Gas Flow Models of Shale: A Review

Farzam Javadpour,* Harpreet Singh, Arash Rabbani, Masoud Babaei,* and Samira Enayati

Cite This: https://dx.doi.org/10.1021/acs.energyfuels.0c04381

ABSTRACT: Conventional flow models based on Darcy’s flow physics fail to model shale gas production data accurately. The failure to match field data and laboratory-scale evidence of non-Darcy flow has led researchers to propose various gas-flow models for the shale reservoirs. There is extensive evidence that suggests the size of the pores in shale is microscopic in the range of a few to hundreds of nanometers (also known as nanopores). These small pores are mostly associated with the shale’s organic matter portion, resulting in a dual pore system that adds to the gas flow complexity. Unlike Darcy’s law, which assumes that a dominant viscous flux determines a rock’s permeability, shale’s permeability leads to other flow processes besides viscous flow such as gas slippage and Knudsen diffusion. This work reviews the dominant gas-flow processes in a single nanopore on the basis of theoretical models and molecular dynamics simulations, and lattice Boltzmann modeling. We extend the review to pore network models used to study the gas permeability of shale.

1. INTRODUCTION

Permeability models generally describe the relationship between the fluid flux and the parameters that control the flux, e.g., pressure gradient and gas and rock properties. The conventional model to predict rock permeability is based on Darcy’s law, which assumes a constant permeability of a rock for a Newtonian fluid flowing through that rock over a constant pressure gradient. However, shale permeability does not adhere to Darcy’s law due to tiny pore sizes and heterogeneity that affect fluid flow in many ways not described by Darcy’s law. In other words, shale permeability is dynamic such that it does not necessarily remain constant and is impacted by different mechanisms of fluid transport besides advective flow.1,2 The vast majority of expressions in the literature focus on predicting the permeability of the matrix. This work reviews gas transport in shale at two spatial scales: in a single nanopore and in a network of nanopores. There are many models in the literature, and a detailed review of each model is lengthy. Instead, we chronologically tabularize various shale permeability models with their pros and cons. We review essential gas-flow regimes and different physical processes of the gas flow in a single pore. Next, we review published models based on first-principles, molecular dynamics (MD) simulations, lattice Boltzmann methods (LBM), and pore network.

2. GAS-FLOW PROCESSES

Flow regimes are generally defined on the basis of the range of Knudsen numbers. Different flow regimes differ in terms of their physics and the type of applicable models. Knudsen number (Kn) is a ratio of the mean free path (λ) of a gas molecule to a characteristic length (s) of the flowing medium (e.g., channel height, pore size, and so on), where λ is a function of the temperature of the flowing gas (T) and the average gas pressure (p) as follows:

\[ \text{Kn} = \frac{\lambda}{s} = \left( \frac{k_BT}{\sqrt{2} \pi \sigma^2 p} \right) \frac{1}{s} = f(s, p) \]  

(1)

where \( k_B \) is the Boltzmann constant and \( \sigma \) is the molecule size.

Table 1 presents flow regimes as a function of Kn, their physics, and suitable models. Continuum models such as the Darcy equation are applicable for \( \text{Kn} \leq 0.01 \), whereas, for \( \text{Kn} \geq 10 \), free-molecule models should be used. The Kn estimated using eq 1 and the corresponding flow regimes for various characteristic lengths and average flowing pressures are shown in Figure 1.

2.1. Gas Slippage. Knudsen3,4 showed that rarefied gas flows could not adequately describe the compressible form of the no-slip Navier–Stokes–Fourier model.5 A generic approach to defining rarefied gas flow is by revising the basic continuum-scale equations of momentum, mass, and heat transfer for their no-slip boundary conditions. Several techniques include slip boundary conditions, including Maxwell slip6 (first-order approximation from the kinetic theory of gases), second-order slip,7 and Langmuir slip.8–10 The above slip models are not appropriate for the flow in transition and molecular regimes (see Table 1 and Figure 1), and advanced methods such as molecular dynamics simulation (MD), Boltzmann gas–kinetic models,11–15 direct simulation Monte Carlo (DSMC), and Burnett equations set16,17 are needed. If there is an adsorbed water film on the inner pore wall, then the gas slippage should be with the coating water

Received: December 29, 2020    Revised: January 16, 2021
and not the mineral.\textsuperscript{15,16} The section below presents a brief review of the velocity slip in terms of governing equations.

