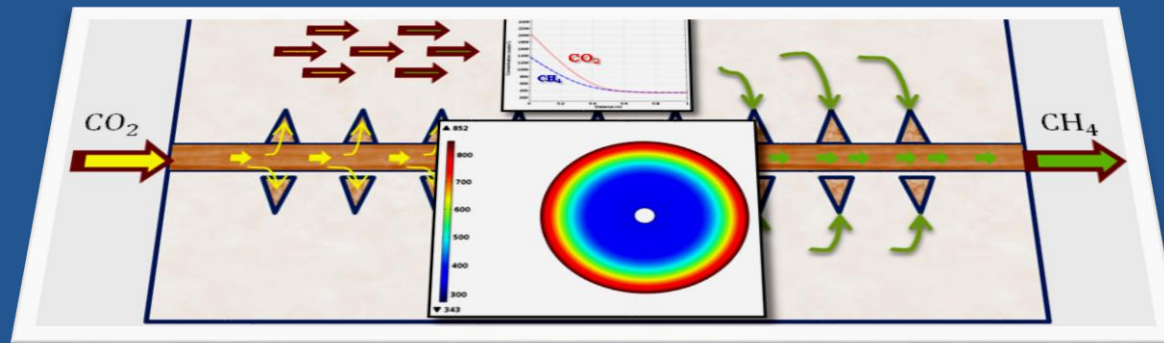


# Numerical Study of Flux Models for CO<sub>2</sub> : Enhanced Natural Gas Recovery and Potential CO<sub>2</sub> Storage in Shale Gas Reservoirs

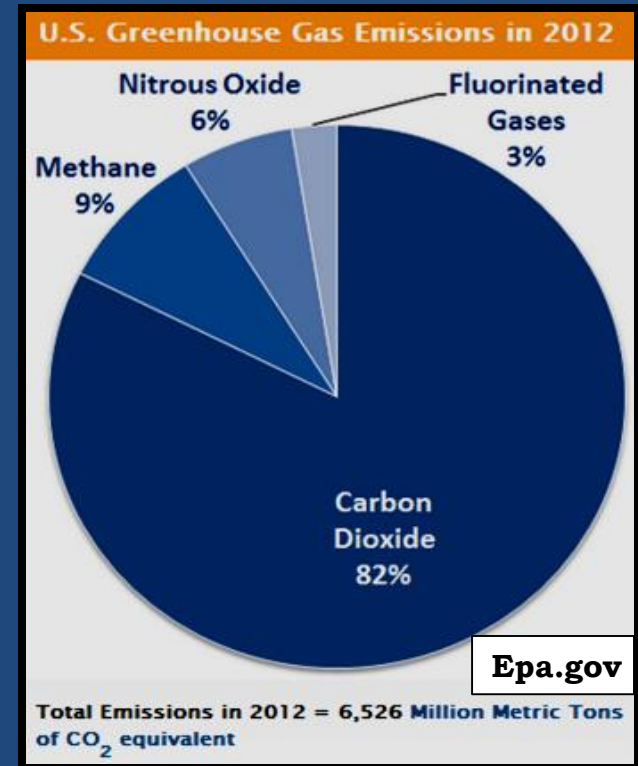
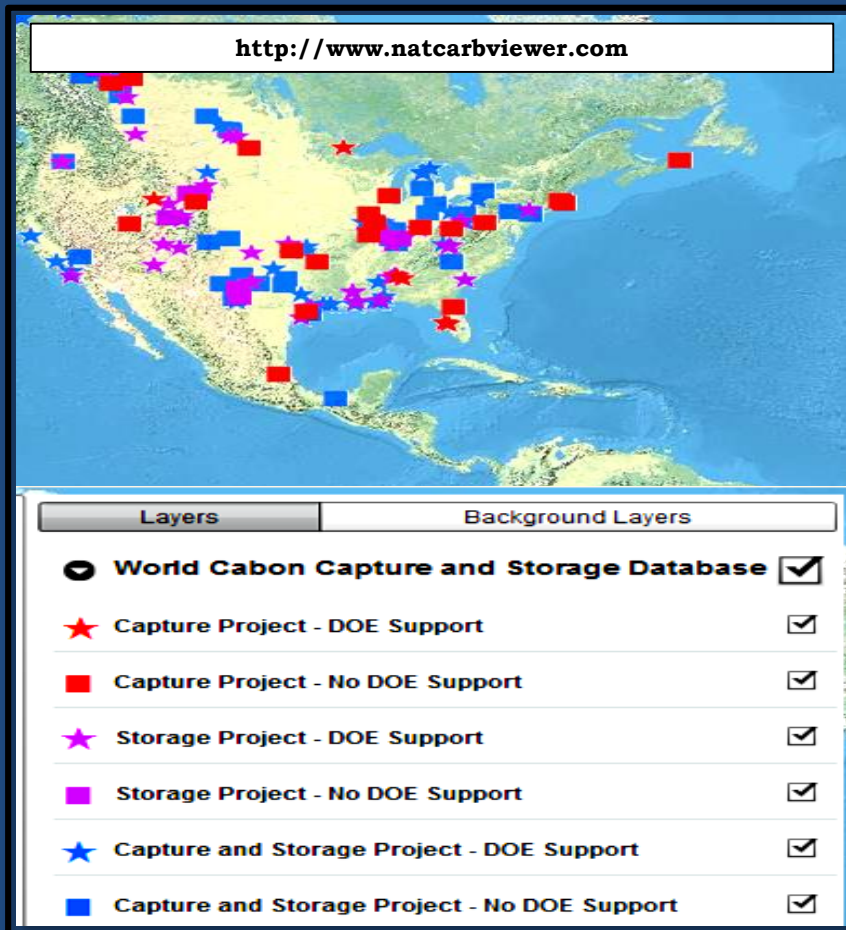
Session : Flow in Porous Media



Nilay J. Prajapati & Patrick L. Mills  
Dept. of Chemical and Natural Gas Engineering  
Texas A&M University - Kingsville

# Introduction

CO<sub>2</sub> is identified by the EPA as a **Primary Greenhouse Gas** and is largely responsible for current global warming trends.



Various USA groups are actively involved in developing technologies for reducing CO<sub>2</sub> emissions by using **capture and storage** methods.

