Application of temperature-dependent adsorption models in material balance calculations for unconventional gas reservoirs

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ABSTRACT

Langmuir isotherm is the most common adsorption model used in the prediction of gas adsorption in most shale and coal bed methane reservoirs. However, due to the underlying assumption of single temperature, it fails to model gas adsorption where temperature differential exists in the reservoir. To address this shortcoming, temperature-dependent gas adsorption models have been incorporated into material balance calculations for accurate prediction of original gas in place as well as determining both average reservoir pressure and future performance in coal/shale gas reservoirs. The material balance equation has been expressed as a straight line with both Bi-Langmuir and Exponential models used in prediction of gas adsorption rather than the Langmuir isotherm. With this methodology, several adsorption capacities can be obtained at multiple temperatures which will allow for better estimation of original gas in place and future gas production. The results from this works show that temperature-dependent gas adsorption models can be used in place of Langmuir isotherm to account for the effect of temperature variations and more accurate representation of the adsorption of gas in coal/shale gas reservoirs.

1. Introduction

Material balance equation has been an important tool for making future reservoir predictions especially future production forecasts in conventional reservoirs. It is seen as one of the most powerful tools used in reservoir engineering (Canel and Rosbaco, 1992). Material balance models uses pressure and production data to determine the volume of hydrocarbons that is originally present. They have been used primarily in the estimation of original hydrocarbons in place and also in determining expected ultimate recovery and remaining reserves in a reservoir. In estimating original gas in place (OGIP) and initial reservoir pressure, several methods including those of King (1993), Jensen and Smith (1997), Seidle (1999), Ahmed et al. (2006), Moghadam et al. (2011) and Firanda (2011) have been proposed. These methods have utilised the application of P/Z plot, which requires cumulative gas production, average reservoir pressure and the properties of the produced gas as the input data (Seidle, 1999).

The success and usefulness of the P/Z plot in conventional reservoir led to its application in unconventional reservoirs such as coal bed methane and shale/tight gas reservoirs. Despite its usefulness, the P/Z plot may give inaccurate results when applied directly to unconventional reservoirs such as coal/shale. This is because in its conventional form, it did not include other sources of gas storage such as connected reservoirs or adsorption which is present in coal/shale reservoirs (Moghadam et al., 2011). This led to the modification of P/Z plot in order for it to be suitably applied to unconventional reservoirs especially for coal/shale gas reservoirs. Unconventional reservoirs such as coal/shale are characterised by gas adsorption, hence incorporating adsorption into the derivation of the P/Z method is necessary for accurate prediction of hydrocarbons in place for such reservoirs. This requires an adsorption model that can correctly represent the adsorption phenomenon within these reservoirs. Langmuir isotherm represented this phenomena for the traditional P/Z plot used in unconventional gas reservoirs. Despite the limitations of Langmuir isotherm such as adsorption being a function of only pressure, it remains the only model currently incorporated in most P/Z plots to evaluate the production performance of unconventional gas reservoirs using material balance. Several P/Z methodology have been developed for use in unconventional reservoirs with the use of classical Langmuir isotherm. Table 1 summarises the different methodologies used in material balance calculations for unconventional gas reservoirs.

