Institution: Cardiff University		
Unit of Assessment: Chemistry (8)		
Title of case study: Improved catalysts to enable air purification in life-saving applications		
Period when the underpinning research was undertaken: 2000 – 2015		
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:**
Stuart Taylor Graham Hutchings	Professor Regius Professor	01/101997 – 31/12/2020 01/08/1997 – 31/12/2020
Period when the claimed impact occurred: 01/08/2013 – 31/12/2020		
Is this case study continued from a case study submitted in 2014? No		

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

Minimising carbon monoxide within challenging environments for the military, mining, and deep-sea exploration is key to keeping people safe. Fundamental research at Cardiff, on the relationship between preparation and performance of catalysts, resulted in improved catalysts, and robust processes for their manufacture, enabling exceptional air purification performance for low temperature carbon monoxide and organic vapour oxidation. Commercialisation of these materials by Molecular Products Group led to new products, increased sales, expansion into new markets, and jobs. This was enabled via use of the catalysts in a wide variety of critical life-support applications in mining, deep-sea diving, medicine and the military.

2. Underpinning research (indicative maximum 500 words)

Catalysts for the conversion of carbon monoxide (CO) to CO_2 at ambient temperature and pressure is a critical process for respiratory protection and life support. They are widely adopted in a diverse range of industries including mining, medicine, deep sea diving, and the military. Addressing this challenge, copper manganese oxide (Hopcalite) heterogeneous catalysts can be used to remove CO and other vapours from life support systems used in these environments. Variability in catalyst performance, however, has hindered commercially available batches from achieving widespread success.

Molecular Products Group, a multi-national UK-based manufacturing company, sought to establish a fundamental understanding of catalyst structure and performance, thereby creating a commercial manufacturing process. Molecular Products collaborated with Cardiff, drawn to the University's extensive heritage in catalyst research, which enabled enhanced knowledge of the underlying concepts in the preparation of Hopcalite catalysts.

2.1 Refining Hopcalite catalysts

Taylor and Hutchings directed and managed the research, exploring oxidation of CO to CO_2 at ambient temperatures using Hopcalite catalysts, as an alternative to dominant technology established in the 1920s. The key research on the preparation of improved low temperature CO catalysts was carried out at Cardiff between 2000-2015, with Cardiff establishing new catalyst preparation protocols vital for manufacturing the most active catalysts, and Molecular Products facilitating specific application tests and large-scale catalyst manufacturing.

The study of preparation methods was based around the processes of co-precipitation **[3.1]**, thermal calcination **[3.1]** and incorporating cobalt **[3.2]** or gold **[3.3]** to enhance catalyst activity. These preparation studies identified reliable methods of producing catalysts with the most active phases, and consequently the most active surfaces optimised. Maximising the preparation of copper manganese mixed metal oxide phases, avoiding production of separate phases of copper oxide and manganese oxide, is critical to producing the most active catalyst. The research resulted in low temperature catalysts that combined both higher activity and more durability than traditional commercial Hopcalite catalysts.

2.2. Developing improved manufacturing processes

The collaborative research expanded from the new Hopcalite catalyst towards developing more efficient catalyst preparation routes. The Cardiff team developed novel supercritical anti-solvent preparation methods for Hopcalite to increase understanding of the critical phases and surface structures required for highly active catalysts **[3.4]**. Additional research explored catalyst transformation during thermal manufacturing steps and the resulting impact of catalyst efficacy **[3.5]**. Too low a heat treatment and not much of the mixed phase will be produced, while too high a temperature and highly crystalline low surface area phases are formed: both cases produce poorer catalysts. The Cardiff team were able to identify thermal transformation conditions which optimise active phases and hence catalyst activity.

Additionally, new industry-viable preparation routes for Molecular Products' high performance Sofnocat precious metal-based catalysts were established. An atom-efficient method for synthesising catalysts using tin oxalate was investigated **[3.6]** and, when found to perform favourably, was transferred to Molecular Products to develop a viable new manufacturing route. The Sofnocat catalyst can be used for CO oxidation under particularly demanding conditions, when a Hopcalite catalyst may not provide the required performance (e.g., in mining sites, creating a safe haven in the event of an emergency).