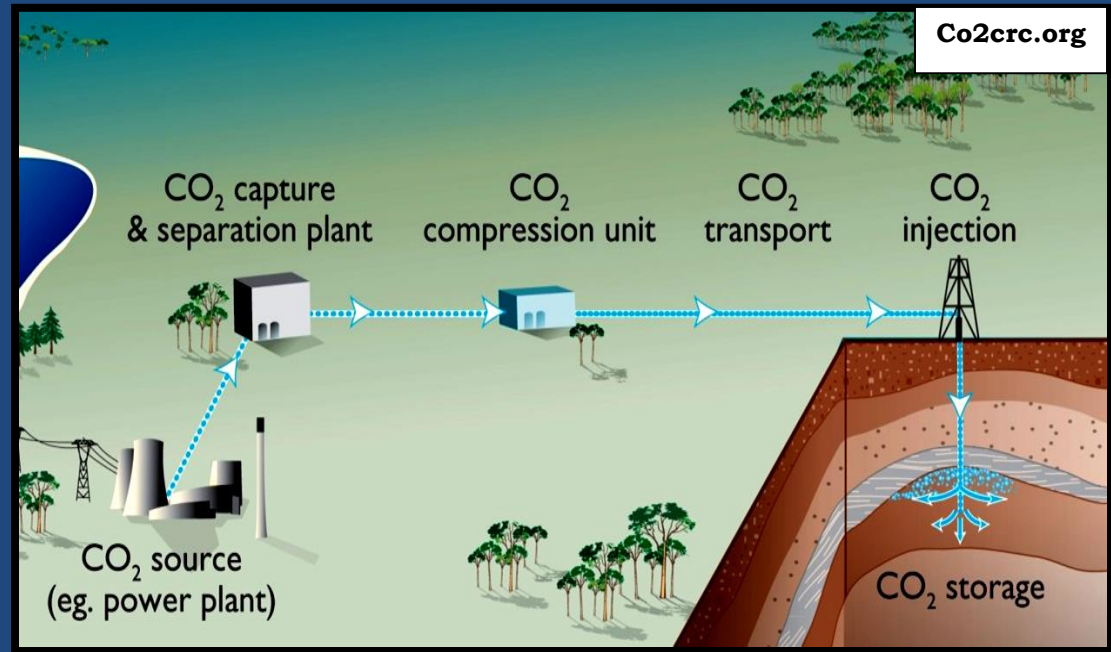
# Geological CO<sub>2</sub> Storage Methods

Technologies being developed for geologic storage are focused on five different approaches:

1. Oil and gas reservoirs
2. Saline formations
3. Coal seams
4. Basalts
- 5. Organic-rich shales**

## Challenges

- Very low inter-pore communication
- Shale characterization
- High drilling and completion costs



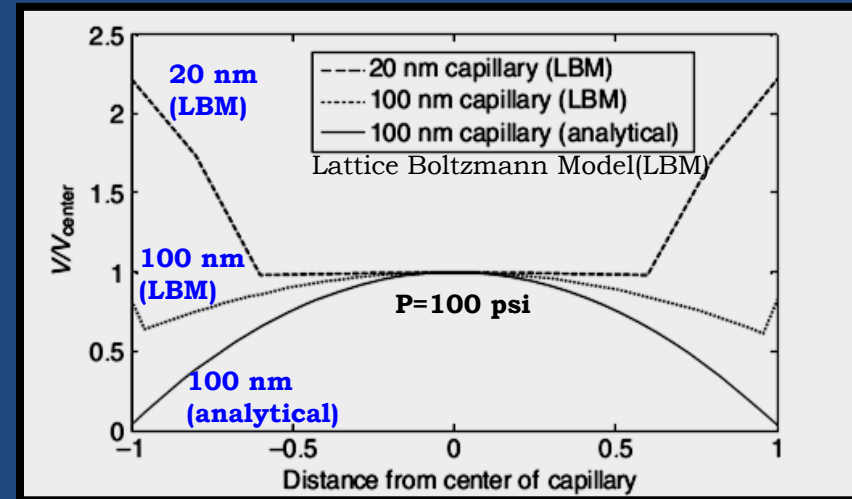
# Motivation

- Shale gas reservoirs would benefit by enhanced recovery methods owing to low recovery factors
- Methane production is primarily limited by shale gas reservoir nano-pores
- No detailed comparison of flux models used for gas transport has been performed
- Performance of various flux models need to be delineated for developing better understanding of gas transport in nano-pores & hence development of higher recovery factors

# Shale Gas Reservoir

## Unique Features

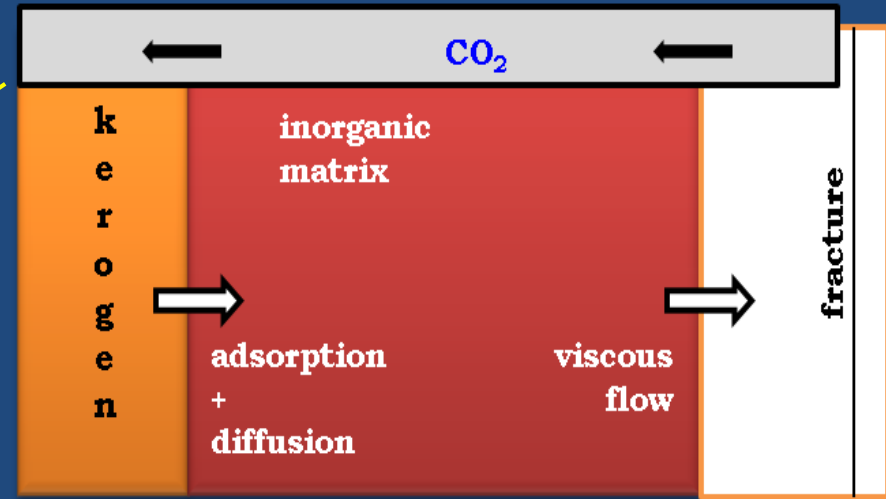
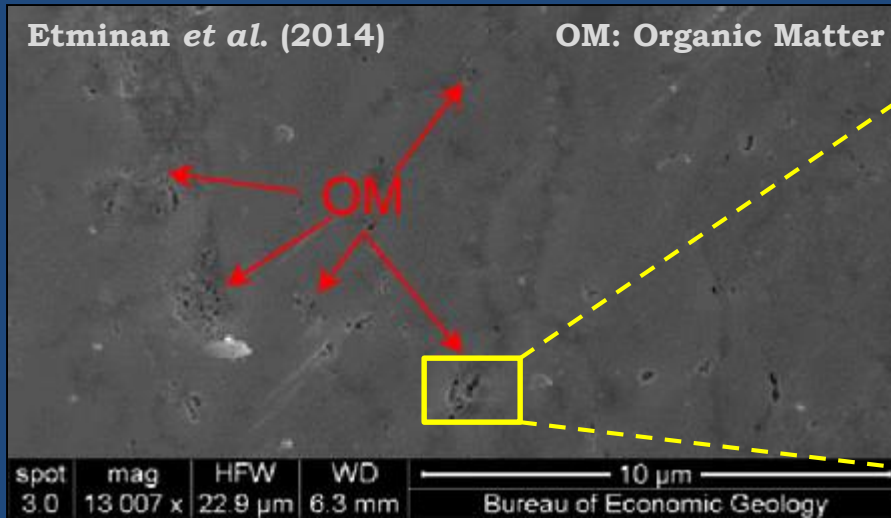
- Low voidage (0.08-0.12) & ultra-low permeability ( $10^{-10}$ - $10^{-12}$  Darcy)
- Significant gas production through adsorption and desorption