2.1.1. Velocity Slip. First-order Maxwell slip condition (slip velocity) for dilute and ideal monatomic gases flowing over a solid boundary surface is as follows:\textsuperscript{6,17,18}

\[
\sigma = -\frac{\partial u}{\partial z} = \frac{\lambda}{\mu} \left( \frac{\partial u}{\partial z} \right)_{w} = \frac{\rho T}{\mu} \left( \frac{\partial u}{\partial z} \right)_{w}
\]

for medium with curvature due to an axial temperature gradient

Here, $\sigma$ is the tangential momentum accommodation coefficient (TMAC), $u_{\text{slip}}$ is the slip velocity of the gas at the solid boundary surface; $u_t$ is the gas velocity in a direction parallel to the solid boundary surface ($x$ direction); $u_z$ is the gas velocity in a direction perpendicular to the solid boundary surface ($z$ direction); $u_w$ is the velocity at the solid boundary surface; $\rho$ is the gas’s density; and subscript $w$ represents the boundary surface (wall). Colin\textsuperscript{19} suggested that for significantly rough surfaces, the expression for slip velocity on curved surfaces is equally applicable.

2.1.2. Measurement of Gas Slip Velocity. There is no consensus on the most appropriate equation to handle gas slip velocity.\textsuperscript{20} Accurate TMAC values are not well characterized as a function of the gas type, material, and rarefaction degree, especially for shale. Maxwell’s equation overcomes these limitations:

\[
u_{\text{slip}} = u - u_w
\]

\[
\left( \frac{\partial u}{\partial z} \right)_{w} = \frac{\lambda}{\mu} \left( \frac{\partial u}{\partial z} \right)_{w} + \frac{\lambda}{\mu} \left( \frac{\partial u}{\partial z} \right)_{w}
\]

Here, $\sigma$ is the tangential momentum accommodation coefficient (TMAC), $u_{\text{slip}}$ is the slip velocity of the gas at the solid boundary surface; $u$ is the gas velocity in a direction parallel to the solid boundary surface ($x$ direction); $u_z$ is the gas velocity in a direction perpendicular to the solid boundary surface ($z$ direction); $u_w$ is the velocity at the solid boundary surface; $\rho$ is the gas’s density; and subscript $w$ represents the boundary surface (wall). Colin\textsuperscript{19} suggested that for significantly rough surfaces, the expression for slip velocity on curved surfaces is equally applicable.

2.1.3. Second-Order Velocity Slip. The linear first-order slip velocity obtained from the original (nonlinear) model in which the slip velocity is directly proportional to the degree of non-equilibrium near the wall surface as follows:\textsuperscript{17}

\[
\frac{2 - \alpha}{\alpha} \left( \frac{\partial u}{\partial z} \right)_{w} = b \left( \frac{\partial u}{\partial z} \right)_{w}
\]
\[ u_{\text{slip}} = u_i - u_w = \frac{2 - \frac{\sigma_g}{\sigma_u}}{\frac{\Pi}{\mu}} (\frac{\Pi}{\mu}) + \frac{3 (\gamma - 1)}{4 \gamma \Pr} (\frac{Q_s}{\rho}) \]

(4)

Here, \( \gamma \) is the specific heat ratio and \( \Pr \) is the Prandtl number. The first-order slip velocity is obtained when the degree of non-equilibrium is linear with the first-order accuracy, such that shear stress \( \Pi \propto \frac{\partial \sigma}{\partial \varepsilon} \) and tangential heat flux \( Q_s \propto \frac{\partial \sigma}{\partial \varepsilon} \). These first-order terms approximate the well-known first-order slip velocity discussed earlier. The resulting slip velocity model becomes a second-order velocity slip when the constitutive relations are second-order approximations, or in other words \( \Pi \propto \left( \frac{\partial \sigma}{\partial \varepsilon} \right)^2 \) and \( Q_s \propto \left( \frac{\partial \sigma}{\partial \varepsilon} \right)^2 \). Second-order velocity slip models have been developed for their application in the gaseous Knudsen layer’s theoretical analysis, which shows that the Knudsen layer can be described within a continuum framework by considering second-order velocity slip.

