A theoretical model for coal swelling induced by gas adsorption in the full pressure range

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Abstract
The phenomenon of coal swelling caused by gas adsorption is well known. For Enhanced Coal Bed Methane Recovery and carbon storage, coal swelling induced by gases adsorption may cause significant reservoir permeability change. In this paper, based on the assumption that the surface energy change caused by adsorption is equal to the change in elastic energy of the coal matrix, a theoretical model is derived to describe coal swelling induced by gas adsorption in the full pressure range. The Langmuir constant, coal density, solid elastic modulus, and Poisson’s ratio are required in this model. These model parameters are easily obtained through laboratory testing. The developed model is verified by available experimental data. The results show that the presented model shows good agreement with the experimental observations of swelling. The model errors are within 14% for pure gas, and within 20% for mixed gas. It is shown that this model is able to describe coal swelling phenomena for full pressure range and different gas type including pure gas and mixed. In addition, it is also shown that the errors of the presented model and the Pan’s model are almost the same, but the presented model is solved more easily.

Keywords
(E)CBM, gas adsorption, coal swelling, gases, pressure

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Introduction

Coalbed methane (CBM), a form of natural gas trapped within coal seam by sorption, has become an important source of energy. To overcome the low production rate of CBM, a process known as Enhanced Coal Bed Methane Recovery (ECBM) is developed. Injecting CO2 into coal seams is expected to enhance CBM recovery, mainly by the competitive sorption of CO2 over CBM. In addition, storage of CO2 in unminable coal seams may be an option for mitigating climate change. CO2-ECBM have been recognized as economically effective and environmentally friendly technologies to improve the utilization of coal resources (Golzadeh et al., 2018; Vishal et al., 2015a; Yin et al., 2017). However, coal is well known to swell in the presence of CO2; this is likely to affect CO2 injection (Liu et al., 2011). The swelling of coal refers to an increase in its volume, which can result in a reduction in the porosity of coalbed confined by surrounding rocks. It, in turn, can induce a dramatic decrease of permeability of coal seam (Vishal et al., 2015b). So knowledge of how gas adsorption induced swelling of coal is crucially important not only to operations involving the production of natural gas from coalbeds, but also to the design and operation of projects to sequester CO2 in coalbeds.

In recent years, experiments conducted by many authors have shown that coal matrix swells with the adsorption of single gases, as well as gas mixtures (Chen et al., 2012; Cui and Bustin, 2005; Han et al., 2017; Jia et al., 2018; Levine, 1996; Majewska et al., 2009; Reucroft and Patel, 1986; Reucroft and Sethuraman, 1987; Staib et al., 2014). However, the theoretical research works have been reported relatively less. Hence, a reliable, physically based model describing the sorption and swelling behaviour of coal exposed is pre-requisite. Harpalani and Chen (1995) found a linear relationship between the volumetric strain and the adsorbed gas volume in coal. However, in their model, the ratio of volumetric strain and the adsorbed gas volume is a constant that depends on the characteristics of the type of coal. This assumption is not reasonable for coal matrix swelling caused by the adsorption of different gases onto coal at high pressures. Levine (1996) found that the linear relationship would overestimate the impact from swelling/shrinkage, especially at relative high pressures and used a Langmuir form of equation to describe the swelling behavior based on experimental observations. This approach of Langmuir form of equation to describe swelling strain has been widely applied (Shi and Durucan, 2004; St. George and Barakat, 2001). In order to describe swelling induced by mixed-gas adsorption, an extended Langmuir form of equation is applied by some researchers (Connell, 2009; Connell and Detournay, 2009; Cui and Bustin, 2005). However, all these approaches of Langmuir form of equation to describe swelling strain are empirical and can only be applied at lower pressure levels. Cui et al. (2007) observed a linear relation between the volumetric strain and the adsorbed amount in the pressure range of 0–6 MPa. Day et al. (2008) measured CO2-induced swelling in three Australian bituminous coals at pressures up to 15 MPa and temperatures up to 55°C. There is a relationship between coal swelling and the amount of CO2 adsorbed by the coal. Below a few atmospheres pressure, swelling is low and generally unaffected by the amount of gas adsorbed, but at increased pressure, swelling becomes roughly linearly proportional to the amount of CO2 adsorbed. Above about 8 MPa, this relationship was no longer linear; adsorption continued to increase but swelling did not. In brief, all these approaches of Langmuir form of equation to describe swelling strain can only be applied in a certain pressure range.

