Abstract
Energy resources and generation of energy have always been popular topics since the industrial revolution. While the necessity for increased energy generation stands out clearly, debates have been arising pertaining to different energy resources, methods of extraction of resources, and processing techniques with environmental and health safety concerns. Shale gas is one of those resources, which became more favored after the application of hydraulic fracturing (hydrofracking) method for extraction of it. However concerns came along with this technique due to high-pressure injection of fracking fluid which consists of water, sand, and numerous chemicals some of which have high toxicity such as methanol. This study investigates the upward flow of methanol from the hydrofracking zone. Three case studies are conducted for the shale basins in Marcellus, Pennsylvania and Bakken, North Dakota in USA, and Bowland in UK. Theoretical analysis was conducted employing governing equations for incompressible, turbulent flow of methanol. Numerical analysis of the flow was also performed through a computational fluid dynamics (CFD) software using finite volume method. Stratigraphic data including layer thickness, permeability, porosity, and inertial resistance for all three basins were implemented into the model. Analysis was done on a transient basis and pressure and velocity distributions of methanol were obtained for all pilot basins studied.

Keywords: shale gas, hydrofracking, methanol, migration, CFD analysis
Introduction

Shale is a fine-grained, sedimentary rock which is a mix of clay and small fragments of other minerals. Shale gas is an important source of natural gas trapped within the shale formation. The residual amount of oil and gas within shale can be predicted using existing quantitative evaluation method of source rocks. The hydrocarbon content in the shale varies, depending upon the depositional environment, and the abundance, type, maturity, and expulsion efficiency of organic matter. Shale gas is difficult to exploit when compared to conventional gas and oil because of tight nature, low porosity and low permeability. To extract shale gas lot of chemicals, water and sand are pumped through pipes into the shale. Some portion of the chemicals cannot be recovered back. The left over chemicals which cannot be recovered can travel upwards. Shale has low matrix permeability, so production requires fractures to provide permeability. Hydraulic Fracturing (fracking) is the most common way of extracting natural gas and oil from shale formations. This technique involves injecting fracturing fluid into the shale to create fractures in the body of rock from which natural gas and oil can be extracted.

Fracking is done both vertically and horizontally. Vertical fracking does not use extensive lateral components. The term vertical fracking can also refer to conventional fracking methods that preceded horizontal fracking. Horizontal fracking on the other hand allows wells to move laterally instead of going straight down. Larger area can be covered without boring as many holes into the surface. A horizontal well can stretch up to two miles along a shale deposit, unlike a vertical well. High volume hydraulic fracturing is possible with the lateral structure of the horizontal drilling. The high volume hydraulic fracturing uses less gelling agents and more friction reducing chemicals. Initially after completing the drilling work and wellbore casing installation a perforating gun is sent into the wellbore for the purpose of making perforated holes into the target rock.
Natural fracture development can affect recovery potential of shale gas reservoir and can also determine the quality of shale gas reservoir and gas production. Fracture development is conducive to the volumetric increase of free natural gas, desorption of adsorptive gas and the increase of total gas accumulation in shale. Fracture development in shale is controlled by non-tectonic and tectonic factors [2].

The major non-tectonic factors that can influence fracture development are lithology and mineral composition, rock mechanism, total organic carbon and abnormal high pressure [3-5].

The conditions which are helpful for fracture formation are single shear strength, dual shear strength, triple shear strength, strain energy density and maximum tension stress strength. The most widely accepted among these conditions is the Coulomb-Mohr generalized single shear strength principle and Griffith generalized maximum tension stress strength principle [6]. The parameters such as Young’s modulus, shear strain modulus, volumetric elastic modulus and Poisson’s ratio, which reflects rock tensile strength, shear strength, compressive strength and lateral relative compressibility, respectively are used to describe elastic deformation of the rocks. Rock shear rupture
depends on both shear stress and normal stress on the rupture surface. The stress condition at each point can be determined by tectonic stress field.

High-volume hydraulic fracturing technique is used to extract shale gas from the reservoir. Large amount of water, sand and chemicals are pumped at high pressure into the shale to induce fractures in the rocks to initialize the gas flow. Within few days after injection, a certain amount of water returns to the surface as a flow-back. The flow-back water is accompanied by high quantities of methane [7].

Table 1: Methane emissions over the lifecycle of a well [8].