### 2.2. Gas Diffusion

Diffusive transport in shale formations can occur through three different types of diffusion mechanisms, which are (i) molecular bulk diffusion, (ii) surface diffusion (sorption), and (iii) Knudsen diffusion.\(^{23}\) The relative magnitude of each diffusion mechanism depends on the value of Knudsen number, where medium with large \( Kn \) experiences a relatively larger magnitude of Knudsen diffusion in comparison to the other two types of diffusion mechanisms. Knudsen diffusion exists when the molecules interact more often with the pore’s wall than with each other. The diffusive flux of the gas is the entire molar flow rate from the two opposite directions \( \bar{n} = \frac{1}{6} \lambda A \bar{v} \frac{\partial c}{\partial \varepsilon} \) across an axis with a cross-sectional area \( (A) \), which is mathematically defined as follows:

\[ J = \frac{\bar{n}}{A} = \frac{1}{3} \lambda A \bar{v} \frac{\partial c}{\partial \varepsilon} = -D \frac{\partial c}{\partial \varepsilon} \]

(5)

Here, \( D \left( \frac{1}{3} \bar{v} \right) \) is the diffusivity coefficient that depends on the type of diffusion mechanism. For Knudsen diffusion \( (D_{Kn}) \), \( A \) is the cross-sectional area, \( \bar{v} \) is the average velocity of gas molecules, and \( c \) is the gas concentration in mole per unit volume. In Knudsen diffusion, a medium’s characteristic length \( (\lambda) \) is generally equivalent to \( \lambda \) and \( \bar{v} \) follows Maxwellian distribution given by \( \nu = \frac{\sqrt{8RT}}{\pi M} \). The Knudsen diffusion coefficient is

\[ D_{Kn} = \frac{1}{3} \lambda A \bar{v} \]

(6)

Here, \( M \) is the molar mass of gas and \( R \) is the universal gas constant.

The effective diffusive flux is the summation of all three types of diffusive flux terms:\(^{22,23}\)

\[ \frac{1}{J_{eff}} = \frac{1}{J_m} + \frac{1}{J_{Kn}} + \frac{1}{J_{sorp}} \]

(7)

Here, \( J_{eff} \) is the effective diffusive flux that is the harmonic average of flux terms due to molecular diffusion \( (J_m) \), Knudsen diffusion \( (J_{Kn}) \), and sorption \( (J_{sorp}) \).

Among the discussed diffusion mechanisms, the significance of the surface diffusion in gas transport within the micropores has been a controversial subject.\(^{24,25}\) On the one hand, several studies have shown that surface diffusion can dominate methane transport in an organic matter.\(^{24,26,27}\) Some simulation studies\(^{26,28,29,30,31}\) have considered the surface diffusion an essential gas transport process in shale due to the strong adsorptive nature of the organic matter in shale. Other researchers\(^{32–35}\) argued that many adsorption sites would be occupied or discontinued due to the pore’s water layers. Therefore, surface diffusion cannot be the leading player in gas transport. Table 2 summarizes the reported surface diffusion coefficients of methane in organic pores. Except for Yang et al., most measured surface diffusion values are between \( 10^{-8} \) and \( 10^{-6} \) m\(^2\)/s. Although the surface diffusion coefficient depends on the gas pressure, Wu et al.\(^{36}\) showed that the dependency is negligible. Increasing the gas pressure 5 orders of magnitude only doubles the surface diffusion coefficient. The limited adsorption sites on the pore walls at elevated pressures explain the mentioned trend.\(^{36}\)

### 3. PERMEABILITY MODELS

The effective permeability observed in the field is a combination of its matrix and induced fractures. Some models have proposed an expression to predict the combined permeability of matrix and fracture;\(^{1,2}\) however, most works focus on predicting the matrix’s permeability. Table 3 summarizes shale permeability models in chronological order. Table 3 presents a brief description of each model with its pros and cons.

