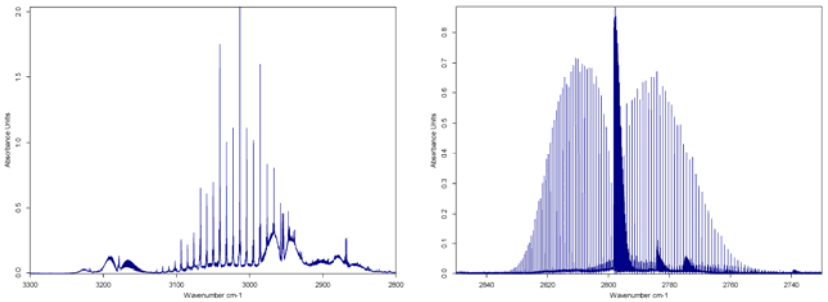
Future observations of climate gases will require both high spatial resolution and high accuracy, e.g. for gases such as water vapour, ozone and methane. These requirements can be met by the next generation of infra-red sounding spectrometers utilising two-dimensional detector arrays. This Centre for Earth Observation Instrumentation project, led by Astrium and University of Leicester, characterised an enhanced detector processing system and performed extensive tests on array performance.



Right: Multiple single channel (top) and transmittance spectra (centre) of N_2O recorded with the detector array operating in a "super-pixel" mode appropriate for atmospheric chemistry observations. (Bottom) Maps of the array window, showing integrated intensity for each chemistry mode super-pixel. Left to right: without N_2O; with N_2O; and transmittance. The orange and blue scales range from 50 to 100(arbitrary units) and 0.8 to 1.0in transmittance respectively.

Atmospheric chemistry from space

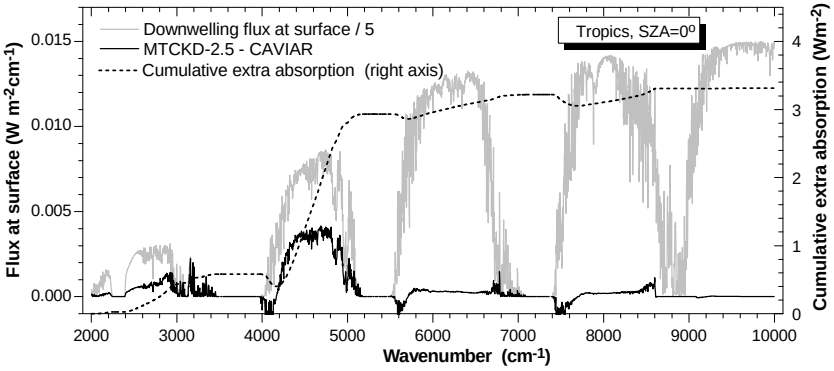
University of York have measured cross section data on acetonitrile and methanol. The former is a relatively long-lived minor constituent of the Earth's atmosphere, its largest source being biomass burning. The long lifetime makes it a useful tracer for biomass burning and other atmospheric transport processes. Methanol is the second most abundant organic molecule in the troposphere and indirectly leads to the production of tropospheric ozone, which is associated with poor air quality and is a greenhouse gas. The budget and emissions of methanol are poorly constrained. Infrared cross section measurements of these molecules recorded at the MSF will allow more accurate global observation of these species from space.



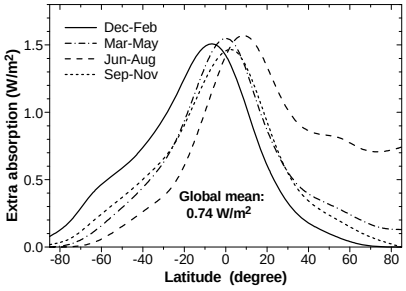
Above: (Left) Example acetonitrile absorbance spectrum between 2800 and 3300 cm^{-1} recorded at 0.015 cm^{-1} resolution using the SPAC at room temperature and a vapour pressure of 3 Torr in a 760 Torr mixture with zero air. (Right) Example methanol absorbance spectra between 2730 and 2850 cm^{-1} recorded at 0.015 cm^{-1} resolution using the SPAC at 190 K and a vapour pressure of 0.01 Torr.

