# A Novel Multiphysics Multiscale Multiporosity Shale Gas Transport Model for Geomechanics/Flow Coupling in Steady and Transient States

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## Summary

A novel multiphysics multiscale multiporosity shale gas transport ($M^3ST$) model was developed to investigate shale gas transport in both transient and steady states. The microscale model component contains a kerogen domain and an inorganic matrix domain, and each domain has its own geomechanical and gas transport properties. Permeabilities of various shale cores were measured in the laboratory using a pulse decay permeameter (PDP) with different pore pressure and confining stress combinations. The PDP-measured apparent permeability as a function of pore pressure under two effective stresses was fitted using the microscale $M^3ST$ model component based on nonlinear least squares fitting (NLSF), and the fitted model parameters were able to provide accurate model predictions for another effective stress. The parameters and petrophysical properties determined in the steady state were then used in the transient-state, continuum-scale $M^3ST$ model component, which performed history matching of the evolutions of the upstream and downstream gas pressures. In addition, a double-exponential empirical model was developed as a powerful alternative to the $M^3ST$ model to fit laboratory-measured apparent permeability under various effective stresses and pore pressures. The developed $M^3ST$ model and the research findings in this study provided critical insights into the role of the multiphysics mechanisms, including geomechanics, fluid dynamics and transport, and the Klinkenberg effect on shale gas transport across different spatial scales in both steady and transient states.

Key Points:

- An $M^3ST$ model accounts for the coupling of geomechanics and gas transport in shale.
- Microscale parameters fitted to laboratory data lead to successful history matching of gas pressure evolutions at the core scale.
- A double-exponential empirical model successfully describes apparent permeability changes under various effective stress and pore pressure.

## Introduction and Background

Production of hydrocarbon energy resources from shale, a fine-grained, low-permeability geological formation, has changed the global energy outlook. Recovery of shale oil and gas has become economically viable due to the development of hydraulic fracturing and horizontal drilling (Montgomery and Smith 2010; Chen et al. 2013; Gu and Mohanty 2014; Stringfellow et al. 2014; Wang et al. 2018). Compared with conventional enhanced oil and gas recovery (Li et al. 2016b; Wang et al. 2017; Zhao et al. 2017; Tang et al. 2019), unconventional resource development is generally associated with a wide range of benefits such as job growth and improved infrastructure and municipal developments.

Extensive research on the correlation between effective stress and shale permeability has been conducted using both laboratory experiments and analytical models (Akkutlu and Fathi 2012; Alnoaimi and Kovscek 2013; Mehmani et al. 2013; Heller et al. 2014; Chen 2016; Ghanbarian and Javadpour 2017; Guo et al. 2018; Sheng et al. 2018; Wang et al. 2019; Zhang et al. 2021). It is generally expected that the permeability of a shale formation decreases with increasing effective stress due to compressed pore space and closure of microscale fractures. In addition to effective stress, the apparent (i.e., measured) permeability of a shale formation depends on the pore pressure if the testing fluid is a gas. This phenomenon is caused by nanoscale pores in shale and is referred to as the Klinkenberg effect. In 1941, Klinkenberg developed the gas slippage theory (i.e., the Klinkenberg effect) to explain the enhancement of measured apparent permeability for gas flow in nanopores (Klinkenberg 1941). The Klinkenberg effect occurs when the mean-free path of the measured gas molecules is longer than the diameter of the nanopore through which they travel. Consequently, gas molecules collide with the pore walls more frequently than with one another, leading to Knudsen diffusion that causes a slip-velocity boundary condition on the pore walls, which enhances the apparent permeability of the nanopore. Therefore, the Klinkenberg effect has a critical impact on gas flow in porous media having ultralow permeability (Wu et al. 1998). Although the Klinkenberg effect may not influence the apparent permeability under in-situ high reservoir pressures (Civan 2020), it plays an important role in the interpretation of laboratory measurements because pore pressures used in laboratory experiments can be at the levels where the Klinkenberg effect is noticeable (Soeder 1988; Li et al. 2020).

The Knudson number (Kn) is an important dimensionless number relevant to the Klinkenberg effect. Kn is calculated as the ratio of the gas mean-free-path length $\lambda$ to the effective pore width $h$. The Navier-Stokes equations can be used to describe gas flow with a no-slip boundary condition on the pore walls when Kn is smaller than 0.001. When the Kn is increased to the range between 0.001 and 0.1, the gas flow is in the slip flow regime in which the noncontinuum effect at the solid/fluid boundary can be accounted for using a velocity slip on the pore walls; the Navier-Stokes equations can still be used to describe the bulk gas flow (Beskok and Karniadakis 1999). The continuous increase of Kn into the range between 0.1 and 10 will lead to the transitional flow regime, followed by the free molecular flow regime when Kn is larger than 10, in which the Navier-Stokes equations cannot be used to describe gas flow in the pores (Tian et al. 2019).

Because of the important implication of the Klinkenberg effect to shale gas transport, a variety of analytical approaches have been developed to describe gas flow subjected to the Klinkenberg effect in tight porous media (Wu et al. 1998; Innocentini and Pandolfelli

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2001; Zhu et al. 2007; Hu et al. 2009; Hayek 2015; Li et al. 2019, 2020; Yuan et al. 2020). In addition, many studies have been conducted to investigate the Klinkenberg effect and its role on multiphase flow (Blanchard et al. 2007), the dynamic Klinkenberg coefficient (Wang et al. 2014), and fractal theory (Li et al. 2016a). All these studies confirmed that the permeability of tight reservoir rocks depends closely on effective stress and the Klinkenberg effect.

Despite numerous previous studies on the relationship between shale's apparent permeability, effective stress, and pore pressure, a mechanistic model is still needed to adequately describe the multiphysics multiscale processes that regulate shale gas transport in tight formations. The lack of such a mechanistic, theoretical model was due to several challenges. First, the model needs to have a multiporosity geometry to differentiate kerogen (i.e., organic matter) and inorganic matrix at the microscopic scale (Chen 2016), because it is the nanopores in kerogen that cause the Klinkenberg effect in shale. Second, the model needs to account for multiphysics mechanisms, including geomechanics, fluid flow and transport, and the Klinkenberg effect, because the effective stress and pore pressure in a shale gas reservoir influence the apparent permeability of the formation through these multiphysics mechanisms. Third, the model should be multiscale and also reasonably simple so that it can be easily calibrated by laboratory core permeability measurements and upscaled to history match continuum-scale pore pressure evolutions. To solve these challenges, in this study, a novel $M^3ST$ model was developed to describe shale gas transport in both transient and steady states, which provides mechanistic insight into the dependence of shale's apparent permeability on effective stress and pore pressure.