<table>
<thead>
<tr>
<th>Emissions during well completion</th>
<th>Conventional gas</th>
<th>Shale gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Routine venting and equipment leaks at well site</td>
<td>0.01%</td>
<td>1.9%</td>
</tr>
<tr>
<td>Emissions during liquid unloading</td>
<td>0.3 to 1.9%</td>
<td>0.3 to 1.9%</td>
</tr>
<tr>
<td>Emissions during gas processing</td>
<td>0 to 0.26%</td>
<td>0 to 0.26%</td>
</tr>
<tr>
<td>Emissions during transport, storage, and distribution</td>
<td>0 to 0.19%</td>
<td>0 to 0.19%</td>
</tr>
<tr>
<td>Total emissions</td>
<td>1.4 to 3.6%</td>
<td>1.4 to 3.6%</td>
</tr>
</tbody>
</table>

The above table gives the information about the methane emissions during well completion, liquid unloading, gas processing, transport, storage, distribution and routine venting and equipment leaks at well site. The significant difference in the methane emissions between conventional gas and shale gas can be observed during well completion. The emissions from conventional natural gas wells during well completion are very low as they have no flow-back and no drill out. Considering all the emissions during life cycle of an average shale gas well, about 3.6% to 7.9% of total production of the well is emitted as methane into the atmosphere, which is twice as great as the methane emissions from the conventional gas wells, 1.7% to 6%. Methane gas has more potential as greenhouse gas when compared to CO2. The effect of methane gas on global warming attenuates more rapidly as it has shorter residence time in the atmosphere. The greenhouse gas footprint of shale gas is larger than conventional gas, due to methane emissions with back-flow and drill outs [8].

Faults are the naturally existing fissures, which are long and narrow line of breakage in the earth. The hydraulic fracturing process activates the dormant fractures and faults present in the area between the shale gas reservoir and aquifers, creating the pathway for the upward migration of the fracturing fluid and gases into the aquifers [9].
This paper focuses on the potential upward flow of methanol present in the fracking fluid. Three shale gas basins are considered as the case studies:

1. Marcellus formation, Pennsylvania, USA
2. Bakken formation, North Dakota, USA
3. Bowland formation, UK

**Theoretical Analysis**

Solid matrix combined with voids is present in the porous medium. The arrangement of pores in a natural porous medium is irregular proportional to the size and shape of the porous medium [10]. In hydraulic fracturing technique the flow of the unrecovered fracturing fluid upwards from the shale gas reservoir can be considered as the flow through porous medium as, it is related to ground water hydrology, oil reservoir engineering and soil mechanics [11]. The flow through porous medium can simply be described by the Darcy’s law for laminar flow. Darcy’s law is the proportion between the flow rate and the applied pressure difference, which can be expressed as

\[
V = -\frac{k}{\mu} \Delta P
\]  

where, \(V\) is Darcy-Velocity or flow rate per unit area, \(\Delta P\) is applied pressure difference in the flow direction, \(\mu\) is Dynamic viscosity of the fluid and \(k\) is Specific
permeability of the medium. The value of $k$ is independent on the nature of the fluid, it is related to the geometry of the medium and is scalar for isotropic medium [10]. Homogenization techniques are used to derive Darcy’s equation from the Navier-Stokes equations. The conservation of mass equation along with Darcy’s equation defines the groundwater flow equation. Gas, oil and water flow through petroleum reservoirs can also be explained by Darcy’s Law.

Continuity, Navier-Stokes and energy equations govern the incompressible turbulent flow of methyl alcohol. Reynolds number through the porous media is

$$Re = \frac{\rho v D}{(1 - \Phi) \mu}$$  \hspace{1cm} (2)

where, $\rho$ is density of fluid flowing through porous media, $v$ is velocity of fluid in the porous media, $D$ is diameter of particles in the porous media, $\Phi$ and $\mu$ are porosity and dynamic viscosity respectively. Equation 3.2 represents the Reynolds number for determining the flow regime in fluid flow through porous media. The critical value of Reynolds number at which flow begins to change to turbulent flow from laminar flow approximately ranges from 3-10. Reynolds number for Marcellus, Bowland, and Bakken formations are 633, 1270 and 2576 respectively, indicating turbulent flow. The equations can be solved using a suitable turbulence model. These governing equations of a flow can be expressed as following:

**Continuity Equation:**

$$\frac{D\rho}{Dt} + \rho \frac{\partial U_i}{\partial x_i} = 0$$  \hspace{1cm} (3)

