# Mathematical modeling of methane flow in coal-matrix using COMSOL



Production through Normal fractures , gas desorption and diffusion<sup>1</sup>.

1. Composite Energy: www.composite-energy.co.uk/cbm-formed.html

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#### **Introduction:**

Almost all geological strata contain gases. These gases maybe released by underground mining activities often in concentrations too small to be of concern<sup>1</sup>. Coalbed methane (the gas emitted from coal which is primarily methane with minor amounts of heavier hydrocarbons, carbon dioxide, nitrogen, oxygen, hydrogen and helium)<sup>2</sup> is a chief component of fire damp in a coal mine<sup>3</sup>.CBM is viewed as a fuel with many environmental advantages because of the lower level of sulfur oxides, hydrocarbons and carbon monoxides it releases when combusted<sup>4</sup>. The Methane primarily resides in the phyteral Pores and micro pores, as well as in the adsorbed state on the carbon complexes in the coal matrix<sup>5</sup> and hence the diffusion rate is very low at the temperature found in mines<sup>3</sup>. The adsorption potential of coal is awesome, allowing it to contain very large amount of gas. A 0.45kg of coal can have up to 46,500 m<sup>2</sup> of adsorptive surface area and estimates that the Canadian Elmworth coals in Alberta can contain up to 14m<sup>3</sup>/tone of free adsorbed material<sup>6</sup>. Residual gas levels may be as great as 32% for highvolatile bituminous coals<sup>7</sup>. Methane bearing coals are considered to be a significant gas resource. Al though coal is a porous medium, permeability is usually guite low and the pore structure is considerably more complex than the usually found in conventional clastic reservoirs<sup>8</sup>. Therefore, the increasing importance of coal seams as gas reservoirs, attention is being focused on fracture patterns in coal matrix<sup>9</sup>. The principal natural fractures permeability is the pathways for the flow of gas and water through the cleat systems. Cleats are the systematic fractures in coal that are equivalent to joints in other sedimentary rocks<sup>10,11</sup>. Cleat system is often the reservoir characteristic that has the greatest influence over the economic success or failure of coal gas exploration and development program<sup>12</sup>. Cleats are natural fractures in coal that serve as permeability avenues for Darcy flow of gas and water to a wellbore depressurization<sup>13,14</sup>. Two cleat sets in orthogonal pattern are designated Face and Butt cleat. Face cleats are commonly planar, smooth-sided fractures that usually comprise the most prominent fracture set<sup>9</sup>. Coalbed permeability may be 3-10 times greater in the face cleat direction than in the other directions<sup>11</sup>. There are two phases of methane flow from coal matrix

to well-bore. Firstly, the adsorbed methane must diffuse through the micro pores of the coal matrix until it reaches a natural fracture (cleat) and secondly methane flows through the cleat network to the well-bore in response to a pressure gradient (Darcy Flow)<sup>15</sup>. Methane flow from the coal is dependent on upon the effective permeability of the coal. According to some mathematical and computer models of methane drainage, the spacing of the macro-fractures (cleats) plays the primary role in the transport of methane through coal<sup>16,17</sup>. Since the coal has very low permeability coalbed methane reservoir generally requires stimulation treatment for increasing the production per well. Two Common methods are used to increase the production viz. a) Increase in wellbore contact area by horizontal drilling and b) Increase the permeability by fracturing<sup>8</sup>.



Fig 1: Flow of methane through the coal microstructure $^{18}$ .

The conventional primary CBM recovery process begins with a production well that is often stimulated by fracturing to connect the well bore to the coal natural fracture system via an induced fracture<sup>19</sup>. When the pressure in the well is reduced by pumping water from the well by using an artificial lift mechanism, the pressure in the induced fracture is reduced which in turn reduces the pressure in the natural coal fracture system. Initially when the operation is started, water begins to move in the direction of the pressure gradient. When the natural fracture system pressure drops below the critical desorption pressure, methane starts to desorb from the primary-secondary porosity interface and is released into the secondary porosity system<sup>20</sup>. As a result, the adsorbed gas concentration in the primary porosity system

near the natural fractures is reduced. This reduction creates a concentration gradient that results in mass transfer by diffusion through the micro and meso-porosity<sup>19</sup>. Adsorbed gas continues to be released as the pressure is reduced.

