Chemistry Update

ISSUE 357 • JULY/AUGUST 2023

Calendar of Events

York Chemistry Postdoctoral Seminars Inaugral Event
ECR Speaker: Dr Anabel Lantern University of Nottingham
PDRA Speaker: Dr James Sherwood
Date: Thursday 7 September
Time: 1pm-3pm
Location: C/B/102

Department Open Day
Date: Saturday 8 September
Time: 9am-4pm

Department Open Day
Date: Sunday 9 September
Time: 9am-4pm

RSC-CRSI UK-India Symposium in Chemical Sciences
Date: Tuesday 12 September
Time: 9am-5pm
Location: C/A/101

EDI Beacon Event - Enhancing Research Culture in the Chemical Sciences through Mentorship
Date: Wednesday 13 September
Time: 11am-4.15pm
Location: C/A/101

Research Seminar
Speaker: Erwin Reisner, University of Cambridge
Date: Wednesday 20 September
Time: 1pm-2pm
Location: C/A/101

Retirement Celebration BBQ
Date: Friday 29 September
Time: 6pm

Research Seminar
Speaker: Dr David LeBoeuf, Université de Strasbourg
Date: Thursday 5 October
Time: 1pm-2pm
Location: C/B/101

Eleanor and Guy Dodson building opening event & lecture
Date: Thursday 5 October
Time: 7pm
Location: Eleanor and Guy Dodson building

Professor Brian Sutcliffe Memorial Symposium
Date: Wednesday 11 October
Time: 1pm-5.30pm
Location: C/A/101

This issue:

New study highlights the effects of extreme air pollution in Delhi

A collective team of researchers led by Wolfson Atmospheric Chemistry Laboratories (WACL) at the Department of Chemistry, the National Centre for Atmospheric Science (NCAS) and other research institutes have discovered the first evidence of the absence of nocturnal oxidation chemistry in the urban megacity of Delhi during highly polluted events.

Delhi, India is one of the most polluted megacities in the world. Levels of multiple pollutants regularly exceed World Health Organisation (WHO) limits. Previous studies have shown that high concentrations of pollutants have led to increased morbidity and premature mortality.

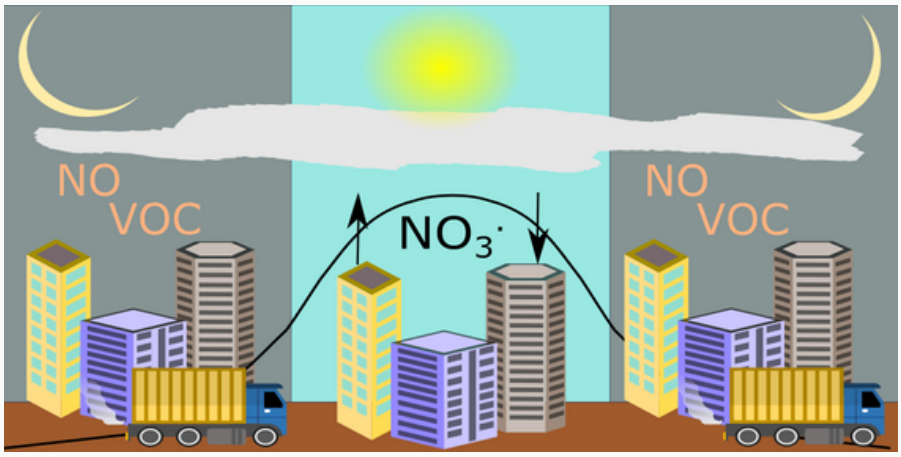
Beth Nelson and Dan Bryant working together with a team of national and local partners from across the DelhiFlux project, collected a comprehensive suite of primary (directly emitted) pollutants, including nitrogen oxides (NO and NO2) and > 80 different species of volatile organic compounds during two field sites in Delhi, this took place place during the pre and post-monsoon seasons, May-June and October-November 2018. The research was funded by the Air Pollution and Human Health in a Indian Megacity programme, a four year research programme jointly funded by the Natural Environment Research Council (NERC), the Medical Research Council (MRC), the Newton–Bhabha Fund, and the Ministry of Earth Sciences (MoES) and Department of Biotechnology (DBT).

Recent decades have seen accelerating invention and deployment of chemical and biophysical methods to answer questions in biology and medicine, including molecular graphics and modelling, chemoinformatics, imaging, and high-throughput crystallography and more recently cryo-electron microscopy. There are great opportunities for early stage, inventive scientists to make significant contributions in the development and deployment of these methods, which can have real impact on their personal development as well as scientific research and benefit to wider society.