To more accurately describe the swelling strain induced by gas adsorption, the key is to understand the interactions between gas and coal that cause the swelling. Levine (1996)
suggested that coal swelling in CO$_2$ is elastic with no permanent deformation after exposure. Larsen (2004) concluded that CO$_2$ dissolves in coal and acts as a plasticiser enabling rearrangements in the coal physical structure that swells the coal. Day et al. (2008) also suggested that swelling was completely elastic, even after the coal had been subject to multiple exposures to CO$_2$. In addition, Ozdemir et al. (2004) found that CO$_2$ adsorption in coal was a physical adsorption behavior. Hence, the cause of adsorption-induced coal swelling must be the force induced by the gas molecules adsorbed on the surface. Pan and Connell (2007) developed a theoretical model for describing coal swelling by considering the changes in surface potential energy due to gas adsorption. In their work, they utilized an energy balance approach that assumes equality between the surface potential and the elastic energy change of a solid adsorbent or coal. Further, the compression effect on coal due to gas pressure was combined with an existing surface potential expression. The Pan and Connell coal swelling model (Pan’s model) is capable of describing the effects of coal swelling and coal compression as a function of gas pressure. However, their model was very complex. The model must be solved by numerical method under high pressure conditions. For better application, a simple and effective model for gas adsorption-induced coal swelling must be established.

In this paper, a new model should be developed to describe adsorption-induced swelling based on an energy balance approach. The developed model assumes that the surface energy change caused by adsorption is equal to the change in elastic energy of the coal matrix. The model is tested by experimental data of gas adsorption-induced coal swelling.

Modeling

Coal consists of a matrix material, cleats and fractures. These cleats and fractures allow the gas flow within coalbed. The swelling and shrinkage of coal matrix may reduce or increase the apertures, which will cause profound changes in the cleat porosity and permeability of the reservoir system. In this paper, a system consists of coal matrix, cleats, fractures, adsorbed phase gas and free phase gas. It assumes that the surface energy change caused by adsorption is equal to the change in elastic energy of the coal.

Surface potential energy

An adsorption system contains two macroscopic phases: a gas phase and a solid phase. In order to divide the adsorbed molecules and their properties into two phases, the problem of defining a boundary between the adsorbed and gas phases was solved by Gibbs (Myers, 2002). Figure 1(a) shows the density profile close to the surface for the case of single-component adsorption. Figure 1(b) illustrates the Gibbs model in which the actual interface is replaced by a single dividing surface located somewhere within the interfacial region.

The adsorption phase volume ($V_a$) can be described by the thickness of the adsorption layer and the specific surface area (Clarkson et al., 1997; Marinin et al., 1992). The adsorption layer thickness of coal adsorbed gas is generally less than 0.6–0.7 nm, and the most adsorbed form is single layer or double layer adsorption (Clarkson et al., 1997). The adsorption phase volume ($V_a$) is much smaller than the empty volume. In addition, with the increase of gas pressure, the compression deformation of the adsorbed phase volume ($V_a$) is larger, so the thickness of the adsorbed layer will be further reduced. Hence, it is reasonable and scientific to introduce the Gibbs interface into the solid–gas interface of coal absorbs gas.
It is assumed that the adsorption system is Gibbs model of interface, and the equilibrium values of temperature ($T$) and pressure ($P$) are given. According to Figure 1(b), the basic parameters of system under isothermal conditions can be expressed as

$$U = U^a + U^s$$  \hspace{1cm} (1)

$$dU = dU^a + dU^s$$ \hspace{1cm} (2)

$$S = S^a + S^s$$ \hspace{1cm} (3)

$$dS = dS^a + dS^s$$ \hspace{1cm} (4)

$$V^a = V - V^s$$ \hspace{1cm} (5)

$$dV = dV^a + dV^s = dV^s$$ \hspace{1cm} (6)

$$\gamma = \gamma^a + \gamma^s$$ \hspace{1cm} (7)

$$d\gamma = d\gamma^a + d\gamma^s$$ \hspace{1cm} (8)

$$n = n^a + n^s = n^a$$ \hspace{1cm} (9)