For incompressible flow, as the density is constant the equation becomes

$$\frac{\partial U_i}{\partial x_i} = 0$$  \hspace{1cm} (4)

**Momentum Equation:**

$$\rho \frac{\partial U_j}{\partial t} + \rho U_i \frac{\partial U_j}{\partial x_i} - \frac{\partial P}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_i} + \rho g_i$$  \hspace{1cm} (5)

$$\tau_{ij} = -\mu \left( \frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) + \frac{2}{3} \delta_{ij} \mu \frac{\partial U_k}{\partial x_k}$$  \hspace{1cm} (6)

**Energy Equation:**

$$\rho c_v \frac{\partial T}{\partial t} + \rho c_v U_i \frac{\partial T}{\partial x_i} = -P \frac{\partial U_i}{\partial x_i} + \lambda \left( \frac{\partial}{\partial x_i} \left( \frac{\partial T}{\partial x_i} \right) \right) - \tau_{ij} \frac{\partial U_i}{\partial x_i}$$  \hspace{1cm} (7)

**Numerical Analysis**

Domain geometries for three different cases were created in ANSYS. The data includes the porosity, permeability, thickness and inertial resistance of each layer between the aquifer and the shale gas extraction layer. Stratigraphic information for each basin including physical properties of the layers are presented in Figures 3-5.
Figure 3: Marcellus stratigraphy.

Permeability (k) = 1e-15
Porosity (φ) = 0.34
Inertial Resistance (Ir) = 4.55e+7

Permeability (k) = 1e-16
Porosity (φ) = 0.28
Inertial Resistance (Ir) = 2.15e+8

Permeability (k) = 1e-15
Porosity (φ) = 0.34
Inertial Resistance (Ir) = 4.55e+7

Permeability (k) = 1e-16
Porosity (φ) = 0.36
Inertial Resistance (Ir) = 2.15e+8

Permeability (k) = 9.6e-18
Porosity (φ) = 0.015
Inertial Resistance (Ir) = 2e+11

Permeability (k) = 1e-16
Porosity (φ) = 0.26
Inertial Resistance (Ir) = 2.15e+8
Figure 4: Bakken stratigraphy.
Figure 5: Bowland stratigraphy.

Computational Fluid Dynamics (CFD) analyses for all three geographic locations considering the cases of formations with and without fault are listed in Figure 6.

Figure 6: CFD results.
As can be concluded from the velocity distributions of methanol originating from the hydrofracking zone which is the horizontal pipeline at the bottom center of each domain presented in Figure 6, methanol was not observed to reach the water aquifers for the assumed cases of with and without fault. However, it should be noted that this study does not account for additional and/or unexpected faults and fractures in the overburden, nor does it consider the migration of the fluid in the long run.

Conclusion

Three different geological locations were investigated for their stratigraphies and rock properties such as permeability, porosity and inertial resistance. In each geological location types of rock layers, thickness of each layer and depth of the layers beneath the groundwater aquifers were estimated. Stratigraphic models for each case were designed in the ANSYS with appropriate data, so that the flow behaves as the flow through the porous media. A fault was introduced in the most resistant layer of each stratigraphy to study the flow in the presence of a naturally occurring fault. Numerical simulations have been proposed for the estimation of the velocity range of methyl alcohol between the shale reservoir and the ground water aquifers of Marcellus (USA), Bakken (USA), and Bowland (UK) formations.

In this study methanol is taken into consideration among all the chemical additives used in the fracking fluid, as it is one of the toxic chemicals used in the hydraulic fracking technique and also it can be a potential source for methane gas, which is very harmful to the atmosphere (greenhouse effect). In real time the fracking fluid is injected into the shale rock with certain velocity for small period of time to create fractures, so user defined function was introduced in such a way that the inlet-velocity after certain time period becomes zero. The simulation results suggest that, as methyl alcohol travel upwards its velocity decreases rapidly at each layer until 300 seconds and after 300 seconds, methyl alcohol doesn’t travel upwards which means its velocity is completely zero. This also means that methyl alcohol is trapped in the layers with zero velocity after 300 seconds and also this scenario is similar with other toxic chemicals.

When a fault was introduced in the most resistant layers of the stratigraphies a little high velocities are observed when compared to the no-fault model, but methyl alcohol doesn’t reach to the top layer in all the three cases. This consolidates that there should be more than one naturally occurring fault present in the stratigraphy for the chemicals to reach the groundwater aquifer else the chemicals cannot travel all the way up to the aquifers.
References


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