PhD GRANT

ÉCOLE DOCTORALE SCIENCES EXACTES ET LEURS APPLICATIONS - ED 211 / NATURAL SCIENCES DOCTORAL SCHOOL

Avenue de l'université BP 1155 64 013 PAU Cedex – France

PhD SUBJECT

TITLE:

Modeling and Multiscale HPC Simulation of CO2 Storage in Saline Aquifers

ABSTRACT: Global warming is one of the major concerns of humankind and many scientists are alerting the need of actions to be taken here and now to limit the greenhouse gas emissions to the atmosphere. A worldwide effort is put in place, but solutions need to be validated and improved. The program Carbon Capture, Utilization and Storage (CCUS) is one of the viable solutions for reducing CO_2 concentration in the atmosphere. CO_2 storage in different conditions is a promising action and a big effort is devoted to foresee its multiple effects. Various CO_2 trapping mechanisms contribute to the overall CO_2 storage in a generic reservoir as a function of time. How fast and efficient these mechanisms are, is still poorly understood, and this project will address mainly the impact of convection on the solubility of CO_2 in brines, which could be much faster than anticipated due to the concurring hydrodynamic instabilities. Experimental activities are currently performed within the CO2ES Industrial Chair. This project will be focused on simulations about the convective dissolution of CO_2 in brine after injection in deep salted aquifers.

Keywords: Geological CO2 storage, multiphase flow, reactive transport, HPC, finite volume

WORKING CONDITIONS

Laboratory: Laboratoire de Mathématiques et de leurs applications (LMAP) et Laboratoire des Fluides Complexes et leurs Réservoirs (LFCR)
Website : https://lma-umr5142.univ-pau.fr/fr/index.html et https://lfc.univ-pau.fr/fr/index.html

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In Collaboration with: Sylvain Thibeau and Mahmoud Jazayeri (TOTAL), Igor Bogdanov (CHLOE), Brahim Amaziane (LMAP), Henri Bataller (LFCR)

Place: LMAP - Pau (FR)

Starting date: October 2020	**Duration: 3 years**

Employer: E2S Université de Pau et des Pays de l'Adour (UPPA)

Monthly salary before taxes: 1883 €

HOST LABORATORY PROFILE

LMAP: The Laboratory of Mathematics and its Applications of Pau is part of the CNRS and of the University of Pau and Adour Region. It is a member of the IPRA Federation FR 2952. The LMAP has four groups covering a broad spectrum in pure and applied mathematics: algebra and geometry, optimization, analysis and numerical simulation, partial differential equations, probability and statistics.
LFCR: From the nanometer to hundreds of kilometers, from the nanosecond to a million years, from the physics and chemistry of interfaces, through the thermodynamics of fluids under flow, to reservoir geology, geomechanics and geophysics, status as an "industrial" UMR (Joint Research Unit), supervised by TOTAL, the CNRS and the UPPA, the LFCR is an innovative and remarkable research unit in more than one way. Its specific focus, essentially based on the study of fossil georesources, and totally in phase with the local socio-economical context, sets it apart regarding applications and enables it to host internationally-recognized teams.

MISSION – PRINCIPAL ACTIVITIES

I. *Scientific Context*

Many mechanisms contribute to the global storage of CO2 in a generic reservoir as a function of time. The trapping of CO2 by capillarity under the cover rock dominates during the first decade after the end of the injection. Its importance gradually diminishes in favor of other safer storage mechanisms: the storage of CO2 as a residual phase when the water re-imbibes the reservoir; by dissolution in the underlying aquifer; and by reaction with or as minerals. The speed and effectiveness of these latter mechanisms are still poorly understood, and this project will attempt to address these issues primarily for solubility trapping, which could be much faster than expected due to the occurring hydrodynamic instabilities and thermal effects. This subject is at the heart of the CO2ES Chair project and falls within the scope of the E2S project (Energy and Environment Solutions) of the Université de Pau et des Pays de l'Adour.