Coal adsorbs gas is the physical adsorption. The fundamental differential form for specific internal energy ($U$) can be expressed as

$$dU = TdS - PdV + \sum_{i=1}^{C} \mu_i dn_i + \gamma dm$$ \hspace{1cm} (10)
The total specific internal energy \((U)\) can be expressed as

\[
U = TS - PV + \sum_{i=1}^{C} \mu_i n_i + \gamma m \tag{11}
\]

According to equations (1) to (11), the differential form and integral form of the internal energy for the solid adsorbent can be derived as

\[
dU^s = TdS^s - PdV^s + \gamma^s dm \tag{12}
\]

\[
U^s = TS^s - PV^s + \gamma^s m \tag{13}
\]

According to equations (10) to (13), the differential form and integral form of specific internal energy \((U^a)\) of the solid phase can be derived as

\[
dU^a = TdS^a + \sum_{i=1}^{C} \mu_i dn_i^a + \gamma dm \tag{14}
\]

\[
U^a = TS^a + \sum_{i=1}^{C} \mu_i n_i^a + \gamma^a m \tag{15}
\]

The differential form and integral form of Gibbs free energy \((G^a)\) for the adsorbed phase can be written as

\[
G^a = U^a - TS^a \tag{16}
\]

Substituting equation (15) into equation (16), the integral form of Gibbs free energy can be described as

\[
G^a = \sum_{i=1}^{C} \mu_i n_i^a + \gamma^a m \tag{17}
\]

The integral form of the surface energy \((\Phi)\) caused by adsorption can be written as

\[
\Phi = (\gamma - \gamma^a)m = \gamma^a m \tag{18}
\]

Substituting equation (18) into equation (17), it can be described as

\[
\Phi = G^a - \sum_{i=1}^{C} \mu_i n_i^a \tag{19}
\]
Hence, the differential form of the surface energy change (\( \Phi \)) for the adsorbed phase can be written as

\[
d\Phi = dG^a - \sum_{i=1}^{C} \mu_i dn_i^a - \sum_{i=1}^{C} n_i^0 d\mu_i
\]  

When the mass (\( m \)) of adsorbent is constant, the differential form of \( U \) and \( U^s \) can be written as

\[
dU = TdS - PdV + \sum_{i=1}^{C} \mu_i dn_i
\]  
\[
dU^s = TdS^s - PdV^s
\]

Subtracting equation (22) from equation (21), the another form of \( dU^a \) can be expressed as

\[
dU^a = TdS^a + \sum_{i=1}^{C} \mu_i dn_i^a
\]

The differential form of Gibbs free energy (\( G^a \)) for the adsorbed phase can be written as

\[
dG^a = dU^a - TdS^a
\]

Substituting equation (23) into equation (24), the differential form of Gibbs free energy (\( G^a \)) can be described as

\[
dG^a = \sum_{i=1}^{C} \mu_i dn_i^a
\]

Substituting equation (25) into equation (20) results in

\[
d\Phi = -\sum_{i=1}^{C} n_i^a d\mu_i
\]

It resumes that the gas mixture is an ideal gas. Therefore, the chemical potential (\( \mu \)) can be written as

\[
\mu_i = \mu_i^0 + RT \ln \left( \frac{P_i}{P_0^i} \right)
\]
Substituting equation (27) into equation (26), we get

$$d\Phi = -RT\sum_{i=1}^{C} n_i^d d\ln\left(\frac{P}{P_0}\right)$$

(28)

The integral form is

$$d\Phi = -RT\sum_{i=1}^{C} n_i^d d\ln P$$

(29)

Hence, the surface energy (\(\Phi\)) caused by adsorption can be written as

$$\Phi = -RT\int_{0}^{P} \sum_{i=1}^{C} n_i^d d\ln P$$

(30)

