Numerical Prediction of Gas Breakthrough in Boom Clay

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ABSTRACT

In Belgium, Boom clay has been studied as a potential host rock for storage of high-level radioactive waste. This work aims at the numerical prediction of gas migration properties in the very low-porosity formation of Boom clay. Considering the meso/microscopic scale of pore network, the analyses based on macroscopic approaches or homogeneous transport properties are no longer appropriate. In this study, the 3D pore space morphological model of Boom clay which possesses a similar pore size distribution (PSD) with experimental results is generated through the union of excursions of Gaussian random fields. Essentially, the extraction of accessible pores for a given gas pressure is feasible via the purely geometric analysis of morpho-mathematical operations. Then this work numerically predicts the capillary induced gas entry and gas breakthrough pressures (GEP and GBP) in Boom clay.1

INTRODUCTION

In Belgium, the investigation of disposal of high-level radioactive waste is ongoing with Boom clay. Boom clay has been chosen for its favorable properties in repository performance, for instance, the low hydraulic conductivity [1], the high adsorption capacity for many radio nuclides [2] and the self-sealing properties due to its elasto-plastic behavior [3]. During the long term of repository, due to humid

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corrosion of metallic parts, radioactive waste decay and radiolysis of water, a
significant amount of hydrogen gas may produce and form a single gas phase if gas

migration is restricted by the low fluid conductivity of rock [4]. In this case, after a
long period of gas accumulation, the increasing gas pressure may create micro-
chronic stress, fracture the compacted clay rock then damage the repository formation.
Consequently, the investigation of gas transport is of high relevance.

In fact, gas migration occurs even at low gas pressure through Brownian
movement of dissolved parts, but the efficiency of this transport mechanism is
significantly limited by the low hydraulic conductivity of the studied rock [5].
Therefore, the capillary induced two-phase flow is the only investigated gas
transport mode in this work. Gas injection tests show that the GBP is estimated
about 5MPa [6][7]. The applied gas pressure firstly reaches the entry threshold when
evident water drainage process begins, then reaches the breakthrough threshold
when continuous gas flow paths form across the pore space.

The numerical simulation of gas migration process has been performed using
finite element model coupled to mechanical strains and stresses with Biot’s effective
stress theory under isothermal conditions [8] or embedding pre-existing fractures to
simulate the localized gas preferential pathways [9]. However, considering the
randomly formed pore space, simulation studies based on homogeneous
macroscopic approaches are not persuasive. In this work, due to the lack of real
image of porous network with micro/nanovoxel size, the 3D pore space
morphological model of Boom clay is generated through the union of excursions of
Gaussian random fields. This method can not only build randomly shaped pore
structure, but can also respect the experimental PSD. It has been used to simulate
pore space of concrete [10] and COx argillite [11]. Based on the generated model,
purely image analyses are conducted using morpho-mathematical operations.
Subsequently, two-phase flow mechanism and geometric information of model are
sufficient to give the numerical prediction of GEP and GBP.

Figure 1. PSD curve of Boom clay [7].
Figure 2. Excursion set (Left: initial Gaussian random field; Right: excursion with a given t).
3D MODEL GENERATION

In order to construct the pore space morphological model and verify its 3D connectivity, the basic information of pore space needs be firstly investigated. The measured total porosity based on water content (by drying at 100°C) is in a range of 36-39%. Standard bulk porosity measurements using mercury injection porosimetry on dried Boom clay samples provide interconnected porosity between 23 and 40% [7][12]. Mercury intrusion porosimetry tests which are performed on freeze-dried samples show that the PSD in Boom clay possesses one dominant value about 90nm [7], see Figure 1.

Excursion set which is in essence a thresholding process, can transform continuous fields to binary ones and meanwhile possess a good control of geometric and topological properties. An excursion \( E_t \) is defined by a threshold \( t \) where Gaussian random field \( f(x) \) takes its values above \( t \):

\[
E_t = \{ x \in M | f_x \geq t \}
\] (1)

Figure 2 illustrates the excursion result. In fact, the defined threshold \( t \) governs the volume fraction of excursion and the correlation length \( L_c \) of random field assigns a certain characteristic length-scale thus represents the average pore size in the generated excursion [10]. In other words, a single excursion is not able to comprise the large interval of pore size of Boom clay between 10nm and 1000nm. In this case, an union of several independent excursions with different correlation lengths (illustration in Figure 3) is indispensable to guarantee the accuracy of PSD.

Based on the experimental result in figure 1, the morphological model is decided to include 10 single excursions with correlation lengths of 20nm, 50nm, 70nm, 90nm, 200nm, 400nm, 600nm, 800nm, 1μm, 1.5μm. Size of cubic domain is chosen as 5μm. Thus, a mesh with 800 points on each side gives the voxel size of 6.25nm. The
volume fraction of each excursion has been modified several times to get better accordance with the experimental trend. A realization is presented in Figure 4 with pores in blue and matrix in grey and with the total interconnected porosity of 25%.

NUMERICAL PREDICTION OF GEP AND GBP IN BOOMCLAY MODEL

According to Young-Laplace equation, the capillary two-phase flow is governed by the gas pressure and the capillary pressure at the interface. For a cylindrical pore totally saturated, the minimum applied gas pressure $P$ for pore water movement is determined by the surface tension $\gamma$ (0.072N/m at 25°C [13]), the wetting angle $\theta$ (hypothesis of complete wettability of media in presence of gas) and the radius $r$ of pore, it is given as:

$$P = \frac{2\gamma \cos \theta}{r}$$  \hspace{1cm} (2)

Gas preferentially migrates in interconnected pores with the least capillary resistance to be overcome. Thus gas breakthrough pathways involve the largest pore throat whose size is defined as the effective pore radius ($r_{\text{eff}}$).