In this study, an effort is made to visualize the methane flow during degasification of coal seam. In a virgin coal seam, methane molecules remain absorbed in the micro pores of the coal matrix. In this two dimensional model, coal matrix is considered as rectangular blocks surrounded by two way conduits viz. Face cleats and Butt cleats. It is assumed that there is only four micro-pores per coal matrix block. This methane diffuses through micro pores and however meets the cleats. These cleats allow it to flow up to the bore well. FEMLAB is used for modeling purpose.

#### **Governing Equations:**

#### a) Assumptions:

- 1. Fractures are sufficiently wide and there are no coal particles inside the created fractures. If they are very small then flow would become capillary flow.
- 2. Flow of methane inside the cleats is considered as laminar and hence Darcy law is applicable.
- 3. There is no change of temperature in coal seam during the degasification process.
- 4. The width and cleat spacing remains constant during the gas flow period.
- 5. Cleats are straight and there is no tortuocity in them.
- 6. Coal matrix is in continuous equilibrium with the fracture system i.e. there is no accumulation of methane at the fracture surface.
- 7. There is no matrix shrinkage in the network during desorption of methane.
- 8. Permeability is assumed to be constant while it varies as per the 'Klinkenberg Law'.



Figure 2: Exaggerated schematic of methane flow through coal matrix.

## **b)** Mathematical Equations:

A two dimensional system is considered for this problem. Micro-pores are represented as small circle. These are the potential sites for methane diffusion. Methane molecules desorbed from these sites, diffuse through the coal matrix till they find a cleat. After entering in a cleat system, this flow follows the Darcy's law and come out.

#### Flow through cleats:

For 1D radial cylindrical flow the continuity equation can be written for a gas-phase fluid

$$-\left(\frac{1}{r}\right)\left(\frac{\partial}{\partial r}\right)\left[\frac{rP_{a}}{Z_{p_{a}}}\vec{v}\right] + \underbrace{\frac{RT}{M}\frac{q_{m}}{V_{ba}}}_{M} + \underbrace{\frac{RT}{M}\frac{q_{ai}}{V_{ba}}}_{M} = \phi_{a}\frac{\partial}{\partial t}\left[\frac{P_{a}}{Z_{p_{a}}}\right]$$
.....(1)

(Neglecting these terms for study)

Darcy law for a fracture flow

$$\vec{v} = -\left[\frac{k}{\mu}\right] \left(\frac{\partial P_a}{\partial r}\right)$$
 .....(2)

By substituting equation (2) in equation (1)

$$\left(\frac{1}{r}\right) \left(\frac{\partial}{\partial r}\right) \left[\frac{krP_a}{Z_{p_a}\mu} \left(\frac{\partial P_a}{\partial r}\right)\right] + \underbrace{\frac{TP_{sc}}{T_{sc}} \frac{q_{sc}}{V_{ba}}}_{T_{sc}} + \frac{RT}{M} \frac{q_{ai}}{V_{ba}} = \phi_a \frac{\partial}{\partial t} \left[\frac{P_a}{Z_{p_a}}\right] \dots (3)$$

(Neglecting these terms for study)

#### Flow through Micro-pores:

Fick's law for diffusion

$$\left(\frac{1}{r}\right)\left(\frac{\partial}{\partial r}\right)\left[rD\left(\frac{\partial C}{\partial r}\right)\right] = \left(\frac{\partial C}{\partial t}\right).$$
(4)

Adsorption and desorption rates under equilibrium condition is given by Langmuir equation

The total volume concentration of matrix gas on a per volume basis

$$C = \left(\frac{PM\phi_i}{ZRT}\right) + \left[\frac{V_{\infty}P}{P+P_L}\right].$$
(6)