Substituting equation (18) into equation (30), we get

$$\gamma^d = -\frac{1}{m} RT\int_{0}^{P} \sum_{i=1}^{C} n_i^d d\ln P$$

(31)

**Elastic energy**

When the specific surface energy changes by gas adsorption, the coal matrix might be deformed. The deformation requires mechanical work, and the energy thus expended is provided. To calculate accurately the strain caused by gas adsorption, several basic assumptions are used in the theoretical modeling of gas adsorption-induced coal swelling. These assumptions include: (1) the porous medium is at a constant uniform temperature; (2) the porous medium is assumed to be isotropic elastic body (Day et al., 2008; Larsen, 2004; Levine, 1996), and the discontinuous model of porous coal is developed, as illustrated in Figure 2; (3) the surface energy change caused by adsorption is equal to the change in elastic energy of the coal matrix.

Hence, the swelling strain (\(\varepsilon_{sw}\)) and swelling stress (\(\sigma_{sw}\)) induced by gas adsorption can be expressed as

$$\sigma_{sw} = \sigma_{sw}^x = \sigma_{sw}^y = \sigma_{sw}^z$$

(32)

$$\varepsilon_{sw} = \varepsilon_{sw}^x = \varepsilon_{sw}^y = \varepsilon_{sw}^z$$

(33)

According to Hooke’s law, the relationship of the swelling strain (\(\varepsilon_{sw}\)) and swelling stress (\(\sigma_{sw}\)) can be written as

$$\sigma_{sw} = E_s \varepsilon_{sw}$$

(34)
To more accurately explain the change in elastic energy, a schematic of gas adsorption-induced matrix swelling should be provided, as illustrated in Figure 3. From Figure 3, the change of the elastic energy ($W$) can be expressed as

$$W = \frac{\sigma_{sw}^x}{C_{0}} \int \varepsilon_{sw}^x \int \varepsilon_{sw}^y \int \varepsilon_{sw}^z \, dz \, dy \, dx \, dx \, dy \, dz$$

(35)

Substituting equations (29) and (30) into equation (32), we get

$$W = -6\sigma_{sw} \varepsilon_{sw} \, dx \, dy \, dz$$

(36)

**Swelling strain**

The adsorption of gas can be described by the extended Langmuir adsorption isotherm model

$$n^a = \sum_{i=1}^{C} n_{ij}^a = m \sum_{i=1}^{C} \frac{c_i A_i B_i P}{1 + c_i B_i P}$$

(37)
Substituting equation (37) into equation (31), we get

\[ \gamma^a = -RT \sum_{i=1}^{C} \frac{c_i A_i B_i P}{1 + c_i B_i P} \text{d} \ln P = -RT \sum_{i=1}^{C} A_i \ln(1 + c_i B_i P) \tag{38} \]

According to the discontinuous model of porous coal, there are six interfaces of each matrix. If the surface energy change caused by adsorption is equal to the change in elastic energy of the coal, elastic energy \( W \) also can be derived as

\[ W = 6 \gamma^a \rho^\sigma \varepsilon_{sw} \text{d}x \text{d}y \text{d}z \tag{39} \]

Subtracting equation (38) from equation (39), we get

\[ W = -6 \rho^\sigma RT \sum_{i=1}^{C} A_i \ln(1 + c_i B_i P) \varepsilon_{sw} \text{d}x \text{d}y \text{d}z \tag{40} \]

According to equations (36) and (40), the linear swelling stress can be derived as

\[ \sigma_{sw} = \rho^\sigma RT \sum_{i=1}^{C} A_i \ln(1 + c_i B_i P) \tag{41} \]

Substituting equation (41) into equation (34), the linear swelling strain can be derived as

\[ \varepsilon_{sw} = \frac{\rho^\sigma RT}{E_s} \sum_{i=1}^{C} A_i \ln(1 + c_i B_i P) \tag{42} \]

It does not consider gas pressure influence in equation (42). The change of surface energy caused by adsorption is just equal to the mechanical work caused by swelling stress, and does not include gas pressures.