Fathi and Akkutlu (2013)

- Desorption occurs as pressure decreases during production and becomes part of the free gas in the natural fractures.
- Javadpour (2009), Fathi and Akkutlu (2011), Kang *et al.* (2011) proved the existence of nano-pores in shales.
- This resulted in the introduction of Knudsen diffusion and slit flow to describe species transport in nano-pores.

# Gas Flow in Shale Nano-pores



- In thermodynamic equilibrium, gas molecules are found in three layers:

1. **Adsorption layer**
2. **Transition layer**
3. **Free gas layer**

- Application of DP (drilling & production)

- **Slippage** (transition region) and
- **Surface diffusion** (adsorbed layer)

Nano-pore (10 nm)



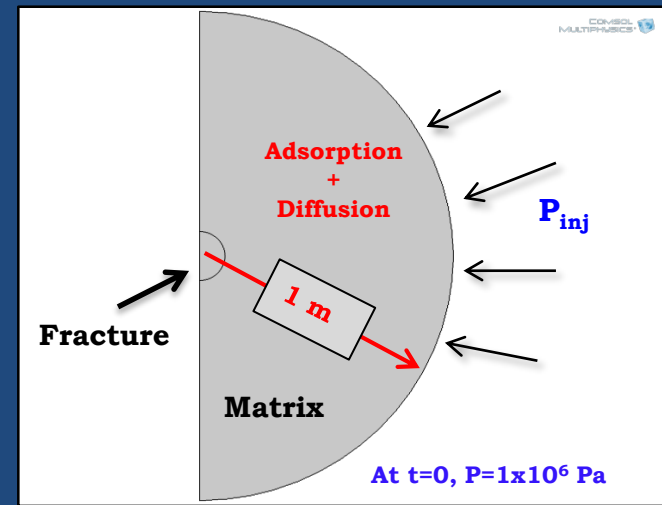


# Model Description

## Assumptions

1. Ideal gas behavior
2. Constant reservoir temperature
3. Single-phase gas flow
4. Constant rock compressibility
5. Isotropic & homogeneous matrix
6. Constant matrix & fracture voidage

- **Physics: COMSOL PDE Module**
- **Solver: Time Dependent PARDISO Solver**
- **Tolerance Factor: 0.1**
- **Maximum Iterative Steps: 5**



COMSOL model geometry with initial boundary conditions

## Reservoir Parameters

Molar mass of $\text{CH}_4$ , kg/mol	0.016
Molar mass of $\text{CO}_2$ , kg/mol	0.044
Permeability, $\text{m}^2$	$1.0 \times 10^{-19}$
Voidage	8.0 %
Rock density, $\text{kg}/\text{m}^3$	2560
Absolute temperature, K	353
Compressibility factor ( $Z_s$ )	1.0
Rock compressibility, $\text{Pa}^{-1}$	$1 \times 10^{-5}$
Langmuir pressure of $\text{CH}_4^*$ , Pa	$3.05 \times 10^6$
Langmuir pressure of $\text{CO}_2^*$ , Pa	$1.68 \times 10^6$
Langmuir volume of $\text{CH}_4^*$ , $\text{std.m}^3/\text{kg}$	$9.80 \times 10^{-4}$
Langmuir volume of $\text{CO}_2^*$ , $\text{std.m}^3/\text{kg}$	$1.91 \times 10^{-3}$

# Governing Multiphysics Equations

## Kerogen-Matrix Species Mass Balance

$$\frac{\partial(\rho\phi_m + \rho_q(1 - \phi_m))_i}{\partial t} + \nabla \cdot (\rho u)_{m,i} = 0$$

where,  $i = 1$  (Methane, CH<sub>4</sub>)  
 $i = 2$  (Carbon Dioxide, CO<sub>2</sub>)

$$\rho_i = \frac{P_i M_i}{Z_i R T} \quad \& \quad P_i = x_i P$$

## Adsorbed Gas Density

$$\rho_{q,i} = \frac{\rho_s M_i}{V_{std}} \times q_{ads,i}$$

## Extended Langmuir Adsorption Isotherm

$$q_{ads,i} = \frac{V_{L,i} B_i P_i}{1 + \sum_{j=1}^n B_j P_j}$$

**Binary Diffusion Coefficient** : Chapman-Enskog Theory

**Knudsen Diffusion Coefficient** : Sun et al. (2014)

## Flux Models

### Wilke Model

$$N_i = (-D_{ei,m} \nabla C_i), \quad D_{ei,m} = \frac{1}{\left( \sum_{j=1, j \neq i}^n \frac{x_j}{D_{ij}^e} \right)}$$

### Wilke-Bosanquet Model

$$N_i = (-D_{i,eff} \nabla C_i), \quad \frac{1}{D_{i,eff}} = \frac{1}{D_{ei,m}} + \frac{1}{D_{ei,k}}$$

### Maxwell-Stefan Model

$$N_i = \frac{-\nabla C_i + \sum_{j=1, j \neq i}^n \frac{x_i N_j}{D_{ij}^e}}{\sum_{j=1, j \neq i}^n \frac{x_j}{D_{ij}^e}}$$

