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A Stochastic Permeability Model for the Shale-Gas Systems

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Abstract

The pore network in shale reservoirs consists of pores associated with both organic matter and inorganic matrix. The range of pore sizes within the organic matter is usually an order of magnitude smaller than pore sizes within the inorganic matrix, causing a bimodal pore-size distribution for the total system revealed in nitrogen adsorption tests. We use a stochastic classification method based on a mixture of Gaussian assumption to separate two distributions of pores in organic matter and inorganic matrix. We construct an ensemble-based stochastic model conditioned to Total Organic Content (TOC) and the characteristics of pore-size distributions in organic and inorganic media. This treatment of different pore sizes in organic and inorganic enables us to assign sorption process only in organic matter. The model can be used to calculate the apparent gas permeability (AP) in shale from a combination of nitrogen-adsorption and SEM-image data. We validate the model with data from the literature, and use it to determine permeability and tortuosity from pulse-decay experimental data. The model results show that AP is more sensitive to the mean of pores within inorganic matrix than within organic matter. These results suggest pore sizes corresponding to each compartment; organic and inorganic should be considered to estimate permeability. The model results also confirm permeability enhancement owing to the sorption process in organic matter below critical sorption pressure.

Keywords: mixture of Gaussian classification, pore-size distribution, micro/nano fluid dynamics, ensemble-based stochastic modeling, shale permeability, porous media

1 Introduction

Unconventional resources, such as ultra-tight shale-gas reservoirs, play a significant role in securing hydrocarbon energy because of their potential to offset declines in conventional gas production. Because of the existence of very small pores (in nanoscale) in shale reservoirs, using conventional approaches (such as Darcy’s law) for fluid flow is challenging. The Knudsen number, defined as the ratio of the mean free path of the molecule to the pore diameter, determines which flow-regime equation is valid. Table 1 shows transition criteria for different flow regimes based on the Knudsen number (Beskok and Karniadakis, 1999; Roy et al., 2003;
There are two approaches for determining the permeability of porous materials: indirect and direct. Both steady-state and unsteady-state flow experiments can be performed using the indirect approach, and corresponding steady-state and unsteady-state solutions can be used to relate experimental data to the permeability of the medium. For the steady-state method, pressure gradient, flow rate, fluid viscosity, and sample dimensions are used in Darcy’s equation to determine permeability. For the unsteady-state method (also known as the pulse-decay method), the slope of pressure-gradient change over time will be used in a more sophisticated formulation to calculate permeability (Cui et al., 2009; Darabi et al., 2012). The direct approach estimates permeability from grain size and pore size using the Carman–Kozeny and Hagen–Poiseuille equations, respectively. In many conventional systems, there is good agreement between the direct and indirect determinations of permeability. However, in shale systems, the measured permeability from indirect methods (mostly pulse-decay tests) cannot simply be matched with the permeability determined using direct methods. The mismatch is caused by the complicated physics of the fluid flow and the small-scale heterogeneities of the shale samples. To address the issue, we begin by identifying controlling properties, such as pore-size distribution and total organic content (TOC), for which we have reliable data, and then try to study unknowns such as permeability and tortuosity.

In this paper, we use a stochastic, ensemble-based model for calculating apparent permeability (AP) in ultra-tight shale-gas reservoirs that takes pore-size distribution and TOC into account. Shale pore networks contain pores associated with both organic and inorganic matter (Akkutlu and Fathi, 2012; Singh et al., 2014). The inorganic-matter pore size varies widely, from nanometer to micrometer scale (10 nm–100 μm), while the organic-matter pore-size distribution mainly falls within the nanometer scale (10–500 nm) (Darabi et al., 2012; Kuila and Prasad, 2013; Loucks et al., 2010, 2012). Because of the difference in the size ranges of these pores, the total pore-size distribution shows bimodal behavior, where each mode represents a pore-network type. Figure 1 shows a scanning electron microscope (SEM) image of a sample from Eagle Ford Shale. The image is taken from a sample normal to the bedding planes. The darker parts of the image represent organic matter. The proposed model accounts for pore-size distribution within organic matter and inorganic matter in shale samples. Table 2 compares the methodology proposed in this paper with other models (Klinkenberg, 1941; Brown et al., 1946; Javadpour, 2009; Civan, 2010; Darabi et al., 2012; Akkutlu and Fathi, 2012; Mehamani et al., 2013; Rezaveisi et al., 2014; Singh et al., 2014).

This paper is organized as follows: In the “Model Description” section, we present an ensemble-based stochastic model conditioned to the pore-size distribution as well as the TOC to calculate AP. We modify the Darabi et al. (2012) model for AP of tortuous ultra-tight shale systems to account for pore-size distribution. Afterward, we implement a stochastic method—using a mixture of Gaussian classification—by which the two different distributions within the total pore-size can be separated and the properties of each distribution found. This method has also been used in the oil industry to determine facies type at reservoirs (John et al., 2008). Figure 2 shows the flowchart of the methodology. We use two separate sources of information, SEM images and nitrogen adsorption test data, to characterize the system. The first step is to generate a stochastic ensemble of realizations for both organic and inorganic matter in the system, conditioned to organic-matter patch size distribution. Organic-matter patch size
distribution is determined from digitized SEM images using the mathematical morphology technique (Najman and Talbot, 2010) in “ImageJ” software. Then, from the nitrogen adsorption data, we separate pore-size distribution within organic and inorganic matter by using a mixture of Gaussian classification. Next, in a numerical model, we assign a pore size to each cell and calculate each cell’s permeability. Finally, we solve for the flow and calculate the AP of the sample. In the “Results and Discussion” section, we begin by validating the model with experimental data and showing that the proposed model matches the data well. Then, we draw different realizations to show that although the method is stochastic, it does not suffer from uncertainty in permeability calculation. Finally, we discuss the sensitivity of the AP to parameters such as TOC, tortuosity, average pressure, and characteristics of pore-size distribution.