#### 3.1. Applicability of Klinkenberg Model

Several studies have proposed various expressions to predict shale’s permeability since the boom in energy production from shale resources in the United States. Before that, there was only one well-known model proposed by Klinkenberg\(^{37}\) that applies to shale to some extent. It includes the effect of gas slippage on gas permeability through a linear relationship between the inverse of pressure and apparent gas permeability. The simple form of the Klinkenberg expression combined with its long legacy made it a popular model to predict shale’s permeability. It is still used widely in the industry as a standard model to predict gas permeability. Few studies\(^{38–41}\) that compared the Klinkenberg permeability of shale with their proposed models found that Klinkenberg permeability represents the permeability due to combined flux of Knudsen diffusion and slip flow. Although the Klinkenberg model works better than Darcy’s law, it still does not account for other mechanisms that impact the apparent gas permeability. Specifically, a gas flow mechanism that is not captured by the Klinkenberg model is surface diffusion. Moreover, there is a strong interaction between the gas and shale matrix (e.g., stress—strain, double-slip, g and as type, etc.) not captured by the Klinkenberg model.
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<th>ref</th>
<th>description</th>
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<tbody>
<tr>
<td>Javadpour129</td>
<td>The model developed using the slip flow assumption, represented by Maxwell’s theory. Accounts for Knudsen diffusion. Modeled only for straight capillary tubes.</td>
<td>Simple.</td>
<td>Limited to straight tubes. Ignores desorption and stress—strain effect.</td>
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<td>Civan130</td>
<td>The model developed using the slip flow assumption, represented by a simplified second-order slip model. Contains several empirical parameters.</td>
<td>Higher-order slip flow.</td>
<td>Several empirical parameters. Ignores stress—strain effect.</td>
</tr>
<tr>
<td>Sakhase-Pour and Bryant139</td>
<td>The model developed using the Navier—Stokes equation and kinetic theory (no-slip flow assumption). Accounts for Knudsen diffusion.</td>
<td>The geometry of porous media included.</td>
<td>Needs TMAC values. Does not explicitly account for desorption.</td>
</tr>
<tr>
<td>Wu et al.141</td>
<td>The model was developed by coupling slip flow and Knudsen diffusion.</td>
<td>Accounts for different pore shapes.</td>
<td>Ignores slip flow, and stress—strain effect.</td>
</tr>
<tr>
<td>Singh and Javadpour143</td>
<td>The model developed using the Langmuir slip condition and it does not carry several shortcomings associated with the use of Maxwell slip; Reliably predict apparent permeability in shale.</td>
<td>Simple and analytic. Gets slip coefficient from sorption data.</td>
<td>Ignores local heterogeneity and slip flow.</td>
</tr>
<tr>
<td>Cao et al.144</td>
<td>The model was developed by coupling viscous flow, Knudsen diffusion, and surface diffusion that also accounts for the stress—strain effect.</td>
<td>Accounts for stress—strain effects.</td>
<td>Ignores local heterogeneity, slip flow, and desorption.</td>
</tr>
<tr>
<td>Wang et al.145</td>
<td>The model developed by coupling viscous flow and Knudsen diffusion also accounts for the stress—strain effect.</td>
<td>Accounts for the spatial distribution of OM at a given scale. Accounts for stress—strain effects. Accounts for multiphase flow in fractures.</td>
<td>Requires spatial distribution of matrix and fractures in the rock. Ignores slip flow.</td>
</tr>
<tr>
<td>Singh and Cai146</td>
