Institution: University of York
Unit of Assessment: 8, Chemistry

a. Context

During 2008-13, Chemistry's impact spanned diverse areas that encompass public and private sectors, society and schools, with tangible benefits in economic, health, public policy, and environmental arenas. The impact reached international policy, global companies, schools throughout Britain, and UK government. Many of these impacts arose from our multidisciplinary research. We highlight our policies and the links between research and impact as follows:

1) Economic impacts with global reach arising via commercial exploitation (*e.g.* enzymes, biofuels);
2) Spin-out companies and links with SMEs with consequent regional benefit;
3) Impacts on environmental policies of the UK, EU and UN through atmospheric chemistry;
4) Societal and health impacts in food security through collaboration with a government agency;
5) Outreach impact linked to research in green chemistry, liquid crystals and solar energy.

b. Approach to impact

Mechanisms and evidence for our engagement and interaction with key research users

The Department's wide view of chemistry embraces core areas plus structural biology, soft matter, atmospheric, archaeological and green chemistry. Long-term strategic decisions to invest in multidisciplinary fields have enabled our impact and, during 2008-13, we renewed investment in this distinctive view of chemistry. New multidisciplinary areas have been supported, notably linking magnetic resonance to neuroscience. The coherent, multidisciplinary teams have complementary skills and qualities, and the cultural norms of different disciplines merge productively for impact generation. Our multifaceted approach to impact involves both strategic leadership and bottom-up initiatives to form sustainable, long-term relationships. Multidisciplinary centres of excellence are a major tool for generating our impact, linking Chemistry to all York Sciences, Management and Archaeology departments. Those that have generated impact in 2008-13 are: *National Centre of Atmospheric Science* (NCAS, supported by NERC), *York Centre for Complex Systems Analysis*, *York Environmental Sustainability Institute*, *Biorenewables Development Centre (BDC), BioArCh* (a Biology-Archaeology-Chemistry centre), *Centre of Excellence in Mass Spectrometry (CoEMS)*, *Centre for Hyperpolarisation in Magnetic Resonance (CHyM)*, *York Nanocentre, Centre for Chronic Diseases and Disorders, York Structural Biology Laboratory (YSBL*)*, *Green Chemistry Centre of Excellence*,* and *the Chemical Industry Education Centre* (now CIEC*) (*solely in Chemistry).

Strategic decision making on investment for impact direction and planning are led by the Head of Department advised by Departmental Committees, each with membership of both genders and from across the academic grades – it is the younger colleagues who frequently generate and implement the most innovative ideas. Further advice is provided by our External Advisory Group, chaired by a senior industrialist and including other industrialists, academics and schoolteachers.

Evidence of relationships, agility, responsiveness and follow-through (2008-13)

1. Economic impacts with global reach. The relationships forged by York Chemistry enable us to achieve impact through products used worldwide. We illustrate how they develop from long-term collaborations based on exceptional research quality nurtured in multidisciplinary centres.

(i) *Enzymes for detergents and biofuels, and crystallographic software. YSBL*, a Chemistry grouping, has sustained excellence in determining the crystal structures of biological macromolecules (three Case Studies). **Davies** and **K. Wilson** collaborated with global company, Novozymes A/S ($1.5bn turnover, 47% industrial enzyme market share), to target structure determination of enzymes for detergents and biofuels. **Davies** and **Walton** consult for Novozymes. In a complementary approach, software for macromolecular crystallography was written by **Cowtan** and others with **K. Wilson** as lead. It is a major component of the CCP4 software suite, which earns >£1m p.a. in commercial user fees (www.ccp4.ac.uk). This is one of two suites used worldwide by global drug companies such as GSK, and SMEs such as Astex. York's long-term support of YSBL in posts and equipment has enabled it to maintain its international pre-eminence.

(ii) Sensitisation of NMR for medical imaging. **Duckett** has discovered new methods to enhance the sensitivity of magnetic resonance based on *para*-hydrogen, offering new prospects for magnetic resonance imaging with great medical potential (five patents submitted). His partnership with Medicine, Biology and Psychology has been pivotal and all participate in the resulting centre, CHyM. Bruker Biospin, a global instrument company, was selected competitively as partner, and has provided funding in cash (PDRA, studentship, equipment) and kind, undertaking in-house R&D

from 2008, and seconding a member of R&D staff to York. End-users AstraZeneca, GSK, FERA and Oxford Instruments have supported research students. This example illustrates the importance of fundamental research in generating impact as well as the Department's agility: the key paper was published in *Science* in 2009; by Nov 2012 two major Wellcome Trust grants and two EPSRC grants, including Follow-On funding (total *ca* £15m) had been won and a new building completed. The first product of Bruker-CHyM partnership, a *para*-hydrogen polariser, was released in 2013.

