Thesis project description

Title: Multiscale modelling and optimization of CO_2 storage in coalbed methane reservoir

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Doctoral school	SIMPPE

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I. Context of the project

As part of the LUE StoCO2 doctoral project, this thesis project deals with the CO_2 storage potential in unminable coalbed methane reservoirs. The coalbed methane reservoir referring to an unconventional reservoir presents a specific geologic formation composed of a natural fracture networks (cleats) of low permeability and coal seam matrix characterized by abundant adsorption sites for gas. The latter offers a huge potential of gas storage within the micropores with a pore size typically of several nanometers.

CO_2 storage in the coal seam consists in using preferential adsorption of CO_2 compared to other gases. When injecting CO_2 into coal reservoirs, CO_2 is adsorbed at the adsorption sites within the coal matrix and the coalbed methane is released and recovered as free gas (see Fig. 1). On the one hand, CO_2 remains stored within the coal seam and on the other hand, this procedure enhances the methane production as more CH_4 can be desorbed from the micropores due to high adsorption potential of CO_2 [1]. However, high gas pressure injection may close the natural fractures and stop the injection procedure. Understanding these complex phenomena by modelling is very important to enhance the injection procedure and to optimize different parameters as injection gas pressures, injection time, gas composition, etc., considering the multiphysical mechanisms.

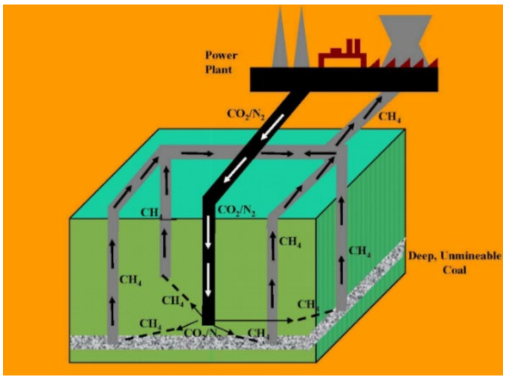

Figure 1: Diagram of coalbed methane production with CO_2 injection

II. Objectives and Methodology

The thesis project aims at developing multiscale models for transport and mechanical problems of the gas mixture from the molecular scale to the reservoir scale in order to simulate the process of CO_2 storage in coal seams and enhanced methane production. Based on this model, parameters optimization will be carried out to find the best scenario for CO_2 storage in a given coal seam reservoir. Several scientific barriers need to be overcome.

- **Porosimetry by NMR (task 1):**

Pore size distribution and corresponding porosity of coal will be measured by low-field NMR relaxometry. These measurements will be corroborated by NMR cryoporometry, which allows us to link the NMR relaxation time distribution to the pore size distribution. This technique is capable of characterizing pore sizes of several nanometers.

- **Adsorption phenomena (task 2)**

Instead of using Langmuir isotherm empirical law, the Density Functional Theory (DFT) will be used for computing the distribution of gas molecules in the nanopores and the solvation force acting on the solid phase for a given pore geometry [2, 3, 4]. In this project, the DFT approach will be explored to study the adsorption isotherm of a mixture of three gases (CH_4, CO_2 and N_2) with a pore size distribution.

- **Reservoir geomechanics (task 3)**

The geomechanics of the coal matrix will be treated classically by the Biot equations modified by the addition of a solvation force stemming from the adsorption effect. In particular, to determine the fracture aperture change during gas injection/production, the non-linear hyperbolic Barton-Bandis (BB) law, which captures increase in joint stiffness induced by the cleat closure due to the matrix swelling, is postulated for the fracture mechanical response. A reiterated homogenized procedure is pursued capable of providing the constitutive response of the homogenized poromechanical parameters at the reservoir scale.

- **Transport (task 4)**

The gas transport through the fracture network is based on multiphase/multicomponent transport in porous media: gas transport by convection and diffusion. The macroscopic conservation laws at the reservoir scale can be then derived by a second upscaling procedure.

- **Numerical modelling (task 5)**

In order to study the couplings between the various processes and to obtain results in realistic geometries, the development of a numerical code is essential. A commercial software, COMSOL for example, will be used. It can be used for the study of transport and geomechanics of coal gas reservoirs during CO_2/N_2 injection process. Based on the numerical code, an optimization procedure needs to be performed to maximize the CO_2 storage quantity in given coal seam reservoir.

In the context of this structured international cooperation, the thesis project will be developed within very close co-working with the team in LNCC (Laboratório Nacional de Computação Científica, Brazil). The work plan with different tasks indicating the mobility period and the involvement of the LNCC partner is shown in the Gantt diagram (Table 1).

Tasks	Team	Year 1				Year 2				Year 3			
T.1: Porosimetry by NMR	LEMTA	■	■										
T.2: Adsorption	LEMTA, LNCC			■	■	■ (mobility)	■						
T.3: Geomechanics	LEMTA, LNCC					■	■	■	■				
T.4: Masse transfer	LEMTA					■	■	■	■				
T.5: Numerical tools	LEMTA							■	■	■	■	■	■
Mobility period (in Brazil)													

Table 1: Gantt diagram

Mobility periods:
The Phd student will have a mobility period of three months in Brazil (at the beginning of the second year). In this occasion, he/she will specifically work with the team in LNCC on the adsorption isotherms and its effect on the poromechanics.

III. Profile and skills required

Profile: Master 2 or engineering school in the fields of fluid mechanics, numerical simulations, multiphase flows and porous media.

Skills required: transport in porous media, continuum mechanics, numerical simulations, knowledge of software (Matlab, COMSOL) would be a plus. Good level of French/English is required.

All applicants to the Doctoral School SIMPPÉ must have successfully completed a Master degree or its equivalent with a grade comparable to or better than the French grade AB (corresponding roughly to the upper half of a graduating class). In all cases (Frenchor foreign Master degree, engineering degree, etc.) the counsel of the doctoral school will examine the candidate's dossier, which must include:
• CV and letter of motivation
• the grades obtained for the Master (or equivalent) degree and a copy of the diploma if it is available
• 2 letters of recommendation, preferably from the director of the Master program and the supervisor of the candidate's research project
• written material (publications, Master thesis or report, etc.) related to the candidate's research project.

The complete application file must be sent to the thesis supervisors by email: tien-dung.le@univ-lorraine.fr and irina.panfilov@univ-lorraine.fr

References

[1] J. Seidle, Fundamentals of coalbed methane reservoir engineering, PennWell Books, 2011.

[2] T. D. Le, C. Moyne, M. A. Murad, I. Panfilov, A three-scale poromechanical model for swelling porous media incorporating solvation forces: Application to enhanced coalbed methane recovery, Mechanics of Materials, 131, 47-60 (2019).

[3] T. D. Le, Q. D. Ha, I. Panfilov, C. Moyne, Multiscale model for flow and transport in CO_2-enhanced coalbed methane recovery incorporating gas mixture adsorption effects, Advances in Water Resources, 144, 47-60 (2020).

[4] Q. D. Ha, T. D. Le, I. Panfilov, C. Moyne, M. Murad, Upscaling poromechanical models of coalbed methane reservoir incorporating the interplay between non-linear cleat deformation and solvation forces, International Journal of Solids and Structures, 262-263, 112083- (2023).