<td>Developed by discretizing shale into the matrix (organic and inorganic parts) and fractures based on a dual medium approach. Considers single-phase and two-phase flow in matrix and fracture, respectively.</td>
<td>Uses a unified diffusion coefficient that transforms its value per the flow regime.</td>
<td>Ignores local heterogeneity and the effect of stress.</td>
</tr>
<tr>
<td>Fan et al.147</td>
<td>The model was developed by coupling viscous flow, diffusion, and surface diffusion.</td>
<td>Accounts for system heterogeneity.</td>
<td>Ignores local heterogeneity. Ignores the effects of stress and strain. Complex numerical model.</td>
</tr>
<tr>
<td>Li et al.148</td>
<td>The model was developed by considering the effect of proppant embedding within hydraulic fractures, including the effect of sorption, stress, and slippage.</td>
<td>Accounts for system anisotropy by introducing permeability along with X and Y directions.</td>
<td>Ignores local heterogeneity.</td>
</tr>
<tr>
<td>Sheng et al.149</td>
<td>The model was developed by coupling viscous flow, diffusion, surface diffusion, and matrix deformation.</td>
<td>Accounts for surface diffusion through monolayer and multilayer.</td>
<td>Ignores stress—strain effect.</td>
</tr>
<tr>
<td>Sheng et al.150</td>
<td>Model adapted from ref 7 and based on fractal tortuous capillary tubes.</td>
<td>Accounts for system heterogeneity.</td>
<td>Complex numerical model and ignores desorption. Ignores stress—strain effect.</td>
</tr>
<tr>
<td>Yuan et al.151</td>
<td>Model adapted from ref 7 and based on fractal tortuous capillary tubes that also account for surface diffusion.</td>
<td>Accounts for system heterogeneity.</td>
<td>Ignores stress—strain effect. Several empirical parameters.</td>
</tr>
<tr>
<td>Wang et al.152</td>
<td>The model developed using viscous flow, and molecular diffusion based on a bundle of fractal tortuous capillary tubes.</td>
<td>Accounts for system heterogeneity.</td>
<td>Ignores slip flow, desorption, and stress—strain effect. Several empirical parameters.</td>
</tr>
<tr>
<td>Song et al.154</td>
<td>The model developed using bulk gas and surface diffusion based on a bundle of fractal tortuous capillary tubes.</td>
<td>Accounts for system heterogeneity.</td>
<td>Ignores stress—strain effect. Several empirical parameters.</td>
</tr>
<tr>
<td>Cai et al.155</td>
<td>The model developed using bulk gas and adsorbed gas based on fractal scale relationships for pore size distribution, the model shapes, tortuosity, surface roughness, and pore size influenced by stresses.</td>
<td>Accounts for the model scale heterogeneity with varying tortuous capillary diameters.</td>
<td>Ignores stress—strain effect. Several empirical parameters.</td>
</tr>
<tr>
<td>Sheng et al.156</td>
<td>The model developed using bulk gas and surface diffusion based on a bundle of fractal tortuous capillary tubes in 3D space.</td>
<td>Accounts for system heterogeneity at different scales. Accounts for stress—strain effects.</td>
<td>Several empirical parameters.</td>
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mechanism the sorption process. The LBM-based modeling of multi-potential to control the local density near the wall to consider implemented the Langmuir slip boundary to address velocity type, e.g., helium versus nitrogen.46 that the measured permeability strongly depends on the gas slippage and surface diffusion53 and multimechanism gas transport in shale.53–57 (ii) the introduction of the long-range force to address sorption;55,58,59 (iii) incorporation of semianalytical or analytical models into REV-scale models;50–62 (iv) consideration of the surface diffusion as a moving boundary;63,64 and (v) the coupling of LBM and molecular dynamics (MD) models.65,59 All of these works are subject to assumptions that require thorough justifications.