## Overview of the Experimental/Modeling Approaches

This section provides an overview of the experimental and modeling approaches used in this paper, including the details for the principle of a pressure PDP and how it measures shale core permeability and the upstream and downstream gas pressure evolutions in the transient state. The section Determination of the Biot's Coefficient introduces basic theories of the Biot's coefficient and Klinkenberg effect, which are relevant to the role of effective stress and pore pressure, respectively, on shale's apparent permeability. The section $M^3ST$ Model develops a novel $M^3ST$ model to study gas transport in shale in both transient and steady states. Particularly, the microscale $M^3ST$ model component was used to fit PDP measurements of shale permeability based on NLSF to determine critical model parameters; the fitted model parameters were used to predict shale permeability under other effective stresses and then imported into the macroscale component of the $M^3ST$ model to history match continuum-scale gas pressure evolutions measured by the PDP. The section A Novel Double-Exponential Empirical Model derives a double-exponential empirical model to describe the dependence of shale's apparent permeability on effective stress and pore pressure. The section Results and Discussion provides experimental and modeling results as well as discussions and implications.

**Fig. 1** illustrates the Eagle Ford and Mancos shale cores used in this study. The two Eagle Ford cores were marked as "Eagle Ford 1A" and "Eagle Ford 1B," and the two Mancos cores were marked as "Mancos 1A" and "Mancos 1B." The cores were 2-in. in length and 1 in. in diameter. The bedding plane direction was parallel to the core axis direction. The total organic carbon contents were 2.02 and 1.37%, respectively, for the Eagle Ford and Mancos cores.

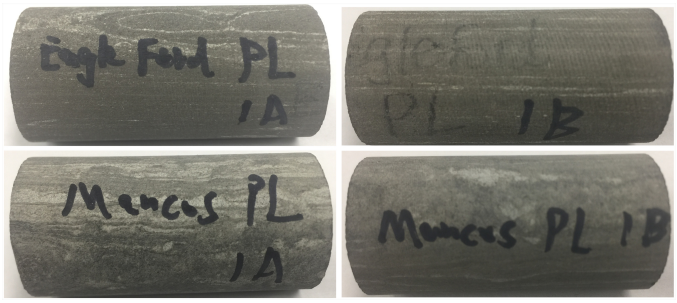


**Fig. 1—Two Eagle Ford shale core plugs (top row) and two Mancos shale core plugs (bottom row) for the PDP permeability measurements. The shale core plugs were 2 in. in length and 1 in. in diameter. The shale bedding plane direction was parallel to the core plug axis direction.**

**Fig. 2** illustrates a schematic plot of the PDP equipment setup, which provides a convenient and dynamic approach for measuring the apparent permeability of tight rocks (Jones 1997). First, with the fill valve and Valves 1 through 4 opened, all the gas reservoirs are filled to the desired starting pressure. The upstream reservoir volume $V_1$ and downstream reservoir volume $V_2$ are both 10 $cm^3$. Next, the fill valve is closed, and after a period of soaking time (usually 300 seconds) Valve 2 is closed. Gas in the downstream reservoir $V_2$ will then be released through the needle valve and shut-off valve to obtain a pressure lower than the upstream reservoir pressure, which is referred to as the differential pressure $\Delta P$. When $\Delta P$ stabilizes, Valves 3 and 4 are both closed. Gas molecules will gradually penetrate through the core sample to migrate from the upstream reservoir to the downstream reservoir, leading to continuously decreasing upstream reservoir pressure and increasing downstream reservoir pressure. In this process, the differential pressure $\Delta P$ continuously decays. The higher the permeability of the core plug, the faster the decay of $\Delta P$. The permeability of the core plug can then be calculated based on the decay rate of $\Delta P$ following the standard procedure of PDP analysis (Dicker and Smits 1988; Jones 1997).

## Determination of the Biot's Coefficient

During the recovery of unconventional hydrocarbon resources, increased effective stress can cause rock matrix deformation, which plays a vital role on the petrophysical properties of the shale formation during production, including permeability (Fan et al. 2018, 2021b), wettability (Guo et al. 2020), and fluid phase behavior (Zhao et al. 2021). Based on the poroelasticity theory from Biot (1941), a porous medium's deformation influences the fluid flow and vice versa. The Biot's coefficient (i.e., Biot's poroelastic term) is a critical concept for the effective stress calculation in a porous medium, which represents the fluid volume change induced by bulk volume changes in the drained condition (Müller and Sahay 2016). The calculation of Biot's coefficient can be based on various correlations, and Civan (2021) summarized these equations used in the literature, which include linear, power-law, exponential, inverse, logarithmic,

and modified power-law correlations. According to Terzaghi et al. (1996), the pore pressure of the fluid reduces the effective stress in a rock mineral matrix, and Biot's coefficient describes the reduction of effective stress quantitatively (Bernabe 1986):

$$P_e = P_c - \chi P_p, \quad \ldots\ldots (1)$$

where $\chi$ is Biot's coefficient; and $P_e$, $P_c$, and $P_p$ are effective stress, confining pressure, and pore pressure, respectively. Previous studies (Warpinski and Teufel 1992; Cheng 1997; Lee 2002; Ojala and Fjær 2007; Tan and Konietzky 2014; Selvadurai 2019) have used both laboratory experiments and theoretical methods to estimate the $\chi$ value in a certain type of rock.