2 Model Description

2.1 Spatial distribution of organic matter in sample

Shale-matrix pore networks consist of pores associated with mineral matrix (inorganic) and organic matter (Loucks et al., 2012). The mineral-matrix pore size varies widely in range on a scale from nanometer to micrometer (10 nm–100 μm), whereas the organic-matter pore size mainly falls within the nanometer scale (10–500 nm). We divide the shale matrix into two constituents: the inorganic matrix constituent (Ω_{in}) and the organic matter constituent (Ω_{o}); *in* and *o* denote the inorganic matrix and organic matter, respectively. Instead of assuming an average pore size throughout the system, we use a stochastic ensemble-based method to assign true pore-size distribution at each organic and inorganic compartment of the medium. Figure 3a illustrates an SEM image (Eagle Ford Shale) that is simplified to the system of most available permeability models (Figure 3b) and our stochastic model (Figure 3c). Darker spots represent organic material in the SEM image and stochastic model. The total volume of the organic material and their patch-size distributions are honored in our stochastic model. The organic matter patch-size distribution is obtained from SEM images. Higher numbers of analyzed SEM images can reduce uncertainties regarding patch-size distributions. We applied a stochastic algorithm conditioned to patch-size distribution to assign organic and inorganic matrices in the system. The algorithm presented in Figure 4 is as follows:

1. Start with defining the length and width of the sample. The sample size can be arbitrary, with any desired length and width. Then, randomly select a node in the sample to assign organic matter.
2. Select a value for the patch size of the organic matter from the patch-size distribution (e.g., Figure 5) using the Monte Carlo sampling method. For the analysis of the SEM images, we found that patch-size distribution is normal. For the samples used in this study, we calculated organic patch size with a mean of 25 μm² and standard deviation of 10 μm². Figure 5 shows the patch-size distribution. Since the algorithm is a stochastic process, one will get different realizations with each run. Figure 6 depicts four realizations. The black color represents organic matter.
3. Assign a selected patch size of organic matter at the randomly selected location.
4. Calculate the total volumetric portion of organic matter in the sample.
5. If the calculated portion is equal to the known TOC (e.g., from SEM image analysis), stop. If it is not equal, go back to Step 1.

This process is usually fast; within seconds a random sample honoring TOC and patch-size distribution can be built.

2.2 Mixture of Gaussian classification of pore-size distribution

There are three methods for determining the pore-size distribution of shale rocks: (1) the mercury intrusion test, (2) analysis of SEM images, and (3) the nitrogen adsorption test. Mercury intrusion tests are time consuming and need to reach extremely high pressures to detect tiny pores. In many cases, these tests fail to detect small nanopores in shale samples. SEM-image analysis reveals useful information about organic patch sizes and pore sizes in both organic and inorganic matrices. The problem with SEM images is that they are very limited and do not give any information about the third dimension (although there are highly sophisticated and expensive techniques that counteract this weakness, such as focused ion beam FIB-SEM imaging). Moreover, because samples are usually taken from a small part of the rock, SEM analysis cannot detect large pores and might lead to biased determination of pore-size distribution. Nitrogen adsorption tests are easy to run and can detect a good range of pore sizes but still lack the ability to detect larger pores (> 300 nm). Nitrogen results also do not distinguish between the pores in organic and inorganic matrices. In order to get the overall spectrum of pore sizes and distinguish between the pores in different media (organic and inorganic), we combine all these sources of data.

Pores in both organic and inorganic media are tiny at the nanoscale, but the range of pore sizes are different in these systems—pores within the organic matter are an order of magnitude smaller than those within the inorganic matter (Figure 7). The contribution of different fluid-flow controlling parameters such as slip flow and Knudsen diffusion depends on pore size and would, therefore, be different in organic and inorganic materials (Loucks et al., 2010, 2012; Darabi et al., 2012; Kulla and Prasad, 2013). In addition, sorption only occurs in pores of the organic matter (Etminan et al., 2014).

As mentioned above, since the ranges of pore sizes within organic and inorganic matter vary, the probability distribution of total (organic and inorganic) pore size is a mixture of individual pore-size distributions whose number, parameters, and proportions are to be estimated. This mixing rule follows from the law of total probability that states

\[
P(Z < z) = \sum_{i=1}^{N} P(F_i)P(Z < z | F_i)
\]

where \(Z\) is a random variable denoting pore size; \(F\) is a categorical random variable denoting whether a pore is in the organic matter or not; \(P(Z < z)\) is the observed probability of pore-size distribution being less than \(z\) (cumulative probability); \(P(F_i)\) is the unconditional probability (prior organic matter proportions) of being in the organic matter zone; \(P(Z < z | F_i)\) is the cumulative probability of observing pore size value \(z\), conditioned to being in organic matter or inorganic matrix; and \(N\) is 2 in this case.

Eq. (1) requires estimation of the conditional probabilities \(P(Z < z | F_i)\). For this purpose, we use the Gaussian distribution parametric model. This choice is based on the assumption that within a region, measured pore sizes are expected to differ only because of random additive
events. Figure 7 shows the pore-size distribution of the sample from the N2 adsorption test. Note that the x-axis is in log scale. The total pore-size distribution shown in Figure 7 confirms a bimodal probability distribution function. The log transform of pore size has a probability distribution function (PDF) with characteristics similar to the mixture of Gaussian distribution. Therefore, we model the pore-size distribution as a mixture of two lognormal distributions. For simplicity in calculation, we model the log transform of the pore size with a mixture of two normal distributions; thus the log transform of the pore size is the random variable being modeled. The assumption of lognormal distribution for pore size in rocks has been reported in several studies (Jendele, 2005; Kutilek et al., 2006). The probability of observing a given value of pore size conditional on being within the organic matter or not is given by

\[ P(Z < z | F_i) = N(\mu_i, \sigma_i) \]  

where \( \mu_i \) and \( \sigma_i \) are the means and standard deviations of the pore-size distribution in each region. Even though the normal distribution is proposed here, any other appropriate parametric distribution such as lognormal can be used.

The left side of Eq. (1) is the probability-density function computed from all the pores without regard to their location, i.e., whether in organic or inorganic matter, which can be measured via nitrogen (N2) adsorption tests. Unknowns to be estimated are the model parameters (means and standard deviations) for the measured attribute and the prior probabilities for each pore type. This estimation uses an optimization procedure that searches for the model parameters that best fit the data distribution. The objective function to be minimized is

\[ R = \sum_{k=1}^{N_{data}} (P_{model}(Z < z) - P_{data}(Z < z))^2 \]  

where \( P_{model}(Z < z) \) is computed using Eq. (1) and Eq. (2), \( P_{data}(Z < z) \) is obtained from the cumulative distribution function measured in nitrogen adsorption experiment, and \( R \) is the residual or error of fit between the model and data.

Figure 7 shows the pore-size distribution of the nitrogen-test sample from the Eagle Ford Shale. As can be seen in this figure, there are two modes in the distribution. We calculate the model parameters by the Expectation-Maximization (EM) algorithm (see Appendix A). Results from the EM algorithm for classifying pore-size distribution are presented in Table 3. It should be noted that pore-size distribution is a mixture of lognormal distributions, which means its logarithm has a bimodal normal distribution. Figure 7 shows the total pore-size distribution in log scale.