Temperature plays an important role in gas adsorption. Hence any adsorption model should be capable of expressing the adsorption as a
Table 1
Summary of methods used in applications of MBE in unconventional gas reservoirs.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
<th>Advantages/Limitation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jensen and Smith Method (1997)</td>
<td>Modified Kings Methodology with a more practical basic evaluation of the estimated recovery and remaining reserves. Neglected the effect of water saturation in their solution. Suitable for reservoirs with high adsorption rate.</td>
<td>Use of Langmuir isotherm meant only single temperature could be used for adsorption calculations.</td>
</tr>
<tr>
<td>Seidle Method –Modified King Method (1999)</td>
<td>Another modification of Kings methodology but with the assumption of constant water saturation over time instead of average water saturation</td>
<td>Avoided the iterative solution adopted by king in its calculation. Langmuir isotherm used to account for gas adsorption.</td>
</tr>
<tr>
<td>Ahmed et al. Method (2006)</td>
<td>Expressed the material balance as an equation of a straight line to enable calculations of original gas in place and also predicting average reservoir pressure</td>
<td>Method is applicable to any coal/shale that behaves according to Langmuir isotherm. Limited to only a single temperature for evaluation of adsorption.</td>
</tr>
<tr>
<td>Moghadam Method (2011)</td>
<td>Similar but more rigorous and advanced form of the material balance proposed by King.</td>
<td>Used to define total compressibility of the system for analysing fluid flow in unconventional gas reservoirs. Adsorption was described by Langmuir isotherm.</td>
</tr>
<tr>
<td>Firanda Method (2011)</td>
<td>Introduced different drive mechanism in the material balance equation proposed by King. These included water expansion, rock compaction, connate water expansion and moisture expansion.</td>
<td>Offered similar methodology used by Ahmed and Roux by expressing material balance as a straight line. Adsorption energy was expressed only as a function of pressure. Material balance calculations can be further improved when the effects of temperature on adsorption is considered. The role of temperature in adsorption has been highlighted by several researchers (Lu et al., 1995; Gasparik et al., 2015; Charoenupanimit et al., 2015; Pashin and McIntyre, 2003).</td>
</tr>
<tr>
<td>New Approach</td>
<td>Similar approach adopted by Ahmed and Roux by expressing material balance as a straight line. Average reservoir pressure as well as future performance of the reservoir can be obtained.</td>
<td>Avoids iterative solution of Kings approach. Adopted Langmuir isotherm and exponential model in its methodology to account for gas adsorption at several temperatures.</td>
</tr>
</tbody>
</table>

function of both pressure and temperature. Majority of gas in shale gas reservoirs is from adsorbed gas and an ample knowledge of gas adsorption behaviour over a wide range of pressure and temperature is needed. Typical sorption capacities for unconventional gas reservoirs requires measurement over extended range of pressures especially for shales gas reservoirs where pressures needs to be greater than 20 MPa and temperatures over 100 °C in order for it to be considered as in-situ reservoir conditions (Gasparik et al., 2015). Therefore, in order to accurately describe the adsorption capacities of these reservoirs, multiple adsorption capacities at different temperatures need to be collected. Langmuir model is limited in providing such adsorption measurements at multiple temperatures.

Since gas adsorption is also a function of temperature, geothermal gradients will contribute substantially to the adsorption capacity of these reservoirs. An example is the black Warrior basin where there is temperature variation of about 26.85 °C–51.85 °C within 0.3–1.8 km depth range (Charoenupanimit et al., 2015; Pashin and McIntyre, 2003). For shale plays with much thinner thickness where temperature might not play crucial role, the use of Bi-Langmuir model could help describe the adsorption phenomenon more accurately (Lu et al., 1995). This is because Bi-Langmuir model takes into account the heterogeneities of the shale play. For example in Devonian shale, both clay and kerogen content plays a significant role in accounting for adsorption (Lu et al., 1995). A key assumption of Langmuir isotherm is the homogeneity of the adsorbent. However, this may not be suitable or true for coal/shale gas systems since different materials such as clay minerals and kerogen content may contribute to gas adsorption on shale (Lu et al., 1995). Hence, the need to introduce temperature-dependent adsorption models in material balance calculations for unconventional gas reservoirs.

2. Methodology

Previous modifications of material balance equation for unconventional gas reservoirs especially for coal and shale have included the adsorption capability of these resources. The additional term of gas adsorption has been modelled based on Langmuir isotherm. Langmuir isotherm describes an equilibrium relation between the free gas and the adsorbed gas under isothermal conditions. Thus gas adsorption has been expressed only as a function of pressure. Material balance calculations can be further improved when the effects of temperature on adsorption is considered. The role of temperature in adsorption has been highlighted by several researchers (Lu et al., 1995; Gasparik et al., 2015; Charoenupanimit et al., 2015; Pashin and McIntyre, 2003).