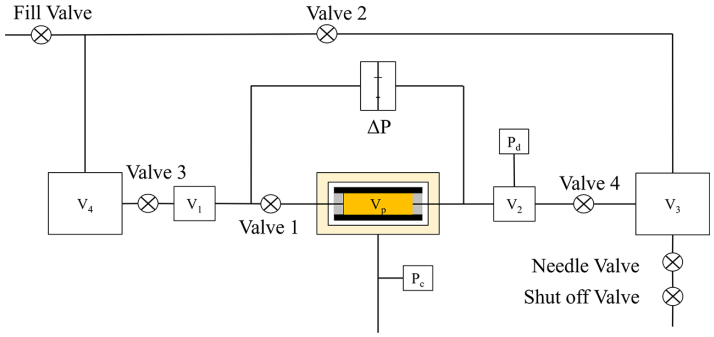


**Fig. 2—Schematic PDP equipment setup, which consists of an upstream gas reservoir having a volume of $V_1$, a high-strength core holder that contains the core sample having a pore volume (PV) of $V_p$, a downstream gas reservoir having a volume of $V_2$, two large gas reservoirs $V_3$ and $V_4$ that stabilize the initial gas pressures in $V_1$ and $V_2$, a differential pressure transducer to continuously measure the differential pressure, $\Delta P$, and a pressure transducer to measure the downstream reservoir pressure, $P_d$. This diagram was modified from the CoreLaboratories, Inc. PDP-200 operation manual.**

In this study, we used the PDP to measure shale's apparent permeability under various pore pressures and confining pressures to calculate the Biot's coefficient based on Geertsma (1957), Kwon et al. (2001), and Civan (2021). Because the apparent permeability $k_a$ depends on both $P_p$ and $P_c$, we express $k_a$ as a function of these two independent variables:

$$k_a = k_a(P_c, P_p), \quad \ldots\ldots (2)$$

Because the permeability of natural geologic formations in general follows a lognormal distribution (Chen and Zeng 2015), we make a logarithm transformation for Eq. 2 and obtain

$$\log(k_a) = \log[k_a(P_c, P_p)]. \quad \ldots\ldots (3)$$

Taking the differential of Eq. 3 leads to

$$\mathrm{d}\log(k_a) = \left(\frac{\partial \log(k_a)}{\partial P_c}\right)\mathrm{d}P_c + \left(\frac{\partial \log(k_a)}{\partial P_p}\right)\mathrm{d}P_p. \quad \ldots\ldots (4)$$

Similarly, taking the differential of Eq. 1 leads to:

$$\mathrm{d}P_e = \mathrm{d}P_c - \chi \mathrm{d}P_p. \quad \ldots\ldots (5)$$

When the pore pressure is sufficiently high, the Klinkenberg effect is inhibited; in this scenario, the apparent permeability is equal to the absolute permeability, which depends only on the pore geometry that is controlled by the effective stress. Therefore, when the change of effective stress $\mathrm{d}P_e$ is zero, the change of apparent permeability $\mathrm{d}\log(k_a)$ is also zero. Therefore, Eqs. 4 and 5 lead to

$$0 = \left(\frac{\partial \log(k_a)}{\partial P_c}\right)\mathrm{d}P_c + \left(\frac{\partial \log(k_a)}{\partial P_p}\right)\mathrm{d}P_p, \quad \ldots\ldots (6)$$

and

$$0 = \mathrm{d}P_c - \chi \mathrm{d}P_p. \quad \ldots\ldots (7)$$

Combining Eqs. 6 and 7, one can solve for the Biot's coefficient $\chi$ as follows:

$$\chi = -\left(\frac{\partial \log(k_a)}{\partial P_p}\right) \Big/ \left(\frac{\partial \log(k_a)}{\partial P_c}\right). \quad \ldots\ldots (8)$$

The Klinkenberg effect) was introduced to explain the difference between measured permeability (i.e., apparent permeability) and absolute permeability in tight rocks. The Klinkenberg coefficient $b$ was applied to quantify the influence of pore pressure and nanopore size on the measured apparent permeability:

$$\frac{k_a}{k} = 1 + \frac{b}{P_p}, \quad \ldots\ldots (9)$$

where $k_a$ and $k$ are apparent permeability ($m^2$) and absolute permeability ($m^2$), respectively, and $b$ is the Klinkenberg coefficient (Pa). The Klinkenberg coefficient depends on the rock's petrophysical properties and can be determined based on the analysis of the mass fluxes contributed by the Knudsen diffusion and viscous flow. The value of $b$ in a planar nanopore can be expressed as (Chen 2016; Li et al. 2020):

$$b = \frac{2\mu}{h}\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + \frac{4\mu}{h}\sqrt{\frac{8RT}{\pi M}}, \quad \ldots\ldots\ldots\

$$Q_i = \frac{k_{ai}}{\mu} \cdot \nabla P_p \cdot h_i = \frac{{h_i}^3}{12} \cdot \frac{\nabla P_p}{\mu} \left(1 + \frac{b_i}{P_p}\right)$$
$$Q_k = N \cdot \frac{k_{ak}}{\mu} \cdot \nabla P_p \cdot h_k = N \cdot \frac{{h_k}^3}{12} \cdot \frac{\nabla P_p}{\mu} \left(1 + \frac{b_k}{P_p}\right). \quad \ldots\ldots (15)$$

In Eq. 15, the Klinkenberg coefficients $b_i$ and $b_k$ are calculated based on Eq. 10:

$$b_i = \frac{2\mu}{h_i}\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + \frac{4\mu}{h_i}\sqrt{\frac{8RT}{\pi M}}$$
$$b_k = \frac{2\mu}{h_k}\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + \frac{4\mu}{h_k}\sqrt{\frac{8RT}{\pi M}}. \quad \ldots\ldots (16)$$

The pore widths in Eq. 15 are subject to the effective stress and calculated as

$$h_i = h_{i0}(1 - \beta_i P_e)$$
$$h_k = h_{k0}(1 - \beta_k P_e), \quad \ldots\ldots (17)$$

where $h_{i0}$ and $h_{k0}$ are the initial (i.e., reference) pore widths in the inorganic matrix and kerogen domain, respectively; $P_e$ is the effective stress and calculated as $P_e = P_c - \chi P_p$; and $\beta_i$ and $\beta_k$ are the isothermal compressibility coefficients for pore width in the inorganic matrix and kerogen domain, respectively, which describe pore width's responses to the change of effective stress.