Based on the model parameters, the pore-size distribution in different organic and inorganic regions can be found. Figure 8 depicts the pore-size distribution within the organic matter and the inorganic matrix in log scale. It should be noted that although the mixture of lognormal distribution is assumed in this study, any other parametric distribution or classification method for separating different uni-modal distributions, such as a mixture of polynomial chaos expansion, can also be applied to separate organic and inorganic pore-size distribution, depending on the total pore-size distribution function (Nouy, 2010).

In the Results section, we show that differences in the means and standard deviations of pore-size distributions of organic and inorganic materials could affect permeability, especially when reservoir pressure is below critical sorption pressure.
2.3 Gas flow in nanopores

Javadpour (2009) defined apparent permeability (AP) for a straight, cylindrical nanotube accounting for slip flow and Knudsen diffusion:

$$k_{app} = \frac{2R_n T \eta M}{3RT \rho_{av}} \left( \frac{8RT}{\pi M} \right)^{0.5} + F \frac{R_n^2}{8}$$  \hspace{1cm} (4)

where $R$ is gas constant, $T$ is temperature, $R_n$ is nanotube radius, $M$ is molar mass, $\eta$ is gas viscosity, $\rho_{av}$ is average gas density, and $F$ is slip coefficient. Later, Darabi et al. (2012) extended the model for porous media as:

$$k_{app} = \frac{\eta M}{RT \rho_{av}} \phi (\delta p f)^{-2} D_k + k_D (1 + \frac{b}{p})$$  \hspace{1cm} (5)

$$b = \left( \frac{8 \pi RT}{M} \right)^{0.5} \frac{\eta}{R_{av}} \left( \frac{2}{\alpha} - 1 \right)$$  \hspace{1cm} (6)

$$D_k = \left( \frac{2R_{av}}{3} \left( \frac{8RT}{\pi M} \right)^{0.5} \right)$$  \hspace{1cm} (7)

where $\phi$ is the porosity of the rock, $\tau$ is the tortuosity of the rock, $R_{av}$ is the average pore radius, $D_f$ is the fractal dimension of the pore surface, $k_D$ is Darcy permeability ($\frac{R_{av}^2 \phi}{8 \tau}$ for a circular channel), and $\delta$ is the ratio of normalized molecular size ($d_m$) to local average pore diameter ($d_p$). Suggested by Agrawal and Probhu (2008), the value of the Tangential Momentum Accommodation Coefficient ($\alpha$) can also be calculated by:

$$\alpha = 1 - \log \left( 1 + K_n^{0.7} \right)$$  \hspace{1cm} (8)

where $K_n$ is the Knudsen number given by:

$$K_n = \frac{\lambda}{R_{av}} = \frac{K_B T}{R_{av} \sqrt{2 \pi \sigma^2 P}}$$  \hspace{1cm} (9)

where $T$ is temperature in Kelvin, $K_B$ is the Boltzmann constant in J/K, $R_{av}$ is average pore size of the porous medium, $\sigma$ is the collision diameter of the molecules, and $P$ is the pressure of the system. It should be noted that Darcy permeability ($k_D$) could have different formulations depending on pore shape (Akkutlu and Fathi, 2012). For example, Darcy permeability of slitlike pores is $\frac{h^2 \phi}{12 \tau}$ where $h$ is the height of the slit (Singh et al., 2014). However, in this study we only consider circular pores because the information on the pore-size distribution from nitrogen adsorption tests is based on circular pores.

The AP models proposed by others do not distinguish between pore characteristics of the organic matter and inorganic matter. Therefore, estimated AP is independent of TOC and pore-
size distribution. We use a stochastic model to calculate AP that is conditioned to TOC and to the individual pore-size distributions in organic and inorganic constituents.

2.4 Estimation of fluid properties

As shown in Eq. (5), we need average gas density ($\rho_{av}$) and gas viscosity ($\eta$). Both these parameters are pressure and temperature dependent. The Peng–Robinson equation of state (PR-EOS) was used to calculate the gas density, and the viscosity is calculated as follows (McCain, 1991):

$$\eta = A \exp (B \rho^C)$$  

where

$$A = \frac{(9.379 + 0.01607M)T^{1.5}}{209.2 + 19.26M + T}$$  

$$B = 3.448 + 0.01009M + \frac{986.4}{T}$$  

$$C = 2.447 - 0.2224B$$

where $\rho$ is gas mass density in g/cc, $T$ is temperature in Rankin, $M$ is molar mass in g/gmol, and $\eta$ is in cp.

2.5 Upscaling and calculating apparent permeability

Apparent permeability at each cell (grid block) is calculated using Eq. (5). Then, the average or effective permeability of the medium can be calculated using the method described in Kelkar and Perez (2002) and summarized in Appendix B. The geometric average of lower and upper bounds for the apparent permeability, assuming no cross flow, is as follows:

$$k_{LB} = \frac{Nc}{Nt} \sum_{i=1}^{Nt} \frac{1}{\sum_{j=1}^{Nc} \frac{1}{k_{i,j}}}$$  

$$k_{UB} = \frac{Nc}{Nt} \sum_{j=1}^{Nc} \frac{1}{\sum_{i=1}^{Nt} k_{i,j}}$$

$$k_{app} = \sqrt{k_{UB}k_{LB}}$$
where \( N_r \) is the number of cells in the vertical direction, \( N_c \) is the number of cells in the horizontal direction, and \( k_{i,j} \) is the permeability of the cell in row \( i \) and column \( j \). The schematic of the system is shown in Figure 9.

In this model, the flow is assumed to be in 1D, and the heterogeneity is assumed to exist only in 2D. The sample is discretized, as shown in Figure 9. The pores within each cell are assumed to have the same pore size, which is calculated by Monte Carlo sampling from pore-size distribution of organic matter (Figure 8a) and inorganic matter (Figure 8b). The permeability of each cell can be calculated by Eq. (5). Then, the average or effective AP of the medium can be calculated by Eq. (16), neglecting the crossflow (justification comes next). In this model, the pressure difference across the sample is assumed to be small enough so that the mean pressure can be applied for calculation of fluid properties and the AP in each cell. In our example, we implemented the method for the sample with the properties listed in Table 4.