![Initial image](image1)

(a). Initial image.

![Geodesic reconstruction](image2)

(b). Geodesic reconstruction from boundaries of (a).

![Erosion](image3)

(c). Erosion of (a).

![Dilation](image4)

(d). Dilation of (c).

Figure 5. Morpho-mathematical methods.

![Scenario](image5)

(a). Initial Image Upstream

(b). Decreasing Structuring Element Size

Case 1 $P_g < \text{GBP}$

Case 2 $P_g = \text{GBP}$

Case 3 $P_g > \text{GBP}$

Figure 6. Scenario to find gas pathways.
The GBP can be defined as the least applied as pressure with which gas leakage firstly happens. When GBP is reached, continuous gas flows appear between the upstream and the downstream sides of pore network. The breakthrough pathways can be given as:

\[
\text{GBP pathways} = \max_x \{ \min[r_i(x)] \}; \quad \min[r_i(x)] = r_{eff}
\]  

\(x\) stands for the different interconnected pores, \(i\) represents the spatial position along the path, \(r\) is the radius of the circular cross-section of pore. From the hypothesis defined above, it is obvious that GBP is obtained by an extraction of the largest effective pore radius along all interconnected pores in the 3D model. This process is performed through purely geometric analysis using morpho-mathematical operations such as the geodesic reconstruction and the morphological opening. According to Vincent [14], the geodesic reconstruction can extract the connected components in a binary image marked by a marker. In the case of pore space model (see Figure 5a), if the boundary is considered as the marker and the entire pore network as the mask, only side-connected pores can be remained and other components will be erased through the transformation of geodesic reconstruction (see Figure 5b). The second operation - morphological opening is derived from the operations of erosion and dilation [15]. Simply speaking, using a
structuring element with defined size, erosion brings a uniform shrinkage to the pore network, pores smaller than the structuring element will be totally erased (see Figure 5c). Subsequently, with the same structuring element, dilation will rebuild the conserved parts (see Figure 5d). As mentioned before, in the context of a simple two-phase flow mechanism, a given gas pressure directly links to an effective pore radius that controls the breakthrough. In order to filter the pore space, conserve the accessible pores and subsequently verify the connectivity between the upstream and the downstream sides, the two operations are numerically implemented. As illustrated in Figure 6, the initial image is obtained through an intersection between two opposite geodesic reconstructions thus only interconnected pores are conserved. In step (a), a morphological opening is performed using a structuring element with size correlated to the gas pressure (i.e. size increases when the applied gas pressure decreases). Following this, a geodesic reconstructions starting from the upstream side is performed on the result of morphological opening to extract the drained porosity. In case 1, the applied gas pressure is lower than GBP thus the gas injection is stopped before arriving at the downstream side. When the breakthrough threshold is reached (case 2), preferential percolation pathways are formed. Additional connected pores will participate in the network of pathway and consequently increase the gas phase permeability if the applied gas pressure continues increasing after the breakthrough.

The drainage process with increasing gas pressure in the initially fully saturated Boom clay model is presented in Figure 7 and the corresponding geodesic distances in breakthrough pathways are illustrated in Figure 8 with the shortest length of 12.07μm and the longest length of 14.92μm. Thus the tortuosity of breakthrough pathways ranges between 2.41 – 2.98. From the obtained results, GEP is about 1.71MPa and GBP is estimated as 4.24MPa thus in good accordance with the experimental GBP value of 5MPa [7]. Numerical prediction enhances that gas leakage may happen through capillary two-phase flow in Boom clay and limit the gas overpressure in the host rock formation of repository. The difference between the predicted value and the experimental value is thought to be acceptable since the morphological model can take account of the PSD and the porosity but not be able to reconstruct some aspect characteristics which are determined during the sedimentation history and the diagenetic evolution such as the bedding plane. A real space model obtained by direct imaging techniques with sufficient voxel size will be helpful to get more accurate numerical prediction.

CONCLUSIONS

In this work, focus is mainly drawn to the numerical point of view: using morphological model to determine the required gas pressure for the creation of drained pathways across the pore network of Boom clay. A detailed characterization of the pore space down to nanometer scale is required for a full microphysical understanding of the material's transport properties.
The union of independent excursions of Gaussian random fields is capable to provide a realistic morphological model in good accordance with the experimental PSD. The basic mechanism of gas transport is suggested as the capillary two-phase flow. In order to determine the GEP and the GBP, the smallest accessible pore radius and the preferential interconnected pathways are extracted via purely geometric analyses using the numerical implementation of morpho-mathematical operations. The predicted GBP of 4.24MPa (experimental value of 5MPa) indicates that hydrogen gas (produced by humid corrosion of metallic parts) can escape through the open porosity and limit the gas overpressure in repository.

However, the lack of capacity to involve natural properties of rock may influence the accuracy of numerical prediction. A real model of sample derived from imaging techniques with sufficient voxel size is always a good alternative. Moreover, stress-strain state analysis and damage or fracture models when considering materials with relatively higher proportion of small pores could be further improvements in this simulation work.

REFERENCES