In Eq. 14, the total porosity $\phi$ can be calculated as

$$\phi = \frac{h_i + Nh_k}{h_i + Nh_k + S} = \frac{h_{i0}(1 - \beta_i P_e) + Nh_{k0}(1 - \beta_k P_e)}{h_{i0}(1 - \beta_i P_e) + Nh_{k0}(1 - \beta_k P_e) + S}. \quad \ldots\ldots (18)$$

Plugging Eqs. 14–18 into Eq. 13, one can rewrite Eq. 13 as:

$$\overline{k_a} = \frac{[h_{i0}(1 - \beta_i P_e)]^3 \left[1 + \frac{2\mu\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + 4\mu\sqrt{\frac{8RT}{\pi M}}}{h_{i0}(1 - \beta_i P_e)P_p}\right] + N \cdot [h_{k0}(1 - \beta_k P_e)]^3 \left[1 + \frac{2\mu\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + 4\mu\sqrt{\frac{8RT}{\pi M}}}{h_{k0}(1 - \beta_k P_e)P_p}\right]}{12[h_{i0}(1 - \beta_i P_e) + N \cdot h_{k0}(1 - \beta_k P_e) + S]}. \quad \ldots\ldots (19)$$

Eq. 19 is the microscale component of the M$^3$ST model based on our previous work (Li et al. 2020) for predicting the overall apparent permeability $\overline{k_a}$ for a shale sample that consists of an inorganic matrix and a kerogen domain. This model takes two independent input variables on the right-hand side of Eq. 19, which are the effective stress $P_e$ and the pore pressure $P_p$.

Using the same approach, one can calculate the apparent permeabilities of the inorganic matrix and kerogen domain as follows:

$$k_{ai} = \frac{[h_{i0}(1 - \beta_i P_e)]^3}{12[h_{i0}(1 - \beta_i P_e) + (1 - \varepsilon_{ks}) \cdot S]} \cdot \left[1 + \frac{2\mu\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + 4\mu\sqrt{\frac{8RT}{\pi M}}}{h_{i0}(1 - \beta_i P_e)P_p}\right]$$
$$k_{ak} = \frac{N \cdot [h_{k0}(1 - \beta_k P_e)]^3}{12[N \cdot h_{k0}(1 - \beta_k P_e) + \varepsilon_{ks} \cdot S]} \cdot \left[1 + \frac{2\mu\left(\frac{2}{\alpha} - 1\right)\sqrt{\frac{8\pi RT}{M}} + 4\mu\sqrt{\frac{8RT}{\pi M}}}{h_{k0}(1 - \beta_k P_e)P_p}\right]. \quad \ldots\ldots (20)$$

Similarly, these two equations take $P_e$ and $P_p$ as model inputs on the right-hand side. The model outputs are the inorganic matrix apparent permeability $k_{ai}$ and kerogen apparent permeability $k_{ak}$ separately.

The parameters in the microscale M$^3$ST model component (Eq. 19) were determined through PDP data fitting and then plugged into Eq. 20 to determine $k_{ai}$ and $k_{ak}$, which were then used in the continuum-scale M$^3$ST model component (Eqs. 21 through 23) to simulate the transient-state pressure evolutions at the larger (inch) scale. Particularly, the continuum-scale M$^3$ST model component is based on the fully coupled, two-porosity transport model published in our previous study (Chen 2016), and gas transport processes in the kerogen domain and inorganic matrix are described by Eqs. 21 and 22, respectively:

$$\varepsilon_{kp}\phi\frac{\partial C_k}{\partial t} + \varepsilon_{ks}(1 - \phi)\frac{\partial C_\mu}{\partial t} = \frac{\partial}{\partial x}\left[zRTC_k\frac{k_{ak}}{\mu}\frac{\partial C_k}{\partial x}\right] + \Gamma, \quad \ldots\ldots (21)$$
$$(1 - \varepsilon_{kp})\phi\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x}\left[zRTC_i\frac{k_{ai}}{\mu}\frac{\partial C_i}{\partial x}\right] - \Gamma, \quad \ldots\ldots (22)$$

where $\varepsilon_{kp}$ is kerogen PV per unit total PV and can be written as $\varepsilon_{kp} = (N \cdot h_{k0})/(N \cdot h_{k0} + h_{i0})$; $C_k$ and $C_i$ are the molar concentrations of free gas within the kerogen and inorganic matrix in the unit of moles per kerogen PV and inorganic PV, respectively (mol/m$^3$); $C_\mu$ is adsorbed gas molar concentration within kerogen in the unit of moles per kerogen solid volume (mol/m$^3$); $\phi$ is the total porosity accounting for interconnected pores within both kerogen and inorganic matrix; $x$ is the distance in the longitudinal direction (m); $t$ is time (seconds); $z$ is the compressibility factor; $\Gamma$ is the mass transfer rate between kerogen and inorganic matrix (mol/m$^3$/s), which can be written as $\Gamma = m(C_i - C_k)$, where $m$ is the mass exchange rate coefficient (1/seconds). Based on the Langmuir adsorption model, the mass exchange in the kerogen domain between adsorbed gas and free gas can be expressed as

$$\frac{\partial C_\mu}{\partial t} = K_{\text{des}}\left[K(C_{\mu\max} - C_\mu)C_k - C_\mu\right], \quad \ldots\ldots\ldots\

