PhD position at EPFL in Swiss national foundation Project No. 2OOO21_179O76

Atomistic Modelling of the Impact of Minor elements on Cement Hydration

Probable Starting date April 1st 2019

Brief overview

The aim of this project is to study the impact of minor elements (particularly zinc) on the hydration of cement. Low concentrations of minor elements (e.g. Zn) can drastically increase the amount of reaction in the first day. This indicates a potential to increase the reactivity of cement and so allow higher amounts of CO_2 intensive clinker to be substituted by more environmentally friendly materials with lower reactivity, such as granulated blast furnace slag, coal fly ash or calcined clay. The main impact is on the growth of calcium silicate hydrate (C-S-H the main hydrate phase in cement). Recent work at EPFL, has developed a new precipitation route for the production of C-S-H of the same composition as found in real cements from simple chemical precursors[1]. The use of NMR and atomistic modelling on these synthetic C-S-Hs has given new insights into their structure at the atomic level [1]. A combined population balance and thermodynamic model has given new insights on the mechanisms of nucleation and growth [2]. This project builds on this success to study the impact of minor elements on cement hydration: elucidating the mechanisms acting and providing a basis for a technological breakthrough in the reactivity of cement. There are two Ph.D positions one will be directed towards the synthesis and collection of kinetic data and the second will try and unravel the growth mechanisms from an atomistic modelling and thermodynamic point of view.

This research is closely related to sustainability, and environmental issues. Concrete is used in huge quantities and although is inherently low in carbon footprint its production contributes to up to 8% of CO_2 emissions. This proposal aims to answer this problem by understanding the fundamental chemistry of the impact of minor elements on the hydration process and so provide the knowledge for further substantial reduction in the environmental impact of cementitious materials – possibly by up to 50%!

PhD position

Atomistic Simulation of doped Calcium Silicate Hydrates(C-S-H)

Director Prof. Karen Scrivener, co-director Prof. Paul Bowen

The key role of the atomistic simulations will be to unravel the atomistic scale mechanisms behind these accelerating effects of minor elements. One key factor will be to integrate surfaces into the C-S-H atomistic model and investigate the interaction of minor elements as ions or aqueous complexes with these surfaces. The use of the brick model recently developed at EPFL [3] will facilitate this challenging task. ***Molecular dynamics (MD) Metadynamics (MTD) transition state theory (TST) combined with Kinetic Monte Carlo (KMC)*** *modelling will be used to investigate the interaction of ions and* molecules with C-S-H surfaces and their incorporation into the bulk structure.

The candidate should have a degree in Materials Science, Physics or Chemistry and prior knowledge or experience in basic atomistic modelling e.g. molecular dynamics.

Interested candidates should contact Prof. Paul Bowen with full CV, publication list and 3 references (paul.bowen@epfl.ch)

References

[1] A. Kumar, B. J. Walder, A. K. Mohamed, A. Hofstetter, B. Srinivasan, A.J. Rossini, K. Scrivener, L. Emsley and P. Bowen "The Atomic-Level Structure of Cementitious Calcium Silicate Hydrate", J.Phys.Chem.C 121(32) 17188–17196 (2017). **DOI:** 10.1021/acs.jpcc.7b02439

[2] . M.R.Andalibi, A.Kumar, B. Srinivasan, P. Bowen, K. Scrivener, C. Ludwig, A. Testino, "On the Mesoscale Mechanism of Calcium-Silicate-Hydrate Precipitation: A Population Balance Modeling Appraoch", J.Mater.Chem.A,6, 363-373, 2018. DOI: 10.1039/c7ta08784e

[3] A. Kunhi Mohamed, S.C. Parker, P. Bowen, S. Galmarini,, “An atomistic building block description of C-S-H - Towards a general C-S-H model”, CCR,107, 221-235, 2018