For pure gas, adsorption of gas can be expressed by the Langmuir adsorption isotherm model

\[ n^a = \frac{mABP}{1 + BP} \tag{43} \]

Hence, equation (38) can be written as

\[ \gamma^a = -RT \frac{ABP}{1 + BP} \text{d} \ln P = -ART \sum_{i=1}^{C} \ln(1 + BP) \tag{44} \]

The linear swelling stress of pure gas adsorption can be described as

\[ \sigma_{sw} = \rho^\sigma ART \ln(1 + BP) \tag{45} \]
Hence, the linear swelling strain of pure gas adsorption can be described as

\[
\varepsilon_{sw} = \frac{\rho A R T \ln(1 + BP)}{E_s} \tag{46}
\]

**Compressive strain**

The linear swelling strain differs from the observed swelling linear strain through laboratory testing, because coal swelling is a comprehensive phenomenon caused by swelling stress and gas pressure. However, equation (42) does not consider the gas pressure influence. At high pressures, the coal matrix compression induced by gas pressure should not be ignored.

To more accurately explain the comprehensive phenomenon caused by gas pressure, schematic of gas pressure-induced matrix shrinkage should be provided, as illustrated in Figure 4. It assumes that the adsorbed gas is He, because it cannot be adsorbed by coal. Hence, the linear compressive strain (\(\varepsilon_P\)) induced by gas pressure can be derived as

\[
\varepsilon_P = -\frac{P}{E_s} (1 - 2v) \tag{47}
\]

**Observed swelling strain**

The observed swelling through laboratory testing is a comprehensive phenomenon caused by swelling stress and gas pressure. The observed swelling represents the difference between two opposing effects that volumetric swelling of the coal matrix due to the adsorption of gas and the matrix compression as a result of pore pressure. In the isothermal process, the observed swelling strain consists of two parts, namely, swelling strain caused by swelling stress and compressive strain caused by gas pressure. Hence, the observed swelling linear strain can be expressed as

\[
\varepsilon = \varepsilon_{sw} + \varepsilon_P \tag{48}
\]
Substituting equations (42) and (47) into equation (48), the observed swelling linear strain can be derived as

\[
\varepsilon = \frac{\rho^sRT}{E_s} \sum_{i=1}^{C} A_i \ln(1 + c_i B_i P) - \frac{P(1 - 2\nu)}{E_s}
\]  

(49)

For pure gas, equation (49) can be written as

\[
\varepsilon = \frac{\rho^sART}{E_s} \ln(1 + BP) - \frac{P(1 - 2\nu)}{E_s}
\]  

(50)

**Modeling results and discussion**

To verify the accuracy of models, the predictions of models are compared with the available experimental data. The swelling ratio is closely related to the adsorption capacity of the coal and its elastic properties. The model parameters include the elastic modulus, Poisson’s ratio, coal density, gas pressure, gas concentration, and Langmuir constant, and these were estimated or regressed from the swelling experiment data.

**Pure gas adsorption-induced coal swelling**

For pure gas, equation (50) is verified by available experiment data of three pressure levels. Three pressure levels include low pressure \((P < 10 \text{ MPa})\), medium pressure \((P < 20 \text{ MPa})\) and high pressure \((P > 20 \text{ MPa})\).

1. **Low pressure.** Levine (1996) measured CO\(_2\) and CH\(_4\) adsorption and swelling on a sample of Fruitland coal. Swelling strain was around 0.17% in CH\(_4\) at 5.17 MPa and 0.41% in CO\(_2\) at 3.10 MPa. The model parameters are given by Pan and Connell (2007), and are listed in Table 1. Cui et al. (2007) measured CH\(_4\) adsorption and swelling on a sample of Wolf Mountain coal. Swelling strain was around 0.26% at 7.42 MPa. The density of Wolf Mountain coal is assumed to be 1400 kg/m\(^3\), which is reasonable for coals. The Poisson’s ratio regressed is 0.40, which is reasonable since the Poisson’s ratio for coal is typically from 0.2 to 0.4 (Levine, 1996). Other parameters are given in Table 1. The experiment data of Levine and Cui et al. are provided in Figure 5.