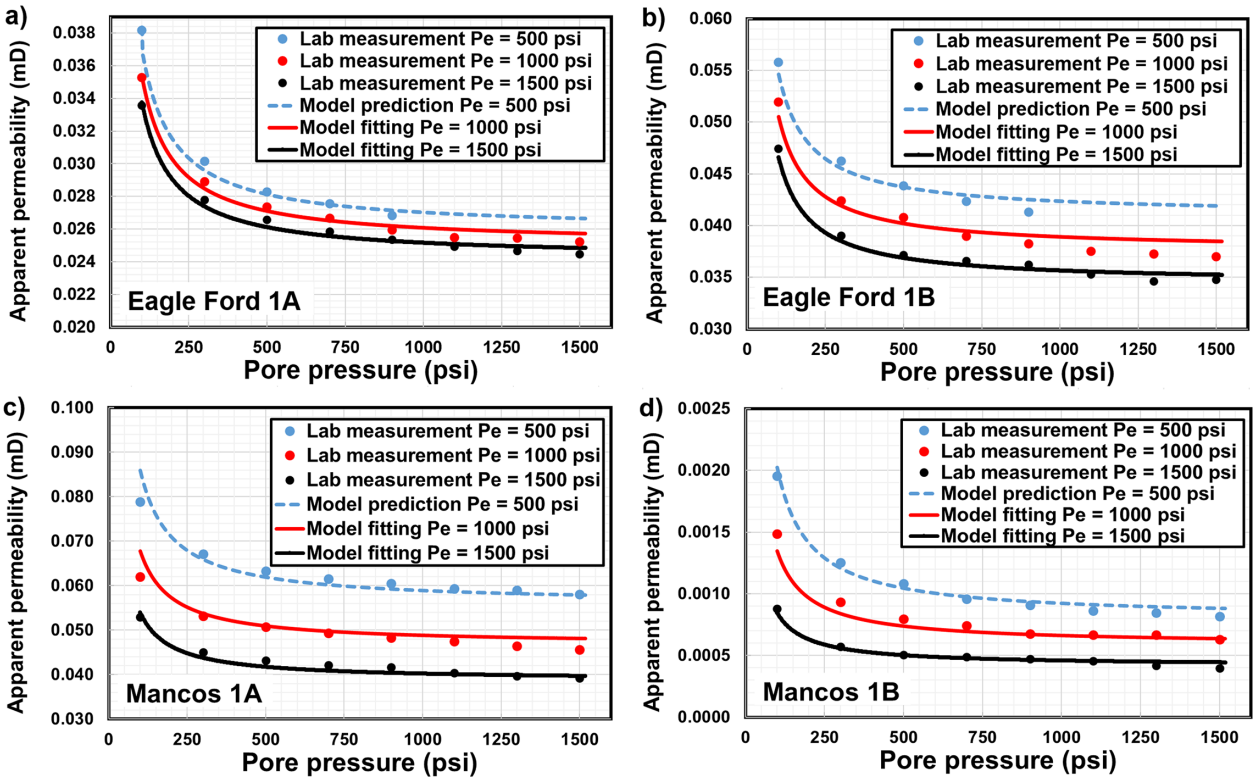


**Fig. 4—PDP-measured apparent permeability (scatter data points) as a function of pore pressure and effective stress. The solid-line curves were obtained by fitting the M$^3$ST model to the PDP measurements at $P_e$ = 1,000 and 1,500 psi based on NLSF. The dash-line curve was the M$^3$ST model prediction of the apparent permeability at $P_e$ =500 psi using the model-fitted parameters.**

Fig. 4 also illustrates the M$^3$ST model fitting and predictions. Specifically, the two solid-line curves are the fitting curves based on the M$^3$ST model, and the dash-line curve is the model prediction. Particularly, PDP-measured apparent permeability values as a function of pore pressure under effective stresses of 1,000 and 1,500 psi were fitted using the M$^3$ST model with NLSF, and the fitted parameters were then used in the model to predict the apparent permeability values under effective stress of 500 psi. **Table 2** demonstrates the six unknown parameters in the M$^3$ST model that were determined by fitting experimental PDP data. In this study, the Gauss-Newton method, an iteration-based algorithm for solving NLSF problems, was used to determine the six unknown parameters in the M$^3$ST model through data fitting. Particularly, the vector of the unknown parameters $\boldsymbol{\beta}$, which has six elements in this case, is calculated by

$$\boldsymbol{\beta}^{n+1} = \boldsymbol{\beta}^{n} + \left(\mathbf{J}^T\mathbf{J}\right)^{-1}\mathbf{J}^T\mathbf{r}, \quad \ldots\ldots\ldots\

where $k_{ai}$ is the $i$th PDP measurement of apparent permeability, $\hat{k}_{ai}$ is the corresponding prediction using the M$^3$ST model, and $N$ is the total number of measurements. The NMSE is a measure to evaluate the relative error of model predictions compared to experimental observations. The smaller the NMSE value, the lower the relative error. The parameters fitted using the measurements under effective stresses of 1,000 and 1,500 psi led to accurate predictions of apparent permeability as a function of pore pressure under the effective stress of 500 psi for all four shale samples. This NMSE result indicates that the microscale M$^3$ST model component successfully accounted for the mechanistic, multiphysics mechanisms that regulate shale's apparent permeability in the steady state.

| $P_e$ | Eagle Ford 1A | Eagle Ford 1B | Mancos 1A | Mancos 1B |
|---|---|---|---|---|
| 500 psi | $7.85\times10^{-5}$ | $3.47\times10^{-4}$ | $1.69\times10^{-3}$ | $1.73\times10^{-3}$ |

Table 3—NMSE values for M$^3$ST model predictions of shale's apparent permeability under effective stress of 500 psi.

**Fig. 5** illustrates the laboratory PDP measurements as well as the double-exponential empirical model (i.e., Eq. 24 fitting based on NLSF for all four shale core samples). The data point at $P_e = 500$ psi and $P_p = 100$ psi was selected as the reference point, so $P_{e0}$ and $P_{p0}$ were 500 and 100 psi, respectively. $k_0$ was the PDP-measured apparent permeability at the reference point. $k_{a0}$ was the absolute permeability when $P_e = 500$ psi (i.e., stable value of apparent permeability at the right end of the blue solid lines in Fig. 5). The double-exponential empirical model can overall capture the apparent permeability variation as a function of both pore pressure and effective stress.

