Pore Network Modeling Study of Gas Transport Temperature Dependency in Tight Formations

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ABSTRACT: Temperature's effects on rock permeability are ambiguous; both positive and negative correlations have been reported in the literature. Temperature can affect the geomechanical behavior of porous media, as well as influence the mode of fluid transport. Rocks are subject to deformation, compaction, and chemical alteration at elevated temperatures. Conversely, confined fluids can undergo augmented non-Darcian mechanisms. In this research, a multiscale, multiphysical study of temperature's effects on gas permeability in tight formations is presented.

INTRODUCTION

Both positive and negative correlations between rock permeability and temperature have been reported in the literature. Increasing the temperature can increase the degree of rock compaction and hence decrease the permeability. A temperature rise may also cause chemical alteration of the minerals, restricting the flow paths of fluids. The mechanical integrity of rock is subject to change at high temperatures. Geomechanical properties can be significantly influenced by temperature variations of injected fluids during hydraulic fracturing. The major focus of the aforementioned studies was the effects of temperature on rocks; exploration of how temperature changes affect fluids being transported has been limited to analyses of viscosity and thermal expansion. Recently, researchers pay attention to the significance of coupling rock and fluid modeling of temperature's effects for a more accurate description of transport in porous media.

Tight formations, classified as unconventional resources, exhibit non-Darcian transport mechanisms. Recent studies have shown that such mechanisms can be augmented at elevated temperatures. Enhanced diffusion can counteract thermal loading, indicating that the permeability of tight formations may either positively or negatively correlate with temperature. The objective of the present research is to couple the stress-related aspects of rocks with non-Darcian transport mechanisms to better understand the temperature's effects on the permeability of tight formations through pore network modeling.

THERMAL STRESS

In general, effective stress relates the pore pressure of rocks to applied stresses through Biot's coefficient

\[ \sigma_e = \sigma_a - nP_f \]

where \( \sigma_a \) is the effective stress, \( \sigma_a \) is the applied stress, \( P_f \) is the pore pressure, and \( n \) is Biot's poroelastic term, defined based on the bulk's modulus of a given rock.

At elevated temperatures, a thermal stress component is added to the above equation, following the Duhamel–Neumann approach

\[ \sigma_e = \sigma_a - nP_f + \beta T \]

where \( \beta \) is the thermal stress coefficient. This is related to the thermal expansion coefficient \( a_T \), Young's modulus \( E \), and Poisson's ratio \( \nu \), assuming a plane-strain deformation

\[ \beta = \frac{a_T E}{1 - 2\nu} \]

NON-DARCIAN TRANSPORT

Temperature reflects internal energy on a molecular level. As the temperature increases, molecule-to-molecule and molecule-to-wall collisions become more frequent. The average distance a molecule can travel before colliding with another molecule, known as the mean free path \( l \), is a parameter that has been used to address the likelihood of deviation from continuum flow to transition and free molecular diffusion regimes

\[ l = \frac{k_B T}{\sqrt{2} \pi d_i^2 P} \]

The mean free path \( l \) is proportional to \( T \) and inversely proportional to the pressure \( P \) and molecular size \( d_i^2 \) through Boltzmann's constant \( k_B \). In the case of ultratight rocks where pores are sized on micro- and nanoscales, the mean free path of...
lighter molecules is of a magnitude close to the pore size. Consequently, molecule-to-wall interactions become significant and can govern the overall transport.

Knudsen’s number $\text{Kn}$, which is the ratio of the mean free path $l$ to the pore size $L$, is used to characterize the mode of transport

$$\text{Kn} = \frac{l}{L} = \frac{k_B T}{\sqrt{2} \pi d^2 P L}$$

A Knudsen’s number $\text{Kn}$ greater than 0.01 indicates a deviation from the continuum flow (i.e., Darcy’s law is insufficient to describe the transport). The Knudsen’s number for ultratight formations is expected to be relatively large and positively correlated with temperature. Hence, the non-Darcian effects of tight formations are more pronounced at higher temperatures.

This deviation from Darcy’s law has been addressed in the literature by introducing the apparent permeability. Klinkenberg (1941) presented a permeability model as

$$k_{\text{app}} = k \left( 1 + \frac{b}{P} \right)$$

where $k_{\text{app}}$ is the apparent permeability. This is related to intrinsic permeability through the $b$ factor, which has been modeled to account for the slippage and Knudsen’s diffusion.

The correction factor $b$ in eq 6 can change with shifts in temperature and pressure. At reservoir conditions where linear and nonlinear thermal gradients exist, the temperature’s effect on $b$ can be significant. In the following section, the non-Darcian effect and thermal stress are discussed on the pore-scale level.