High levels of pollutants were observed during both studies. During the post-monsoon period, extremely high concentrations of pollutants were measured at night. In particular, very high levels of nitrogen oxide (NO) were detected, which were around 400 times higher in the post-monsoon than in the pre-monsoon at night.
The study models the effect of the extreme night-time concentrations of NO, predominantly emitted from fossil fuel combustion processes such as vehicular emissions, and reveals an unusual night-time radical “desert” where all radical species are suppressed, leading to no oxidation chemistry at night.

The research suggests that this suppression of chemical activity at night could be contributing towards a build-up of primary pollutants in the evening, which then undergo rapid chemical reactions when the sun rises. This leads to a shift in peak secondary pollutant production, with major pollutants such as ozone peaking at midday rather than later in the afternoon, which is more typical. The high levels of pollution observed at night may also be exacerbated by pollution abatement strategies restricting the movement of Heavy Goods Vehicles (HGVs) during the day, which could lead to more HGV activity at night.

Beth Nelson, project lead said "The research highlights the importance of pollution reduction strategy design in urban centres such as Delhi and a need for emission reduction policies which focus on reducing emissions throughout the entire 24 hour period."



This research has been published in Environmental Science & Technology Letters.

National Student Survey reveals the strengths of Chemistry at York

The results of a nationwide survey have revealed that the Department of Chemistry is home to some of the happiest chemistry students in the UK.

We placed 1st for 'Learning opportunities' among the Russell Group universities included for Chemistry in the 2023 National Student Survey (NSS), with a score of 89%. We received 91 per cent for Q05 To what extent have you had the chance to explore ideas and concepts in depth?, 93 per cent for Q06 How well does your course introduce subjects and skills in way that builds on what you have already learned? and 93 per cent for Q07 To what extent have you had the chance to bring together information and ideas from different topics?.

We also ranked highly within the Russell Group in the following areas:

2nd for 'Student voice' in chemistry
Including:

- Q22 To what extent do you get the right opportunities to give feedback on your course? 92 percent
- Q23 To what extent are students' opinions about the course valued by staff? 85 percent
- Q24 How clear is it that students' feedback on the course is acted on? 82 percent

Professor Caroline Dessent, the Head of Department, said "We are proud that the Department of Chemistry in York is a unique learning community which allows students to study at the frontiers of the subject. We are delighted to see that our students value the learning opportunities we provide and are empowered to work with us to build the best course possible".

York's overall position
York performed strongly in this year's National Student Survey, featuring in the top 10 for multiple categories among Russell Group universities.The University as a whole placed 4th in the Russell Group for Learning Resources, 5th for Academic Support and 6th for Organisation and Management. Thirteen subjects featured in the top three in the Russell Group for Academic Support, while a further 12 were placed in the top three for Teaching On My Course. Read more about York's excellent NSS results.

Deep Neural Network Predicts Time-Resolved Spectroscopic Data

A team of researchers from the University of York and Newcastle University have trialled an 'on-the-fly' deep neural network (DNN) training protocol that can be used to simulate the spectroscopic signals from ultrafast molecular processes.

The latest high-brilliance light sources at particle accelerator facilities have transformed the kind of science that it is possible to do today, unlocking a universe of ultrafast high-resolution time-resolved experimental techniques that are able reveal fine details about the excited-state dynamics of molecules and materials on the atomic scales of length and time.

Many of these techniques (eg. ultrafast (multidimensional) spectroscopy, stimulated Raman, and electron and X-ray scattering experiments) offer complimentary insights into the coupled nuclear and electronic dynamics that underpin the functional properties of the molecules and materials that are able to be studied. Connecting the experimental observables to the operational chemistry and physics through computational simulations is the best way to understand these physical phenomena and, ultimately, an important step towards harnessing them for practical applications. The complexity of these techniques is such that this is an incredibly tall order, however, and there is real demand for approaches to computational simulation that are fast, accurate, affordable, and generally-applicable enough to act as a 'limited-experience-necessary' starting point.

In the new research, Dr Conor Rankine, Prof. Tom Penfold, and Clelia Middleton (the PhD student who led the work) have shown that their XANESNET DNN for X-ray absorption and emission spectroscopy can be used with an 'on-the-fly' training protocol, allowing it to analyse a limited quantity of computational simulation data and converge quickly to meaningful solutions. Their machine-learning approach is able to sidestep what would otherwise involve days/weeks of time-consuming quantum-chemical calculations and expert oversight, allowing the experimental observables of an ultrafast excited-state dynamic process to be predicted using only a limited sample of geometries explored in the process.

Speaking about the research, Dr Conor Rankine said: "I'm sure that people will remember (and perhaps be sick of!) the ultrafast ring-opening dynamics of 1,2-dithiane [a small, cyclic disulfide] that we used as a test bed in this research – I presented countless posters and talks on this system when I was a postgraduate student at York! It's great to see Clelia carrying the torch for these disulfide systems – she's put a Herculean amount of effort into driving this research forwards and putting this out as her first [PhD] publication, and it couldn't be in safer hands as far as I'm concerned. Congratulations Clelia!"

