Institution: University of York		
Unit of Assessment: 8 - Chemistry		
Title of case study: Software and instruments supporting air pollution management		
Period when the underpinning research was undertaken: 2005 - 2018		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
David Carslaw Alastair Lewis James Lee Pete Edwards Andrew Rickard Lucy Carpenter	Reader Professor Professor URF Senior Research Fellow Professor	Apr 2015 - present May 2003 - present Sep 2003 - present Mar 2014 - present Jan 2012 - present Sep 2000 - present
Period when the claimed impact occurred: 2014-2020		
Is this case study continued from a case study submitted in 2014? N		

1. Summary of the impact (indicative maximum 100 words)

A highly influential set of software and measurement tools have been developed at the University of York that are used globally to support practitioners undertaking research, policy development and regulatory activities around air pollution. *Openair* is the world's most widely used data analysis software for air pollution visualisation and statistical analysis with >260,000 GitHub downloads. The *Master Chemical Mechanism* is the leading reference model for air pollution chemistry and is used in more than 40 countries. Atmospheric instrument technologies developed in York have been adopted into official global guidelines on measurement and been commercialised into new products supporting global sales in excess of USD50,000,000.

2. Underpinning research (indicative maximum 500 words)

The University of York has the largest laboratory in the UK working on research related to atmospheric chemistry and air pollution; it is consistently the top UK chemistry department for NERC research income. Research over the assessment period has resulted in the development of scientific tools and techniques for atmospheric chemistry that have subsequently been adopted and used world-wide, both for research and by applied users responsible for emissions control and air quality management.

1. **Software and data**

Research by **Rickard** over the past decade into the oxidation pathways of volatile organic compounds (VOCs) and associated chemical mechanisms (>35 publications) has underpinned the latest science contained in the *Master Chemical Mechanism (MCM)*, the most detailed and advanced description of gas phase tropospheric chemistry, used in ~40 countries for air pollution management and policy development. Notable has been research in York to develop a new isoprene degradation mechanism for the MCM, a fundamental set of > 1000 reaction steps that describe the oxidation and fate of the most significant VOC in the atmosphere [3.1].

A body of research by **Carslaw** into statistical methods for air pollution data analysis led to the creation of a range of powerful open-source tools used for research, policy and public engagement, initially funded by a NERC grant. This has included new visualisation approaches [3.2], new statistical methods for air pollution trend analysis, source apportionment, and machine learning removal of meteorological effects when detecting air pollution change due to policy, behavioural or natural interventions [3.3]. Research outputs have included academic papers, reports to government and commercial users and the publication of *R* software tools for public use on the *Openair* community GitHub platform, supporting a large global community of users.

2. **Instruments and measurement science**

Measurement science research has generated new capability for the trace detection of NO_x and VOCs in the atmosphere and provided insight into the performance and calibration of a new generation of lower cost compact sensors. Laboratory and field research by **Lee** and **Carpenter** on the measurement of ultra-trace part-per-trillion mixing ratios of NO and NO_2 has led to new techniques capable of automated measurements in the clean maritime tropical atmosphere [3.4], resolving outstanding long-standing problems associated with measurement certainties at very low concentrations.

Research into new methods for the detection of VOCs by **Lewis** led to the development of high sensitivity but robust methods for the simultaneous quantification of both non-methane hydrocarbons and oxygenated volatile organic compounds in a single analysis [3.5], enabled through innovative controls of water in the sample and methods of calibration of polar compounds. Research by Lewis and Carpenter subsequently adapted these methods of VOC detection for application in maritime environments, generating new insight into global long-term trends of ethane and propane and the impacts of shale gas extraction on the North Atlantic atmosphere.

Research by **Lewis** and **Edwards** lead to new scientific insight into the factors influencing the performance of lower cost compact air pollution sensors [3.6], including the quantification of uncertainties, discovery of key measurement interferences, and the development of technical strategies that could improve data quality. Underpinning research in the area of sensors has included the development of new approaches to atmospheric measurement using sensor clustering and data improvement using machine learning methods.

3. References to the research (indicative maximum of six references)

3.1. Jenkin, M.E., Young, J.C., **Rickard, A.R**. (2015) The MCM v3.3.1 degradation scheme for isoprene. Atmospheric Chemistry And Physics, **15**, 11433-11459. DOI: 10.5194/acp-15-11433-2015.