Over the years, several researchers have modified the classical Langmuir model to include a temperature term that makes it appropriate to describe the adsorption capacity of shale/coal. Lu et al. (1995) proposed the use of Bi-Langmuir model to describe the adsorption of gas at several temperatures. One term of the model describes gas adsorption on clay minerals while the other accounts for gas adsorption on kerogen. The model, therefore, is suitable for non-homogeneous adsorbents especially in the Devonian shale where two mineral composition of clay and kerogen are said to be mainly responsible for gas storage. Ye et al. (2016) also proposed a variation of the classical Langmuir isotherm equation by introducing an exponential relation that expresses the Langmuir volume ($V_L$) as dependent on temperature. Thus, the constant Langmuir volume ($V_L$) as expressed in the Langmuir equation is replaced by a $V_L$ that is a function of temperature. Based on applying the models to different sets of shale gas data, it has been established that modified Langmuir model with temperature dependency can accurately describe shale gas adsorption under various pressures and temperatures (Fianu et al., 2018; Lu et al., 1995; Ye et al., 2016).

Bi-Langmuir model is expressed as:

$$V = V_L \left[ f_1 + \frac{k_1 T^{-1/2} \exp\left(-\frac{E_1}{RT}\right)p}{1 + k_1 T^{-1/2} \exp\left(-\frac{E_1}{RT}\right)p} + \frac{(1 - f_1) k_2 T^{-1/2} \exp\left(-\frac{E_2}{RT}\right)p}{1 + k_2 T^{-1/2} \exp\left(-\frac{E_2}{RT}\right)p} \right]$$

(1)

$$k_1, k_2 = \text{constants independent of temperature.}$$

$$f_1 = \text{fraction of adsorption site.}$$

$$E_1, E_2 = \text{adsorption energy.}$$

All variables with the exception of pressure (P), and Temperature (T) are obtained by matching the adsorption data using regression analysis. Hence,

$$V = V_L \left[ f_1 b_1 p \left(1 + b_1 p\right) \right] + \frac{(1 - f_1) b_2 p}{1 + b_2 p}$$

(2)

$$b_1 = k_1 T^{-1/2} \exp\left(-\frac{E_1}{RT}\right), \quad b_2 = k_2 T^{-1/2} \exp\left(-\frac{E_2}{RT}\right)$$

Exponential model for adsorption is given as:

$$V = V_L \exp\left(-\frac{E_3}{RT}\right)$$

(3)
\[ \beta = 1/c, \quad c = \sqrt{\frac{F}{A \exp(\theta)}} \]

The coefficients \( A \) and \( B \) are obtained by matching the adsorption data through regression analysis.

To incorporate Eqs. (1) (Bi-Langmuir model) and 3 (Exponential model) into the material balance equation, Ahmed et al., 2006 approach has been adopted expressing the material balance as an equation of a straight line with \( x \) and \( y \). The use of this method provides the advantage of not using an iterative process as employed by the other methods in solving the resulting equations. It offers the advantages of minimizing cost associated with obtaining pressure survey data since the average reservoir pressures can be easily obtained by using the initial reservoir pressure, Langmuir isotherm and cumulative gas production.

Produced gas can be expressed as

\[ G_r = G + G_p - G_A - G_b \]  

(4)

\( G, G_r \), and \( G_b \) have been defined in Appendix. \( G_A \) is the gas adsorbed and can now be expressed as a function of both pressure and temperature. Inserting both the Bi – Langmuir and exponential formulae into \( G_A \) yields the following equations respectively:

\[ G_A = 1359.7Ah_p\left\{ \frac{V_L}{1 + h_p} \left( \frac{1 - f_i}{h_p} \right) \right\} \]  

(5)

\[ G_A = 1359.7Ah_p\left\{ \frac{V_L \exp(-D_T/\beta p)}{1 + \beta p} \right\} \]  

(6)

The general material balance equation in Eq. (4) have been used to derive both the Bi-Langmuir model and Exponential model. In order to test the sensitivity of estimating the original gas in place to water and fluid compressibilities, a case of including compressibilities were tested and another without compressibilities also tested (Ahmed et al., 2006).

For Bi-Langmuir model, the modified material balance equation can therefore be expressed as:

**Bi-Langmuir model**

\[ G_r + B_e W_e E_t \frac{1}{(\gamma_f \Delta P)} = Ah_p\left[ \frac{1359.7h_p\left( G_r - V_L \left( \frac{f_i b_p}{1 + b_p} + \frac{(1 - f_i)c_p}{1 + b_p} \right) \right) + 7758Ah_p(1 - S_m)E_t}{1 - (\gamma_f \Delta P)} \right] \]  

(7)