2. **Middle pressure.** Day et al. (2008) measured CO\(_2\)-induced swelling in three Australian coals. The maximum swelling of the three coal samples was around 0.6% at pressures up to 15 MPa. The data of Day and Sakurovs are provided, as illustrated in Figure 6. The model parameters are listed in Table 1. Langmuir constants are regressed by adsorption and pressure values, which are reasonable value, and these results are consistent with other estimates for Australian coal. Keshavarz et al. (2017) suggested that the Langmuir constant \(a\) of Australian coal ranges from 1.24 mol/kg to 2.50 mol/kg, and Langmuir constant \(b\) ranges from 0.85 mol/kg to 1.62 mol/kg. The density is assumed to be 1400 kg/m\(^3\), which is reasonable for coals. The elastic modulus and Poisson’s ratio are estimated by experience value, which are reasonable value, because the Poisson’s ratio for
coal is typically from 0.22 to 0.42, and the elastic modulus for coal is from 1 to 14 GPa (Levine, 1996).

3. High pressure. It is well known that the adsorption capacity of coal is limited. From the experimental results of Day and Sakurovs, the adsorption deformation capacity is limited. This means that the change of surface potential energy caused by adsorption is less than the work produced by gas compressing matrix. Hence, the matrix volume should be shrunk after reaching a swelling maximum. This behaviour was also confirmed by Moffat and Weale (1995). Moffat and Weale measured CH$_4$-induced swelling at pressures up to 70 MPa, and their test data were provided, as illustrated in Figure 7. The model parameters are given by Pan and Connell (2007), and are listed in Table 1.

### Table 1. Summary of model parameters for pure gas adsorption-induced coal swelling.

| Pressure level | Data source      | Coal type       | Gas type | A (mol/kg) | B (MPa$^{-1}$) | $\rho^s$ (kg/m$^3$) | $E_s$ (GPa) | $\nu$ |
|---------------|------------------|-----------------|----------|------------|----------------|---------------------|------------|-------|
| Low pressures | Levine Fruitland | CH$_4$          | 1.257    | 0.249      | 1300           | 1.54                | 0.372      |       |
|               | Levine Fruitland | CO$_2$          | 1.488    | 0.953      | 1300           | 1.54                | 0.372      |       |
|               | Cui et al Wolf Mountain | CH$_4$    | 0.599    | 2.380      | 1400$^a$       | 1.80                | 0.400      |       |
| Middle pressures | Day and Sakurovs Coal sample 1 | CO$_2$    | 1.938    | 1.115      | 1400$^a$       | 1.80$^a$            | 0.400$^a$  |       |
|               | Day and Sakurovs Coal sample 2 | CO$_2$    | 1.804    | 1.105      | 1400$^a$       | 1.80$^a$            | 0.400$^a$  |       |
|               | Day and Sakurovs Coal sample 3 | CO$_2$    | 1.753    | 1.105      | 1400$^a$       | 1.80$^a$            | 0.400$^a$  |       |
| High pressures | Moffat and Weale Coal sample G | CH$_4$    | 1.260    | 1.890      | 1300           | 2.65                | 0.403      |       |
|               | Moffat and Weale Coal sample H | CH$_4$    | 1.890    | 0.338      | 1298           | 2.65                | 0.371      |       |
|               | Moffat and Weale Coal sample J | CH$_4$    | 2.483    | 0.237      | 1321           | 1.16                | 0.450      |       |

$^a$Value assumed.

**Figure 5.** Modeling of adsorption-induced swelling at low pressure level.
Figure 5 shows the observed and calculated swelling ratio with respect to low pressure. The model results are in excellent agreement with the data. The model errors are 3.47% for Levine’s data of CH$_4$, 2.98% for Levine’s data of CO$_2$, and 10.30% for Cui et al.’s data of CH$_4$. This means that new model is able to describe this behaviour accurately. In addition, the swelling behaviour for a given coal also varies with respect to gas type even though the pressure adsorbed is the same.

It presents the observed and modeling swelling ratio with respect to middle pressure in Figure 6. The presented model shows good agreement with the experimental data of Day.

Figure 6. Modeling of adsorption-induced swelling at middle pressure level.