### Dusty Gas Model

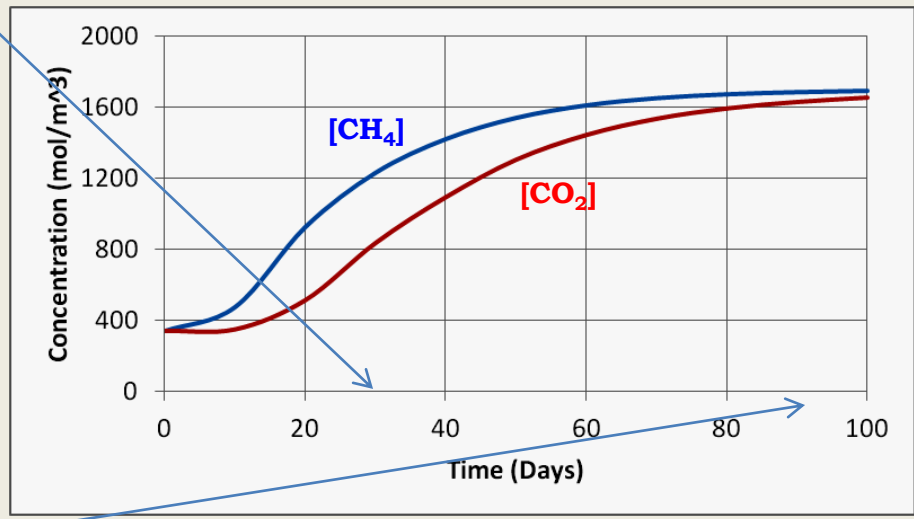
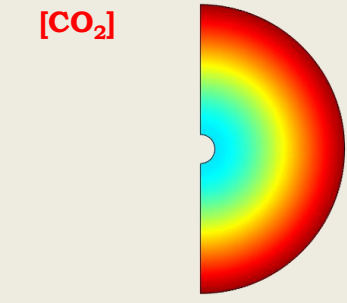
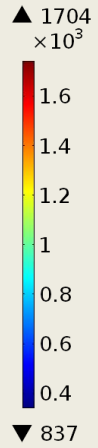
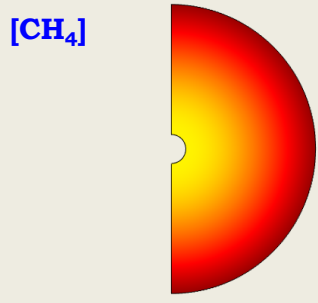
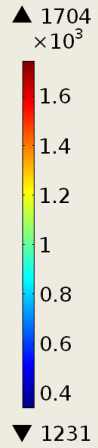
$$N_i = \frac{\sum_{j=1, j \neq i}^n \frac{x_i N_j}{D_{ij}^e} - \frac{C_i v^*}{D_{ei,k}} - \nabla C_i}{\sum_{j=1, j \neq i}^n \frac{x_j}{D_{ij}^e} + \frac{1}{D_{ei,k}}}, \quad v^* = -\frac{\varepsilon d_{pore}^2}{32 \tau \mu} \nabla P$$



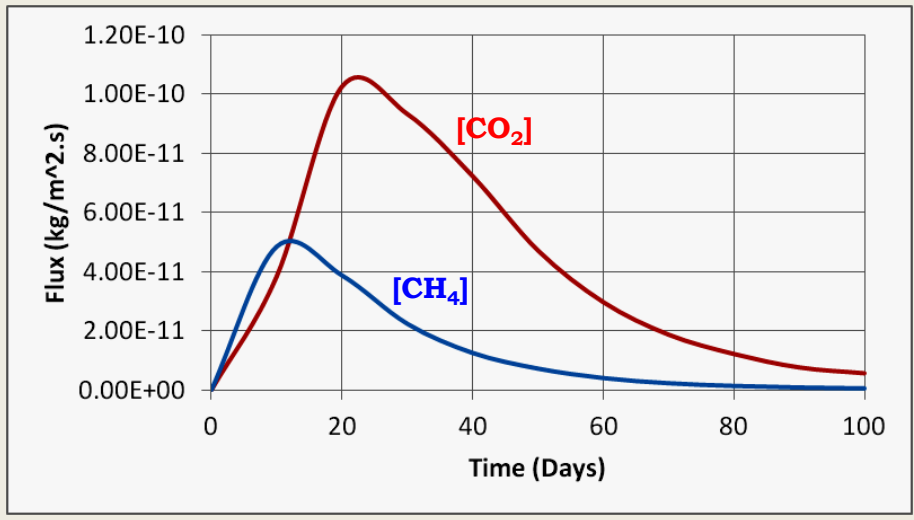
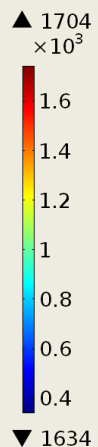
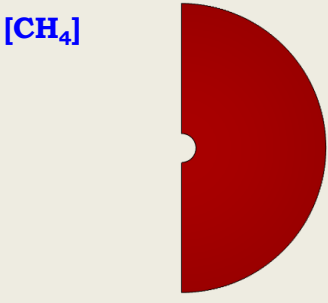
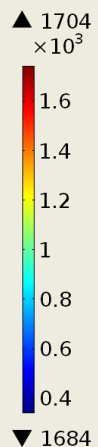
# Key Results

**Wilke Flux Model:**  $N_i = (-D_{ei,m} \nabla C_i)$ ,  $D_{ei,m} = \left( \sum_{j=1, j \neq i}^n (x_j / D_{ij}^e) \right)^{-1}$