When supercritical CO2 (s-CO2) is injected into an aquifer, a layer of s-CO2 is rapidly formed over the salt water by means of buoyancy forces. The interface between the two layers induces a strong molecular diffusion rapidly forming a layer of CO2 / brine mixture. Since this layer is generally denser than the brine itself, convection can be initiated by density fluctuations, thereby providing an accelerated dissolution rate. All the phenomena described occur naturally in the host rock, i.e. in a porous material. Different parameters can influence the speed of these phenomena, in particular the composition of the host fluid, the injection pressure, the phase of the components, the thermodynamic conditions, the chemical reactions between CO2 and the dissolved salts, the presence of a gradient temperature, and the structure and composition of the porous medium. Experimental studies of the effects of convection on the dissolution of CO2 in real reservoir conditions (high pressure, s-CO2, 3D) cover a part of the experimental activities of the CO2ES project. Here the main scope is to perform numerical simulation activities to compare and complement the experimental results.

II. *Objectives*

This work aims at developing and implementing a parallel code coupling approach for multiphase multicomponent flow and reactive transport simulation in the framework of the parallel open-source platform DuMuX. Modelling such problems leads to a highly nonlinear, coupled system of partial differential equations to algebraic or ordinary differential equations requiring special numerical treatment. The major difficulties related to this model are in the nonlinear degenerate structure of the equations, as well as in the coupling in the system. The PhD student will contribute developing an efficient parallel algorithm implementing the discrete model based on a conservative finite volume method. The approach will employ a fully implicit treatment in time in order to preserve the nonlinear coupling of flow, transport, reactions, mass transfer across phases and to increase the time step size. Accurate description of the interface separating the gravity current from the brine is necessary for reliable predictions of the transport behaviour of CO2 plumes, and this poses significant challenges for numerical models of the large-scale flow systems of interest. Parallel computing offers an opportunity for building detailed models for such problems and in providing the capability of solving larger, more realistic and practical problems faster. The accuracy and effectiveness of the approach will be demonstrated through 2D and 3D numerical simulations. At the end of this project, the defined methodology will be applied to a larger scale model, representative of an industrial CO2 storage pilot.

III. *Work plan*

The selected PhD student will integrate the LMAP laboratory at the Pau site of the Univesrity of Pau, working in close collaboration with the LFCR laboratory at the Anglet site of UPPA. Specifically, he/she will contribute to the development and validation of cited codes within the DuMuX platform.

IV. *References*

- Ahusborde, E., Amaziane, B., El Ossmani, M. Improvement of numerical approximation of coupled multiphase multicomponent flow with reactive geochemical transport in porous media. Oil & Gas Science and Technology - Rev. IFP Energies nouvelles 73, 73 (2018).
- Niemi A., Bear J., Bensabat J. (2017) Geological Storage of CO2 in Deep Saline Formations, Springer.
- Zhang F., Yeh G.T., Parker J.C. (2012) Groundwater Reactive Transport Models, Bentham e–books.

REQUIRED COMPETENCES

The candidate must hold a Master or equivalent degree with a strong background in applied mathematics and Computational Fluid Dynamics including multiphase flow and porous media. Good programming skills with fluency in C++ are expected and be interested in physics and team working are mandatory. Knowledge of DuMuX and interest in geochemistry are a plus. Good knowledge in English and good writing skills are required.

CRITERIA USED TO SELECT CANDIDATE

Selection process steps:
- Establishment of the selection comittee.
- Evaluation of the applicants cv's.
- Interview with the selected candidates and ranking.

Criteria used in selection of the candidate:
- The candidate's motivation, scientific maturity and curiosity.
- Candidate knowledge in optics and experimental fluid dynamics.
- Candidate marks and rankings in M1 and M2.
- English proficiency.

REQUIRED DOCUMENTS, DEADLINE

Envoyer par email un dossier de candidature comprenant (send an e-mail with your candidature containing):
- CV (CV)
- lettre de motivation (cover letter detailing candidate's motivations)
- relevé de notes et classements en Master (candidate's MSc marks and ranking)
- lettres de recommandation (any letters of recommendation)
- coordonnées des personnes du milieu professionnel (minimum two) à contacter (contact details for 2 referees)

Deadline:	**31/06/2020**

CONTACTS

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