### PORE-SCALE COMBINED TRANSPORT MODEL

The transport equation for gas in single nanocapillaries has frequently been cited. In general, this approach is based on combining viscous and transition regimes. A nonempirical transport equation for nanopores that accounted for slippage and molecular diffusion effects is given as

$$q = \left( \frac{F \pi r^4}{8 \mu} + \frac{1}{P_p} \pi r^2 D_{\text{Kn}} \right) \frac{dP}{dx}$$

where $r$ is the radius of the nanopore, $P_p$ is the pore pressure, $\mu$ is the viscosity, and $D_{\text{Kn}}$ is Knudsen’s diffusivity coefficient.
\[
D_{Kn} = \frac{2r}{3} \sqrt{\frac{8RT}{\pi MW}}
\]

(8)

\[F = 1 + \left( \frac{8\pi RT}{MW} \right)^{0.5} \mu \left( \frac{2}{P_d^{0.5\alpha}} - 1 \right)\]

(9)

where \(\alpha\) is between 0 and 1 and related to the parts of molecules reflected diffusively from the walls, similar to a mirror-like reflection.\(^{22}\)

The transport described in the above equation is an explicit function of the pressure and pore radius. It is also a function of temperature as Knudsen’s diffusivity coefficient \(D_{Kn}\) and the slip velocity factor \(F\) are temperature-dependent.

The permeability of nanotubes is related to their radii, as given by the Hagen–Poiseuille relationship. Hence, the capillary size \(r\) is subject to change through the exponential relationship of the effective stress, including thermal loading (see eq 2)\(^{23}\)

\[r^2 = r_0^2 \exp[-c_s(r_0 - nP + \beta T)]\]

(10)

where \(c_s\) is the compressibility of the pores, and \(r_0\) is the pore size at zero effective stress.

**PORE NETWORK MODELING**

Performing experimental work on rock samples at varying temperatures is quite challenging and associated with a high degree of uncertainty due to heating/reheating hysteresis and the length of time it takes to reach the thermal equilibrium.\(^{24}\)

The concept of “digital rocks” or pore network models (PNMs) where pores are interconnected by throats provides an alternative means of performing parametric analysis. Pores are where fluid is stored, while throats or capillaries are the conduits for transport among those pores. A 3D arrangement of a pore/throat system can serve as a representation of a particular porous medium.\(^{3}\)

Similar to a previous research study on this topic, mass balance can be written for each pore as follows\(^{26}\)

\[\sum_{i=1}^{n} \rho q_i + \frac{d(\rho V)}{dt} = 0\]

(11)

where the first term is the sum of all fluxes entering the pore through \(n\) number of capillaries, with the flow rate \(q\) usually given by the classical Hagen–Poiseuille equation for cylindrical geometry. In our case, transport in the throats is governed by eq 7 to account for the non-Darcian transport mechanism. The second term of eq 11 indicates the accumulation of fluid inside the pores. Discretization of the mass balance yields a set of nonlinear equations that determine the total flow rate in the system.

**SENSITIVITY ANALYSIS AND DISCUSSION**

Temperature’s effects on gas transport on a nanoscale were studied across a range of pore sizes at relatively high and low pore pressures. The analysis was carried out for single capillaries without considering the thermal stress effect to investigate how temperature changes can influence transport. Equation 7 was used to obtain the velocity for different scenarios, with Darcian velocity serving as a reference. The results are given in Figure 1.

The velocity of methane positively correlated with temperature. Temperature was found to enhance the non-Darcian mechanisms that increase the overall velocity. The effects of temperature were more pronounced at lower pressures, where slippage and diffusion were dominant. As the capillary sizes increased, transport became less dependent on temperature, indicating the predominance of viscosity-driven transport.
The individual effects of slippage and Knudsen diffusion at elevated temperatures are presented here as a Darcian velocity multiplier for a single capillary with a size of 2 nm at 500 psi. The results given in Figure 2 indicate the temperature dependency of both mechanisms.

Next, thermal stress was coupled with the transport model to study the net effect of temperature on the permeability of tight rocks. In this stage, a pore network modeling approach involving pores interconnected by throats was used to mimic rock samples. At each pore, the mass balance given in eq 11 was solved with the flux determined by eq 7. The radius $r$ of the capillary was subject to change as a function of pressure and temperature, as given by eq 10. Throats and pores were sampled from predefined distributions to build a network through which gas could be transported. The pressure gradient was imposed by setting the value of the downstream to be lower than that of the upstream. The apparent permeability value was obtained from the flow rate, area, and pressure gradient. Detailed discretization of eq 11 is given in the Appendix, and a description of the model appears in Figure 3.