By putting the value of C in equation (4)

$$\left(\frac{1}{r}\right) \left(\frac{\partial}{\partial r}\right) \left[ rD\left(\frac{\partial}{\partial r} \left\{ \left(\frac{PM\phi_i}{Z_p RT}\right) + \left[\frac{V_{\infty}P}{P+P_L}\right] \right\} \right) \right] = \frac{\partial}{\partial t} \left[ \left(\frac{PM\phi_i}{Z_p RT}\right) + \left[\frac{V_{\infty}P}{P+P_L}\right] \right] \dots (7)$$

Real Gas law

$$P = CZRT.....(8)$$

#### c) Boundary and Initial Conditions:

The initial condition is given by as the pressure distribution of the methane gas in the cleat system at t=0. The pressure distribution is uniform throughout the coal seam and is equal to initial reservoir pressure. Methane gas concentration on the external surface of the matrix elements is evaluated at the gas pressure in the cleats. The micro-pore and macro-pore systems are coupled by the boundary conditions specified along the cleat walls that the two systems share. Matrix and fracture transport equations are coupled at the external surface of the matrix elements where the micro-pore gas concentration is evaluated at the gas fracture pressure.

Initial P =  $P_a$  and Final  $P = P_{sc}$ 

Variable	Value	Variable	Value
Macro pore porosityø <sub>a</sub>	.02	Macro pore permeability k(D)	2.47E-15
Rock density $\rho$ (Kg/m <sup>3</sup> )	1370	Initial seam pressure $P_a$ N/m <sup>2</sup>	3.4E+6
Seam Temperature T(K)	313	Micro pore porosity $\phi_i$	.025
$P = P_{sc} N/m^2$	10E+5	<i>Т<sub>sc</sub></i> К	298
Diffusion Constant(m <sup>2</sup> /s) D	3.75X10E-11	Langmuir's constant $V_{\infty}$	13.9E-3
Langmuir's pressure $P_L$	1.2E+6	Gas Molecular weight M	16.043
$Z_{p_a}$	0.93	$Z_p$	1

# 3. Formulation:

Most numerical models developed are based on physical phenomenon. The most commonly used model is shown in figure 3, where side of the square shows fracturing surface.



Figure 3: Illustration of Coal matrix unit and methane dissusion<sup>15</sup>.

A coalbed is shown to be made up of small cubic blocks, or units separated by fractures. The spacing of the fractures determines how far the gas has to diffuse before reaching the fracture and the dimensions of the fractures decide the quantity of gas that can flow through<sup>15</sup>.

# a) Micro-pores and coal matrix:

A small unit of coal matrix with side 0.005m is considered. This unit is isotropic in nature and pressure and temperature is assumed to be constant, though they may vary from point to point. Theoretically, there are millions of billions of micro-pores present in coal unit of this size. Four micro-pores (representative of same pore volume of millions of billions of micro-pores) of

0.37mm radius were considered for this study. There location is set as per the symmetry of the block. Assumption made in describing this model has been mentioned previously in this paper. Boundaries of the coal matrix are set at a concentration given by Langmuir isotherm at 1.25 Mpa. Concentration inside the coal matrix sub domain is fixed as 50 mole/  $m^3$ . Representative micro-pore are assumed as constant source of very high methane concentration (6000 mole/ $m^3$ ) and there diffusion coefficient is very high in comparison of coal-matrix diffusion coefficient (D=3.75X10<sup>-11</sup>m<sup>2</sup>/s). In the matrix, diffusion of methane is governed by diffusion constant D. Coal-matrix boundaries directly communicate with face and butt cleats. With above mentioned assumptions and nature of the model, the convection and diffusion model under chemical engineering in mass balance section seems to be best fit. An application mode as shown in figure 4 was designed for boundary conditions paired with initial conditions.

The boundaries of the matrix are at fixed concentration as the methane molecule arrived there taken out via cleats. There is no accumulation of gas and pressure remains constant. Gas constant R, M,  $V_{\infty}$ ,  $P_L$  were defined into constant section under option menu. Langmuir adsorption equation was fitted in to the scalar expressions available in the option menu. Since, there is no reaction taking place in the system the value of R is kept zero. Also, initial conditions and boundaries conditions are defined as a scalar or constant expression under option menu.

