## DIADEM ACADEMY







## Master thesis proposal

## In situ SAXS/WAXS analysis of sustainable cement carbonation curing

Keywords: energy transition, low-carbon cement and concrete, SAXS, microfluidics, automation

## **SCIENTIFIC DESCRIPTION:**

The production of ordinary Portland cement (OPC) clinker accounts for up to 8% of global  $CO_2$  emissions. Approximately 40% of this  $CO_2$  comes from the energy expended by heating the raw limestone and clays needed to produce the clinker, while the remaining 60% is released from the carbonates trapped within the limestone. Unfortunately, only a small fraction of this released  $CO_2$  is re-captured when cements are hardened through standard hydration processes. To reduce net  $CO_2$  emissions, a growing number of researchers and start-up companies (e.g., CarbonCure, Fortera) are working to cure cements through a combination of hydration and carbonation to re-capture released  $CO_2$ . However, the carbonation of cements is a poorly understood phenomenon that can proceed through complex multi-step pathways.

Due to its density, hardness, and opacity, cement setting processes are extraordinarily difficult to study. To overcome this challenge, our lab recently developed a cement "microreactor" that enables real-time analysis of cement curing (**Figure**) and used it to study the evolving structure of cements using X-ray diffraction (XRD). The goal of this internship is to adapt the microreactor for use on the new DIADEM FastNano automated small-angle X-ray scattering (SAXS) platform. In addition to obtaining structural information by XRD, SAXS will enable us to uncover the evolving porosity of cements during early curing stages, which is crucial to CO<sub>2</sub> transport and mechanical strength. The intern will help us to develop microreactor hardware for performing *in situ* SAXS analysis and accompanying scripts for the automated collection and treatment of SAXS data.

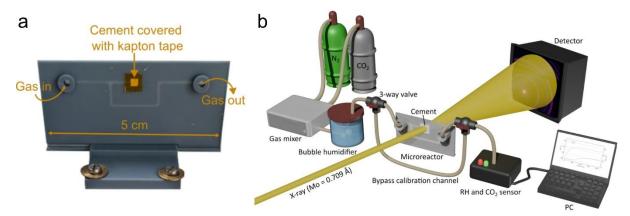


Figure: Millifluidic device (a) for studying cement carbonation in situ with X-ray scattering (b).

**Techniques/methods in use :** Small- and wide-angle X-ray scattering (SAXS/WAXS), micro/millifluidics, 3D printing, computer-aided design (CAD), Python/Jupyter Notebook

Budget description and use: M2 student stipend

**Applicant skills :** Good experimental, analysis and reporting skills are mandatory. The ideal candidate would have a high English level, previous XRD/SAXS experience, and some knowledge of Python coding.

**Industrial partnership:** N

Internship supervisor(s): Dr Mark LEVENSTEIN, mark.levenstein@cea.fr, 01 69 08 57 34, Web

Dr David CARRIERE, david.carriere@cea.fr, 01 69 08 54 89, Web

Ms Emeline COURNEDE, emeline.cournede@cea.fr, 01 69 08 57 34

Internship location: FastNano Liquid, NIMBE/LIONS UMR 3685, CEA Paris-Saclay, 91191 Gif-sur-Yvette

Possibility for a Doctoral thesis: Yes