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The ratio of permeability at a given temperature to permeability at a reference temperature (i.e., ratio $= k_{app}(T)/k_{app}(T_0)$) was obtained for a range of pressure values and capillary size distributions, as shown in Figures 4–6. In general, the Knudsen and slippage diffusions increase with rising temperatures at a rate that depends on the pressure and size of the capillary. At high pressures, the molecule-to-wall interactions are insignificant compared to the molecule-to-molecule collisions, a condition that hinders slippage and diffusion. Hence, increasing the temperature favors thermal stress over non-Darcian effects, as shown in Figure 4. As the pressure decreases, the slippage and Knudsen’s diffusion become more significant, positively impacting the apparent permeability with the temperature increase (see Figures 5 and 6).

Conversely, capillary size negatively correlates with Knudsen’s number. Larger capillaries exhibit viscous transport over slippage and diffusion, which makes them more vulnerable to thermal stress at elevated temperatures (Table 1).

### CONCLUSIONS

Laboratory measurements of petrophysical parameters such as permeability are essential for optimum exploitation and reservoir management. The permeability of ultratight rocks is an active subject of study because of its dependency on pressure. In this research, it was shown that the permeability of ultratight rocks also correlates with temperature. This occurs through the two counteracting mechanisms of thermal stress and enhanced diffusion. The prevalence of one mechanism over the other is determined by pore pressure and the degree of confinement. A positive correlation between gas permeability and temperature was observed in the low to intermediate range of pressure in ultratight formations, while a negative correlation is expected as the formations become more permeable.

### APPENDIX A

#### A.1. Discretization of Mass Balance for Pore Network Modeling

1. Accumulation.

$$\frac{\partial (M V_p)}{\partial t} = \frac{PM V_p}{z_{avg, in}} \left( P_{z_t} - P_{z_{t-1}} \right)$$

2. 1D mass flux.

mass, in = $A_{inf} P_{avg, in}$

$$= \frac{M}{z_{avg, in}} \left[ P_{avg, in} \left( \frac{r_{avg, in}}{P_{avg, in}} + \frac{1}{P_p} D_{Kn} \right) \right] \left( P_{z_t}^2 - P_{z_{t-1}}^2 \right)$$

mass, out = $A_{inf} P_{avg, out}$

$$= \frac{M}{z_{avg, out}} \left[ P_{avg, out} \left( \frac{r_{avg, out}}{P_{avg, out}} + \frac{1}{P_p} D_{Kn} \right) \right] \left( P_{z_{t+1}}^2 - P_{z_t}^2 \right)$$

where

$$P_{avg, in} = \frac{P_{z_{t-1}} + P_{z_{t}}}{2} \text{ and } P_{avg, out} = \frac{P_{z_{t}} + P_{z_{t+1}}}{2}$$

3. Combination of terms.

$$V_p \frac{P_{z_{t+1}}^2 - P_{z_t}^2}{\Delta t} = \frac{1}{z_{avg, in}} \left[ P_{avg, in} \left( \frac{r_{avg, in}}{P_{avg, in}} + \frac{1}{P_p} D_{Kn} \right) \right] \left( P_{z_{t-1}}^2 - P_{z_{t-1}}^2 \right)$$

$$- \frac{1}{z_{avg, out}} \left[ P_{avg, out} \left( \frac{r_{avg, out}}{P_{avg, out}} + \frac{1}{P_p} D_{Kn} \right) \right] \left( P_{z_t}^2 - P_{z_{t+1}}^2 \right)$$

4. Simulation and convergence. The final equation is nonlinear with respect to pressure. A Newton–Raphson iterative method was used to obtain the solution. Convergence was achieved after five to seven iterations.

$$P_{z_{t+1}} = P_z + J^{-1}(P_z)$$

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**Notes**

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#### NOMENCLATURE

$n$ Biot’s number

$P_p$ pressure (psi)

$E$ Young’s modulus (psi)

$T$ temperature ($°R$)

$D_{Kn}$ Knudsen’s diffusivity coefficient (nm/s)

$r$ pore throat radius (nm)

$R$ gas constant

$b$ Knudsen’s diffusion factor

$L$ organic materials’ intrinsic permeability (μD)

$k_{app}$ organic materials’ apparent permeability (μD)

$V_p$ pore volume (nm$^3$)

$q_i$ volumetric flow rate (nm$^3$/s)

$C_r$ compressibility of the throats (1/psi)

$C$ concentration (mol/m$^3$)

$MW$ molecular weight (g/mol)

$\alpha_v$ thermal expansion coefficient

#### Greek Letters

$\mu$ dynamic viscosity of natural gas (psi-s)

$\sigma_e$ effective stress (psi)

$\sigma_a$ applied stress (psi)

$\beta$ thermal stress coefficient (1/psi)

$\nu$ Poisson ratio

$\rho_g$ gas density (g/cm$^3$)

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