Abstract of the thesis

The thesis presents some mathematical and numerical models developed for the modelling of multiphase flows in naturally fractured rocks. In particular, the context is the recovery of coalbed methane or reversely the storage of carbon dioxide in coalbeds. The thesis is entitled:

Hydro-mechanical modelling of multiphase flow in naturally fractured coalbeds applied to CBM recovery or CO₂ storage

The first part of the thesis presents the context of the research. In this part, the reader will understand that changes of coal properties during methane production or carbon storage are a critical issue and that hydro-mechanical couplings can likely affect the permeability of the reservoir. Indeed, on the one hand, the increase in effective stress after the reservoir depletion tends to decrease the permeability. On the other hand, the matrix shrinkage following gas desorption tends to increase the permeability.

The second part of the thesis highlights these phenomena with some remarkable experimental results from the literature. However, this part of the thesis was not limited to a literature review, an experimental study was also carried out to highlight the hydro-mechanical couplings in coal with an emphasis on fracture (called cleat) permeability changes. The material was characterized via a suite of mechanical tests and sorption isotherm measurements. The cleat spacing of the specimens was also investigated with a tomography imaging and some thin sections.

The main work of the thesis was the development of some numerical models to properly take into account the permeability evolution during the gas production/storage. As coal is rarely dry *in situ*, constitutive models were developed for unsaturated conditions. In existing CBM models, sorption- and stress-induced coal permeability alteration is a remarkable aspect which is improperly simplified. Ideally, a numerical model would detail the material microstructure with separate descriptions of each constituent. However, direct modelling of the entire microstructure is usually not possible due to the high computational expense it would require at the scale of a reservoir. In consequence, large-scale models are generally phenomenological in nature: the behaviour of all the constituents is represented collectively by closed-form macroscopic constitutive equations. The phenomenological approach has limits because improving the macroscale models by taking into account more and more micromechanical effects makes it more and more difficult to formulate.

This thesis presents three models at different scales. The first model is developed at the macroscale, as generally followed in the literature for reservoir modelling. Then, with the second model, we directly model the fractures and the matrix blocks. Finally, this microscale model is integrated in a multiscale approach with the finite element square method. These models were implemented in the finite element code Lagamine developed at the University of Liège.

1 Macroscale model

The macroscale model is presented in the third part of the thesis. This part consists in four sections. The first one presents some general concepts used for the modelling of geomaterials. Then, the hydro-mechanical model is presented detailing the mechanics, the hydraulic and the

hydro-mechanical couplings. Then, the formulation of the model with the finite element method is presented. Finally, the last section presents the application of the model to coalbed methane production.

This hydro-mechanical model captures the sorption-induced volumetric strain or the dependence of permeability on fracture aperture, which evolves with the stress state. Note this part is more than a literature review, it presents a consistent model taking advantages of different models from the literature. Due to the particular structure of coal, this model is based on a dual-continuum approach (Figure 1) to enrich the macroscale with microscale considerations. A novelty is to consider simultaneously a dual-continuum approach for both mechanical and hydraulic behaviours in order to, contrary to many models in the literature, directly link the permeability evolution to the fracture aperture instead of the porosity evolution. A remarkable feature of the model is that it does not consider desorption strain is necessarily fully converted into a fracture opening. Moreover, the model was developed for multiphase flows in the fractures. Beside advective flows in the cleats, the model considers the influence of the kinetics of diffusion on the mass transfer between the matrix and the fractures. Indeed, shape factors are employed to take into account the geometry of the matrix blocks in the mass exchange between matrix and fractures. The Langmuir's isotherm is used to evaluate the gas content in the matrix. It appears in the mass transfer equation between the matrix and cleats, it is not usual.



Figure 1 – Dual-continuum approach for the hydraulic modelling.

This model was applied to the modelling of the CBM production at the scale of one well. Simulations on a reservoir showed it is interesting not to drop the pressure at the well too fast in order to reduce the closure of the fracture due to the increase of effective stress. However, in the case the reservoir does not store the maximal adsorbed gas capacity, it is advisable to apply a first pressure drop until the desorption mechanism is activated.

2 Microscale model

In the fourth part of the thesis, the model is written at the scale of the coal constituents: matrix blocks and cleats. Methane is mainly stored in the coal matrix as adsorbed gas but once the pressure is decreased in the cleats, the coal becomes less capable of retaining the methane (orange dots in Figure 2) and gas molecules diffuse through the matrix to reach the cleats where water is also present (blue dots in Figure 2).