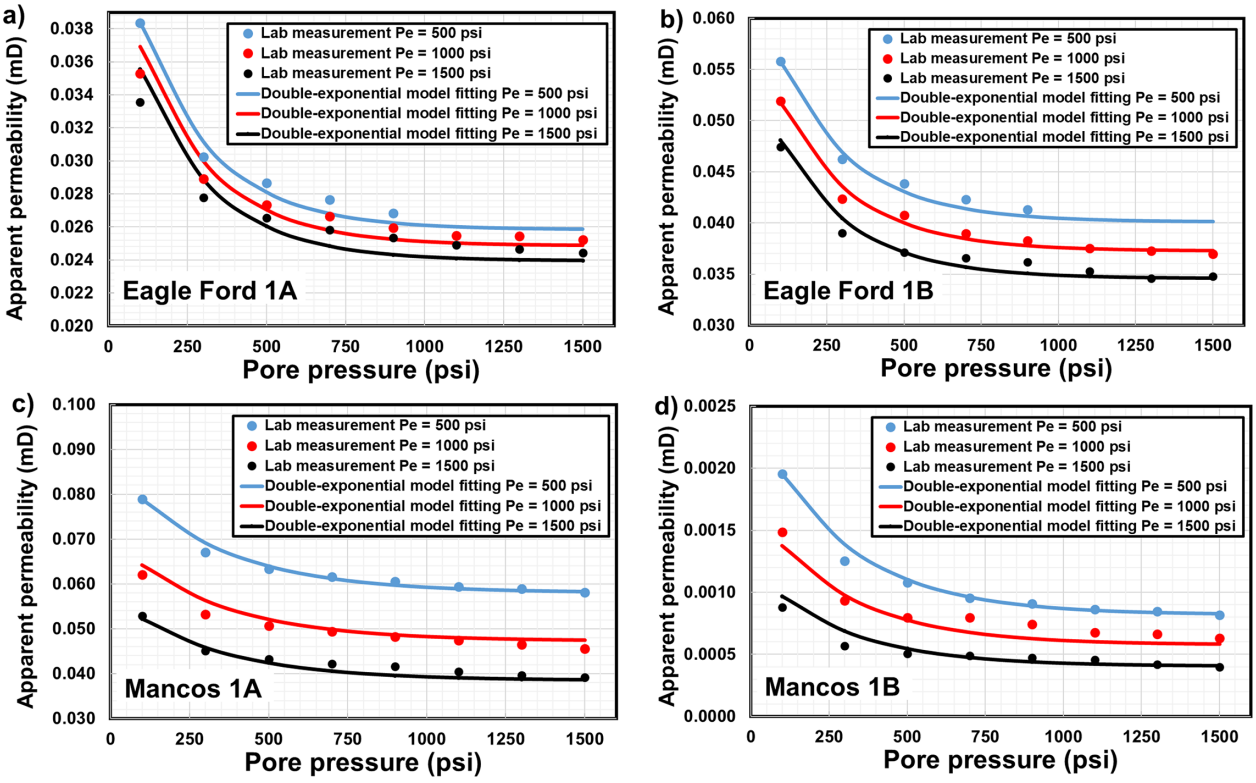


**Fig. 5—PDP-measured apparent permeability (scatter data points) as a function of pore pressure and effective stress. The solid-line curves were obtained by fitting the double-exponential empirical model to the PDP measurements based on NLSF.**

**Table 4** demonstrates the comparison of the NMSE values for global data fitting using the M$^3$ST model (i.e., Eq. 19) and the double-exponential empirical model (i.e., Eq. 24). Global data fitting means that the model was used to fit all the laboratory PDP measurements under effective stresses of 500, 1,000, and 1,500 psi. Therefore, the NMSE value was calculated based on the experimental measurements under all the effective stresses. Table 4 shows that the NMSE measures of the M$^3$ST global data fitting were overall lower than those for the global data fitting using the empirical model, which confirms that the M$^3$ST model was based on the first principles and thus successfully accounted for the mechanistic, multiphysics processes that regulate shale's apparent permeability under various combinations of pore pressures and effective stresses.

| Sample | NMSE of M$^3$ST Global Fitting | NMSE of Empirical Model Global Fitting |
|---|---|---|
| Eagle Ford 1 A | $1.27\times10^{-4}$ | $1.10\times10^{-3}$ |
| Eagle Ford 1B | $2.18\times10^{-4}$ | $3.04\times10^{-4}$ |
| Mancos 1 A | $1.13\times10^{-3}$ | $6.32\times10^{-4}$ |
| Mancos 1B | $4.24\times10^{-3}$ | $6.60\times10^{-3}$ |

Table 4—NMSE values for global fitting using the M$^3$ST model and the double-exponential empirical model.

In practice, however, the double-exponential empirical model has some advantages because of its simplicity. **Table 5** illustrates the modulus values in Eq. 24, determined by fitting all the laboratory PDP measurements using NLSF based on the Gauss-Newton method. The values of $\gamma_2$ were in general higher than those of $\gamma_1$. This implies that the pore pressure influenced shale's apparent permeability more noticeably than effective stress in the current range of pore pressure. The double-exponential empirical model can be used as a powerful alternative to the M$^3$ST model to fit laboratory-measured apparent permeability under various pore pressures and effective stresses because of its simple formulation and small number of undetermined parameters.

| Sample | $\gamma_1$ (psi$^{-1}$) | $\gamma_2$ (psi$^{-1}$) |
|---|---|---|
| Eagle Ford 1 A | $7.61\times10^{-5}$ | $4.30\times10^{-3}$ |
| Eagle Ford 1B | $1.49\times10^{-4}$ | $4.10\times10^{-3}$ |
| Mancos 1 A | $4.12\times10^{-4}$ | $3.10\times10^{-3}$ |
| Mancos 1B | $7.03\times10^{-4}$ | $3.40\times10^{-3}$ |

Table 5—Fitted values of $\gamma_1$ and $\gamma_2$ in the double-exponential empirical model.