Neglecting rock and fluid compressibility:

\[ G_r + B_e W_e E_t = Ah_p\left[ \frac{1359.7h_p\left( G_r - V_L \left( f_i b_p + \frac{(1 - f_i)c_p}{1 + b_p} \right) \right) + 7758Ah_p(1 - S_m)E_t}{1 - (\gamma_f \Delta P)} \right] \]  

(8)

Eq. (7) can be expressed as an equation of a straight line, i.e \( y = mx + a \), where

\[ y = G_r + B_e W_e E_t \frac{1}{(\gamma_f \Delta P)} \]  

(9)

\[ x = 1359.7h_p\left( G_r - V_L \left( f_i b_p + \frac{(1 - f_i)c_p}{1 + b_p} \right) \right) + 7758Ah_p(1 - S_m)E_t \frac{1}{(\gamma_f \Delta P)} \]  

(10)

Neglecting rock and fluid compressibility:

\[ y = G_r + B_e W_e E_t \frac{1}{(\gamma_f \Delta P)} \]  

(11)

\[ x = 1359.7h_p\left( G_r - V_L \left( f_i b_p + \frac{(1 - f_i)c_p}{1 + b_p} \right) \right) + 7758Ah_p(1 - S_m)E_t \frac{1}{(\gamma_f \Delta P)} \]  

(12)

When \( x \) is plotted against \( y \), this will yield a straight line with slope \( m \) and \( a \) as intercept.

\[ a = 7758Ah_p(1 - S_m)E_t \frac{1}{(\gamma_f \Delta P)} \]  

(13)

**Exponential Model**

For the exponential model, the modified material balance can be expressed as:

\[ G_r + B_e W_e E_t = Ah_p\left[ \frac{1359.7h_p\left( G_r - V_L \exp(-D_T/\beta p) \right) + 7758Ah_p(1 - S_m)E_t}{1 - (\gamma_f \Delta P)} \right] \]  

(14)

Neglecting rock and fluid compressibility:

\[ G_r + B_e W_e E_t = Ah_p\left[ \frac{1359.7h_p\left( G_r - V_L \exp(-D_T/\beta p) \right) + 7758Ah_p(1 - S_m)E_t}{1 - (\gamma_f \Delta P)} \right] \]  

(15)

\[ y = G_r + B_e W_e E_t \frac{1}{(\gamma_f \Delta P)} \]  

(16)

\[ x = 1359.7h_p\left( G_r - V_L \exp(-D_T/\beta p) \right) + 7758Ah_p(1 - S_m)E_t \frac{1}{(\gamma_f \Delta P)} \]  

(17)

Neglecting rock and fluid compressibility:

\[ y = G_r + B_e W_e E_t \frac{1}{(\gamma_f \Delta P)} \]  

(18)

**2.1. Average reservoir pressure**

Ahmed et al., 2006 method of expressing the material balance as an equation of a straight line with variables \( x \) and \( y \) can be used in estimating the average reservoir pressure based on historical production data alone. The proposed method by Ahmed et al., 2006 assumed a single layer reservoir system with a knowledge of the initial reservoir pressure, Langmuir relationship and an initial gas in place. By replacing the Langmuir relationship with temperature-dependent Langmuir model, the material balance equation using both Bi-Langmuir and Exponential model can be expressed as:

Bi Langmuir model:
\[
\left( \frac{1}{\frac{h_{m,n}}{h_{m,n}^2}} + \frac{(1-t)h_{m,n}}{1 + t^2h_{m,n}^2} \right) \left( \frac{f_i b_1 p_i^2 + (1-f_i)b_2 p_i^2}{1 + b_1 p_i + b_2 p_i^2} \right) + \frac{1}{G} \left( G_p + \frac{198.69B_L W_e}{Z_f} \right) - 1 = 0
\]

(19)

**Exponential Model**

\[
\left[ \frac{p}{p_i} \right] \left[ \frac{1 + \beta p}{1 + \beta p_i} \right] + \frac{1}{G} \left( G_p + B_L W_e \right) - 1 = 0
\]

(20)

Eqs. (19) and (20) can be solved iteratively for the average reservoir pressure using the Newton Raphson method.

2.2. Prediction of reservoir production performance

The ability to predict future reservoir production performance can be achieved with the modified methodology which includes the temperature-dependent gas adsorption models. A finite difference scheme can be adopted with the modification to predict future reservoir performance.