In order to justify the assumption of no crossflow and the use of Eq. (16), we numerically solved the steady state gas flow in 2D considering crossflow \((\nabla . u = 0)\) where \( u \) is Darcy velocity and is calculated by Darcy’s law \((u = -k \nabla p)\), where \( k \), \( \mu \), and \( p \) are local permeability, fluid viscosity, and pressure, respectively. Combining these equations leads to Eq. (23) and finally Eq. (19). It should be noted that the gas viscosity is a function of location, since it depends on pressure, which changes locally. Eq. (19) is spatially discretized as shown in Eq. (20). Eq. (20) combined with Eq. (21) (boundary conditions) is used to compute the 2D pressure map. The boundary conditions are constant pressure at inlet and outlet, and no flow at the top and bottom boundaries (Figure 9). The pressure map is shown in Figure 10.

\[
\nabla \cdot \left( \frac{k(x,y)}{\mu(x,y)} \nabla p(x,y) \right) = 0
\]

\[
\frac{\partial}{\partial x} \left( \frac{k}{\mu} \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{k}{\mu} \frac{\partial p}{\partial y} \right) = 0
\]

\[
\frac{k}{\mu} \frac{\partial^2 p}{\partial x^2} + \frac{\partial}{\partial x} \left( \frac{k}{\mu} \frac{\partial p}{\partial x} \right) + \frac{k}{\mu} \frac{\partial^2 p}{\partial y^2} + \frac{\partial}{\partial y} \left( \frac{k}{\mu} \frac{\partial p}{\partial y} \right) = 0
\]

\[
\frac{1}{(\Delta x)^2} \left( p_{i+1,j} \left( \frac{k_{i,j} + k_{i+1,j}}{4\mu_{i,j}} - \frac{k_{i-1,j}}{4\mu_{i,j}} \right) - p_{i,j} \left( \frac{2k_{i,j}}{\mu_{i,j}} \right) + \right)
\]

\[
\frac{1}{(\Delta y)^2} \left( p_{i+1,j} \left( \frac{k_{i,j} + k_{i+1,j}}{4\mu_{i,j}} - \frac{k_{i-1,j}}{4\mu_{i,j}} \right) - p_{i,j} \left( \frac{2k_{i,j}}{\mu_{i,j}} \right) + \right)
\]

\[
i = 2, ..., N_r - 1, j = 2, ..., N_c - 1
\]
\[ p_{i,1} = p_u, p_{i,N_c} = p_d \quad i = 1, ..., N_r \quad \text{(Constant inlet and outlet pressure)} \]  \tag{21}

\[ p_{1,j} = p_{2,j}, p_{N_r,j} = p_{N_r-1,j} \quad j = 1, ..., N_c \quad \text{(No flow boundary condition)} \]

\[ q = \frac{-kA \frac{\partial p}{\partial x}}{\mu} \bigg|_{x=0}, \quad k_{app} = \frac{q\mu L}{A(p_u - p_d)} \]  \tag{22}

This pressure map can be used to calculate the apparent permeability by Eq. (22) \((L\) is the length of the sample). Using the numerical model, the average permeability calculated for our example is 0.26 \(\mu\)D, which is close enough to the value of 0.28 \(\mu\)D obtained from the no-crossflow model of Eq. (16). This comparison supports the assumption of no crossflow and the applicability of the geometric average of lower and upper bounds, i.e., Eq. (16). In general, there are three forces that control crossflow: viscous, gravity, and capillary. None of these crossflow forces exist in our system of interest. Vertical permeability is very low in shale; therefore, crossflow due to viscous forces is negligible. For the single-phase gas flow, gravity and capillary crossflow are also not important (Kelkar and Perez, 2002).

2.6 Representative equivalent size

In this section, we compared the sensitivity of the total apparent permeability to the local heterogeneity by changing the sample size. To do this, we divided the system shown in Figure 6 into smaller subsystems; we then calculated the total apparent permeability along these smaller systems and determined total apparent permeability of each sample in relation to its size. Figure 11 shows a map of the heterogeneous permeability field for one of the realizations shown in Figure 6. Figure 12 shows the results of permeability change versus sample size. The effective permeability decreases as the sample size increases and reaches a plateau for sample size around 200 \(\mu\)m \(\times\) 200 \(\mu\)m.

### 3 Results and Discussion

We first use our model to simulate pulse-decay experimental data reported in the literature to show the application of our model for pulse-decay permeability analysis. We also present more validation of the proposed model with recent data reported for Pierre Shale and Mancos B Shale samples. Finally, we use the base case data of an Eagle Ford Shale sample to study the sorption effect on permeability and the sensitivity of the method to various parameters, including TOC, tortuosity, pressure, pore-size distribution characteristics, and sample size.

3.1 Implementation of stochastic model for pulse-decay permeability analysis

Pulse-decay permeability measurement is a method most commonly used for ultra-tight systems such as shale gas. The method is based on transient variation of a pressure gradient when loaded with an inert gas such as nitrogen (Figure 13). The pulse-decay permeability method is discussed in more detail elsewhere (Brace et al., 1968; Jones, 1997; Cui et al., 2009; Darabi et al., 2012).
Using pseudo-pressure term \( m(p) \) (Al-Hussaini et al., 1966), the unsteady-state pseudo-pressure equation governing pressure decay for an inert gas (no sorption) in a pulse-decay test is defined as:

\[
m(p) = 2 \int_0^p \frac{k}{\mu z} \dot{p} dp
\]  \hspace{1cm} (23)

\[
\frac{\partial m}{\partial t} = \frac{k}{\mu c_g \phi} \frac{\partial^2 m}{\partial x^2}, \hspace{1cm} 0 < x < L, t > 0
\]  \hspace{1cm} (24)

To solve Eq. (24), we need an initial condition, \( m(x,0) = m_d(0) \) and two boundary conditions: \( m(0,t) = m_u(t) \) and \( m(L,t) = m_d(t) \). The late-transient analytical solution of Eq. (24) is:

\[
\ln(\Delta m_D) = \Psi + st
\]  \hspace{1cm} (25)

where \( \Delta m_D \) is dimensionless pseudo-pressure difference and defined as:

\[
\Delta m_D = \frac{m_u - m_d}{m_u - m_d_0}
\]  \hspace{1cm} (26)

and \( s \) is the slope of the late-transient dimensionless pseudo-pressure difference (Figure 13)

\[
s = \frac{-kfA(1/V_u + 1/V_d)}{\mu L c_g}
\]  \hspace{1cm} (27)

\( V_u \) and \( V_d \) are the volumes of the upstream and downstream vessels, \( L \) is the core sample length, \( A \) is the cross-sectional area, \( \mu \) is the fluid (Helium or Argon) viscosity, and \( c_g \) is the isothermal compressibility. \( f \) is defined as:

\[
f = \frac{\theta^2}{a + b}
\]  \hspace{1cm} (28)

where \( \theta \) is the first solution of the equation

\[
\tan(\theta) = \frac{(a + b)\theta}{\theta^2 - ab}, \begin{cases} a = V_p/V_u \\ b = V_p/V_d \end{cases}
\]  \hspace{1cm} (29)