This research has been published in Physical Chemistry Chemical Physics.

Triple Platinum Award Success for the Green Chemistry Green Impact Team

This year at the University of York's Green Impact Awards the Green Chemistry team celebrated their best ever accomplishment by receiving 3 Platinum Awards. This was the most ever achieved by the team since its creation, the most awards achieved across the whole of the University of York and the first time the team had attempted a specific green impact project.

This year the team was led by Ryan Barker and Richard Gammons. The other team members were; Aobh Hyland, Daniel Inglis, Hannah Chapman, Harry Maslen, James Metcalf, Megan Goss Oliver Stevens, Rebecca Willans and Krista Abbott (Green Impact Project Assistant).

Our target areas this year have included:

- Changing weighing boats from plastic to reusable glass
- Campus Tree Trial Walk for improving Mental Health and Wellbeing
- Sustainability lab methods including waterless condensers and multipoint equipment
- Sustainability lab notice board for all green chemistry announcements
- Charity events raising money for our toilet twinning campaign and food bank collections

The Green Chemistry Centre of Excellence has always been proud of its sustainability work and this year marked an even further leap with our project Greening up GC-FID analysis: From Helium to Hydrogen. This work was completed by just 3 members of the team; Megan Goss, Daniel Inglis and Richard Gammons. The project aims were to Green up Gas Chromatography Analysis, by Investigating the environmental impact and carbon footprint of helium production and transportation, Investigating the environmental impact and carbon footprint of hydrogen production from water and hence, Investigating the economic and carbon footprint implications of switching carrier gas.

The UN sustainability goals we aimed to align with are as follows:
1. Number 7: Affordable and Clean Energy
2. Number 9: Industry, Innovation and Infrastructure
3. Number 12: Responsible Consumption and Production
4. Number 13: Climate Action

What were our successes and outcomes?
As a result of both the long term economic and environmental impacts we have switched carrier gases for our 4 GC-FIDs in the green chemistry centre and we have shared our findings from the project report with the wider university via the Tech York Network. (All of the technical staff across the University of York.)

What does the team hope to do in the future?
In the future we will continue this work and we also aim to complete other lab projects/initiatives in the green impact team including;

1. Cost benefit analysis of installing chillers in the lab (Report by Green Impact Team) rather than using constant running water, in order to save all the galleons of wasted water used for cooling.

2. Green Lab Solutions Day - Jan 2024. A day to bring together suppliers from Industry with Academia to investigate conducting research more sustainably. (Including demos in the lab)

3. Single Use Plastics - track and reduce usage where possible - including pipette tips, centrifuge tubes and other disposable plastics.

4. Calculate the Carbon footprint of our GCCE labs - raise awareness and try to look at solutions to reduce this.

The Green Chemistry Green Impact team would like to thank all members of staff and students in the department who have supported any of our initiatives this year and look forward to an inspiring year next year improving sustainability for all.

Chem@York Research Conference

The first Chem@York Research Conference, organised by Will Unsworth, took place on Thursday 6 July and was a fantastic day of engaging talks from PhDs and PDRAs from across the department, celebrating the wide range of research taking place. David Cole Hamilton, University of St Andrews kicked off the event with his lecture “The role of chemists in a sustainable world”.

A major driver for organising the conference was to bring together the whole department and celebrate our research jointly. The talks were themed across five different research areas with a prize awarded for each area.

The day concluded with a poster session, providing participants who were not giving oral presentations to have the opportunity to present, this was accompanied by a drinks reception and prize giving.

The hope is that the conference will become a regular annual event and one of the highlights of Chemistry calendar.

Chem@York Conference Prize winners:

- Catalysis for a Cleaner Future - Andres Gomez Angel (PAOB)
- Chemical Biology and Biological Chemistry - Charlay Wood (WPU/Lichman)
- Green and Sustainable Synthesis - Kirsten Hawkin (HFS)
- Molecular Materials - Yuzhen Wen (PRM)
- Atmospheric Chemistry - Loren Temple (PME)

Student success at Nuclear Magnetic Resonance conferences

A number of students from Meghan Halse and Simon Duckett's groups participated in the Royal Society Chemistry Nuclear Magnetic Resonance Discussion Group (NMRDG), Postgraduate and Postdoctoral Meeting in Leicester on June 22-23, 2023. Callum Garter (3rd Year PhD with SBD) presented his work at the event and won a poster prize.

Left to right: Ana Silva Terra (PhD with MEH), Izzy Hehir (PhD with MEH), Laura Tadiello (visiting PhD student with MEH), Dan Taylor (PDRA with MEH), James McCall (PhD with MEH), Callum Gater (PhD with SBD) at the NMRDG Postgraduate meeting in Leicester in June 2023.