2. Spin-out companies and links with SMEs. We illustrate regional and wider impacts that were supported by the University Research and Enterprise Office (REO) (patenting and funding).

(i) 2D Detectors for capillary electrophoresis. Paraytec Ltd develops and builds instruments for pharmaceutical bioanalysis. This spin-out, founded by Goodall (emeritus), generated worldwide patents in period. The instruments (75 sold, most in period, revenue ca £1.8m) are marketed through established companies *via* licensing agreements. (ii) *The Biorenewables Development Centre* (BDC), formed in 2009 between the Green Chemistry Centre of Excellence and Biology, provides a microwave biorefinery and bioethanol plant. It works with companies on conversion of biomass to chemicals and materials as a commercial demonstrator. The University established the BDC as a company, which was awarded grants exceeding £7m in 2012 from ERDF, BIS and ETDE Contracting Ltd. With 22 staff and £3m of equipment, the BDC is located on York Science Park. *(iii) Starbons and Green Chemistry KTP.* Starbon® Technologies Ltd, a spin-out founded by **Clark** (2012), manufactures mesoporous carbonaceous materials in the BDC from waste polysaccharides; the materials are used for chromatography, water purification and catalysis. Starbons were invented in Green Chemistry and supported by EPSRC with Follow-On funding (2010). The company sells through Sigma-Aldrich, and has won awards from TSB, DEFRA and Rushlight. A KTP (2007-9) linking Green Chemistry to Brocklesby Ltd, an SME specialising in oil recycling, won the 2009 Yorkshire and Humber Innovator of the Year Award.

3. Impacts on environmental policies. Initiatives with national and international agencies are crucial to our far-reaching impact. The atmospheric chemistry group interacts with DEFRA and the Met Office in the UK and with UN agencies (two Case Studies): (i) *Role of natural organic emissions on UK air quality,* led by **Lewis,** concerns ozone build-up near ground level during a heat wave and informed DEFRA reports in 2008-9 and Met Office forecasts for the public. (ii) *Influence of organohalogens on ozone depletion* concerns satellite observations and the Cape Verde Atmospheric Observatory. The data underpin the Montreal Protocol, and contribute to UK obligations under the UN Convention on Climate Change. **Carpenter** and **Bernath** were reviewers for the UN Environment Programme and members of its Scientific Assessment Panel (2010).

4. Societal and health impacts in food security. Two collaborations with FERA (Food and Environment Research Agency, fera.defra.gov.uk) reveal York Chemistry's impacts in current international challenges *via* multidisciplinary centres. *(i) Animal sources of food products* (Case Study). **Thomas-Oates** collaborated with Collins (Archaeology) to develop a method for identifying the animal source of gelatin *via* collagen analysis. A CASE studentship with Prosper de Mulder, a meat and bone meal company, followed original archaeological applications. FERA validated the methods and uses them to identify food fraud such as use of pork gelatin in chicken products. *(ii) Analysis of food products by NMR spectroscopy.* **J Wilson** (Chemistry-Mathematics) initiated work with FERA (2004-13, three studentships) to develop mathematical routines for processing 2D-NMR metabolomic datasets. The computational routines have been incorporated into FERA's graphical user interface, Metabolab, and are used for identifying biomarkers of animal disease. These methods were central to a £1.7M project for the Food Standards Agency, investigating novel biomarkers of BSE and scrapie and underpin a €15m FP6 project (TRACE) on food authenticity.

5. Outreach for schoolteachers, students and public. We run a distinctive schools outreach programme coordinated by the directors of CIEC-Promoting Science (ciec.org.uk) and a dedicated Outreach Officer, **Hodgson**. It aims to disseminate chemistry to schools pupils of all ages and the public. (i) *Chemistry Review*, (www.hoddereducation.co.uk/magazines) edited in York by Hodgson is a high-quality schools magazine with 7,800 subscriptions and many articles based on York research. (ii) Green Chemistry's public understanding programme was funded by the EPSRC and industry (greener-industry.org.uk). Green Chemistry works with the Ellen MacArthur Foundation and has exhibited at science discovery centres in Bristol and Glasgow. CIEC and Green Chemistry received the 2012 ACS Award for Incorporating Sustainability into Chemical Education from primary age to undergraduates. (iii) In 2008-12, CIEC's *Children Challenging Industry* initiative delivered outreach work featuring green chemistry research into 550 primary schools (16,500

pupils). CIEC obtained £1.5m in 2008-13 from industry and engages captains of industry including CEOs of Thomas Swan and Johnson Matthey. (iv) Research on liquid crystals and on solar fuels featured at The Royal Society Summer Exhibitions in 2010 led by **Goodby**, in 2011 by **Perutz** and in 2013 by **Parkin** (visitor numbers *ca* 50,000, 14,000 and 13,000, respectively).