The modified material balance equation can be expressed in the following form neglecting water and rock compressibility after finite difference approximation.

**Bi Langmuir Gas Adsorption Model:**

\[
G_{n+1}^p - G_p = \left( \frac{\beta_{n+1}^W W_e^e - \beta_{n+1}^\beta W_e^{n+1} E_x^{n+1}}{1 + b_{n+1}^W W_e^e + b_{n+1}^\beta W_e^{n+1} E_x^{n+1}} \right) + a_1 \left( \frac{p^n - p_i^{n+1}}{1 + b_1 p_i^{n+1}} \right)^2 + a_2 \left( \frac{E_x^n - E_x^{n+1}}{1 + b_2 p_i^{n+1}} \right)^2
\]

(21)

**Exponential Gas Adsorption Model:**

\[
G_{p+1} = G_p + \left( \frac{\beta_{n+1}^W W_e^e - \beta_{n+1}^\beta W_e^{n+1} E_x^{n+1}}{1 + b_{n+1}^W W_e^e + b_{n+1}^\beta W_e^{n+1} E_x^{n+1}} \right) + a_1 \left( \frac{p^n - p_i^{n+1}}{1 + b_1 p_i^{n+1}} \right)^2 + a_2 \left( \frac{E_x^n - E_x^{n+1}}{1 + b_2 p_i^{n+1}} \right)^2
\]

(22)

\[
a_1 = 1359.7 Ah \rho \frac{B_V}{\phi} \rho \text{ and } a_2 = 7758 \phi Ah (1 - S_w)
\]

The steps needed to carry out a prediction of future reservoir performance can be outlined below and also by the algorithm in Fig. 1.

**Step 1:** A future reservoir pressure below current reservoir pressure needs to be selected.

**Step 2:** If the current pressure is equal to the initial reservoir, then set current water production and current gas produced to zero.

**Step 3:** Guess or estimate the cumulative water production and solve future cumulative gas production, gas saturation and gas–water ratio.

**Step 4:** Recalculate cumulative gas production by applying Eq. (25).

**Step 5:** If the two values of cumulative gas production in Step 3 and 4 agree, then the assumed value of water production in Step 3 is correct. If not, assume a new value for water production and go through Step 3 to Step 5.

**Step 6:** Next calculate incremental gas production, gas and water flow rates.

**Step 7:** Replace the calculated old values of water production, cumulative gas production, gas and water rate with the new values calculated and repeat steps 1–7.

The following equations are also useful:

![Fig. 1. Algorithm for predicting future production using Temperature-dependent models.](image-url)
The gas saturation equation is given as

\[ S_g^{t+1} = \frac{(1 - S_w) - (p_i - p^{t+1})(\gamma_s + c_w S_w\mu - \frac{\mu}{\mu^t} W^{t+1})}{1 - [p_i - p^{t+1} \gamma_s]} \] (23)

The relative permeability ratio of \( k_{rg} \) at the gas saturation \( S_g^{t+1} \) can be used to estimate the gas water ratio as

\[ (GWR)^{t+1} = \frac{k_{rg}}{k_{rw}} \left( \frac{\mu B_w}{\mu^t B_w^t} \right)^{n-1} \] (24)

\[ G_{p1} = G_P^t + \frac{(GWR)^{t+1} + (GWR)^n}{2} \left( W^{t+1} - W^n \right) \] (25)

Gas and water flow rates are calculated respectively as:

\[ Q_{g}^{t+1} = \frac{0.703hk (k_{rg})^{n-1} (p^{t+1} - p_{ref})}{T(\gamma_s Z)_\text{avg} \ln \left( \frac{Z_s}{Z} \right) - 0.75 + x} \] (26)

\[ Q_{w}^{t+1} = \left( \frac{k_{rw}}{k_{rg}} \right)^{n-1} \left( \frac{\mu B_w}{\mu^t B_w^t} \right)^{n-1} Q_{g}^{t+1} \] (27)

The average gas flow rate as reservoir pressure declines from \( p^n \) to \( p^{n+1} \) is

\[ \langle Q_g \rangle_{avg} = \frac{Q_{g}^n + Q_{g}^{n+1}}{2} \] (28)