Many researchers used the concept of effective viscosity (or relaxation time) correction to study microscale gas flow in the reconstructed porous media via a regularized MRT-LBM.66–73 Note that the MRT-LBM model is a continuum-based CFD solver. In other words, the Navier–Stokes equations (NSE) can be recovered from the MRT-LBM by the multiscale analysis.74 The NSE is only valid for the continuum and slip flow regimes. The introduction of the effective viscosity correction75–79 dramatically extends the applicability of MRT-LBM to the transition and free molecule flow regimes (see Table 1 and Figure 1). However, these viscosity correction models only apply to straight long channels and should be used cautiously for the gas flow in porous media at high Knudsen-number conditions.80–82 Su et al.81 revealed that the MRT-LBM is not suitable to model gas flow at high Knudsen numbers through porous media due to the limited number of discrete velocities (e.g., D2Q9 or D3Q19). Higher-order LBM models, with more discrete velocities and high isotropy, are suitable for the gas flow at high Knudsen numbers.83–86 Nevertheless, higher-order LBM models require more computational resources, thereby having limited applicability in shale reservoirs. Recent studies showed that the discrete unified gas kinetic scheme (DUGKS),87 which combines LBM and the unified gas kinetic scheme, is a promising method to model gas flow in shale.88,89

The LBM—which originated from the kinetic theory of molecules90–94—is a mesoscopic numerical model. LBM with small and limited discrete velocity sets cannot accurately capture the nanoscale gas flow in shale, as pointed out above. The widely used LBM strategies, e.g., the velocity–slip boundary, the effective viscosity correction, and the introduction of interaction forces (such as Shan–Chen forces) between gas and wall, are developed at mesoscopic and macroscopic scales. To accurately model gas flow at the molecular level, the MD simulation is required. The MD’s accuracy comes with an exorbitant computational cost. A few models couple LBM and MD to take advantage of these models.59,65,91,72 Zhao et al.59 employed LBM and the grand canonical Monte Carlo method to predict the shale gas production considering gas sorption. MD is used to determine sorption parameters in these LBM models. Yu et al.65 also employed a similar coupling model approach to study viscous flow, gas slippage, and surface diffusion in shale. Li et al.91 calculated the density and pressure distributions near the pore wall in a different modeling approach. They subtracted the thickness of the adsorbed layer from the pore size before using the data in an LBM. Takbir-Borujeni et al.72 coupled MD, LBM, and the regularized 13-moment method to study multiscale and multimechanism gas transport in shale. Wang et al.92 coupled MD and a pore–network model for developing a multiscale framework for the gas flow in shale.

Many researchers used MD to study gas flow and sorption in shale nanopores.93–96 MD studies included methane diffusion,97–99 adsorption behavior,100–103 and gas transport.104–106 MD models can model gas transport processes in a microscopic spatial domain for a short time. Because of high computation, MD cannot model gas flow in pore

Figure 2. Comparison of Klinkenberg permeability with other permeability models.46 Reproduced from ref 40. Copyright 2016 Elsevier.

![Image](https://dx.doi.org/10.1021/acs.energyfuels.0c04381)

Figure 3. Three main types of the pore network models used for gas flow simulation in porous shales: (a) structured fully connected;109 (b) structured partially connected network;110 and (c) unstructured partially connected network.111

model. Researchers studied these other processes and compared their models with the Klinkenberg model.38–43 The variability in permeability as predicted by the Klinkenberg model and other models impacts gas production analysis from shale resources39,40,44 as shown in Figure 2.

Thorough experimental works support that even though the Klinkenberg relationship holds well for low-permeability rocks, it does not work well for shales.45 Experiments also showed that the measured permeability strongly depends on the gas type, e.g., helium versus nitrogen.46

3.2. LBM and MD Simulations. Ansumali and Kardin47 and Succi48 first initiated and other researchers developed49–52 the lattice Boltzmann modeling (LBM) of the gas flow in small pores. The fundamental strategy is to incorporate the first-order or second-order velocity-slip boundary condition into LBM to achieve a finite slip velocity along the tangential direction of a rigid wall. The exploitation of shale reservoirs involves complex multiscale33 and multimechanism flow, e.g., continuum flow, slip flow, transition flow, free molecule flow, and surface diffusion53 caused by methane adsorption and desorption. Fathi and Akkutlu47 first employed LBM to study slippage and surface diffusion’s coupling effects. They implemented the Langmuir slip boundary to address velocity slip along the wall. They also used the Shan–Chen interaction potential to control the local density near the wall to consider the sorption process. The LBM-based modeling of multimechanism flow includes (i) the incorporation of the Langmuir slip model into LBM;55–57 (ii) the introduction of the long-range force to address sorption;55,58,59 (iii) incorporation of semianalytical or analytical models into REV-scale models;50–62 (iv) consideration of the surface diffusion as a moving boundary;63,64 and (v) the coupling of LBM and molecular dynamics (MD) models.65,59 All of these works are subject to assumptions that require thorough justifications.
networks but can provide important parameters for the upscaled models.94,59,65