Mechanisms to enable, encourage and reward staff to generate impact

The Department encourages staff to create impact by providing support and approving flexible working arrangements (*e.g.* timing/loading and replacement cover for teaching), often at short notice, to underpin external initiatives. Recognising the importance of external input to the development of software for macromolecular crystallography and computational methods and fragment-based drug discovery, **Hubbard** is seconded (40%) to pharma company Vernalis (www.vernalis.com), **K Wilson** is appointed (20%) to CCP4 (BBSRC, STFC) and **Cowtan's** appointment is underwritten by the Department. **Lewis** is Deputy Director of NCAS and Director of Composition Science; he was also Technology Strategy Advisor to NERC (2008-13). This staffing flexibility extends beyond academic staff: Bergström (Experimental Officer, EO) is seconded (20%) to spin-out Paraytec, while the Department provided bridging finance for Abbott (EO) to preserve the long-term collaboration between **Moore** and Unilever on commercially important dye research.

In a totally new approach, the Department has enabled the Swiss chemical robotics company, Chemspeed Technologies, to move its UK base to York. The staff, and robotic parallel synthesis platforms worth £750k, are located in Chemistry. The equipment is accessible to chemistry users and the company, while the staff provide expertise and work collaboratively with in-house users.

Academic appointments during the period reflect our determination to strengthen groups with a proven record and further potential for impact generation. Thus, four appointments (including chair, **Evans**) expanded Atmospheric Chemistry, while in Materials Chemistry, **Bates** and **Saez** moved to lectureships and **Cowling** moved to Grade 7 to oversee the new small-angle X-ray facility as well as lead on new projects concerning applications of dyes. In Organic Chemistry, **Fairlamb**'s assimilation as a member of staff enabled the Chemspeed initiative to progress, while there has been an appointment spanning Inorganic Chemistry and Chemical Biology (**Parkin**) and one in Analytical Chemistry (**Lucquin**), the latter enhancing our high impact work with Archaeology.

Impact is highlighted in promotion. Outreach's importance is recognised by paying the salary of the Outreach Officer and supporting CIEC. The University incentivises inventors through a royalties scheme starting at 100% and decreasing in steps to 33.3%, and through the Vice Chancellor's prizes – winners include Atmospheric Chemistry, Magnetic Resonance and Green Chemistry.

Facilities, Expertise and Resources

Excellent infrastructure underpins our ability to conduct high quality research generating impact. The current period has seen very significant investment in buildings (total investment 2008-13, £17.9m). In prioritising bids, strategic attention was paid to the accommodation of groups with outward-facing research agendas: (a) for liquid crystals within Dorothy Hodgkin Building Phase 2 (completed 2012, University funds), (b) a new atmospheric chemistry laboratory (Q4 2013, Wolfson and donors), (c) a new Centre for Hyperpolarisation in Magnetic Resonance (completed 2012, Wellcome, Wolfson and the University), (d) new labs for Green Chemistry (due March 2014, University and ERDF). The last includes an Industrial Engagement facility purpose-built for industry-academic collaboration in the use of green and sustainable technologies to valorise waste.

We recognise the importance of first-class equipment in our impact generation and have seeded grant applications in the period accordingly. Major equipment with links to impact includes: (i) £1.6M to CoEMS for mass spectrometers (food security impact), (ii) equipment *e.g.* large microwave (£3m) for green chemistry projects, *e.g.* Starbons, (iii) MRI and NMR spectrometers (£4M) for CHyM's hyperpolarised imaging (iv) crystallisation robot for structural biology (£500k).