The incremental time needed for the incremental gas production during the pressure drop is

\[ \Delta t = \frac{\Delta G_{p1}}{\langle Q_g \rangle_{avg}} = \frac{G_{p1}^{n+1} - G_{p1}^n}{\langle Q_g \rangle_{avg}} \] (29)

3. Results and discussion

To verify the application of the modified method, simulation data provided by (Ahmed et al., 2006; King, 1990; Seidle, 1999) have been adopted to confirm the initial gas in place and other historical production data. The model can be described by a 2-D areal model that contains single coal well. A detailed reservoir properties is given in Table 3. The reservoir is described as being homogeneous with the well-draining a 320 acre coal deposit. Initial water saturation is reported as 0.95 with an initial reservoir pressure of 1500 psia. The estimated initial gas in place is 12.763 bscf with an actual production data given in Table 2. The adsorption capacity of this reservoir is expressed by the Langmuir isotherm, with Langmuir parameters given in Table 3.

To obtain the parameters for the adsorption models with temperature dependence, gas adsorption has to be expressed at different temperatures and a regression analysis done on the data to obtain the relevant model parameters. Since no data have been provided relating to the experimental adsorption capacity of the coal reservoir at several temperatures, obtaining the model parameters for the temperature-dependent models was a challenge. To obtain the model parameters for the temperature-dependent adsorption model, similar method to that of (Wang, 2017; Yue et al., 2015) was adopted where unknown independent parameters in Eqs. (2) and (3) are determined from Langmuir isotherm curve at provided temperature conditions by nonlinear regression (see Figs. 2, 3, and 4). In the case where multiple gas adsorption data at different temperatures are available, temperature-dependent models could be easily applied to obtain model parameters to be used in simulation studies.

Tables 4 and 5 shows the model parameters obtained for both Bi Langmuir and Exponential models.

Using the above data, the OGIP has been determined for both temperature-dependent models. By neglecting the formation and water

---

Table 2

<table>
<thead>
<tr>
<th>Time (days)</th>
<th>( G_q ) (MMscf)</th>
<th>( W_q ) (MMscf)</th>
<th>( p ) (psia)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1500</td>
</tr>
<tr>
<td>730</td>
<td>265.086</td>
<td>0.15749</td>
<td>1315</td>
</tr>
<tr>
<td>1460</td>
<td>968.41</td>
<td>0.290238</td>
<td>1021</td>
</tr>
<tr>
<td>2190</td>
<td>1704.033</td>
<td>0.368292</td>
<td>814.4</td>
</tr>
<tr>
<td>2920</td>
<td>2423.4</td>
<td>0.425473</td>
<td>664.9</td>
</tr>
<tr>
<td>3650</td>
<td>2992.901</td>
<td>0.464361</td>
<td>571.1</td>
</tr>
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</table>

Table 3

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Langmuir's pressure constant</td>
<td>b = 0.00276 psi⁻¹</td>
</tr>
<tr>
<td>Langmuir volume constant</td>
<td>( V_1 = 428.5 \text{ scf/ton} )</td>
</tr>
<tr>
<td>Average bulk density</td>
<td>( \rho_b = 1.70 \text{ g/cm³} )</td>
</tr>
<tr>
<td>Average thickness</td>
<td>h = 50 ft</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>( S_w = 0.95 )</td>
</tr>
<tr>
<td>Drainage area</td>
<td>A = 320 acres</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>( p_i = 1500 \text{ psia} )</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>( p_c = 1500 \text{ psia} )</td>
</tr>
<tr>
<td>Temperature</td>
<td>T = 105 °F</td>
</tr>
<tr>
<td>Initial gas content</td>
<td>( G_c = 345.1 \text{ scf/ton} )</td>
</tr>
<tr>
<td>Formation volume factor</td>
<td>( B_w = 1.00 \text{ bbl/STB} )</td>
</tr>
<tr>
<td>Porosity</td>
<td>( \phi = 0.01 )</td>
</tr>
<tr>
<td>Water compressibility</td>
<td>( c_w = 3 \times 10^{-6} \text{ psi}^{-1} )</td>
</tr>
<tr>
<td>Formation compressibility</td>
<td>( \gamma_s = 6 \times 10^{-6} \text{ psi}^{-1} )</td>
</tr>
</tbody>
</table>

Fig. 2. Regression with Langmuir isotherm parameters (data from Ahmed et al., 2006).
A plot of $x$ and $y$ will yield a straight line on a Cartesian scale (see Figs. 5 and 6). The slope of the straight line can then be used to determine the drainage area and subsequently the initial gas in place. A slope of 15,946 acre-ft. and 15,933 acre-ft. was obtained for Bi-Langmuir and Exponential model respectively, at the current reservoir temperature. Table 7 shows the corresponding drainage area and OGIP (see Figs. 7 and 8).

