French Polytech network form for PhD Research Grants from the China Scholarship Council

This document describes one of the PhD subjects proposed by the French Polytech network. The network is composed of engineering schools/universities. The document also provides information about the supervisor.

Supervisor information

Family name	RAMEZANI
First name	Hamidréza
Email	hamidreza.ramezani@univ-orleans.fr
Web reference	https://orcid.org/0000-0001-7657-1430
Lab name	Interfaces, Confinement, Matériaux et Nanostrcutures (ICMN), UMR7374 CNRS
Lab web site	https://icmn.cnrs.fr/
Polytech name	Polytech Orléans
University name	University of Orléans
Country	France

PhD information

Title	Role of activated carbon on Interfacial Zone Stiffness in Composite Cement/Activated Carbon Materials
Main topics regards to CSC list (3 topics at maximum)	IV. Science of materials and new material IV-12. Environmental behavior and failure of materials.

Required skills in science and engineering	Cement-based materials, 3D FEM modeling and simulation, Molecular simulations, programming, fluent in English and ability to work in an international research group.

Subject description (two pages maximum including biblio)

Problem statement:

Natural carbonation of cement-based materials occurs throughout the lifespan of buildings and concrete structures. This process entails several disadvantages regarding their structural integrity and reliability. The main concern stems from the decline in concrete pH and subsequent corrosion of steel reinforcement bars [1-2]. However, carbonation itself absorbs carbon dioxide from the air through a series of chemical reactions well-known in the cement and concrete industry in the case of natural carbonation [3-5]. Interestingly, the incorporation of a small amount of activated carbon in cement and concrete has been observed to increase their mechanical strength, a phenomenon not well understood in current literature. One of the main reasons for this enhanced mechanical strength in both bending and compression arises from changes in the Interfacial Zone (IZ) located between cement paste and activated carbon in cement-based materials.

Ph.D. program description:

To study such a composite material containing cement and activated carbon, it is necessary to investigate activated carbon (AC) at both the continuum and nanometric scales. Activated carbon is a porous material often used for trapping gases (CO_2, CH_4, N_2, and mixed gases) [6-8]. Its use in cement-based materials has proven to be highly effective in trapping CO_2. Experimental results clearly demonstrate a significant improvement in CO_2 adsorption in concrete with the addition of a small amount of activated carbon (less than 2% by weight). The objective of this Ph.D. proposal is to study this behavior at the molecular level and verify it against experimental data from the literature. Additionally, the structure of cement-based materials will be examined at the nanoscale with different CaO/SiO_2 ratios to develop a realistic representation of CSH and $Ca(OH)_2$ in cement paste [9-11]. By performing reactive molecular dynamics simulations [12] on random mixtures of CSH/$Ca(OH)_2$/AC incorporating natural carbonation phenomena, we aim to obtain the atomic structure for our numerical experiments. These experiments will assess the modulus of elasticity, Poisson's ratio, tensile and compressive strength, and thermal expansion coefficient of carbonated mixtures of cement and activated carbon in the IZ. Large-scale simulations can also be conducted using the mechanical properties obtained from nanoscale numerical simulations and characterizations. The numerical results will be validated against experimental data from the literature and supplemented by laboratory experiments (including X-ray diffraction and TEM analyses).

Co-supervisor: Nathalie Mathieu (ICMN UMR 7374 CNRS)

References :

[1] A. Steffens, D. Dinkler, and H. Ahrens, “Modeling carbonation for corrosion risk prediction of concrete structures,” *Cement and Concrete Research*, vol. 32, no. 6, pp. 935–941, 2002, doi: 10.1016/S0008-8846(02)00728-7.

[2] A. V. Saetta and R. V. Vitaliani, “Experimental investigation and numerical modeling of carbonation process in reinforced concrete structures: Part I: Theoretical formulation,” Cement and Concrete Research, vol. 34, no. 4, pp. 571–579, 2004, doi: 10.1016/j.cemconres.2003.09.009.

[3] V. G. Papadakis, C. G. Vayenas, and M. N. Fardis, “Fundamental modeling and experimental investigation of concrete carbonation,” *ACI Materials Journal*, vol. 88, no. 4, pp. 363–373, Jul. 1991.

[4] J. Jeong, H. Ramézani, and E. Chuta, “Reactive transport numerical modeling of mortar carbonation: Atmospheric and accelerated carbonation,” *Journal of Building Engineering*, vol. 23, pp. 351–368, 2019, doi: https://doi.org/10.1016/j.jobe.2019.01.038.

[5] J. Jeong, H. Ramézani, V. G. Papadakis, J. Colin, and L. Izoret, “On CO2 sequestration in concrete aggregate via carbonation: simulation and experimental verification,” *European Journal of Environmental and Civil Engineering*, vol. 26, no. 12, pp. 6076–6095, Jun. 2021, doi: 10.1080/19648189.2021.1928555.

[6] T. X. Nguyen, N. Cohaut (Mathieu), J.-S. Bae, and S. K. Bhatia, “New Method for Atomistic Modeling of the Microstructure of Activated Carbons Using Hybrid Reverse Monte Carlo Simulation,” *Langmuir*, vol. 24, no. 15, pp. 7912–7922, 2008, doi: 10.1021/la800351d.

[7] D. N. Kouetcha, H. Ramézani, N. Mathieu-Cohaut, and S. K. Bhatia, “Carbon dioxide adsorption through carbon adsorbent structures: Effect of the porosity size, chemical potential and temperature,” *Computational Materials Science*, vol. 151, pp. 255–272, 2018, doi: https://doi.org/10.1016/j.commatsci.2018.04.029.

[8] Z. E. Oufir, H. Ramézani, N. Mathieu, and S. Delpeux, “Impact of adsorbent carbons and carbon surface conductivity on adsorption capacity of CO2 , CH4 , N2 and gas separation,” *Computational Materials Science*, vol. 199, p. 110572, 2021, doi: https://doi.org/10.1016/j.commatsci.2021.110572.

[9] R. K. Kammeugne, “Simulation moléculaire sur la capacité d’adsorption de gaz CO2 dans C-S-H,” Université d’Orléans, CNRS, ICMN, UMR 7374, Orléans, France, 2018.

[10] W. Taleb, “Capacité d’adsorption de CO2 dans un matériau hybride,” Université d’Orléans, CNRS, ICMN, UMR 7374, Orléans, France, 2021.

[11] F. Fayad, “Etude numérique de la captation de CO2 dans un matériau hybride carbone-béton,” 2023.

[12] H. Manzano, R. J. M. Pellenq, F.-J. Ulm, M. J. Buehler, and A. C. T. van Duin, “Hydration of Calcium Oxide Surface Predicted by Reactive Force Field Molecular Dynamics,” *Langmuir*, vol. 28, no. 9, pp. 4187–4197, 2012, doi: 10.1021/la204338m.C