Figure 7. Modeling of adsorption-induced swelling at high pressure level.
Table 2. Summary of error of new model and Pan’s model.

| Pressure level | Pressure range (MPa) | Data source | Coal type | Gas type | New model | Pan’s model |
|---------------|----------------------|-------------|-----------|----------|-----------|-------------|
| Low pressures | 0–10                 | Levine      | Fruitland | CH₄      | 3.47      | 3.52        |
|               |                      | Levine      | Fruitland | CO₂      | 2.98      | 3.65        |
|               |                      | Cui et al.  | Wolf Mountain | CH₄ | 10.30     | 12.32       |
| Middle pressures | 0–20                | Day and Sakurovs | Coal sample 1 | CO₂ | 10.92     | 10.58       |
|               |                      | Day and Sakurovs | Coal sample 2 | CO₂ | 7.32      | 9.52        |
|               |                      | Day and Sakurovs | Coal sample 3 | CO₂ | 6.47      | 8.57        |
| High pressures | 0–70                 | Moffat and Weale | Coal sample G | CH₄ | 13.81     | 13.91       |
|               |                      | Moffat and Weale | Coal sample H | CH₄ | 12.33     | 12.41       |

and Sakurovs. The model errors are 10.92% for Coal sample 1, 7.32% for Coal sample 2, and 6.47% for Coal sample 3. From Table 2, the elastic modulus, Poisson’s ratio and coal density are same, but there are also some differences in adsorption capacity of each sample. The curves for the similar rank Australian coals are quite similar, but swelling ratio also is different, as illustrated in Figure 6.

Figure 7 presents the measured and calculated swelling ratio with respect to high pressure. From Figure 7, the model is confirmed by evaluating the quality of the fit to the individual data points of Moffat and Weale. The model errors are 13.81% for Coal sample G, 12.33% for Coal sample H, and 5.10% for Coal sample J. Hence, these high-pressure measurements indicate that the model can be able to describe the swelling behavior for full pressure range. They also demonstrated that swelling ratio is the combined effect of the swelling induced by gas adsorption and matrix compression due to gas pressure.

In this paper, the model error also is analyzed, which can be expressed as

$$X = \frac{1}{N} \sum_{j=1}^{N} \left| \frac{\varepsilon_{Mo} - \varepsilon_{Lab}}{\varepsilon_{Lab}} \right| \times 100\%$$

(51)

where $\varepsilon_{Mo}$ is swelling ratio of model, $\varepsilon_{Lab}$ is swelling ratio of measurements, $N$ is number.

To further demonstrate the advantages of the new model, a comparative study was conducted between the new model and the Pan’s model. The Pan’s model can be expressed as

$$\varepsilon = \frac{\rho^s ART\ln(1+BP)f(q, vs) - P(1-2\nu)}{E_s} - \frac{3f(q, vs)}{(1-\phi)E_s} \int_0^{P_0} \varepsilon dP$$

(52)

Table 2 presents the new model and the Pan’s model error with respect to full pressure range. From Table 2, the new model error is smaller than Pan’s, but all the results of model error are within 14%. Hence, these results indicate that these models are able to describe the swelling behavior for full pressure range. However, compared to the new model, Pan’s
model is very complex, which must be solved by numerical method under high pressure conditions.

For mixed gas, the model is validated by the available experiment data of Syed et al. (2013). They selected three coal types of different ranks from the Scottish coalfields, and measured mixed gas sorption and swelling characteristics of coals at pressures up to 7 MPa. Swelling strain was around 0.23% for Coal A, 0.26% for Coal B, and 0.11% for Coal C. The data of Syed et al.’s are provided, as illustrated in Figure 8. The model parameters are listed in Table 3. Langmuir constants are regressed by Syed et al. The density is assumed to be 1400 kg/m³. Of course, the estimated values for $E_s$ and $v$ which also are reasonable for bituminous coal (Levine, 1996).

The observed and calculated swelling ratio with respect to mixed gas pressure is presented in Figure 8. The presented model shows good agreement with the experimental data.