## b) Cleats:

A rectangular element of .005mX.00001m is considered as a vertical cleat<sup>21</sup> (as shown in figure 5). This unit is isotropic in nature and pressure and temperature is assumed to be constant, though they may vary from point to point. Permeability for this cleat is defined as a scalar expression under options menu.  $k = 84.4 \times 10^8 \times (\frac{w^3}{z})$  Darcy;

Where w: width of the cleat (This is calculated by using Boundary distance variable (dist1) available in option menu)

z: separation of the cleat

Density of the gas is also defined as scalar expression. Boundaries (3 and 11) of the cleats are kept at a pressure of 0.1Mpa while other boundaries of cleats are kept insulated. Boundary (4 and 8) is kept at equivalent pressure of 50 mol/m<sup>3</sup> concentration.

Parameter	Density	Porosity	Viscosity	p(t0)	w	Z
Value(MKS)	.68	.3	1.0×10 <sup>-4</sup>	1.01×10 <sup>5</sup>	1×10 <sup>-5</sup>	1×10 <sup>-3</sup>



Figure 4: Geometry (up to the scale) drew in COMSOL representing Micro-pores, coal-matrix and cleat.

# 4. Solution Using COMSOL:

Outputs were obtained from the simulation with above mentioned value.

#### a) Micro-pores and coal matrix:

Surface map for diffusive flux and concentration contours were plotted at T= 864000s (10 days). surface that the value of flux keeps on decreasing while going away from micro-pores. For the same model concentration-contours for methane were observed. It can be seen from plot (figure 5) that concentration decreases with distance from the micro-pore.



Figure 5: Diffusive flux surface map and concentration contours for a single coal matrix unit.

## b) Cleats:

Surface map of velocity field (m/s) and pressure-contours were plotted at T= 864000s (10 days). Velocity varies from zero (at coal matrix bottom end) to high (at upper end) as shown in figure 6.



Figure 6: Velocity field surface map and pressure contours for a cleat.

## 5. Validation of Model:

Validation is an important part of a model. To validate for the overall solution, the concentration in the matrix was set to zero. Concentration was plotted across a vertical line passing through the centre of the micro-pores. The nature of the curve is compared the curve in similar literature.

#### a) Micro-pores and Matrix:

The breakthrough profile for concentration was obtained across a line passing through the centre of the two micro-pores. The concentration for the micro-pores was set to zero. Reverse flux pattern was shown by following profile.



**Figure 7:** Surface, showing concentration (arrow showing direction of reverse flow inside the micro-pores) and a breakthrough profile of total flux across a cross-section.

This confirms the validity of the model of micro-pores. Now concentration profile was observed from source to boundary. This profile matches with the profile found in literature work for Fick's diffusion.



**Figure 8:** Typical concentration profile of Fick's diffusion (right) obtained from literature and profile obtained from model (left).

#### **b)** Cleats:

Validation of the cleats model was done by changing the pressure differential. Pressure

differential was set as  $\Delta P$ ,  $2\Delta P$  and  $3\Delta P$ . Darcy law states that velocity is directly proportional to pressure differential which is apparent from Figure 9 and hence validates the results.



**Figure 9:** Velocities profile across the length of the cleat at  $\Delta P$ ,  $2\Delta P$  and  $3\Delta P$ .

## 6. Parametric Study:

Parametric study was done by varying the values of diffusion coefficient, concentration of methane in micro-pores and concentration of methane in coal matrix.

#### a) Micro-pores and matrix:

**6.1 Varying Diffusion coefficient:** Diffusion coefficient was varied in a range of  $10^{10} (10^{-10}, 10^{-15}, 10^{-20})$  and the concentration/diffusive flux profile was observed.



**Figure 10.** Concentration across a line passing through the centre of the two micro-pores at T=86400s and D=  $10^{-10}$ ,  $10^{-15}$ ,  $10^{-20}$  (from right to left then down)

It was apparent from the concentration profile that the Diffusion coefficient is the guiding factor for diffusion of methane in coal matrix. If the value of diffusion coefficient is high then the methane diffuses fast and tries to make the concentration uniform everywhere in the matrix.