The fitted parameters in the microscale M$^3$ST model component (Eq. 19) were used to calculate the apparent permeabilities of kerogen and inorganic matrix based on Eq. 20, which were then imported into the continuum-scale M$^3$ST model component (i.e., Eqs. 21 through 23) for large-scale, transient-state simulations of gas pressure evolutions in the core. Other known parameter values used in the continuum-scale M$^3$ST model component were $C_{\mu\max} = 1800\,\text{mol/m}^3$, $\text{K} = 1.7\times10^{-4}\,\text{m}^3/\text{mol}$, $K_{\text{des}} = 1.4\times10^{-7}\,\text{s}^{-1}$, $M = 0.028\,\text{kg/mol}$, $m = 3.0\times10^{-6}\,\text{s}^{-1}$, $T = 298\,\text{K}$, and $\mu = 1.75\times10^{-5}\,\text{Pa·s}$. We used these parameter values from previous studies (Pribylov et al. 2014; Chen 2016) because the variations of these parameter values did not noticeably affect the numerical model output at the experimental time scale, which was dominated by the apparent permeability of the inorganic matrix $k_{ai}$, because viscous flow in the inorganic matrix was the dominant mechanism that regulated core-scale pressure evolutions at the time scale of interest. **Fig. 6** illustrates the transient-state M$^3$ST simulations that were used to history match the PDP-measured upstream and downstream gas pressure evolutions. Experimental conditions used in the laboratory PDP measurements are shown in **Table 6.** Particularly, the values of downstream gas pressure $P_d$ and pressure difference $\Delta P$ were experimental readings from the pressure transducers. The confining pressure in these PDP measurements was fixed at 1,500 psi. In the continuum-scale simulations, the pore pressure in each gridblock was solved in each timestep using the implicit finite difference scheme, and then the effective stress in each gridblock was determined using Eq. 1. Therefore, the pore pressure and effective stress in each gridblock continuously changed. Consequently, the kerogen permeability and inorganic matrix permeability of each gridblock were updated in each timestep using the updated pore pressure and effective stress values based on Eq. 20. However, it should be noted that the variations of kerogen permeability and inorganic matrix permeability were minimal because the value of $\Delta P$ was much lower than that of $P_d$. In practice, we only needed to make minor adjustments on $h_{i0}$, $h_{k0}$, $\beta_i$, and $\beta_k$ based on their fitted values shown in Table 2 to match the simulated pressures to the PDP-measured pressures. Overall, the continuum-scale M$^3$ST simulations managed to history match the PDP-measured evolutions of upstream and downstream gas pressures. This indicates that the kerogen and inorganic matrix permeabilities, determined through the microscale M$^3$ST-model-fitted parameters, can successfully match the laboratory PDP experimental data using large-scale, transient-state pressure predictions based on the continuum-scale M$^3$ST model component (i.e., Eqs. 21 through 23). This suggests that the M$^3$ST model is able to account for the dominant mechanisms that regulate geomechanics and gas flow at both the microscopic and continuum scales.

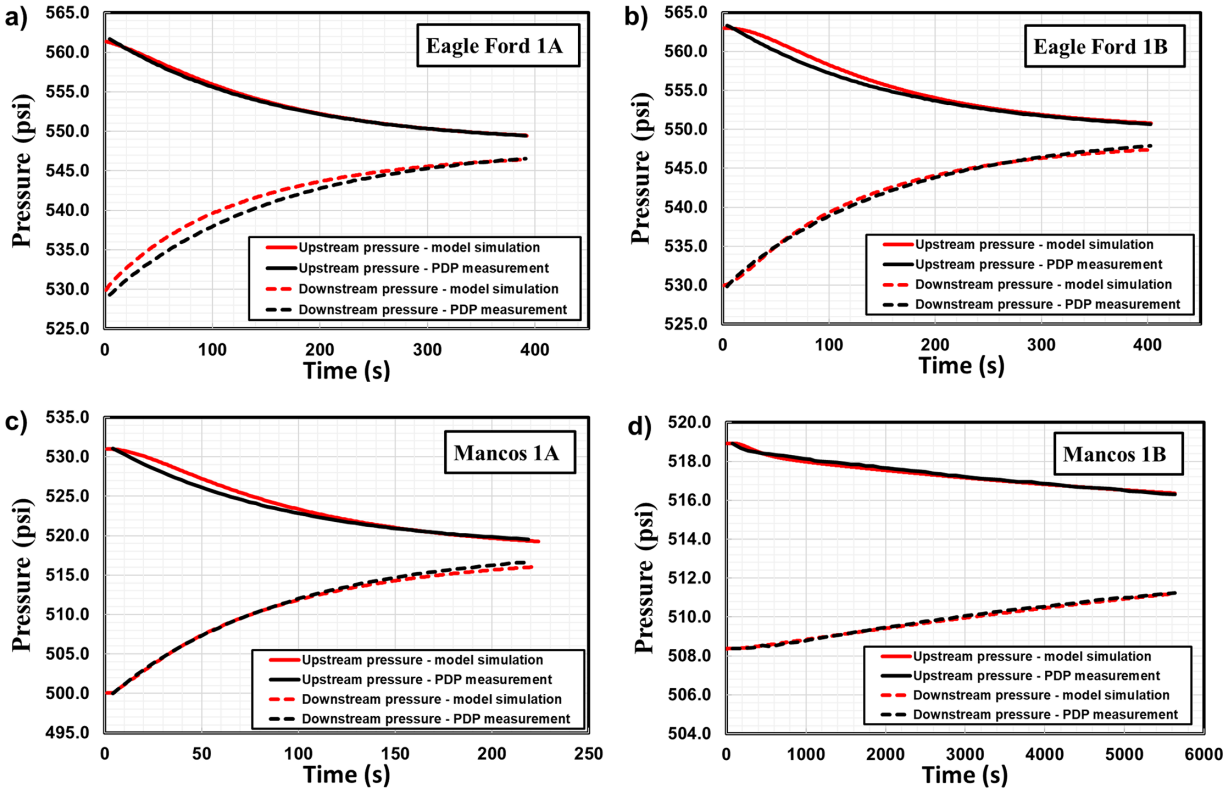


**Fig. 6—History matching of PDP-measured upstream and downstream gas pressures using the continuum-scale M$^3$ST model component.**

| Parameter | Eagle Ford 1A | Eagle Ford 1B | Mancos 1A | Mancos 1B |
|---|---|---|---|---|
| Initial $\Delta P$ (psi) | 32.4 | 33.4 | 31.0 | 10.5 |
| Initial $P_u$ (psi) | 561.7 | 563.3 | 531.0 | 518.9 |
| Initial $P_d$ (psi) | 529.3 | 529.9 | 500.0 | 508.4 |

Table 6—Experimental conditions in PDP measurements. $P_u$ and $P_d$ are gas pressures in the upstream and downstream reservoirs, respectively. $\Delta P$ is the difference between $P_u$ and $P_d$.

**Fig. 7** illustrates a sensitivity analysis that studied the effect of the apparent permeability of the inorganic matrix $k_{ai}$ on upstream and downstream pressure evolutions, which were simulated using the continuum-scale M$^3$ST model component. Three values of $k_{ai}$ were used in this sensitivity analysis, including $1\times10^{-2}$, $1\times10^{-3}$, and $1\times10^{-4}$ md. The sensitivity analysis demonstrated that the value of $k_{ai}$ significantly influenced the variations of the upstream and downstream gas pressures. A high value of $k_{ai}$ (e.g., $1\times10^{-2}$ md) resulted in relatively fast variations of the upstream and downstream gas pressures, leading to a rapid decay rate of the pressure difference. It was also noticed that the evolutions of upstream and downstream gas pressures were relatively insensitive to other parameters in the continuum-scale M$^3$ST model component. This is because in a shale core plug the overall apparent permeability is primarily contributed by the inorganic pores, and thus a higher inorganic permeability is favorable for faster gas molecule migration from the upstream end to the downstream end, leading to a faster decay rate of the pressure difference.