**Production Time = 30 Days**

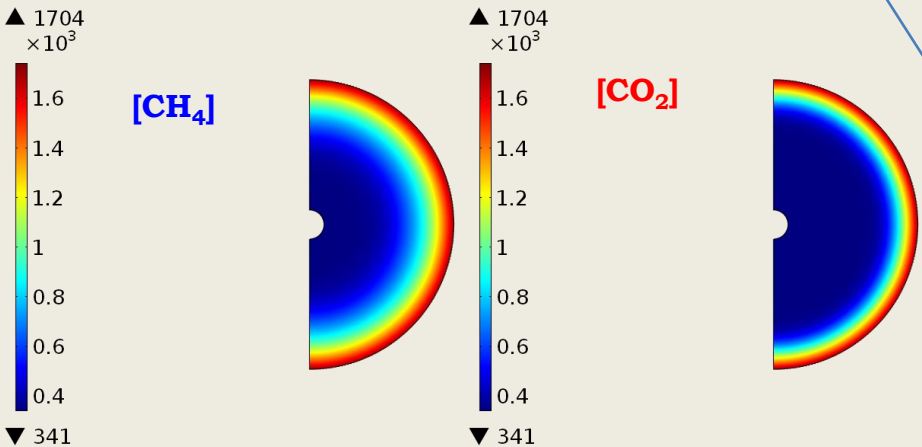


**Production Time = 90 Days**

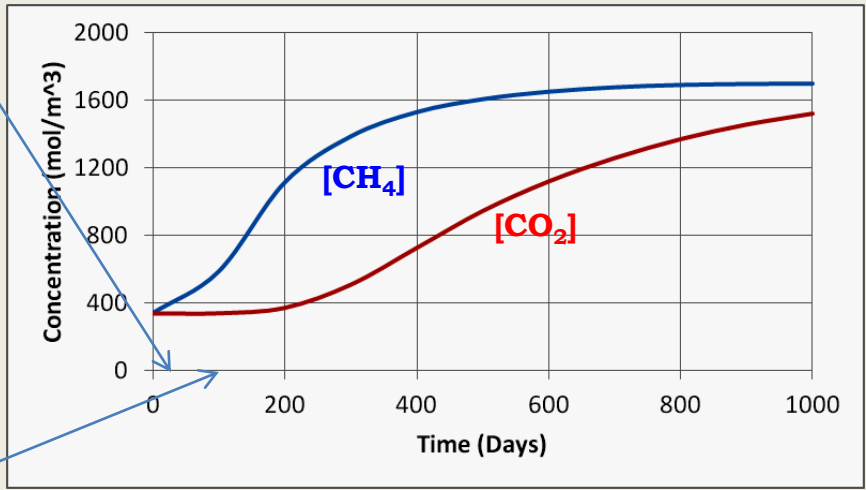


**Wilke-Bosanquet Flux Model:**  $N_i = (-D_{i,eff} \nabla C_i)$ ,  $\frac{1}{D_{i,eff}} = \frac{1}{D_{ei,m}} + \frac{1}{D_{ei,k}}$

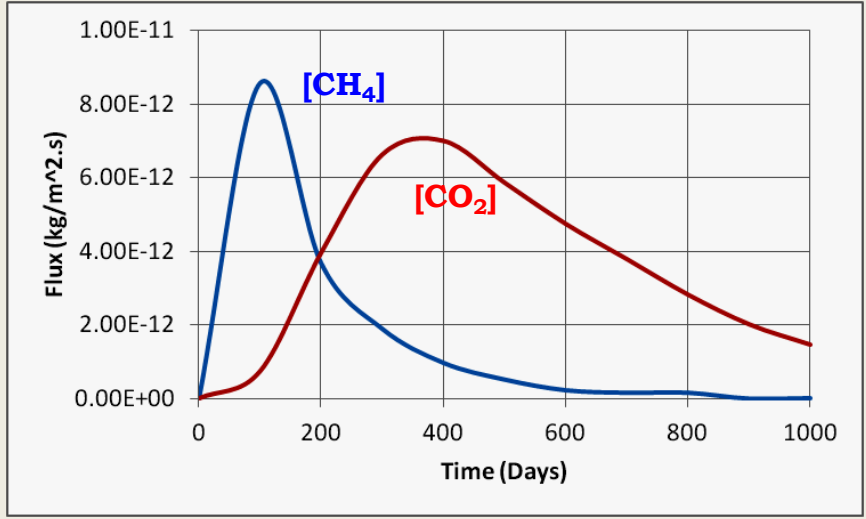
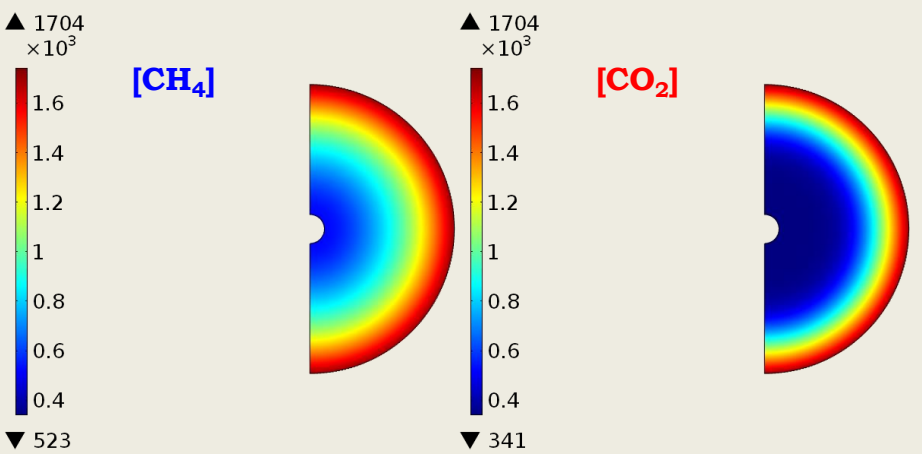
**Production Time = 30 Days**