A plot of \( \ln(\Delta m_D) \) versus time yields to a straight line at late times. Sample permeability can be calculated from the slope of the straight-line “s” using Eq. (27). We used pulse-decay data reported in Darabi et al. (2012) to determine permeability of the system. Then we used a fully implicit finite difference method to numerically solve Eq. (24). Since the estimation of tortuosity (\( \tau \)) and the fractal dimension of the pore surface (\( D_f \)) are not available, we used an optimization scheme to minimize the error between predicted results and experimental data. The optimization problem is given as:
We used the interior-point algorithm (Mehrotra, 1992) to solve Eq. (30). The values of $\tau_{\text{min}}$, $\tau_{\text{max}}$, $D_{f,\text{min}}$, and $D_f$ were set to 1, 4, 2, and 2.5, respectively. The experiment condition parameters and the final values of $\tau$ and $D_f$ are tabulated in Table 5. The results of numerical and analytical solution of the pulse-decay data are shown in Figure 14. In order to show the effect of tortuosity on pressure-decline data, we performed numerical analysis by changing tortuosity values and keeping other parameters constant (Figure 14). Systems with higher tortuosity show lower pressure-decline rates.

3.2 Model validation

To validate our proposed stochastic model, we used the permeability and pore-size distribution, along with other data, for two shale systems (Pierre Shale and Mancos B Shale) reported by Kuila (2013). Figure 15 and Table 6 present the pore-size distribution of these two shale samples and sample parameters, respectively. We used the optimization algorithm presented in Section 3.1 for estimating $\tau$ and $D_f$ to match with the measured permeability. Estimated values of $\tau$ and $D_f$ to match the permeability values are presented in Table 6.

3.3 Effect of sorption on permeability

Apparent permeability in shale systems is a function of pressure and temperature in addition to desorption, since the pore sizes within organic matter change as a result of Langmuir sorption. Because the proposed methodology in this paper distinguishes between organic matter and inorganic matter, we can model the effect of sorption on apparent permeability. If pressure falls below the critical desorption pressure in shale systems, gas molecules detach from the pore walls in organic matter, consequently enlarging the pores and improving permeability. The relative change in pore sizes can be determined by assuming a prescribed pore shape and a volume of adsorbed gas (Aguilera and Lopez, 2013). Gas volume can be determined by the Langmuir sorption isotherm of the shale sample. The algorithm modeling this process is as follows:

Langmuir adsorption isotherm model relates the mass of the sorbed gas to pressure as:

$$\Gamma = \Gamma_{\text{max}} \frac{\xi P}{1 + \xi P}$$  \hspace{1cm} (31)

where $\Gamma_{\text{max}}$ is the volume of adsorbed gas (scf/ton rock), $P$ is the equilibrium pressure of the gas in the system (MPa), $\Gamma_{\text{max}}$ is the maximum amount of the sorbed gas at a certain temperature and infinite pressure, and $\xi$ is the Langmuir coefficient. The values for $\Gamma_{\text{max}}$ and $\xi$ in our base case are listed in Table 4.

Eq. (31) calculates the volume of gas released from the system at any given pressure. The released gas from the inner wall of the pores in organic matter can be related to the receding of the pore wall by updating the new enlarged pore radius as:
where $N$ and $V$ are the number of pores and the new pore volume after certain gas desorption (original pore volume plus the volume of the released gas at a given pressure), respectively. Figure 16 describes the algorithm for incorporating gas desorption to a permeability model. Updated pore radius at each pressure will then be used to calculate new permeability.

### 3.4 Sensitivity analysis

In order to evaluate the uncertainty of our stochastic model, we generated 40 ensembles, using the stochastic algorithm explained in Sections 2.1 and 2.2. Table 7 presents the statistics of the AP results of all 40 realizations. The standard deviation of the permeability of different realizations is 3%, indicating that the method has acceptable uncertainty to generate random realization of organic patch distribution.

We studied the sensitivity of AP to TOC. The value of volumetric TOC varied between 0.05 and 0.25. We assumed that the pore-size distributions within both organic and inorganic matter were constant. Increasing TOC decreases the average pore size in the entire system because of the higher portion of smaller pores within organic matter (Figure 17). Apparent permeability decreases the fraction of organic matter with smaller pores increases. Figure 17 also shows the sensitivity of AP to volumetric TOC for scenarios with and without slip flow and Knudsen diffusion. Models that include additional flow physics of slip flow and Knudsen diffusion show more sensitivity with the TOC variation, which suggests that the contribution of slip flow and Knudsen diffusion is more pronounced in inorganic matter.

Figure 18 shows the sensitivity of AP to tortuosity. The value of tortuosity varied between 1 and 20. All other parameters remained constant as listed in Table 4. Apparent permeability decreases as tortuosity increases because tortuous channels hinder the flow of gas molecules. Figure 18 also suggests that variation of AP is more pronounced when slip flow and Knudsen diffusion are included in the model.

Figure 19 shows the sensitivity of AP to average system pressure, both with and without sorption. The Langmuir adsorption curve is added to Figure 19 to better describe the behavior of the system. Average pressure ranged from 1 MPa to 30 MPa. As can be seen in Figure 18, a decrease in average reservoir pressure does not affect Darcy permeability. However, when we include slip flow and/or Knudsen flow, AP shows dependency on average pressure. This pressure dependency has been reported by others in the past (Javadpour, 2009; Civan, 2010; Darabi et al., 2012). However, the interesting finding here is the effect of sorption on AP. The model results suggest an increase in AP, especially below the critical sorption pressure.

Next, we present the sensitivity of AP in a shale sample to the characteristics of pore-size distribution. We changed the mean and standard deviation of pore-size distribution within both organic matter and inorganic matter. Figure 20 shows the sensitivity of AP to the mean ($\mu$) and standard deviation ($\sigma$) of pore-size distribution in organic matter. The increase in the mean pore size increases AP, but the slope of the increase in AP decreases as the mean pore size increases. Figure 20 also suggests that an increase in standard deviation of the pore-size distribution decreases AP. The increase in $\sigma$ increases the uncertainty of pore size and decreases the impact of the pores with larger diameter. Note that the curve corresponding to zero standard deviation

\[ r = \frac{1}{N} \left( \frac{3V}{4\pi} \right)^{1/3} \]
falls within the realizations where the pore sizes within organic-matter patches are constant in the sample.

Figure 21 shows the sensitivity of AP to the mean and standard deviation of pore-size distribution in inorganic matter. Similar to the case of organic matter, the curve corresponding to zero standard deviation falls within the realization where the pore sizes within the inorganic matrix are constant in the entire system. Figure 21 shows the trend that increasing the mean of pore size increases the AP of the sample. Although AP increases with the increase of mean pore size in the inorganic matrix, the trend is different when compared to the case of organic matter. The increase in AP is small at small-mean pore sizes, and the slope of change in AP increases as the mean pore size increases in the inorganic matrix. This trend is more pronounced in the smaller standard deviation of the pores in the inorganic matrix. The increase in the standard deviation of pores in the inorganic matrix decreases AP because it increases the uncertainty of pore size and decreases the impact of the pores with larger diameter.

