IDENT: Identification without Separation: Novel approaches to the measurement of complex atmospheric VOC mixtures using soft chemical-ionisation mass spectrometry - drift-tube techniques

Fully Funded NERC-CASE PhD Studentship, University of Birmingham
-School of Geography, Earth & Environmental Sciences (Dr W Bloss / Prof AR MacKenzie)
-School of Physics & Astronomy (Dr C Mayhew)
-Kore Technology Ltd.

Background: Natural and anthropogenic processes emit a wide variety of volatile organic compounds (VOCs) into the atmosphere. Many have different chemical properties, affecting their contribution to the production of ozone and secondary organic aerosol (SOA), and their toxicity. There is a critical need for analytical approaches to distinguish such compounds in the complex mixture that is ambient air. Traditional chromatography methods have limited scope to study rapidly changing atmospheric composition, which may arise from emissions, chemical processing and meteorology. Alternatively, an ionisation technique coupled to a mass spectrometer, through which most VOCs can be measured (almost) simultaneously, and at high temporal frequency, such as PTR-ToF-MS (Proton Transfer Reaction – Time of Flight - Mass Spectrometry) may be used - however compound identification using MS approaches is challenging, as is not always clear which compounds are contributing to a given mass-charge ratio (*m*/*z*): many VOCs may be isobaric – *i.e.* have the same whole-number molecular mass (or are isomeric, with identical molecular masses), and may fragment.

The **aim of this project** is to develop a new approach to distinguish between isobaric / isomeric atmospheric VOCs, using the PTR-MS approach. Our proof-of-concept work shows that the fragmentation patterns of such VOCs vary in a systematic manner with the operating parameters of the PTR-MS system. Within this project, the PhD student / Doctoral Researcher will characterise the dependence of VOC fragmentation upon PTR-MS operating parameters; develop algorithms to analyse (or fit) these fragmentation patterns to series of mass spectra collected under different conditions, and establish operational protocols to most effectively probe the controlled fragmentation dependence of a given set of target analytes, at high time resolution. You will then apply the improved analytical capability to key challenges in atmospheric chemistry: (a) detection of isoprene, and studies of (aspects of) its degradation chemistry, and (b) resolution between the isobaric monoterpene isomers, and between isobaric aromatic compounds.

Isoprene (C_5H_8) is the dominant biogenic VOC emitted globally, and a major contributor to O_3 and SOA production, however within the atmosphere potential interferants are frequently present at the $C_5H_9^+$ protonated parent peak mass of m/z 69, making identification using PTR-MS difficult. Furthermore, the isoprene degradation products methyl vinyl ketone (MVK) and methacrolein (MACR) are also key atmospheric components, but as these are both C_4H_6O structural isomers, conventional MS approaches cannot distinguish between them. The $C_{10}H_{16}$ monoterpenes differ widely in their structure, and hence in their reactivity and atmospheric chemical role. Isobaric aromatic VOCs such as ethylbenzene and o/m/p-xylene again differ in their atmospheric impacts, sources and perhaps most significantly in their toxicity – the project will demonstrate the capability to distinguish between these species, initially using test mixtures, followed by atmospheric measurements at background and roadside locations.

Training and Development Opportunities
The project will provide a comprehensive interdisciplinary training in analytical science and mass spectrometric techniques, and in atmospheric composition and chemistry. The studentship coincides with and will benefit from an EC-funded Initial Training Network on Proton Ionisation Molecular Mass Spectrometry, coordinated by

Dr Mayhew and involving 16 other academic, industrial and governmental partners from across Europe; while on the atmospheric side you will have the opportunity to network with atmospheric chemists, ecologists, and climate scientists through our affiliation to the National Centre for Atmospheric Science (NCAS). The project will also involve working with our industrial CASE Partner, Kore Technology Ltd which will provide exposure to a fast-moving commercial R&D environment to complement the academic training.

The project is a collaboration between the Environmental Health Sciences research group in the School of Geography, Earth & Environmental Sciences, and the Molecular Physics group in the School of Physics and Astronomy, together with CASE Partner Kore Technology Ltd. The student will spend time working with each research group at Birmingham, and at Kore's facility in Ely, Cambridgeshire. Details of the activities of the project team may be found at the links below.

http://www.birmingham.ac.uk/research/activity/environmental-health/index.aspx
http://www.birmingham.ac.uk/research/activity/physics/quantum/molecular/index.aspx

Who should apply

Applications are invited from candidates who have, or expect to obtain, a good honours degree in a relevant subject (*e.g.* Chemistry, Physics, Environmental Science, Engineering). You must have demonstrable potential for creative, high-quality, PhD research and relish problem-solving. An eagerness to develop skills in instrumental analytical techniques, molecular physics, and atmospheric chemistry, is essential.

Funding

The project is fully funded (fees, maintenance grant etc.) through a NERC-RSC funding award, which will be supplemented by a further payment to the student from the CASE partner, Kore Technology Ltd.*

For further information, please contact either
Dr William (Bill) Bloss, GEES – w.j.bloss@bham.ac.uk, Tel. 0121 414 2558
Dr Chris Mayhew, Physics – c.mayhew@bham.ac.uk Tel. 0121 414 4729

To apply for this project, please use the link below. Please advise Dr Bloss by email of your candidate ID number after completing your application. Applications will be reviewed on a monthly basis until the studentship is filled.

Application Link :
http://www.birmingham.ac.uk/students/courses/postgraduate/research/gees/environmental-sci-risk-mgt.aspx

*Full funding available to UK students – funding may be available for EU students, please contact us. Unfortunately funding for this studentship is not available to applicants from outside the EU.