**Simulation Time = 1000 Days**



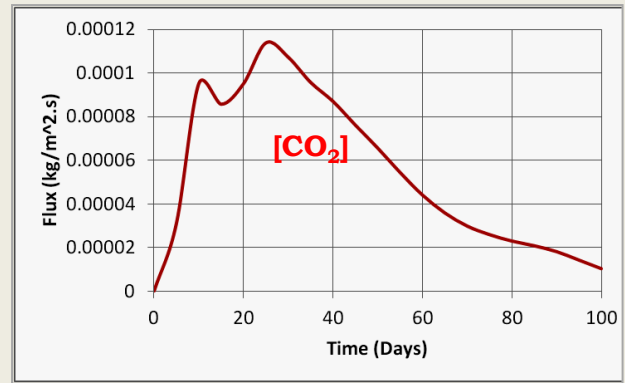
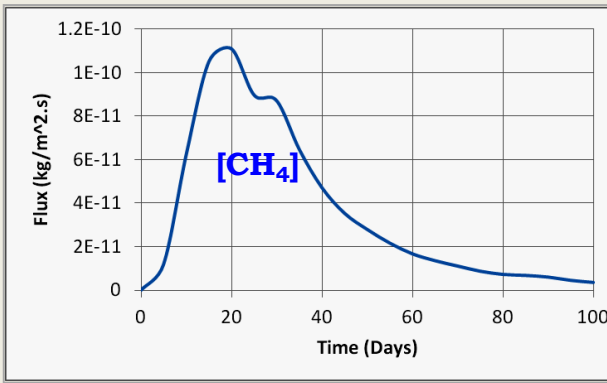
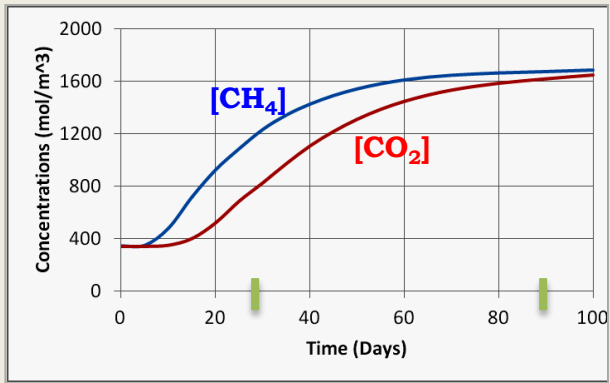
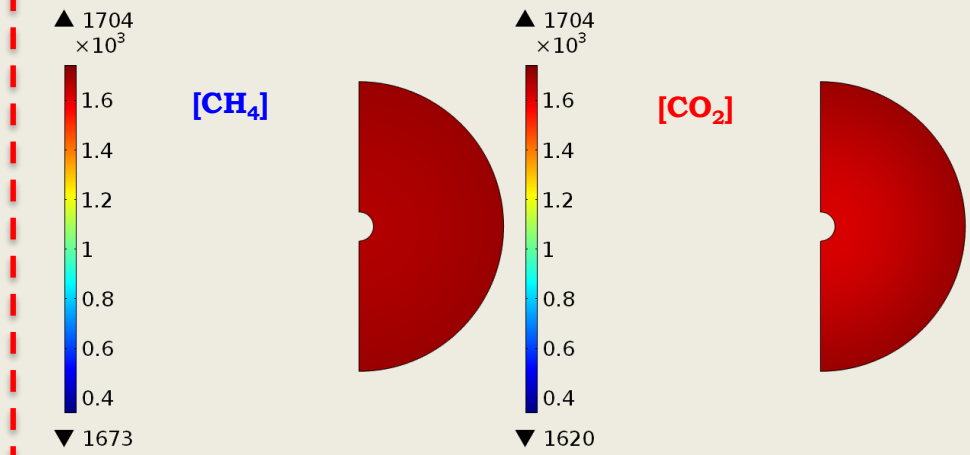
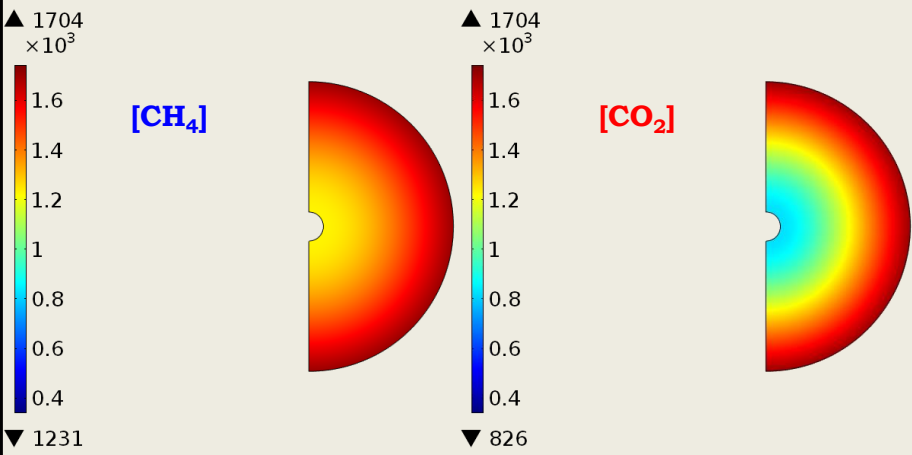
**Production Time = 90 Days**



$$\text{Maxwell-Stefan Flux Model: } N_i = \left( -\nabla C_i + \sum_{j=1, j \neq i}^n \frac{x_i N_j}{D_{ij}^e} \right) \times \left( \sum_{j=1, j \neq i}^n \frac{x_j}{D_{ij}^e} \right)^{-1}$$

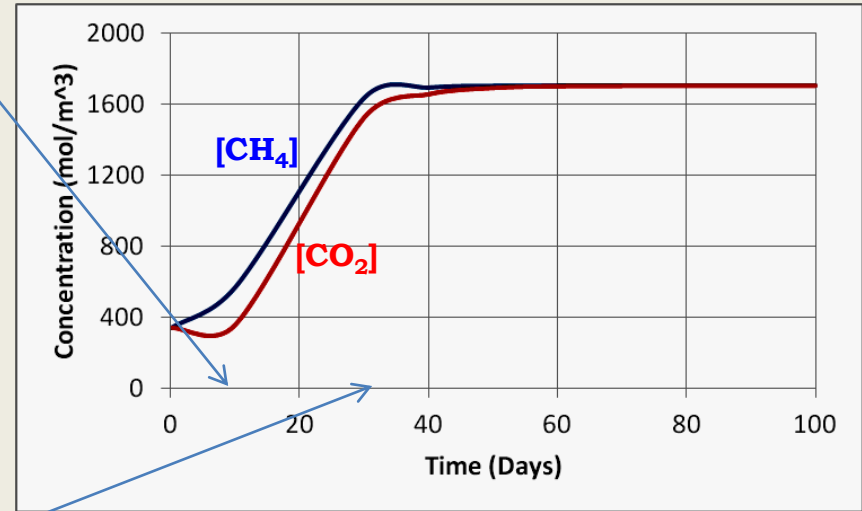
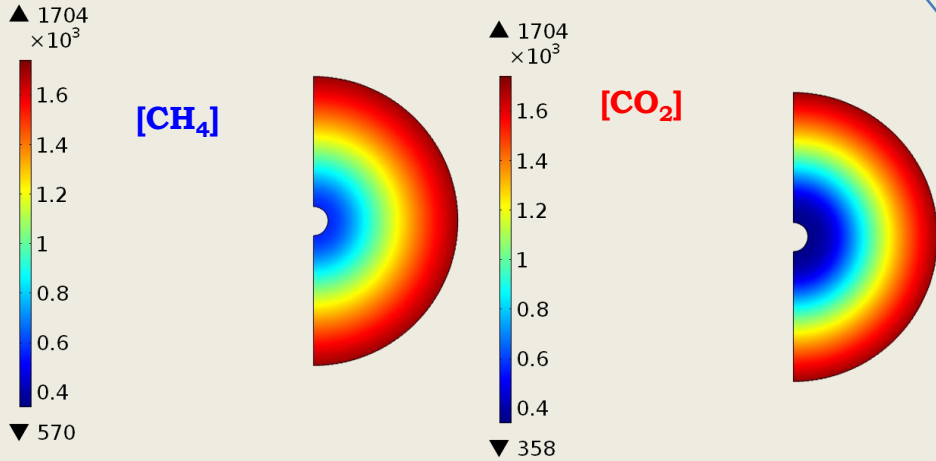
**Production Time = 30 Days**

