University of Glasgow | School of Chemistry

**Ph.D. Studentship: The development of kinetic models for phosgene synthesis over heterogeneous catalysts**

Phosgene is an important intermediate used in the industrial manufacture of polyurethanes, polycarbonates, pharmaceuticals and agrochemicals. It is typically manufactured industrially via the gas phase reaction between carbon monoxide and chlorine over an activated carbon catalyst.

$$CO_{(g)} + Cl_{2(g)} \rightleftharpoons COCl_{2(g)}$$

The reaction is strongly exothermic ($\Delta H$=-107.6 kJ $mol^{-1}$). Despite wide industrial application, there are surprisingly few laboratory studies of phosgene synthesis catalysis reported in the literature.

The project, commencing in October 2024, will utilise a unique experimental facility that is housed in the School of Chemistry's Chemical Process Fundamentals Laboratory, which is designed to handle the hazardous reagents associated with the production of phosgene [1]. A major thrust of the workplan involves determining kinetic models for the synthesis of phosgene over a series of high surface area activated carbon catalysts. Product and reagent analysis will be undertaken using a combination of infrared spectroscopy, UV-visible spectroscopy and mass spectrometry. Product selectivity will be monitored under a variety of reaction conditions in order to determine optimum operating arrangements for particular catalyst formulations.

Mass balance measurements of reference industrial grade catalysts reveal a significant degree of chlorine retention as being part of the phosgene formation process. A secondary goal of the project will be to apply the technique of temperature-programmed reaction spectroscopy to quantify and characterise the varying degrees of chlorine laydown exhibited by different catalyst formulations. It is envisaged that these measurements will provide new information on the distribution of active sites responsible for phosgene production.

Collectively, the project will provide the student with a sound grounding in the development of industrially relevant heterogeneously catalysed reaction systems, as well as experience in modern catalyst characterisation techniques.

The project is ideally suited to high-calibre graduates in Chemistry, Chemistry and Medicinal Chemistry and/or Chemical Physics. A tax-free stipend of *ca*. £18,622 *p.a*. for 3.5 years is provided alongside the payment of all University fees. *Eligibility is restricted to UK citizens only.*

Reference

1. Operational parameters relevant to the examination of phosgene synthesis catalysis, R. Hughes, G.E. Rossi and D. Lennon, *Reaction Chemistry and Engineering*, 2023, DOI: 10.1039/D3RE00354J.

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