The results in Figures 20 and 21 confirm that permeability estimation in shale systems based on an average pore size could be erroneous. Pore sizes corresponding to each compartment, organic and inorganic, should be considered.

4 Summary and Conclusion

We studied gas flow in ultra-tight shale reservoirs in which pores exist in both organic matter and inorganic mineral matrix. The range of pore sizes within organic matter is usually an order of magnitude less than the range of inorganic-matter pores, making the pore-size distribution bimodal. We used an ensemble-based stochastic model to relate pore-size distribution characteristics to the apparent permeability (AP) of shale reservoirs. The stochastic model honors the TOC as well as the pore-size distribution of the sample.

We used our stochastic model to analyze pulse-decay permeability experimental data. We used an optimization method to estimate the tortuosity of the sample and validated our model with data reported in other studies.

We performed sensitivity analyses of AP to various parameters, including TOC, tortuosity, average pressure, and characteristics of pore-size distributions (mean and standard deviation) in organic matter and inorganic matrix. The model results show that an increase in any of these parameters—TOC, average pressure, tortuosity, standard deviation of pore-size distributions—decreases AP, whereas an increased mean value of pore-size distribution increases AP. AP is more sensitive to the mean of pores within inorganic matrix than within organic matter. These results suggest that permeability estimation in shale systems solely based on average pore size could be erroneous. To estimate permeability, pore sizes corresponding to each compartment, organic and inorganic, should be considered.

Notation

\[ A \] \quad \text{cross-sectional area, m}^2

\[ D_f \] \quad \text{fractal dimension of pore surface}

\[ D_k \] \quad \text{Knudsen diffusion coefficient, m}^2/\text{s}

\[ K \] \quad \text{permeability, m}^2

\[ k_D \] \quad \text{Darcy permeability, m}^2
L  Length, m
M  molar mass, g/gmol
P  pressure, Pa
Q  molar flux, mol/s
R  universal gas constant (= 8.314 J/gmol.K)
R_{nt}  nanotube radius, m
T  temperature, K
\alpha  tangential momentum accommodation coefficient, dimensionless
\rho  Langmuir gas adsorption capacity, Scf/ton
\delta  ratio of normalize molecular size to local pore diameter
\eta  gas viscosity, Pa.s
\mu  mean pore diameter, nm
\xi  Langmuir coefficient, 1/MPa
\rho  density, g/cm^3
\sigma  standard deviation of pore diameter, nm
\tau  Tortuosity, dimensionless, (>1)
\phi  porosity, dimensionless

Acknowledgments

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References


Appendix A: Expectation-Maximization Algorithm

We use the Expectation-Maximization (EM) algorithm for the Gaussian mixtures in our study. The algorithm is an iterative algorithm that starts from initial estimate of parameters and proceeds to iteratively update those parameters until convergence is detected. Each iteration consists of an E-step and an M-step.

**E-Step:** Denote the current parameter values as \( \theta \). Compute \( w_{ik} \) using Eq. (A-1) for all data points and all mixture components.

\[
w_{ik} = \frac{p_k(x_i|\theta_k)\alpha_k}{\sum_{m=1}^{K} p_m(x_i|\theta_m)\alpha_m}, \quad 1 \leq k \leq K, 1 \leq i \leq N \tag{A-1}
\]

Where \( K \) is the number of total classes, \( N \) is the total number of data, \( \alpha_k \) is the prior probability of \( k^{th} \) class, \( \theta_k = \{\mu_k, \Sigma_k\} \) where \( \mu_k \) is the mean of \( k^{th} \) class, and \( \Sigma_k \) is the covariance of \( k^{th} \) class. \( p_k(x_i|\theta_k) \) is calculated using Eq. (A-2).

\[
p_k(x_i|\theta_k) = \frac{1}{(2\pi)^{d/2} |\Sigma_k|^{-1/2}} \exp \left( -\frac{1}{2} (x_i - \mu_k)^T \Sigma_k^{-1} (x_i - \mu_k) \right) \tag{A-2}
\]

**M-Step:** Now use the \( w_{ik} \) weights and the data to calculate new parameter values. Let \( N_k = \sum_{i=1}^{N} w_{ik} \), i.e., the sum of the membership weights for the \( k^{th} \) component (which is the effective number of data points assigned to component \( k \)).

Then, the parameters are updated using Eqs. (A-3) to (A-5).

\[
\alpha_k^{new} = \frac{N_k}{N} \tag{A-3}
\]
\[
\mu_k^{new} = \left( \frac{1}{N_k} \right) \sum_{i=1}^{N} w_{ik} \cdot x_i 
\]  

(A-4)

\[
\Sigma_k^{new} = \left( \frac{1}{N_k} \right) \sum_{i=1}^{N} w_{ik} \cdot (x_i - \mu_k^{new}) (x_i - \mu_k^{new})^t 
\]  

(A-5)

**Appendix B: Upscaling and Calculating Total Apparent Permeability**

In order to calculate the total apparent permeability, we simplify the problem by assuming the flow is in 1D and neglecting the cross flow. Kelkar and Perez (2002) proposed that the upscaled permeability is the geometric average of the lower and upper bounds. The lower and upper bounds can be calculated as follows:

Using Eq. (B-1), the lower bound of the average permeability can be calculated (see the lower bound averaging at the left side of Fig. B.1). In order to calculate the upper bound (Eq. [B-2]), the series layers can be upscaled to calculate the total apparent permeability as depicted in the righthand side of Fig. B.1:

\[
k_{LB} = \frac{N_c}{N_r} \sum_{i=1}^{N_r} \frac{1}{\sum_{j=1}^{N_c} \frac{1}{k_{i,j}}} 
\]

(B-1)

\[
k_{UB} = \frac{m}{n} \frac{1}{\sum_{j=1}^{N_c} \sum_{i=1}^{N_r} k_{i,j}} 
\]

(B-2)

where \(N_c\) is the number of columns and \(N_r\) the number of rows in the system.