**Production Time = 90 Days**

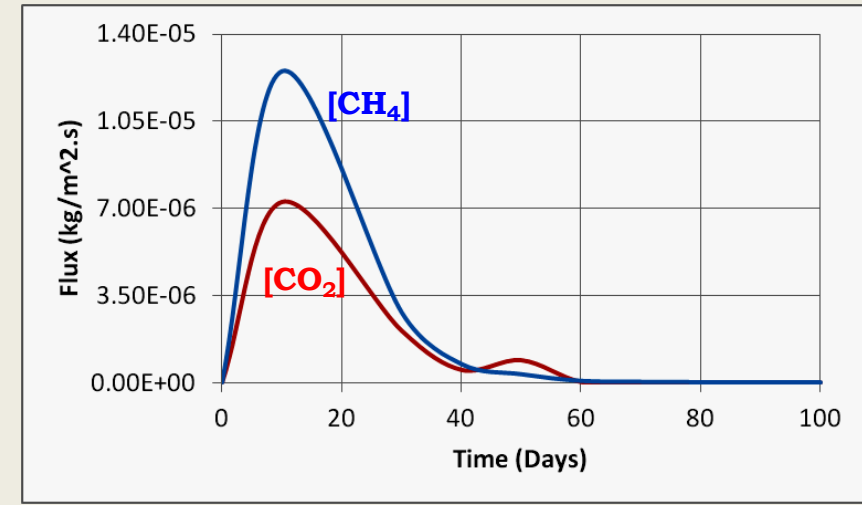
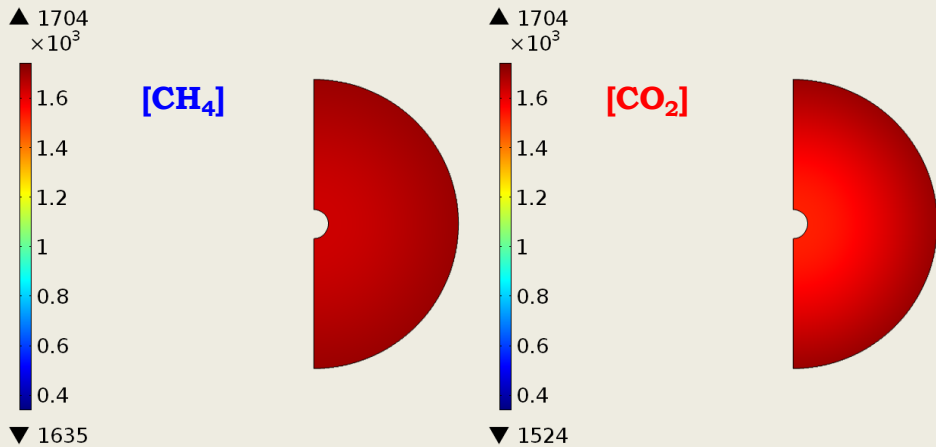


$$\text{Dusty Gas Flux Model: } N_i = \left( \sum_{j=1, j \neq i}^n \frac{x_j N_j}{D_{ij}^e} - \frac{C_i v^*}{D_{eik}} \cdot \nabla C_i \right) \times \left( \sum_{j=1, j \neq i}^n \frac{x_j}{D_{ij}^e} + \frac{1}{D_{eik}} \right)^{-1}$$