At this scale, a channel flow model is directly derived from Navier-Stokes equations and cleats are represented with interface elements. It means that the permeability evolution is not based on a porosity model and that the use of shape factor is not required since the geometry is explicitly represented. From a mechanical point of view, the coal matrix is assumed linearly elastic and the complex non-linear behaviour of the material is obtained from the assembly with the fractures.



Figure 2 – Conceptual hydraulic microscale model.

The hydro-mechanical model for both the matrix and the cleats is presented in details. The sorption isotherm is innovatively included in the formulation of the gas transfer between the matrix and the cleats to account for the change of state. The swelling/shrinkage of the matrix is linked to its gas content and, depending on the boundary conditions, this sorption-induced strain may impact the fracture aperture. It is considered that the normal stiffness evolves with the fracture closure. This closure modifies the permeability of the fracture and impacts the fluid flow in the fracture. As a multiphase flow may be encountered in the cleats in the context of coalbed methane recovery, the applicability of unsaturated formalism to a single fracture (modelled with an interface finite element) is investigated. The implementation in the finite element code is briefly presented with a special attention paid to interface elements. Then, the implementation of the model is validated by comparison with analytical solutions. The model can be used for both gas production and gas injection. In the last section of this part of the thesis, it is used for modelling the permeability alteration due to CO_2 for different boundary conditions on a few blocks.

These few blocks combine horizontal and vertical fractures that impacts differently the permeability evolution if anisotropic boundaries conditions are encountered. In this case, it was shown that models based on the porosity evolution largely deviates from the direct fracture aperture model, such it is supposed to be in the reservoir. Note the computational cost of the direct modelling of the full microstructure would be highly expensive at the scale of the reservoir. However, the model presented in this part of the thesis is very useful for the modelling of the representative elementary volume which, using homogenization techniques, defines the macroscale behaviour of the material. This microscale model was therefore integrated into a multiscale approach.

3 Multiscale model

The idea is to model the micromechanical effects explicitly on their specific length scale through a direct modelling and couple their homogenized effects to the macroscale. Homogenization from the microscale to the macroscale avoids the use of some constitutive laws at the reservoir scale. When solving the boundary value problems at both scales using a finite element method, the approach is termed the Finite Element Square Method (Figure 3). To our knowledge, this method has never been applied to coal before.



Figure 3 – Multiscale approach.

The first section outlines the Finite Element Square Method (FE^2) . This method is then applied to develop a hydro-mechanical model with multiphase flows in a coal reservoir. In order to integrate the microscale model in the doublescale scheme and compute a consistent stiffness matrix for the macroscale, some adaptions of the microscale model were required. For instance, the REV boundary value problem is formulated under steady-state conditions given the separation of the scales between the microscale and the macroscale. Thus, a double porosity effect is not directly taken into account by the modelling of diffusive flows in he matrix but by introducing a sorption time coefficient in the macroscopic storage term. Finally, 2D-axisymmetric conditions are used for the modelling of a well production scenario.

My contributions to this model are of different kinds. Compared to previous FE^2 models, I introduced a new degree of freedom for gas to deal with multiphase flows, I implemented the adsorption and the swelling/shrinkage mechanisms for the modelling of coalbed methane production and CO_2 storage in coal seams, I introduce some initial stresses and axisymmetric conditions useful for reservoir modelling. This model was applied to the modelling of one production well. The sensitivity study highlights the role of the main parameters on the response of the model to a pressure drop at the well. Parameters affecting the cleat aperture play of course a significant role in the production curves. But the influence of the boundary conditions on the hydro-mechanical couplings was also highlighted.

Compared to the macroscale model, any fracture network could be used in the REV geometry of the multiscale model. Indeed, the macroscale model is limited to a matchstick geometry while, despite simple unit cells were used in our modelling, this is not a limitation of the multiscale model. Moreover, as physical phenomena are written at the fracture scale, the formulation is sometimes simplified. For instance, there is no Biot's coefficient appearing in the effective stress equation.

In conclusion, this thesis allowed to develop and implement new models taking into account the hydro-mechanical couplings influencing the reservoir permeability during methane production or carbon storage. However, these new modelling tools are certainly useful for a wide range of applications, also outside coal-related applications. Indeed, the questions that have arisen in this thesis on multiphase flows in multiscale model may also find applications in other media.