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A multi-scale model to study gas transport processes in clay materials

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In the field of radioactive waste confinement, the question of gas transfers in clay formations is a crucial issue [1]. A certain amount of gas, such as Hydrogen may be generated during the exploitation phase in the nearfield by the deterioration of the metal components of the system. Since the host medium is characterised by a very low permeability, the mechanisms of gas transport by advection and diffusion within the groundwater remain insufficient to evacuate the gas generated and a free gas phase is formed. If the gas pressure keeps increasing and reaches the minimum principal stress acting on the rock, micro-fractures, known as preferential gas pathways could develop through the rock mass [2], and affect the clay barrier integrity.

There is a growing body of experimental evidences [3, 4] that separation planes such as bedding planes or pre-existing fractures and heterogeneities in clay-rich materials represent preferred weaknesses for the process of opening discrete gas-filled pathways. Capturing the related transport mechanisms therefore requires to go from macroscopic to microscopic scale. In this context, the adopted numerical approach would ideally take into account the effect of each constituent of the material microstructure on the macroscopic gas flow. Yet, direct modelling of the entire microstructure using small-scale models is usually not possible due to the huge computational costs it would require at the scale of a repository. Conversely, indirect modelling of the behaviour of all the micro-constituents by collective closed-form macroscopic constitutive equations using large-scale models [5] has also limits in terms of assumptions formulation and parameters identification. Hence, the use of a multi-scale approach that models the micro-scale effects explicitely on their specific length scale and couples their homogenized effects to the macro-scale is proposed in the present work. Based on a periodicity assumption of the microstructure, the physical and geometrical properties of the microstructure are embedded on a Representative Element Volume (REV) which contains a detailed model of the microstructure constituents, i.e. the pore network, the bedding planes and the bridging planes, while eluding a complex description of the whole microstructure over the domain. From this local description of the material, the macroscopic response to loading can be derived using numerical homogenisation techniques [6].

The multi-scale model proposed here has been implemented in the finite element code Lagamine, and validated against a well established and documented macro-scale THM coupled model [7]. The size and structure of the REV comes from experimental data acquired from scanning images in clay material, like for instance the Boom Clay formation which is envisaged as a potential host rock for a deep geological disposal in Belgium. Such scans reveal the opening of large aperture with a repeated distance in-between, which make it possible to extrapolate a physical idealisation of the microstructure (Figure 1a), built with one of these fractures corresponding to the bedding planes (red) and the pore network substituted by an assembly of tubes (green). Narrow-aperture fissures, known as the bridging planes (blue) were also identified to contribute to the flow normal to the predominant direction of fissure [4], by connecting the natural discontinuities which were initially closed. These micro-scale constituents are defined in such a way as to satisfy the conditions of pore size distribution, macroporosity and intrinsic permeability. For the mechanical behaviour, a simple linear elastic constitutive law was introduced for the tube network while a non-linear stress-strain relationship was used for the interfaces defining the bedding and bridging planes. Concerning the hydraulic behaviour, gas diffusive fluxes were considered and modelled by a Fick's law while a channel flow based on the Navier-Stokes equations was used for the multiphase flow in the different constituents.

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The model has been subsequently applied to simulate a gas injection test parallel and perpendicular to the bedding of initially saturated samples of Boom Clay [4]. This analysis provides a rather good agreement with the experimental results in terms of injection and outflow pressure response, outflow volume and average axial strain along the sample height. In addition, it allows to simulated the creation of a preferential flow pathway along the sample axis (Figure 1b, top), which serves as basis to numerically reproduce the development of random pathway through the sample in plane strain state (Figure 1b, bottom), and aims to improve the mechanistic understanding of the gas transport processes at play in clayey barriers [8].

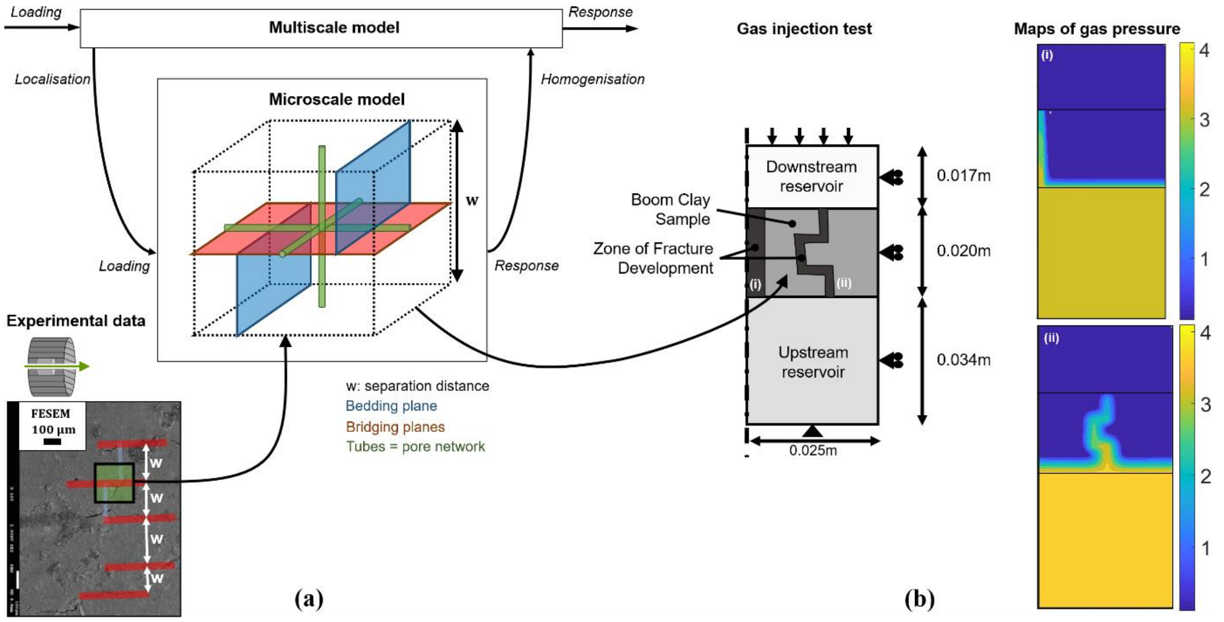

Figure 1: (a) Multi-scale approach. (b) Modelling of a gas injection experiment with preferential pathway development.

Contributor statement

Gilles Corman: Conceptualisation, Methodology, Implementation, Validation, Writing. **Frédéric Collin:** Conceptualisation, Supervision, Funding acquisition, Project management, Review and Feedback.

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