CHEMISTRY MASTER - M2 INTERNSHIP **2022-2023** (end of January – end of June)	
TITLE	**CO2 adsorption/desorption kinetics in kerogen: multi-scale simulation and in situ IR/Raman spectroscopy**
COMPETENCES / INTERESTS	Physical Chemistry/Thermodynamics/Numerical Modeling/Spectroscopy /CO2 storage
SUBJECT	The internship will consist in carrying out an original joint experimental and numerical study of the adsorption/desorption kinetics of CO_2 in kerogen within the context of geological CO_2 sequestration. The experimental part will take place under the direction of Thierry Tassaing (molecular spectroscopy group) and the numerical part under the direction of Amaël Obliger (theoretical chemistry group). Kerogen is the microporous organic phase of non-conventional hydrocarbon reservoirs. This phase, which contains hydrocarbons, is responsible for the very high CO2 adsorption capacity that makes these so-called source rocks reservoirs interesting for CO_2 sequestration. In view of the great structural complexity of these kerogens, whose porosity is amorphous and can sometimes give rise to strong swelling effects, experimental results are scarce and numerical studies struggle to take into account the multiple spatial and temporal scales that influence the adsorption/desorption kinetics of these materials and that can play a significant role on a possible CO_2 sequestration process. Indeed, non-Fickian behaviors are observed during the expulsion of fluid (desorption) from these matrices: the total amount of fluid recovered evolving as t^n (where t is time) with $n < 0.5$ whereas Fick's law predicts $n = 0.5$ [Monteiro_PNAS_13, Kang_AIPA_15]. Poromechanical effects as well as the multiscale nature of porosity in kerogens could be responsible for these behaviors. In order to elucidate the link between these phenomena and the adsorption/desorption kinetic properties of kerogens, the objectives of the internship will be to experimentally obtain adsorption properties and adsorption/desorption kinetic time curves as well as their interpretations, and secondly, to attempt to reproduce these results using a multiscale numerical transport model. This study will allow to clarify the importance of the non-Fickian effects on the kinetics and to explain its physical origin which remains unknown and which cannot be revealed by the usual transport models.

	[Monteiro_PNAS] P. J. M. Monteiro, C. H. Rycroft, G. I. Barenblatt, *Proc. Nat. Ac. Sci. USA*, 2013, *110*, 6241. [Kang_AIPA_15] J. Kang, F. Zhou, G. Ye, Y. Liu, *AIP Adv.*, 2015, *5*, 127119.
TECHNIQUES USED	The thermodynamic and transport properties of kerogen-gas mixtures will be determined using an innovative method based on in situ infrared and Raman microscopy. This method also allows to gain informations on adsorption and swelling kinetics on samples of micrometer to millimeter size [Champeau_JSF_14, Dubois_JSF_18, Ongkasin_IJP_20]. The experiments will be performed with demineralized kerogen samples of intermediate maturity. To allow the comparison between these experimental results and those of molecular dynamics recently obtained in the group, we will develop a multiscale transport model accounting for the diffusion/poromechanics coupling via the model of Edwards and Cohen [Edwards_AIC_95], solved by the finite element method (code developed by Amaël Obliger) [Champeau_JSF_14] M. Champeau, J. M. Thomassin, C. Jérôme and T. Tassaing, *J. Supercrit. Fluids*, 2014, *90*, 44-52. [Dubois_JSF_18] J. Dubois, E. Grau, T. Tassaing and M. Dumon, *J. Supercrit. Fluids*, 2018, *131*, 150-15. [Ongkasin_IJP_20] K. Ongkasin, Y. Masmoudi, T. Tassaing, G. Le-Bourdon and E. Badens, *Int. J. Pharm.*, 2020, *581*, 119247. [Edwards_AIC_95] Edwards, D. A.; Cohen, D. S., *AIChE J.* 1995, *41* (11), 2345–2355.
HOST LABORATORY	Institut des Sciences Moléculaires de Bordeaux
TEAM	Theoretical chemistry and modelling group / Molecular spectroscope group
SCIENTIFIC DIRECTOR	Dr. Amaël OBLIGER Tel : Mail : amael.obliger@u-bordeaux.fr Dr. Thierry TASSAING Tel : 05 40 00 28 92 Mail : thierry.tassaing@u-bordeaux.fr Adress : Institut des Sciences Moléculaires, Bât. A12, 3ème étage, Bureau B15
Possibility to pursue the internship until the end of August: YES ☐ / NO ☒ **Possibility to offer the internship to a M1 if not attributed to a M2: YES ☐ / NO ☒**	