Callum Gater presenting his work at the NMRDG in Leicester.

The groups also attended the Euromar conference in Glasgow on July 9-13, where Simon Duckett gave the opening keynote lecture and Ana Silva Terra (3rd year PhD with MEH) won a Best Flash Presentation prize from the Institute of Physics (IoP) British Radiofrequency Spectroscopy Group (BRSG). Euromar is the leading annual European Magnetic resonance conference. The last time it was hosted in the UK was in 2006 in York.

Simon Duckett's keynot lecture at the Euromar conference in Glasgow

Left to right: Vicky Leadley (technical support in CHyM with SBD), Callum Gater (PhD with SBD), Ana Silva Terra (PhD with MEH), Dan Taylor (PDRA wth MEH) at Euromar in Glasgow.

Chemistry Graduation

We were pleased to welcome honorary graduand Professor Amilra (AP) de Silva to the graduation cerenomy in July. It was great to hear from both Professor Duncan Bruce and Professor AP de Silva at the event. Born in Sri Lanka, AP studied at both the University of Colombo, Sri Lanka, and Queen's University Belfast, UK, where he is now an Emeritus Professor of Chemistry. His influential research includes the development of low-cost PET sensors & the invention of molecular logic-based computation. His work has saved thousands of lives worldwide.

Professor Duncan Bruce and Honorary Graduand AP de Silva

The departmental celebration provided the annual opportunity to acknowledge the achievements of all our new graduates along with their friends and families. Huge congratulations!

Goodbye to Clare Docking

The Centre for Industry Education Collaboration (CIEC) will soon be saying goodbye to the CCI advisory teacher for the East of England, Clare Docking. Clare has spent the last 5 years working with primary school teachers and children to make science engaging and meaningful. A large part of her job has involved working with local science-based industries and helping children to see the links between science in real life industrial contexts and the science that they learn in school. She has led training for teachers and lessons for children. Shehas also worked with STEM professionals in partner industries to give them the skills needed to work effectively with young people.

She told us: “It has been a real privilege to have met and worked with Sartorius Stedim Biotech and Johnson Matthey, our partners in the region, and support them to raise the aspirations of children. CIEC is committed to breaking down stereotypes and educating children about opportunities in science and engineering and I am proud to have been part of this important work.”

We will be very sad to see Clare go. She puts her heart and soul into the work, and we know that she will be greatly missed by the schools and companies that she has worked with as well as by the whole CIEC team. She is not however going to be letting the grass grow under her feet. Earlier this year she got married and she and her husband plan to spend their retirement touring in their camper van.

Dr Charles Barry Thomas RSC Obituary

Dr Charles Barry Thomas’s obituary has been published by the RSC. It is available to read here

Thanks to Professor Bruce Gilbert for writing the piece.

Upcoming events in the department

RSC-CRSI UK-India Symposium in Chemical Sciences 2023

Tuesday 12 September • C/A/101 • 9am-5pm
The Royal Society of Chemistry (RSC) and Chemical Research Society of India (CRSI) are proudly presenting a free one-day symposium, to be hosted in the Department on Tuesday 12 September. This event aims to bring together researchers from the UK and India, fostering research collaborations focusing on sustainable chemistry. Learn more and register.

Please note: despite any indications in the sign-up process, this symposium is completely free to attend. The RSC's registration system might mention directing you towards a payment page, however, no payment information is required.

EDI Beacon Event - Enhancing Research Culture in the Chemical Sciences through Mentorship

Wednesday 13 September • 11am-4.15pm • C/A/101
Join us for this symposium which will bring together some excellent speakers to discuss mentorship and its role in addressing inequalities and promoting a positive research culture in chemistry and the physical sciences. All student and staff groups are welcome and encouraged to attend. Please register your attendence via the eventbrite link.

Speakers include:

- *Dr Laura Reyes & Laura Woodward, Royal Society of Chemistry*
- *Dr Karen Clegg, University of York*
- *Professor Robin Perutz, University of York*
- *Professor Jennifer Heemstra, Washington University in St. Louis, USA*
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Panel discussion | Post-meeting reception & networking from 4.15pm onwards
Contact: john.slattery@york.ac.uk

Eleanor and Guy Dodson Building opening event & lecture

Thursday 5 October • 7pm • Eleanor and Guy Dodson Building
Public lecture given by Nobel Laureate, Richard Henderson

Professor Brian Sutcliffe Memorial Symposium

Wednesday 11 October • 1.00pm-5.30pm • C/A/101
In celebration of the life of our colleague Brian Sutcliffe, the department is organising a memorial symposium.The event will take place from 1.00pm-5.30pm and will be followed by a drinks reception.