3.2. Grange S.K., **Carslaw D.C**. and **Lewis A.C.** (2016). Source apportionment advances using polar plots of bivariate correlation and regression statistics**.** Atmospheric Environment, 145, 1**28-134**. DOI: 10.1016/j.atmosenv.2016.09.016.

3.3. Grange S.K. and **Carslaw, D.C**. (2018) Using meteorological normalisation to detect interventions in air quality time series, Science of the Total Environment, **653**, DOI: 578-588. 10.1016/j.scitotenv.2018.10.344.

3.4. **Lee, J.D**., Moller, S.J., Read, K.A., **Lewis, A.C**., Mendes, L.M., and **Carpenter, L.J**. (2009) Year-Round Measurements Of Nitrogen Oxides And Ozone In The Tropical North Atlantic Marine Boundary Layer. Journal of Geophysical Research (Atmospheres), 114, D21302. DOI: 10.1029/2009JD011878

3.5. **Lewis, A.C**., Hopkins, J.R., Read, K.A., Carpenter, L.J., Pilling, M.J., and Stanton, J. (2005) Sources and sinks of acetaldehyde, acetone and methanol in North Atlantic marine boundary layer air. Atmospheric Chemistry and Physics, **5**, 1963-1974. DOI: 10.5194/acp-5-1963-2005

3.6. **Lewis, A.C.,** Lee, J.D., Edwards, P.M., Shaw, M.D., Evans, M.J., Moller, S.J. Smith, K., Ellis, M., Gillott, S., White, A., and Buckley J.W. (2016) Evaluating the performance of low cost chemical sensors for air pollution research. Faraday Discussions, **189**, 2016, 85-103. doi.org/10.1039/C5FD00201J

All references have been peer reviewed. [3.1] and [3.6] are being returned to REF2021.

4. Details of the impact (indicative maximum 750 words)

A substantial body of research from the University of York has influenced multiple areas of international air pollution practice through creation of a set of highly influential ***software tools*** and ***instrumental techniques*** that have been adopted globally. The users of these tools include practitioners working in the fields of air pollution policy and management, regulatory agencies, industrial users, national laboratories and the public. Impact has been achieved through the take up of open source software, the adoption of analytical methods into international guidelines, and the direct commercialisation of new instruments.

1. **Impact from software and data that supports air pollution management.**

Since its launch in 2012 *Openair* has grown to become the world's most widely used data analysis software for air pollution visualisation and statistical analysis, with >260,000 downloads (as of Dec 2020). The software package was created and then expanded from basic research and is shared open-source *via* the GitHub repository and via a UK Government website [5.1]. These software and data tools are used by organisations including the Environment Agency, Defra and the Department for Transport in the UK, the European Environment Agency, US Environmental Protection Agency, and international bodies including the World Health Organisation, World Meteorological Organisation and UN-Environment [e.g software downloads shown at 5.1]. Visualisations developed by Carslaw such as polar plots of bivariate statistics now appear in thousands of figures in air pollution-related documents and analyses. Statistical methods for the quantification of long-term atmospheric trends are used for regulatory analysis and reporting in dozens of countries.

The ability of data tools developed at the University of York to account for the effects of variable meteorology when assessing change points in air pollution came to the fore during the COVID-19 outbreak. It was used widely to support public communication about air quality, including a front-page story in The Guardian (print and online editions) [5.2] and reporting by other outlets (e.g. BBC, The Times, Daily Telegraph, Daily Mail). Weather-corrected air pollution effects during COVID-19 were a central component of an urgent evidence review commissioned by the Minister of State for the Environment, and published by Defra in June 2020 [5.3].

The *Master Chemical Mechanism* (MCM) is an explicit description of gas phase tropospheric reactions and York leads its scientific development [5.4]. It is considered the global gold standard reference for tropospheric chemistry and is used around the world as a benchmark against which air pollution models for forecasting and prediction are tested. Research at York into chemical mechanisms has maintained the scientific pre-eminence of the MCM over the last decade. The MCM has >1000 registered users in >40 countries. A key end-user application of the MCM has been for the evaluation of policies for tropospheric ozone management and the predicted impacts of specific regulatory actions on NO_x reductions from vehicles, and VOC emissions from solvents and industry.

The global reach of the MCM is evidenced through more than 2,000 papers and reports which cite the mechanism, and that it is used by environmental agencies in China, India, the US EPA and industries who must manage air pollution emissions. For example, from the Ford Motor Company, "*Commercial organisations like Ford look to detailed chemical mechanisms to support the development of cleaner vehicles which have the lowest possible impacts on the environment. Being able to model the detailed chemistry of tailpipe pollutants such as* NO_x *and VOCs is a vital part of that development process. The continual integration of the latest laboratory and theoretical science into the MCM is a major pathway by which the latest research finds its way into practical use, in particular here through the long-standing essential links between the MCM and IUPAC databases*." [5.5].