**6.2 Varying Time:** Breakthrough profile for concentration and diffusive flux was drawn across the cross section line passing through the centre of the two micro-pores at different times. It is clear from Figure 11 that, the concentration of the methane in coal matrix (central part) keeps on increasing with time. It can be concluded that the methane concentration is higher in central part of the coal matrix unit. However, if one more fracture can be induced in the central part of the matrix then the recovery of methane could be increased. Methane gas received at cleats travels up to the upper boundary and hence concentration of methane decreases sharply as we go towards cleats and remains constant in the cleat.



**Figure 11.** Total flux and concentration across a line(as shown in figure 10) passing through the centre of the two micro-pores at d(T) = 1000s.

#### b) Cleats:

**6.3 Varying permeability:** Permeability of the cleat was varied by changing the width of the cleat (2w, 3w and 4w) in turn varying the permeability in multiples of (8, 27 and 64). Pressure Surface and velocity field profile was drawn. Here w stands for width of the cleats. Widening of the cleat represents high permeability and high permeability allows large velocities. Large flowing velocities results in higher rate of methane extraction.





**Figure 12.** Velocity field across the cleat at w, 2w and 3w in turn changing the permeability 8, 27 and 64 times (from right to left then down)

**6.4 Varying concentration at cleats boundaries:** Pressure was varied as (2P, 3P and 4P) at the cleats boundaries and velocity profile was drawn. Here P stands for pressure at cleat. Methane concentration at the coal matrix boundaries increases with pressure (refer equation (8)). Velocity increase with pressure rise (refer figure 13). This again suggests the enhanced recovery of methane. Concentration at the coal matrix boundaries can be increased by increasing the temperature of the coal matrix unit.





**Figure 13.** Velocity field across the cleat at different pressure differentials P, 2P and 3P (from right to left then down).

## 7. Conclusions:

It was clear from the modeling studies that the amount of methane diffused through the coal matrix per unit time can be increased by reducing the distance (a diffused atom has to travel before finding a Cleat to escape). This will increase the production rate of the methane. COMSOL seem to provide a reasonable breakthrough profile for concentration and diffusive flux behavior. Since a good fundamental study on parameters are not readily available, values were to be assumed to get a breakthrough profile for concentration, diffusive flux and velocity field. It was clear from the model that the extraction rate from a coal block can be increased by widening up the existing cleats. More widened cleats reflect enhanced permeability. Anyhow, if pressure of the methane gas can be increased inside the coal unit (in turn at the cleat boundary) it will enhance the extraction rate (increased velocity) as seen in the breakthrough profile.

Since, no values can be found in literature for such a model, it became quite complicated to arrive at the real time situation with this model and hence model is in developing stage. Also, the program routinely crashes/takes longer time to solve for small size geometries and varied ranges of data. Allocated memory in the systems won't allow for fine mesh sizes.

# **Appendix A**

Nomenclature:

- C = Gas concentration in coal matrix (Kg/ $m^3$ )
- D = Diffusion coefficient ( $cm^2/sec$ )
- k = Permeability, md
- M = Molecular weight (Kg/kmol<sup>3</sup>)
- P = pressure, psi (kpa)
- P<sub>L</sub> = Langmuir pressure constant, psi (kpa)
- q = Volumetric flow rate, (std  $m^3/s$ )
- q<sub>m</sub> = Mass flow rate,(kg/s)
- R = Universal gas constant
- t = Time (s)
- T = Temperature, (K) v
- $V_E$  = Equilibrium isotherm (Kg/m<sup>3</sup>)
- $V_{\infty}$  = Langmuir Volume constant (Kg/m<sup>3</sup>)
- Z = Gas compressibility factor
- $\mu$  = Viscosity, cP
- $\rho$  = Density (Kg/m<sup>3</sup>)
- $\phi$  = Porosity

Subscripts:

- a = Macro-pore
- b = Bulk
- ai = Macro-pore and Micro-pore interaction
- E = Equilibrium
- i = Micro-pore
- L = Langmuir
- r = Radial direction

- sc = standard conditions
- $\infty$  = At infinite pressure

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