3.3. Pore Network Models. Pore network models (PNMs) are simplified realizations of porous microstructures initially designed to accelerate numerical simulations with minimal physical accuracy loss. Shale contains intricate porous microstructures with multiscale nature heterogeneity.107 Researchers used pore network modeling to study different physical problems from nanometer to micrometer length scales of shale.108 Three main types of network models to mimic the microstructure of the shale samples are (i) structured fully connected networks,109 (ii) structured partially connected networks,110 and (iii) unstructured partially connected networks111 as illustrated in Figure 3. Generally, network models with complex microstructures have limited capabilities of considering different gas flow processes. The limitation is because of the computation time. Educated and justified microstructure’s simplification can hold the validity of the PNM for shale.

Table 4 presents peer-reviewed PNM papers published from 2013 to 2020, including the physical, chemical, and morphological aspects of each PNM. The recent increase of the published PNM works devoted to shale indicates the robustness of PNM. Figure 4 shows the prevalence of gas flow processes in the PNM. Most PNM contributions considered only gas slippage and Knudsen diffusion. Surface diffusion, geochemistry, physical deformation, transient simulations, and realistic three-dimensional (3D) tomography received less attention. This section briefly describes the common approaches to simulate each of the mentioned physics in PNMs.

<table>
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<th>Reference</th>
<th>Compressible fluid</th>
<th>Real gas</th>
<th>Physical Deformation</th>
<th>Two-Phase</th>
<th>Transient simulation</th>
<th>Pressure drop</th>
<th>Knudsen diffusion</th>
<th>Slip flow</th>
<th>Surface diffusion</th>
<th>Geochemistry</th>
<th>Realistic 3D tomography</th>
<th>Reconstructed Geometry</th>
<th>Multiscale</th>
<th>Sorption</th>
<th>Pore space characterization</th>
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<td>Mehrmani et al. 114</td>
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Table 4. Summary of the Simulated Physics in Shale Pore Network Models Presented by Peer-Reviewed Papers between 2013 and 2020 (From References 107–116, 118, 119, and 146–166)
Desorption of a layer of adsorbed gas enlarges the OM pore dramatically. For example, desorption of a single layer of methane (with molecule size of 0.38 nm) from a circular cylindrical pore changes pore conductivity $\sim 16\%$. Figure 5 illustrates the pore shapes’ geometrical correction due to the thickness of the adsorbed gas layer. Yu et al. calculated correction factors for pores with four cross-sectional shapes: circle, square, triangle, and slit. Huang et al. and Wang et al. assumed square-shaped and circular cross-sections to derive the effective pore radii based on the gas pressure and sorption capacity.

4. CHALLENGES AND PERSPECTIVES

There were tremendous efforts to model gas flow in nanoporous shale. The biggest challenges are heterogeneity at different scales. Shale is a complex composite natural material. Therefore, the flowing gas interacts with various materials. The overall interaction of the gas molecules and different constituent components, e.g., organic and inorganic materials, control total gas flow. Models should be able to distinguish between these materials. Therefore, identifying these materials and locating them accurately in the models is of great importance. Recent digital shale efforts are to address the issue.

Another challenge is the small size of the controlling pores. To capture the accessibility of the small pores, we need extremely small grid blocks to build a representative elemental volume-scale model. The pores’ small size results in gas flow physics different from the gas flow physics in larger pores. The projection advances more in PNM and other numerical models.

PNM are useful tools to study different gas-flow processes in pore networks representing shale. The main concerns of PNM are the small size of the model (a few micrometers) and sometimes oversimplification of microstructure. PNM can be more realistic if we consider the interplay of in situ water (connate, capillary bound, and interstitial water) and gas molecules. It is better to use three-dimensional microstructures obtained from micro- and nanotomography techniques in PNM. Two-dimensional SEM images are acceptable as long as they are processed to 3D using reliable imaging techniques.