Impacts of water vapour measurements on climate modelling and weather forecasting

The water vapour data recorded at the MSF as part of the CAVIAR project have been used to produce a new model of the water vapour continuum absorption spanning the infrared spectral region from 1 to 5 µm. Preliminary comparisons of calculated clear-sky absorption using the CAVIAR continuum against the widely used MT_CKD-2.5 model of the continuum have been made for a variety of atmospheric conditions. The CAVIAR continuum increases the calculated clear-sky atmospheric absorption of solar radiation by about 1% for the global-mean and 2 to 3% in the tropics relative to MT_CKD-2.5. This increase in our understanding of the radiative properties of water vapour will enable improvements in climate forecasting and numerical weather prediction. The new continuum model will additionally have implications for remote-sensing techniques that use the atmospheric windows between the main water vapour absorption bands to monitor atmospheric composition and other parameters such as sea surface temperature.



Above: The calculated spectrum of downwelling clear-sky solar flux at the surface (grey) and extra absorption (black line) caused by the CAVIAR self-continuum relative to MT_CKD-2.5 model. The dashed line shows the cumulative extra absorption (right axis). Right: The latitudinal dependence of the extra absorption for different seasons.



PUBLICATIONS: Examples of peer-reviewed publications resulting from MSF work appearing during 2010.

Atmospheric chemistry of HFE-7200, HFE-7100, HFE-7000 and $C_3F_7CH_2OH$: Temperature dependence of the kinetics of their reactions with OH radicals, atmospheric lifetimes and Global Warming Potentials, Iván Bravo, Yolanda Díaz-de-Mera, Alfonso Aranda, Kevin Smith, Keith P. Shine and George Marston, Phys. Chem. Chem. Phys., 12, 5115–5125, 2010. [**Impact factor 3.9**]

Infrared Absorption Spectra, Radiative Efficiencies, and Global Warming Potentials of Perfluorocarbons: Comparison between Experiment and Theory, Bravo, I., A. Aranda, M. D. Hurley, G. Marston, D. R. Nutt, K. P. Shine, K. Smith, and T. J. Wallington, J. Geophys. Res., doi:10.1029/2010JD014771, 2010. [**Impact factor 3.6**]

Improved water vapour line parameters, for use in radiation and climate modelling (Water vapour line intensities and self-broadening coefficients in the 5000-5600 cm^{-1} spectral region, I. V. Ptashnik and K. M. Smith, Journal of Quantitative Spectroscopy and Radiative Transfer, 111, 1317–1327, doi:10.1016/j.jqsrt.2010.01.007, 2010). [**Impact factor 2.0**]

FUTURE DEVELOPMENTS/STRATEGIC FORWARD LOOK

Attenuated total reflectance (ATR) spectroscopy: ATR will enable measurements to be made on solids, liquids or gases with minimal sample preparation, making the system ideal for short feasibility studies. The technique would be particularly well-suited to the study of liquid solutions as a precursor to aerosol studies. Funding has been granted to develop this capability during 2011/12.

Development of a supersonic molecular beam source: This will be used to study environmentally relevant clusters such as SO_3/H_2O and SO_3/DMS, to investigate coagulation, cluster growth, reaction and ionisation in order to understand their role in aerosol nucleation, an area where there is a paucity of experimental data. Such data will be used in modelling studies in the sub 3 nm size range, a size regime which bridges the gap between molecular species and embryonic aerosol modes. This work will draw upon expertise in molecular beams, spectroscopy and atmospheric models from the Universities of Southampton and Manchester.

Medium resolution spectrometer renewal: The Bruker IFS 66v/S spectrometer is used extensively for aerosol spectroscopy and is key to a number of current NERC projects. The instrument is about twelve years old and is becoming increasingly unreliable. If capital funding becomes available consideration should be given to replacing this instrument.