Figure B.1. Schematic of lower bound averaging (left-hand side) and upper bound averaging (right-hand side) of the total system (center).
Table 1. Transition of flow regimes based on Knudsen number

<table>
<thead>
<tr>
<th>Flow regime</th>
<th>Darcy flow</th>
<th>Slip flow</th>
<th>Transition flow</th>
<th>Free-molecule flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Knudsen number</td>
<td>$k_n &lt; 10^{-3}$</td>
<td>$10^{-3} &lt; k_n &lt; 10^{-1}$</td>
<td>$10^{-1} &lt; k_n &lt; 10$</td>
<td>$k_n &gt; 10$</td>
</tr>
</tbody>
</table>

Table 2. History of gas-flow models in porous media and shale systems

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Model Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Klinkenberg</td>
<td>Empirical slip flow</td>
</tr>
<tr>
<td>(1941)</td>
<td></td>
</tr>
<tr>
<td>Brown et al.</td>
<td>Theoretical slip flow</td>
</tr>
<tr>
<td>(1946)</td>
<td></td>
</tr>
<tr>
<td>Javadpour</td>
<td>Maxwell slip flow, Knudsen diffusion, single straight nanotube</td>
</tr>
<tr>
<td>(2009)</td>
<td></td>
</tr>
<tr>
<td>Civam</td>
<td>Simplified 2nd order slip model, several empirical parameters</td>
</tr>
<tr>
<td>(2010)</td>
<td></td>
</tr>
<tr>
<td>Darabi et al.</td>
<td>Maxwell slip flow, Knudsen diffusion, surface roughness, average pore size</td>
</tr>
<tr>
<td>(2012)</td>
<td></td>
</tr>
<tr>
<td>Akkutlu &amp; Fathi</td>
<td>Circular pores in organic matter and slit-shape pores in inorganic matter</td>
</tr>
<tr>
<td>(2012)</td>
<td></td>
</tr>
<tr>
<td>Mehmami et al.</td>
<td>Network model of straight nanotubes with Maxwell slip and Knudsen diffusion</td>
</tr>
<tr>
<td>(2013)</td>
<td></td>
</tr>
<tr>
<td>Rezaveisi et al.</td>
<td>Maxwell slip and Knudsen diffusion for multicomponent chromatographic separation</td>
</tr>
<tr>
<td>(2014)</td>
<td></td>
</tr>
<tr>
<td>Singh et al.</td>
<td>Nonempirical model, circular and slit-shape pores in organic matter</td>
</tr>
<tr>
<td>(2014)</td>
<td></td>
</tr>
<tr>
<td>This study</td>
<td>Maxwell slip flow, Knudsen diffusion, surface roughness, PSD in organic and inorganic, TOC, sorption</td>
</tr>
</tbody>
</table>
Table 3. Properties of two distributions: $\mu$ and $\sigma$ are mean and standard deviation of the log transform of the pore size

<table>
<thead>
<tr>
<th>Region/Property</th>
<th>$\mu$</th>
<th>$\sigma$</th>
<th>Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Organic matter</td>
<td>0.4</td>
<td>0.18</td>
<td>0.5565</td>
</tr>
<tr>
<td>Inorganic matter</td>
<td>1.4</td>
<td>0.44</td>
<td>0.4435</td>
</tr>
</tbody>
</table>

Table 4. Base case input parameters of the sample used in analysis

<table>
<thead>
<tr>
<th>Input Data</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample size</td>
<td>200 $\mu$m×300 $\mu$m</td>
</tr>
<tr>
<td>Gas type</td>
<td>Methane, 16.04 g/mol</td>
</tr>
<tr>
<td>$N_c$</td>
<td>600</td>
</tr>
<tr>
<td>$N_r$</td>
<td>400</td>
</tr>
<tr>
<td>$N_2$ adsorption—pore-size distribution</td>
<td>See Figure 7</td>
</tr>
<tr>
<td>Kerogen patch-size distribution</td>
<td>See Figure 5</td>
</tr>
<tr>
<td>Porosity</td>
<td>10%</td>
</tr>
<tr>
<td>Volumetric TOC</td>
<td>12%</td>
</tr>
<tr>
<td>Fractal dimension of the pore surface ($D_f$)</td>
<td>2</td>
</tr>
<tr>
<td>Temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Average pressure</td>
<td>10 MPa</td>
</tr>
<tr>
<td>Tortuosity</td>
<td>2</td>
</tr>
<tr>
<td>Maximum Langmuir adsorption capacity ($I_{max}$)</td>
<td>125 scf/ton</td>
</tr>
<tr>
<td>Langmuir adsorption coefficient ($\xi$)</td>
<td>0.16 1/MPa</td>
</tr>
</tbody>
</table>
Table 5. Core sample and pressure data used in pulse-decay experiment and calculated parameters. Adopted from Darabi, et al. (2012).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core length</td>
<td>6.15 cm</td>
</tr>
<tr>
<td>Core diameter</td>
<td>3.80 cm</td>
</tr>
<tr>
<td>Upstream pressure</td>
<td>13.79 MPa</td>
</tr>
<tr>
<td>Upstream vessel vol.</td>
<td>$30 \times 10^{-6}$ m$^3$</td>
</tr>
<tr>
<td>Downstream pressure</td>
<td>13.10 MPa</td>
</tr>
<tr>
<td>Downstream vessel vol.</td>
<td>$30 \times 10^{-6}$ m$^3$</td>
</tr>
<tr>
<td>Permeability (calculated)</td>
<td>$1.07 \times 10^{-19}$ m$^2$</td>
</tr>
<tr>
<td>Tortuosity (calculated)</td>
<td>2.34</td>
</tr>
<tr>
<td>$D_f$ (calculated)</td>
<td>2.24</td>
</tr>
<tr>
<td>Gas type</td>
<td>Nitrogen, 28.01g/mol</td>
</tr>
<tr>
<td>Temperature</td>
<td>293K</td>
</tr>
</tbody>
</table>

Table 6. Properties of samples (Kuila, 2013)

<table>
<thead>
<tr>
<th>Property</th>
<th>Sample</th>
<th>Pierre Shale</th>
<th>Mancos B Shale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pore-size distribution</td>
<td>Figure 15</td>
<td>Figure 15</td>
<td></td>
</tr>
<tr>
<td>Porosity</td>
<td>0.06</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>TOC (wt %)</td>
<td>18.00</td>
<td>1.36</td>
<td></td>
</tr>
<tr>
<td>Pressure</td>
<td>2000 psi (13.8 MPa)</td>
<td>2000 psi (13.8 MPa)</td>
<td></td>
</tr>
<tr>
<td>Permeability</td>
<td>$1.7 \times 10^{-20}$ m$^2$</td>
<td>$1.6 \times 10^{-20}$ m$^2$</td>
<td></td>
</tr>
<tr>
<td>Estimated tortuosity</td>
<td>2.6</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>Estimated $D_f$</td>
<td>2.23</td>
<td>2.49</td>
<td></td>
</tr>
</tbody>
</table>