The MCM provides the scientific backbone of the Common Reactive Intermediates (CRI) parameterisation, a chemical reaction scheme that is used in regional models for operational air pollution forecasting for the public. The impacts of the science in the MCM are therefore delivered daily through air pollution forecasts issued by national weather services that use the CRI and its derivatives in their models, including the Daily Air Quality Index forecasts issued by the Met Office in the UK.

2. **Impact from instruments that support air pollution monitoring.**

Lee, Carpenter and Lewis played leading roles in setting new global standards for air pollution measurement, with methods being adopted by international bodies and provided as commercial products. Methods for the quantification of NOx and VOCs that were pioneered at York and demonstrated at its Cape Verde Atmospheric Observatory, now form part of the global guidelines for best measurement practice issued by the UN World Meteorological Organisation [5.6]

Novel methods for the analysis of oxygenated VOCs in air, first developed by Lewis through an InnovateUK KTP project, are now manufactured by a UK company, Markes International. This new capability added an integrated water management system for polar VOCs into the Markes product line [5.7 see image] and facilitated additional global instrument sales now in excess of USD40,000,000. The technology has been adopted by both Chinese and US governments as a preferred regulatory method for VOC monitoring, enabling continuous quantification of key VOCs such as methanol, and ethanol. York has published a number of key papers on the calibration of polar VOCs, and developed practical methods for generating real-time gas standards for on-line mass spectrometry measurements. A long-term research collaboration with mass spectrometer manufacturer Syft Technologies, led to York licencing a simple plug-in module for VOC calibration to support Syft products, and underpinned a growth in global sales for air monitoring applications in excess of NZD10,000,000 [5.8].

In 2015 Lewis and Edwards pioneered field evaluation of low cost pollution sensors, a technology that had begun to expand rapidly and that was receiving large venture capital and philanthropic investments. Some critical sensor performance limitations were summarised as a Commentary article by Lewis and Edwards in *Nature*, highlighting many fundamental issues around chemical interferences that degraded performance. This had global influence on the adoption of low-cost technologies by key decision-makers, for example at the request of the UK Government, Lewis authored advice for Local Authorities and the public on use of low cost sensors for air quality assessment [5.9], and an international report commissioned by WMO, UNEP and WHO that provided advice on sensor use to environmental and meteorological agencies. The latter report was published by the United Nations in 2018 with summaries in seven languages [5.10]. York expertise in sensors and air pollution was later called on to inform the investment decisions by two major global philanthropies, the Childrens Investment Fund Foundation (CIFF), and the C40 collaboration of global cities, supported by Bloomberg Philanthropies.

5. Sources to corroborate the impact (indicative maximum of 10 references)

5.1. Github repository link, including download statistics can be found at http://davidcarslaw.github.io/openair/
Tools also disseminated via Defra at https://uk-air.defra.gov.uk/data/openair

5.2. Link to Guardian article: https://www.theguardian.com/environment/2020/jul/10/uk-air-pollution-still-down-despite-return-normal-traffic-study

5.3. Report "Estimation of changes in air pollution emissions, concentrations and exposure during the COVID-19 outbreak in the UK". Department for Environment, Food and Rural Affairs. https://uk-air.defra.gov.uk/library/reports.php?report_id=1005

5.4. Link to MCM homepage: http://mcm.york.ac.uk/home.htt

5.5. Letter of Support from the Ford Motor Company, Research and Advanced Engineering, Dearborn, USA. Dated 29th July 2020.

5.6. WMO measurement guidelines report (for NOx) can be found at: https://library.wmo.int/opac/doc_num.php?explnum_id=3562

5.7. Markes International brochures showing York contributions and commercialised product.

5.8. Letter of Support from Syft Technologies, New Zealand.

5.9. Link to Defra/AQEG advice on the use of 'low-cost' pollution sensors, review and report lead by Lewis. https://uk-air.defra.gov.uk/research/aqeg/pollution-sensors.php

5.10. Access to a copy of the report from World Meteorological Organisation / UNEP report "Low-cost sensors for the measurement of atmospheric composition: overview of topic and future applications" http://eprints.whiterose.ac.uk/135994/1/WMO_Low_cost_sensors_post_review_final.pdf