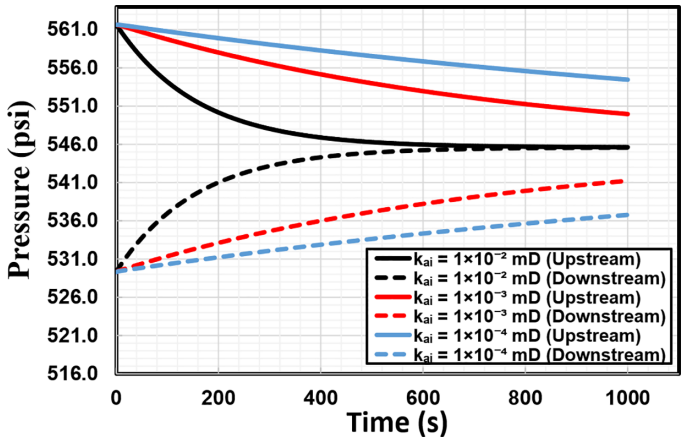


**Fig. 7—Impact of the apparent permeability of inorganic matrix $k_{ai}$ on upstream and downstream gas pressure evolutions.**

## Conclusions

A novel M$^3$ST model was developed to investigate gas transport in shales in both steady and transient states using experimental and modeling approaches. The microscale M$^3$ST model component contains a kerogen domain and an inorganic matrix domain, both of which are subjected to confining stress. Each domain has its respective geomechanical and gas transport properties. We used a laboratory PDP to measure the permeabilities of various shale cores to calibrate the microscale M$^3$ST model component and to quantify the parameters in the steady state. We used the microscale M$^3$ST model component to fit the PDP-measured apparent permeability as a function of pore pressure under two effective stresses based on NLSF, and the fitted model parameters were able to provide accurate model predictions for other effective stresses. We then imported the parameters and petrophysical properties determined in the steady state into the transient-state, continuum-scale M$^3$ST model component, which performed history matching of the evolutions of the upstream and downstream gas pressures as a function of time at the core scale. In addition, we introduced a double-exponential empirical model, which is a powerful alternative to the M$^3$ST model to fit laboratory-measured apparent permeability under various pore pressures and effectives stresses because of its simple formulation and small number of undetermined parameters. The M$^3$ST model and the research findings in this study provided critical insights into the role of the multiphysics mechanisms, including geomechanics, fluid dynamics and transport, and the Klinkenberg effect on the transport of shale gas across different spatial scales in both steady and transient states.

## Nomenclature

$A$ = model total cross-sectional area, m$^2$
$A_i$ = inorganic matrix cross-sectional area, m$^2$
$\mathbf{A_k}$ = kerogen cross-sectional area, m$^2$
$b$ = Klinkenberg coefficient, Pa
$b_i$ = Klinkenberg coefficient of inorganic matrix, Pa
$b_k$ = Klinkenberg coefficient of kerogen, Pa
$C_i$ = molar concentration of free gas within the inorganic matrix, mol/m$^3$
$C_k$ = molar concentration of free gas within the kerogen, mol/m$^3$
$C_\mu$ = adsorbed gas molar concentration within kerogen, mol/m$^3$
$C_{\mu\max}$ = maximum monolayer adsorption of gas molar concentration within kerogen, mol/m$^3$
$h$ = effective pore width, m
$h_i$ = effective pore width in inorganic matrix, m
$h_{i0}$ = reference pore width in inorganic matrix, m
$h_k$ = effective pore width in kerogen, m

$h_{k0}$ = reference pore width in kerogen, m
$k$ = absolute permeability, $m^2$
$k_a$ = apparent permeability, $m^2$
$k_{a0}$ = reference absolute permeability, $m^2$
$\overline{k_a}$ = overall apparent permeability, $m^2$
$k_{ai}$ = apparent permeability of inorganic matrix, $m^2$
$k_{ak}$ = apparent permeability of kerogen, $m^2$
$k_{ap}$ = model-predicted apparent permeability, $m^2$
$k_0$ = reference measured permeability, $m^2$
$K$ = equilibrium partition coefficient, $m^3$/mol
$K_{ads}$ = adsorption rate coefficient, $m^3$/s/mol
$K_{des}$ = desorption rate coefficient, 1/s
$m$ = mass-exchange-rate coefficient, 1/s
$M$ = molar mass, kg/mol
$N$ = number ratio
$P_c$ = confining pressure, Pa
$P_d$ = downstream pressure of measured sample, Pa
$P_e$ = effective stress, Pa
$P_p$ = pore pressure, Pa
$P_u$ = upstream pressure of measured sample, Pa
$Q_i$ = flow rate in the inorganic matrix, $m^3$/s
$Q_k$ = flow rate in the kerogen, $m^3$/s
$R$ = gas constant, J/mol/K
$S$ = model solid cross-sectional area, $m^2$
$t$ = running time, seconds
$T$ = absolute temperature, K
$x$ = distance in the core longitudinal direction, m
$z$ = compressibility factor
$\alpha$ = tangential momentum accommodation coefficient
$\beta_i$ = compressibility of inorganic matrix, 1/Pa
$\beta_k$ = compressibility of kerogen, 1/Pa
$\gamma_1$ = permeability modulus for effective stress, 1/psi
$\gamma_2$ = permeability modulus for pore pressure, 1/psi
$\Gamma$ = mass transfer rate between kerogen and inorganic matrix, mol/$m^3$/s
$\Delta P$ = differential pressure in the PDP measurement, Pa
$\varepsilon_{kp}$ = kerogen pore volume per unit total pore volume
$\varepsilon_{ks}$ = kerogen solid volume per unit total solid volume
$\lambda$ = free gas mean-free-path length, m
$\mu$ = dynamic viscosity, Pa·s
$\rho$ = free gas mass density, Pa·s
$\phi$ = total porosity
$\chi$ = Biot's coefficient

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