3.1. OGIP and average pressure

Firstly, by neglecting rock and fluid compressibility, the value of the OGIP obtained for both Bi-Langmuir and Exponential model are 12.757 Bscf and 12.742 Bscf respectively (See Table 7). Compared with Ahmed and Roux method which gave OGIP as 12.72 Bscf, the new methodology of incorporating temperature-dependent models into material balance calculation resulted in a much closer estimation of the OGIP obtained from the field data of 12.763.

However, the inclusion of compressibility calculation resulted in a slight over prediction of the original gas in place as shown in Table 6. Though, using Bi- Langmuir model in the material balance calculation resulted in the correct estimation of the drainage area of 320 acres, the

compressibility, Table 6 shows the case of bi-Langmuir and that of exponential model.

Table 4

<table>
<thead>
<tr>
<th>Bi-Langmuir parameters.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_i$, scf/ton</td>
<td>428.49912</td>
</tr>
<tr>
<td>$k_1$, 1/psi</td>
<td>0.0657363</td>
</tr>
<tr>
<td>$k_2$, 1/psi</td>
<td>0.0630964</td>
</tr>
<tr>
<td>$E_1$, cal/mol</td>
<td>-0.036275</td>
</tr>
<tr>
<td>$E_2$, cal/mol</td>
<td>-0.012802</td>
</tr>
<tr>
<td>$f_i$</td>
<td>0.97</td>
</tr>
</tbody>
</table>

Table 5

<table>
<thead>
<tr>
<th>Exponential parameters.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_i$, scf/ton</td>
<td>491.88</td>
</tr>
<tr>
<td>$D_r$, 1/F</td>
<td>0.000244</td>
</tr>
<tr>
<td>$A$, °F/psi</td>
<td>0.0655498</td>
</tr>
<tr>
<td>$B$, °F</td>
<td>0.0199987</td>
</tr>
</tbody>
</table>

Fig. 3. Shale gas adsorption capacity at selected temperature using Exponential Model (data from Ahmed et al., 2006).

Fig. 4. Shale gas adsorption capacity at selected temperature using Bi-Langmuir Model (data from Ahmed et al., 2006).
OGIP was slightly higher than actual data reported. Ahmed and Roux method under predicted the OGIP when rock and fluid compressibility was included in the calculation (See Table 8).

Also, an estimate for the initial gas in place can be made at different temperatures of the reservoir, something which cannot be done when Langmuir isotherm is used in the calculation of the adsorption potential of the reservoir. Fig. 9 shows estimated gas in place when both temperature-dependent models are used with decreasing gas in place as the reservoir temperature increases. Thus, it can be concluded that at a much higher reservoir temperature, the original gas in place in a CBM/
shale gas reservoir will be much lower compared with when the reservoir temperature is low. This is because, the contribution by gas adsorption will be smaller at higher temperature since gas adsorption is exothermic.

Using Eqs. (19) and (20), the average reservoir pressure for the reservoir can be determined by only using the historical cumulative production values. An excellent pressure match has been obtained for both cases of temperature-dependent models (see Figs. 10 and 11). The pressure match results is in agreement with both the reported data and Ahmed and Roux method. This shows that the new methodology is capable of predicting average reservoir pressure using historical production data.