The University's REO, with business development managers recruited from industry with departmental participation, has facilitated business engagement in numerous projects including hyperpolarisation, lab-on-a-chip analysis, green chemistry, the spin-out companies, *etc.* Notable features of its activity include its liaison with European Regional Development Fund (ERDF), with Yorkshire Forward (former RDA), Science City York and Technology Strategy Board. The University contributed £380k during 2008-12 into impact-generating projects in Chemistry, supporting patent costs, proof-of-concept studies, teaching buy-out, development of research grants, *etc.* These sums have levered much greater support, for example for CHyM and the BDC.

c. Strategy and plans

Our strategic impact policies in period will be reinforced by new initiatives for the future:

1. Targeting impact through multidisciplinarity. Multidisciplinary centres within and across departments have long driven impact generation through teamwork and complementarity; we thus foster this as best practice (YSBL, CoEMS, NCAS, Green, materials, CHyM) and will actively seek additional connections, *e.g.* Plasma Physics Institute, Health Sciences, History. Our Research Committee and group leaders will support this agenda, link with other departments through joint planning groups, and review impact progress formally and regularly. We recognise the importance of high-quality lab space and equipment for achieving impact. New buildings for Materials and for CHyM are complete and those for Green Chemistry and for Atmospheric Chemistry are under construction, with further building plans in progress. The BDC illustrates design for external engagement. Strategic appointments have been made to nurture impact (*e.g.* **Evans**, Chair global atmospheric models, 2011). In autumn 2013 **North** (Chair, Green Chemistry especially CO_2 conversion), **Dillon** (Lecturer, Atmospheric) and a Research Facilitator with specific brief in impact generation, joined Chemistry. Recruitment is currently being planned in new areas with our sights on impact potential (*e.g.* human-electronics interface, chemical aspects of synthetic biology).

2. Close relationships with end-users. A new strategy for impact that embeds companies or their staff in the Department (*e.g.* Bruker, Chemspeed) as a complement to secondment of our staff to companies (*e.g.* Vernalis, Paraytec) will be developed further beyond the period, with new close collaborations following these models (*e.g.* Green Chemistry with Brocklesby Ltd. and new KTPs (*e.g.* Akros, Q4 2013). We will target studentships and pump-priming funds for collaborative proposals with impact potential, and will lever support through REO. We will instigate impact sandpits with support from EPSRC Industrial Engagement, Impact Accelerator and Departmental funds. We will encourage new spin-out companies, with two starting in Q4 2013.

3. Support for impact-generating staff. We will stress impact in allocating research leave and encourage secondments to industry. We have introduced mechanisms for flexible staff loadings to enable an agile impact response, we recognise impact in promotions and we celebrate impact through magazines and websites. Impact through outreach is supported *via* dedicated CIEC staff (primary education) and our outreach officer (secondary and public). In the future, impact will be discussed specifically in annual performance reviews and we will initiate Impact Fora to highlight current and stimulate new impact, targeting extra financial support for outreach to widen our reach.

Our goals for new economic and policy impact generation and consequent investments include: (i) *New CO_2 chemistry*. CO_2 conversion from power station emissions is an impact goal of **North,** who will join the new building and exploit results through new spin outs. (ii) *Medical applications of hyperpolarisation.* CHyM will capitalise on its collaboration with Bruker and use its new spin-out (Hypernetix Imaging Ltd) to exploit applications of its technology. (iii) *Cellulose oxidising enzymes for biofuels.* **Davies'** and **Walton's** discoveries of the structures of Cu-enzymes have applications for biofuels and will be supported by a chemical biology lecturer appointment, **Fascione** (2014). (iv) *Impacting international environmental policy.* **Carpenter** is to be a lead author of a chapter updating the Montreal Protocol (2014) for the UN Environment Programme. (v) *Polymeric liquid crystals as conducting polarisers for touch-screens*. **Goodby** will have reduced departmental load to work with Dymatic Chemicals Inc., supported by new equipment. (vi) *Structure of insulin bound to its receptor*. New structural discoveries by **Brzozowski** will be exploited in cancer and diabetes therapies. He is supported by new robotics equipment and his IP is protected by patents with REO support. (vii) *Dating of archaeological and palaeontological sites.* A new reliable dating method using amino acid racemisation (**Penkman)** reaches beyond the radiocarbon limit with new equipment. It will be exploited internationally both culturally in museums and commercially.

d. Relationship to case studies

The selected six Case Studies arise directly as a result of the Department's approach to impact laid out in **Section b**. The strategic investment in Analytical Chemistry (RSC/EPSRC initiative, 1999-2002) and YSBL informed our policies during period and going forward. The Case Studies on *Natural organic emissions and summertime European air quality* and on *Ozone-depleting halogens in the atmosphere* show impact on environmental policy at UK governmental and international levels. The Case Study on *Food security and authentication* demonstrates societal and health impacts in food security. The Case Studies on *Crystallographic software development*, on *Sugar-degrading enzymes in the detergent and biofuels sectors* and on *Short and long-acting insulins* have economic impacts with global reach. Moreover, two of the Case Studies have health impacts.