**Production Time = 10 Days**

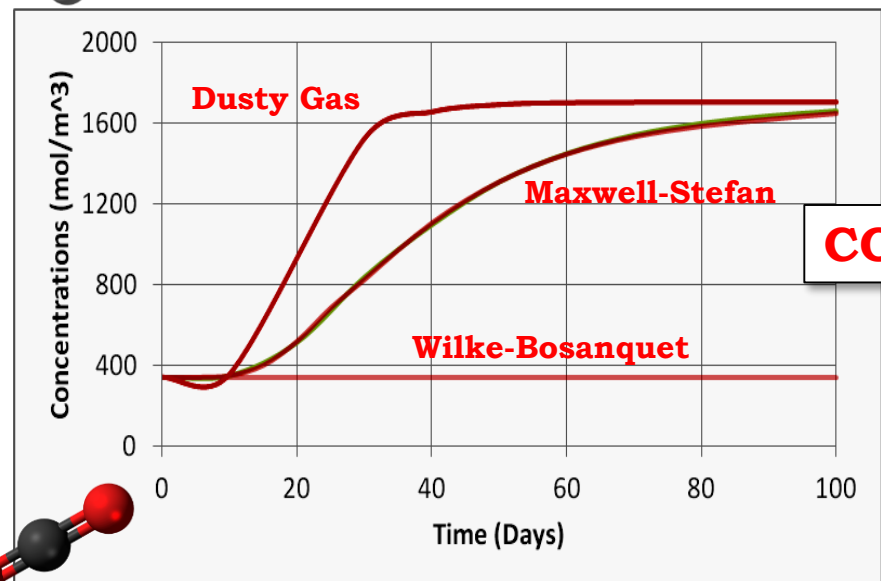
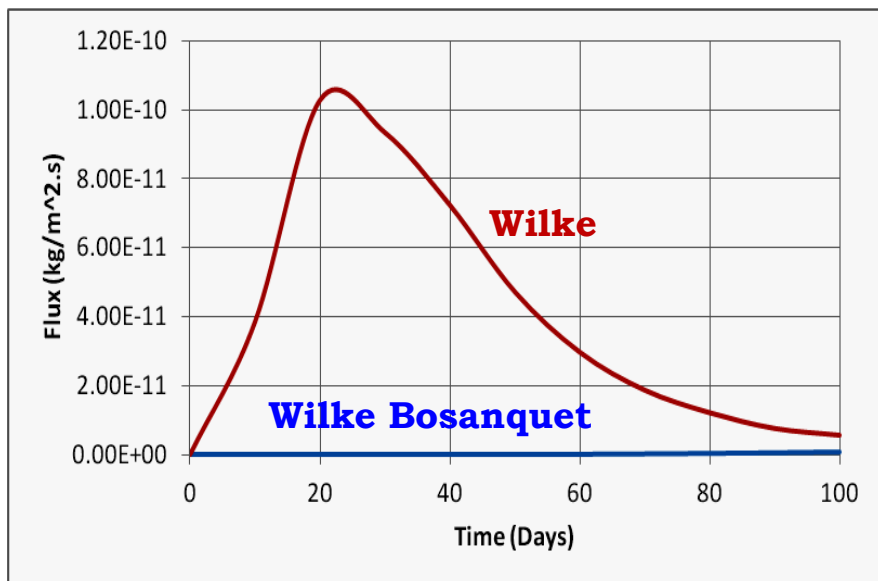
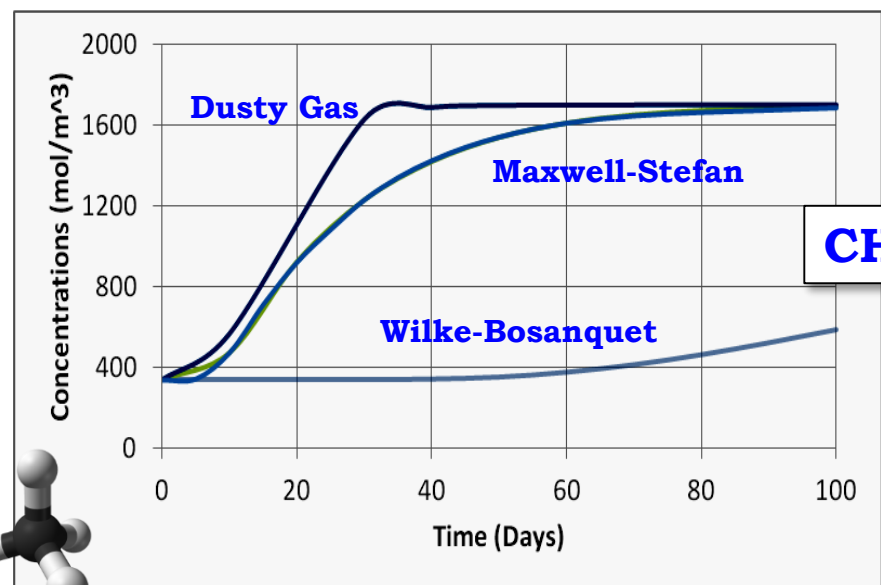
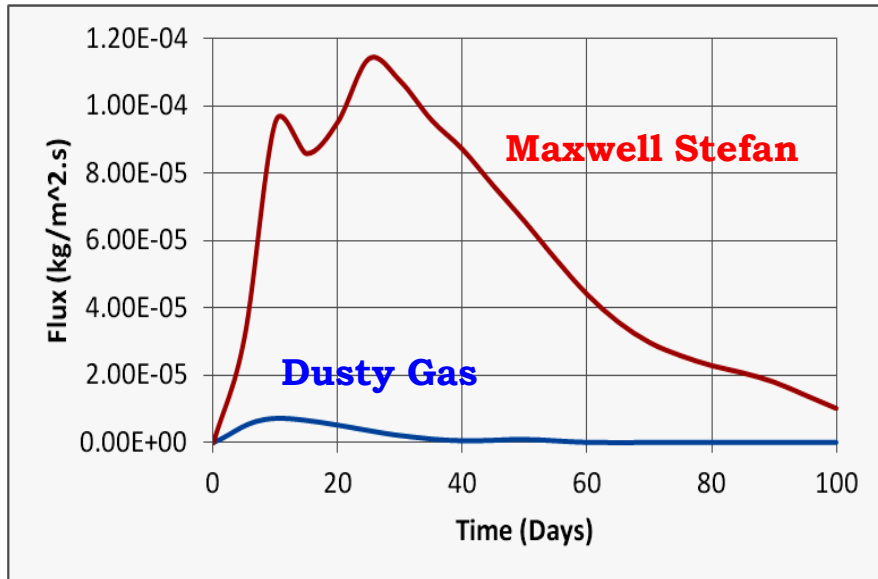


**Production Time = 30 Days**



# FLUX COMPARISON

# CONC. COMPARISON





# Key Adaptations

- Initial difficulties encountered in 2D with Dusty gas and Maxwell-Stefan flux models:
  - Non-smooth conc<sup>n</sup> & flux profiles with increasing time range
  - Convergence errors occurred when  $t > 50$  mins

## Adaptation :

- Reduced DOF by use of 2D-axisymmetric geometry
- Equations for both the above models are highly non-linear
  - Operator :  $(Pz \leq 0) * (Pz \geq 0)$  for efficient computation

# Conclusions & Future Work

- Shale characterization is very important for optimum development of the reservoir. COMSOL has served as a very strong computation engine for solving the non-linear equations associated with shale nano-pores.
- Comparison of various flux models shows that Knudsen diffusion ( $D_k$ ) plays very important role for defining fluid flow in shale nano-pores specially in a fluid mixture with  $\text{CO}_2$ .
- Higher adsorption of  $\text{CO}_2$  is noticed, causing preferential flow of  $\text{CH}_4$  molecules.  $\text{CO}_2$  will stay adsorbed until a threshold pressure is reached.
- Dusty gas model gives the best fit for the considered system as it incorporates pore structure as part of equation along with  $D_k$  and  $D_m$ .
- This model can be extended by including other physical phenomena, such as fracture flow mechanics, other gas species and multi-phase flow due to variable pressure, temperature and water concentration.

**Thank you  
for your  
Attention**

**QUESTIONS??**