### 3.2. Reservoir performance prediction

Both temperature-dependent model has been used to estimate production performance of the well. The validity of the modified methodology with temperature-dependent models has been tested against the cumulative gas production. The performed simulation in MATLAB allowed for different pressure steps to be used and it was found that the choice of smaller pressure steps resulted in much accurate match to the production data. See Figs. 12 and 13 for a match of the simulated results with that of the cumulative production data. Using Bi-Langmuir model and Exponential model in the methodology showed excellent match with the reported cumulative gas production when time step size of 20 psi was chosen. However using real pressure time steps showed higher total prediction for both models. This results is also in congruence with results

<table>
<thead>
<tr>
<th>Method</th>
<th>Slope (acre-ft)</th>
<th>Drainage area (acre)</th>
<th>OGIP (Bscf)</th>
<th>Relative percentage error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data</td>
<td>15957</td>
<td>320</td>
<td>12.763</td>
<td></td>
</tr>
<tr>
<td>Ahmed and Roux</td>
<td>15957</td>
<td>319</td>
<td>12.76</td>
<td>0.023%</td>
</tr>
<tr>
<td>Bi-Langmuir</td>
<td>15996</td>
<td>320</td>
<td>12.800</td>
<td>0.28%</td>
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<tr>
<td>Exponential Model</td>
<td>15989</td>
<td>319.78</td>
<td>12.791</td>
<td>0.21%</td>
</tr>
</tbody>
</table>

Fig. 7. MBE as a straight line for Bi Langmuir model with compressibility.

Fig. 8. MBE as a straight line for Bi Langmuir model with compressibility.
Fig. 9. Graph of OGIP at different temperature using Bi Langmuir and Exponential model.

Fig. 10. Pressure match for new method using Bi-Langmuir model.

Fig. 11. Pressure Match for new method using Exponential Model.
4. Conclusion

Temperature-dependent models have been introduced into material balance equation for unconventional gas reservoirs such as CBM and shale gas reservoirs. Two different temperature-dependent models, namely, Bi-Langmuir model and Exponential model have been introduced and subsequently incorporated into the material balance equation. By modifying the material balance to include a temperature-dependent gas adsorption model, a new model was developed and applied to available data. One of the limitations of this study was the fact that adsorption capacities at several temperatures needed to conduct temperature-dependent modelling were not available. Without this data, the authors recognise that it will be difficult to argue the point of its supremacy over existing models. What we are suggesting is that, in situations where such data is available, it will be appropriate to use temperature-dependent models in material balance calculations since they have been shown to predict the adsorption capacities accurately over a wide range of temperatures compared to a single isotherm. The following conclusions are made based on the results of validation of the model:

1. Accurate adsorption potential of the reservoir can be modelled once several gas adsorption data are available at several temperatures. Langmuir isotherm although useful fails to model gas adsorption at several temperatures. Results compared with earlier methodology like

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**Fig. 12.** Predicted total production versus reservoir pressure for Bi Langmuir model.

**Fig. 13.** Predicted total production versus reservoir pressure for Exponential model.
Ahmed and Roux showed excellent predictions and in some cases closer match to reported gas in place.

2. Extrapolation of adsorption capacity can be made at actual reservoir temperature with temperature-dependent gas adsorption models, thereby giving an accurate representation of adsorption capacity which can ultimately improve the estimation of gas in place values.

3. Accurate estimation of reservoir performance can be made with the use of temperature-dependent gas adsorption models in material balance calculations once the adsorption capacity of the reservoir are expressed at different temperatures.

Declarations

Author contribution statement

John Fianu: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.
Jebraeel Gholinezhad, Mohamad Hassan: Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

Nomenclature

A: drainage area
b: Langmuir constant
$B_w$: water formation volume factor
$B_g$: gas formation volume factor
c_f: compressibility of the formation
c_w: water compressibility
$D_T$: Reduction coefficient
$E_g$: gas expansion factor
$E_{gi}$: initial gas expansion factor
$G_p$: produced gas
G: gas originally adsorbed
$G_f$: original free gas
$G_A$: adsorbed gas currently
$G_R$: remaining free gas
$G_c$: gas content at critical desorption pressure
$GWR$: gas water ration
$G_i$: initial gas in place
h: average thickness
$k_{rg}$: relative permeability of gas
$k_{rw}$: relative permeability of water
P: pressure
$Q_g$: gas flow rate
$Q_w$: Water flow rate
$(Q_g)_{avg}$: average gas rate
R: Universal gas constant
$S_{wi}$: initial water saturation
$S_g$: gas saturation
$S_w$: water saturation
T: Temperature
$: viscosity of gas
$: viscosity of water
$V_L$: Theoretical maximum adsorption capacity
$V_g$: gas content at pressure p
$V_L$: Langmuir Volume
$W_p$: produced water
Z: gas compressibility factor
$: bulk density
$: porosity
References