Most of the developed shale gas flow models consider either the matrix or the fracture. There is a need for unified models to capture both the matrix and fractures on the effective permeability. Current permeability models are not suitable for field-scale studies because of the multiscale heterogeneity in shale. Most of the research on shale gas flow models has focused on modeling microscale behavior of gas in shale, while only a few models focus on the scale-up aspect. More research on this issue is key to the practical applicability of shale permeability models to field scale.

5. CONCLUSIONS

The concluding remarks of the review on gas-flow models in shale are as follows.

- A shale gas permeability model should capture the small size of the pores, their interconnection, and the shale’s material heterogeneity.
- The governing physics in shale gas is different from conventional reservoirs because of the orders of magnitude smaller size of the pores. Gas slippage,
Knudsen diffusion, and surface diffusion are the minimum needed processes.

- Pore network models efficiently upscale the gas flow from nano- to microscale. Recent advances made PNMs computationally affordable and flexible to include several governing physics. They may still suffer from oversimplification of the morphologies. Image-based PNMs can improve realistic geometries in an unprecedented manner.
- Two of the most simulated physics in PNMs are gas slippage and Knudsen diffusion. Other physical processes, such as surface diffusion, geochemistry, and deformation, should be considered in future studies.

## AUTHOR INFORMATION

**Corresponding Authors**

- Farzam Javadpour — Bureau of Economic Geology, Jackson School of Geosciences, The University of Texas at Austin, Austin, Texas 78713, United States; orcid.org/0000-0002-9286-2403; Email: Farzam.javadpour@beg.utexas.edu
- Masoud Babaei — Department of Chemical Engineering and Analytical Science, The University of Manchester, Manchester M13 9PL, United Kingdom; orcid.org/0000-0002-4201-3489; Email: masoud.babaei@manchester.ac.uk

**Authors**

- Harpreet Singh — Bureau of Economic Geology, Jackson School of Geosciences, The University of Texas at Austin, Austin, Texas 78713, United States
- Arash Rabbani — Department of Chemical Engineering and Analytical Science, The University of Manchester, Manchester M13 9PL, United Kingdom
- Samira Enayati — Bureau of Economic Geology, Jackson School of Geosciences, The University of Texas at Austin, Austin, Texas 78713, United States

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.energyfuels.0c04381

**Notes**

The authors declare no competing financial interest.

**Biographies**

Farzam Javadpour is a Research Scientist at the University of Texas at Austin. Javadpour leads research works on novel techniques of permeability estimations. Farzam holds B.Sc., M.Sc., and Ph.D. degrees in chemical and petroleum engineering. He has published 62 peer-reviewed journal papers and 26 conference proceedings. Javadpour teaches Unconventional Reservoirs at UT-Austin. He has received multiple awards from the Society of Petroleum Engineers (SPE) and serves as associate editor of Transp. Porous Media. He has worked on image-based fluid transport modeling in heterogeneous porous materials accelerated with machine learning techniques.

Masoud Babaei is a senior lecturer (Associate Professor) at the University of Manchester and has joined the University of Manchester in 2014. He has a Ph.D. in Petroleum Engineering from Imperial College London, completed in 2013, and an M.Sc. degree in Reservoir Simulation from Sharif University of Technology, Iran, 2008. His expertise is modeling flow and transport in porous media across different length scales.

Samira Enayati has taught micro- and macro-economics at St. Edwards and Concordia Universities. She has worked as a research fellow at the UT-Austin and University of Calgary (Canada). Samira received B.Sc., M.Sc., and Ph.D. in Statistics and Economics from The University of Nice (France). Enayati coauthored a book titled Public Finance and Governmental Financial Strategies and eight papers. She has received awards from the Government and Alpes Maritimes province (France) and Quebec’s province (Canada).

## ACKNOWLEDGMENTS

This work was supported partly by the NanoGeosciences Laboratory and the Mudrock Systems Research Laboratory (MSRL) consortium at the Bureau of Economic Geology (The University of Texas at Austin). We also thank the University of Manchester for the President’s Doctoral Scholarship Award 2018 granted to A.R. to carry out part of this research. Also, M.B. acknowledges the Royal Society Grant No. IEC/NSFC/19002 for partially supporting this research. F.J. appreciates inputs from Hong Zuo in Section 3.2.

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