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

[3.1] C. Jones, K. Cole, **S.H. Taylor**, M.J. Crudace, **G.J. Hutchings**, Copper manganese oxide catalysts for ambient temperature carbon monoxide oxidation: effect of calcination on activity. J. Mol. Catal. A: Chem., 2009, 305, 121-124. https://doi.org/10.1016/j.molcata.2008.10.027

[3.2] C. Jones, **S.H. Taylor**, A. Burrows, M.J. Crudace, C.J. Kiely, **G.J. Hutchings**, Cobalt promoted copper manganese oxide catalysts for ambient temperature carbon monoxide oxidation. Chem. Commun., 2008, 1707-1709. https://doi.org/10.1039/B800052M

[3.3] K.J. Cole, A.F. Carley, M.J. Crudace, M. Clarke, **S.H. Taylor**, **G.J. Hutchings**, Copper manganese oxide catalysts modified by gold deposition: the influence on activity for ambient temperature carbon monoxide oxidation. Catal. Lett., 2010, 138(3-4), 143-147. https://doi.org/10.1007/s10562-010-0392-2

[3.4] Z. Tang, S.A. Kondrat, C. Dickinson, J.K. Bartley, A.F. Carley, **S.H. Taylor**, T.E. Davies, M. Allix, M.J. Rosseinsky, J.B. Claridge, Z. Xu, S. Romani, M.J. Crudace, **G.J. Hutchings**, Synthesis of high surface area $CuMn_2O_4$ by supercritical antisolvent precipitation for the oxidation of CO at ambient temperature. Catal. Sci. Technol., 2011, 1(5), 740-746. https://doi.org/10.1039/c1cy00064k

[3.5] Z. Tang, C.D. Jones, T.E. Davies, J.K. Bartley, A.F. Carley, **S.H. Taylor**, M. Allix, C. Dickinson, M.J. Rosseinsky, J.B. Claridge, Z. Xu, M.J. Crudace, **G.J. Hutchings**, New nanocrystalline Cu/MnOx catalysts prepared using supercritical antisolvent precipitation. ChemCatChem., 2009, 1(2), 247-251. https://doi.org/10.1002/cctc.200900195

[3.6] J.K. Aldridge, L.R. Smith, D.J. Morgan, A.F. Carley, M. Humphreys, M.J. Clarke, P. Wormald, **S.H. Taylor**, **G.J. Hutchings**, Ambient temperature CO oxidation using palladium–platinum bimetallic catalysts supported on tin oxide/alumina. Catalysts 2020, 10, 1223. https://doi.org/10.3390/catal10111223

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

Cardiff research established commercially viable CO-removal catalysts based on robust understanding of relationships between preparation, catalyst structure and activity. These have been sold around the world to produce a breathable atmosphere for people working in extreme environments, including miners, submariners and hospital patients under anaesthesia.

4.1 Commercialising research for Molecular Products

The primary economic beneficiary of the Cardiff-based research is the Molecular Products Group, which has a turnover of £14.4M and over 130 staff (2018). Dr Mandy Humphreys,

former Technical Director of Molecular Products from 2003-14, stated that the research was "*pivotal for our business"* **[5.1]**. As a result, the company adopted the technique of co-precipitation and optimised the formulation and preparation of the Hopcalite-based catalyst, Moleculite **[5.2]**, which is sold worldwide for the oxidation of CO and volatile organic vapours.

Prior to the Cardiff research, the manufacturing process for Moleculite was susceptible to delivering batches of catalyst with varying performance, an unacceptable risk given the planned applications. Molecular Products stated that: "*Prolonged control of low levels of carbon monoxide in breathing systems is often considered the 'holy grail' from an industrial perspective, and this formed a corner stone strategic goal for the business. The fundamental research at Cardiff was required to crack this very difficult nut*" **[5.1]**.

With Cardiff's involvement, Molecular Products achieved a "*step change in the efficacy of our catalytic products*" **[5.1]**. The research supported a significant expansion of Molecular Products' product range and enabled penetration into new markets and novel utilisations of current technology (as noted in Section 4.2, below). Cardiff involvement was also credited with increasing client confidence in the catalysts as Molecular Products stated: "*The research from Cardiff University was essential to allow us to engage with new markets and customers across the globe, which led to forming long-term sustainable relationships leading to strategic contracts for military and commercial applications*" **[5.1]**.

