Accelerating the discovery of low carbon cements using machine learning and thermodynamic modelling

Supervisor (primary) Imperial College London: Dr. Rupert J. Myers

Applications are invited to fill a PhD position funded through internal or external scholarships, or from a student's own funding.

The PhD student will produce and optimise glasses containing Fe(II), Mg, Si, Al, and Ca, or Portland clinker from Ca containing industrial by-products like metallurgical slags, incinerator residues, and demolition concrete waste, for low carbon cements. These materials have the potential to avoid substantial amounts of CO_2 emissions from cement production by reducing use of limestone and thus decomposition of CO_2 in the material. Limestone decomposition in Portland clinker production is responsible for ~4% of global CO_2 emissions. This will be done through experiments, thermodynamic modelling, and machine learning approaches.

The PhD will be based in the Materials Section of the Department of Civil and Environmental Engineering (Skempton Building, South Kensington Campus). On a day-to-day basis they will work alongside ~30 PhD students and ~10 postdoctoral research associates in the Materials Section, including several in their research group, led by Dr. Myers. The Section hosts the Advanced Infrastructure Materials laboratory, which is a world-class facility for concrete materials characterisation.

This PhD project offers excellent training and development opportunities in a highly stimulating environment, as well as access to a network of internationally leading academics, industrial partners, and research facilities.

Project details

The key aim of this PhD project is to optimise the chemical and mineralogical compositions of glasses or Portland clinker produced from uncarbonated CaO containing by-products (e.g., by modifying temperature), and the mix design of cement produced from these materials (e.g., through additions of gypsum), with respect to cement paste properties (e.g., microstructure, compressive strength development). The goal is to create cements with lower carbon emissions that lead to comparable or better cement paste properties than conventional high carbon Portland cement. The material class (glass or clinker) chosen to be studied depends on the interests of the PhD student and will be determined during the initial literature review phase of the PhD, since both routes are promising.

Today, many Ca containing by-products are being generated, including end-of-life cement paste, iron and steel slags (from blast, basic oxygen, electric arc furnaces), coal (fly, bottom) ashes, biomass ashes, incinerator ashes, bauxite residue, phosphogypsum, mining tailings, etc. Many of these materials are inefficiently or incompletely utilised despite their upcycling potential in the production of concrete materials due to their compatible chemical compositions. Recycling these materials offers a way to reduce landfilling and conventional Portland clinker production, and thus associated reduction in land use, resource depletion, and climate change impacts.

This PhD project will use experiments, thermodynamic modelling, and machine learning to study novel low carbon cements, including modelling of the slag composition at high temperatures, and cement paste composition at ambient conditions in concrete. Currently available thermodynamic data and software will be used rather than development of new thermodynamic data, to understand the fundamental physical and chemical properties of the cement (and cement paste), and then use this fundamental knowledge to engineer excellent structural materials. Machine learning models and approaches such as active learning and inverse design will be used to approach optimum feedstocks and process conditions more quickly than through traditional trial-and-error experimentation.

This is a heavily experimental PhD project that will utilise the suite of state-of-the-art materials characterisation equipment available in our Advanced Infrastructure Materials, Structures, and Environmental Laboratories, which is a facility that is essentially unparalleled in terms of quality within the UK.

Academic requirements and experience

Required

- A good first class degree (or international equivalent) in a STEM subject, e.g., Chemistry, Metallurgy, Physics, Materials Science, Chemical Engineering, Environmental Science, Geology), or a course with strong emphasis on chemistry.
- Laboratory experience.
- Programming experience.
- Strong interest in materials research.
- Excellent English communication skills.

How to apply

Applicants wishing to be considered for this opportunity should send the following application documents to Dr. Rupert J. Myers (r.myers@imperial.ac.uk):

1. Current CV including degree result and, if possible, class ranking

Application via the Imperial College Registry is not necessary at this stage.

Applications will be regularly reviewed until the position is filled.

Funding notes

Applicants interested in this project and seeking funding via scholarship schemes (see here: https://www.imperial.ac.uk/study/pg/fees-and-funding/scholarships/) or can self fund are welcome to apply.