Table 7. Apparent permeability (AP) results of all 40 realizations

<table>
<thead>
<tr>
<th>Property</th>
<th>Average AP ($\mu$D)</th>
<th>STD of AP ($\mu$D)</th>
<th>Minimum AP ($\mu$D)</th>
<th>Maximum AP ($\mu$D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.280</td>
<td>0.0084</td>
<td>0.262</td>
<td>0.288</td>
</tr>
</tbody>
</table>
Figure 1. SEM image of an Eagle Ford Shale sample. The image is taken from a sample normal to the bedding planes. The dark parts represent organic matter. The darkest spots in the organic matter are pores.
Figure 2. The flowchart of the proposed methodology to determine apparent permeability (AP) from pore-size and organic matter patch-size distributions. Three sets of input data are needed: nitrogen adsorption data for the pore-size distribution, SEM images to find organic-matter patch-size distribution, and fluid properties. Organic-matter patch-size distribution from SEM images will be used to generate realizations of distributed organic matter in the system. The bimodal PSD from nitrogen adsorption data will be used to find PSD in organic and inorganic matters. In a fluid-flow numerical code, the discretized system will be solved for the velocity field and permeability.
Figure 3. (a) SEM image from Eagle Ford Shale, (b) average model, and (c) stochastic model.
Portion of organic matter is equal to volumetric TOC

Figure 4. Flowchart for generating stochastic realizations of organic-matter patches in the system. The input data are TOC and organic-matter patch-size distribution analyzed from SEM images using ImageJ software. Monte Carlo sampling was used to sample a patch from the distribution. The selected patch is then located at a spot; this continues until all patch sizes are distributed to the system. The TOC of the generated system will then be compared with the original TOC.
Figure 5. Patch-size distribution of organic matter. Based on available SEM images of the Eagle Ford Shale sample, we assumed that the patch-size distribution was normal, with a mean of $25 \mu m^2$ and standard deviation of $10 \mu m^2$. The average patch-size distribution is approximately $5 \mu m \times 5 \mu m$, and the maximum patch-size distribution is approximately $10 \mu m \times 10 \mu m$.

Figure 6. Four different realizations of the proposed algorithm in Figure 4 for Eagle Ford Shale samples in Figure 5. Black indicates organic matter and white indicates inorganic matter.
Figure 7. Log-scale pore-size distribution results of the nitrogen adsorption experiment on the Eagle Ford Shale sample. A bimodal trend is evidenced in data.

Figure 8. Pore-size distribution (a) within organic matter, and (b) within the inorganic matrix of the Eagle Ford Shale sample. Please note that although the pore-size range of organic matter is less than the range within inorganic matter, there is an overlap between their distributions.
Figure 9. Schematic of the discretized medium from the realizations in Figure 6. The grid blocks (cells) are small enough to assure that each cell is either organic matter or inorganic-mineral matrix. A pore diameter is assigned to each cell depending on whether it is organic matter (Figure 8a) or inorganic matter (Figure 8b). The permeability of each cell is calculated with Eq. (5). Then, we calculate the total apparent permeability (AP) with Eq. (16), as shown in Figure 2.

Figure 10. Pressure map of 2D (300µm × 175µm) steady-state fluid flow of a realization in Figure 6 and in discretized form as depicted in Figure 9. The color bar is pressure in MPa. The properties of the sample are shown in Table 4. The pressure gradient in y direction is negligible, and the assumption of no cross flow leads to negligible error.
Figure 11. Permeability map for one of the 2D realizations (left: 30µm × 30µm; right: 300µm × 300µm) shown in Figure 6. The color-scale bar is permeability in µD.

Figure 12. Permeability variation versus sample size. Y-axis is total apparent permeability of the sample in µD. X-axis is the edge length of the sample. The shape of the sample is square. The mean permeability reaches a plateau around sample size of 200 µm and the standard deviation goes approximately to zero, meaning that the REV size could be 200 µm.
Figure 13. Schematic diagram of the pulse decay experimental set. Temporal changes of pseudo-pressure ($m$) in upstream and downstream vessels as well as pseudo-pressure difference ($\Delta m$) across the core are illustrated.

Figure 14. Analytical and numerical solution of the pulse-decay experiment and the experimental data. Our proposed method is used for calculating permeability.
Figure 15. The pore-size distribution of two shale samples (Kuila, 2013).
Find the number of pores using the pore volume and the pore size

Find the volume of sorbed gas using Eq. (31)

Convert the calculated gas volume to the gas volume in reservoir condition using a suitable EOS

Find the expanded pore size using Eq. (32)

Update the pore sizes in organic matter and calculate the apparent permeability

Figure 16. The algorithm for integrating the sorption process in calculating apparent permeability.
Figure 17. Predictions of stochastic model (SM). Sensitivity of apparent permeability (AP) to volumetric TOC. All other parameters are the same as presented in Table 4. The value of AP decreases as TOC increases mainly because pores within the organic matter are smaller than pores within the inorganic matter, causing the permeability to decrease.

Figure 18. Sensitivity of apparent permeability (AP) to tortuosity (τ). All other parameters are the same as shown in Table 4. The trend of permeability change versus tortuosity is the same for both methods because the fluid can flow more easily in a straight tube than in tortuous channels.
Figure 19. Sensitivity of apparent permeability (AP) to average pressure, accounting for adsorption. All other parameters are the same as shown in table 4. Increasing pressure will decrease the AP.
Figure 20. Sensitivity of apparent permeability (AP) to the mean pore diameter of organic matter ($\mu$). As stated above, the pore-size distribution in each medium is lognormal. $\mu$ and $\sigma$ are the mean and standard deviation of the log transformation of pore size. All other parameters are listed in Table 4. The curve corresponding to the zero standard deviation ($\sigma$) represents the realizations in which the pore sizes within organic matter are constant along the whole sample (the mean of organic-matter pore-size distribution). The trends show that increasing the mean of pore size increases the AP of the sample.
Figure 21. Sensitivity of apparent permeability (AP) to the mean pore diameter of inorganic matter (µ). As stated above, the pore-size distribution in each medium is lognormal. µ and σ are the mean and standard deviation of the log transformation of pore size. All other parameters are the same as shown in Table 4. The curve corresponding to the zero standard deviation (σ) represents the realizations in which the pore sizes within inorganic matter are constant along the whole sample (the mean of inorganic-matter pore-size distribution). Increasing the mean of pore size increases the AP of the sample.
Highlights:

- Stochastic model reveals permeability relation to pores in organic and inorganic
- Stochastic model allows selective sorption process in organic pores
- TOC and spatial distribution of organic matter affect permeability