Molecular Products' catalysts business continues to expand at a faster rate than other areas of their business, driving a strong increase in revenue. The collaboration with Cardiff, supporting improved product design and access to expert knowledge, *"significantly contributed to the financial viability of the business"* **[5.1]**. [Text redacted] Molecular Products' financial reports for 2014-2020 reveal that sales and profits continued to increase throughout the REF period, increasing total turnover to £99M between 2014 and 2020, an increase of 14% over the previous seven years **[5.3]**. In 2017, the company won the *Sunday Times* 'Ones to Recognise' award as one of Britain's top 100 private companies with the fastest-growing profits **[5.4]**.

4.2 Widespread applications and benefits for end users

Catalysts for the conversion of CO are widely adopted in mining, medicine, deep sea diving, and the military. Dr Patricia Wormald, Development Chemist at Molecular Products, stated: "*The Moleculite and Sofnocat catalysts underpin our life-maintaining products in a wide variety of applications, which must be of the highest reliability and robustness due to their application in life-supporting activities*" **[5.5]**.

The catalysts are sold by Molecular Products as-is **[5.2**, **5.6]** or combined with oxygen-enriching and CO_2-scrubbing catalysts in a single, all-purpose, atmosphere-treatment product. The enhanced Moleculite formulation has been incorporated within air purification systems such as HiCap CO™ **[5.7]** which can be bought as a single product and deployed to create a breathable atmosphere in emergency situations, such as a mining cave-in, or used in self-contained breathing apparatus, such as those used by firefighters.

Molecular Products stated that HiCap CO™ "*has been a key product for us due to its established status as a comprehensive air-purification system with our customers"* **[5.5]**. Molecular Products also consult on bespoke solutions for their clients, such as atmosphere chambers for a diving company in South Africa, or life support systems for submarines sold to the Malay, Indian and Chinese navies. As the method of alleviating CO poisoning, the Moleculite and Sofnocat catalysts are utilised in the majority of these designs **[5.5]**.

The catalysts developed at Cardiff, therefore, underpin worldwide activity in hazardous environments, and the solutions offered by Molecular Products are "*used every day, across the world, to ensure a survivable atmosphere for end-users*" **[5.5]**. Example applications include:

a. Military use

41 countries operate military submarines, with many more using civilian exploratory and research vessels. Consequently, thousands of people globally are reliant on air purification

catalysts. Molecular Products noted: "*We are unable to confirm which navies are currently supplied by our products for reasons of national security. However, I can confirm that the catalysts created by Cardiff research are currently in submersible vessels in use all over the world*." **[5.5]**

b. The mining sector

High-profile mining incidents (including the 2010 Chilean gold-copper mine cave-in) highlighted the need for secure life support systems within this hazardous sector. Molecular Products developed emergency backup systems using advanced catalysts (including Sofnocat), which prevent CO poisoning in these environments. The systems can be activated in the event of a cave-in to supply breathable air until the mine can be secured and any trapped miners rescued **[5.5]**.

c. Healthcare, hospital, and laboratory safety

Moleculite is also used in the sterilisation of hospital equipment that would otherwise be damaged by traditional heat- or moisture-based sterilisation procedures (e.g., those comprising plastic or rubber). These devices are sterilised with ethylene oxide gas, which must then be treated with Moleculite to render it inert. This application is routinely used in hospitals and laboratories worldwide to remove the danger of toxic gases being released **[5.5]**.

In summary, Cardiff's research was integral to enabling commercialisation of Molecular Products' catalytic life-support products. This underpinned increased success for Molecular Products' catalytic sector, which grew (as described by the company) "*from an embryo to a sustainable 'third leg' of the business*" **[5.1]**.

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

[5.1] Testimonial: Dr Mandy Humphreys, former Technical Director, Molecular Products (2003 – 2014)

[5.2] Details of Moleculite. Moleculite: copper manganese oxide-based carbon monoxide removal catalyst. Molecular Products website

[5.3] Molecular Products' Financial Reports 2014 – 2020 (Obtained from Companies House)

[5.4] Details of Molecular Products wins *Sunday Times* 'Ones to Watch' award. Latest News: Molecular Products is one to watch in the List of UK's fastest Growing companies (2017). Molecular Products website

[5.5] Testimonial: Dr Patricia Wormald, Development Chemist at Molecular Products (2017 – present)

[5.6] Details of high-performance Sofnocat catalysts for carbon monoxide removal. Sofnocat 423. Molecular Products website

[5.7] Details of Moleculite cannisters for carbon monoxide removal applications. Hi-Cap Co Absorber. Molecular Products website