![Figure 8. Modeling of mixed gases adsorption-induced coal swelling.](image)

**Table 3.** Summary of model parameters for mixed gases adsorption-induced coal swelling.

| Coal type | Gas type                  | Adsorption constant of N₂ | Adsorption constant of CO₂ | $\rho^s$ (kg/m³) | $E_s$ (GPa) | $v$   |
|-----------|---------------------------|---------------------------|---------------------------|------------------|-------------|-------|
|           |                           | $A$ (mol/kg)              | $B$ (MPa⁻¹)              |                  |             |       |
| Coal A    | Flue gas (87% N₂ and 13% CO₂) | 0.670                     | 0.310                     | 1.900            | 0.356       | 1400a |
| Coal B    | Flue gas (87% N₂ and 13% CO₂) | 0.580                     | 0.303                     | 3.420            | 0.157       | 1400a |
| Coal C    | Flue gas (87% N₂ and 13% CO₂) | 0.340                     | 0.351                     | 2.180            | 0.126       | 1400a |

*aValue assumed.*
The model errors are 16.54% for Coal A, 19.78% for Coal B, and 10.29% for Coal C. This means that the model can be able to describe the swelling behavior induced by adsorption of mixed gases.

Conclusions

This paper has constructed a theoretical model for adsorption induced swelling of coal exposed to a single pure gas or mixed gases in the full pressure range. This new model is based on an energy balance between the surface energy change caused by gas adsorption and the elastic energy change caused by solid volume change. This provides a predictive basis for shrinkage or swelling behavior with gas adsorption. The model parameters include Langmuir constant, coal density, solid elastic modulus, and Poisson’s ratio, which have a definite physical meaning. Of course, these model parameters are easily obtained through laboratory testing.

The developed model combines swelling due to gas adsorption and matrix compression due to gas pressure; it is able to describe coal swelling behavior for the whole pressure range. This model is verified by available experimental data of gas adsorption-induced coal swelling. The results show that the presented model shows good agreement with the experimental observations for the whole pressure range. It is also able to represent the differential swelling behavior related to gas type including pure gas or mixed gases. In addition, the results also show that the presented model errors are within 14% for pure gas, and within 20% for mixed gas. The errors of the presented model and the Pan’s model are almost the same, but the presented model is solved more easily.

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Appendix

Notation

\( a \) cylinder radius in the pore structure model (m)
\( A \) Langmuir constant (mol/kg)
\( B \) Langmuir constant (Pa⁻¹)
\( c \) component concentration (%) 
\( C \) number of components (–)
\( E_s \) elastic modulus (Pa)
\( G^i \) Gibbs free energy (J)
\( i \) \( i \)th component (–)
\( l \) length in the pore structure model (m)
\( m \) mass of adsorbent (kg)
\( n \) amount adsorbed (mol)
\( n^a \) amount adsorbed of adsorbed phase (mol)
\( n^s \) amount adsorbed of solid phase (mol)
\( P \) gas pressure (Pa)
\( P_0 \) atmospheric pressure (Pa)
\( q \) ratio \( a/l \)
\( R \) gas constant (8.314 J mol⁻¹ K⁻¹)
\( S \) total internal energy (J/K)
\( S^a \) internal energy of adsorbed phase (J/K)
\( S^s \) internal energy of solid phase (J/K)
\( T \) temperature (K)
\( U \) internal energy (J)
\( U^a \) internal energy of adsorbed phase (J)
\( U^s \) internal energy of solid phase (J)
\( V \) volume (m³)
\( V^a \) volume of adsorbed phase (m³)
\( V_s \) volume of solid phase (m³)
\( W \) elastic energy (J)
\( x, y, z \) direction of space coordinates (–)
\( \gamma \) specific surface energy (J/kg)
\( \gamma^a \) specific surface energy of adsorbed phase (J/kg)
\( \gamma^s \) specific surface energy of solid phase (J/kg)
\( \varepsilon \) observed swelling strain (–)
\( \varepsilon_P \) compressive strain (–)
\( \varepsilon_{sw} \) swelling strain (–)
\( \mu \) chemical potential (J/mol)
\( \rho_s \) density of solid phase (kg/m³)
\( \sigma_{sw} \) swelling stress (Pa)
\( \nu \) Poisson’s ratio (–)
\( \Phi \) surface energy (J)
\( \varphi \) porosity