

Comparison of Numerical Simulators for Greenhouse Gas Storage in Coalbeds, Part I: Pure Carbon Dioxide Injection

David H.-S. Law (law@arc.ab.ca; 780-450-5034)

Alberta Research Council (ARC) Inc.
250 Karl Clark Road, Edmonton, Alberta, Canada T6N 1E4

L.H.G. (Bert) van der Meer (l.vandermeer@nitg.tno.nl; +31-30-256-4635)

Netherlands Institute of Applied Geoscience TNO
P.O. Box 80015, 3508 TA Utrecht, The Netherlands

W.D. (Bill) Gunter (gunter@arc.ab.ca; 780-450-5467)

Alberta Research Council (ARC) Inc.
250 Karl Clark Road, Edmonton, Alberta, Canada T6N 1E4

Abstract

The injection of carbon dioxide (CO₂) in deep, unmineable coalbeds is a very attractive option for geologic CO₂ storage: the CO₂ is stored and at the same time the recovery of coalbed methane (CBM) is enhanced. The revenue of methane (CH₄) production can offset the expenditures of the storage operation.

Coalbeds form complex gas reservoirs characterized by their dual porosity: they contain both primary and secondary porosity systems. The primary porosity system contains the vast majority of the gas-in-place volume while the secondary porosity system provides the conduit for mass transfer to production wells. Primary porosity gas storage is dominated by adsorption. Mass transfer for each gas molecular species is dominated by diffusion that is driven by the concentration gradient. Flow through the secondary porosity system is dominated by Darcy flow that relates flow rate to permeability and pressure gradient. A full understanding of all of the process mechanisms is essential to performing a numerical simulation of this CO₂ storage process in which CO₂ is injected into the coalbed to replace the adsorbed CH₄.

Existing CBM numerical simulators which are developed for the primary CBM recovery process, have many important features such as: (1) a dual porosity system; (2) Darcy flows of gas and water (i.e., multiphase flow) in the natural fracture system; (3) pure gas diffusion and adsorption in the primary porosity system; and (4) coal shrinkage due to gas desorption; taken into consideration. However, process mechanisms become more complex with CO₂ injection. Additional features such as: (1) coal swelling due to CO₂ sorption on coal; (2) mixed gas adsorption; (3) mixed gas diffusion; and (4) non-isothermal effect for gas injection; have to be considered.

This paper describes the first part of a comparison study between numerical simulators for CO₂ storage in coalbeds with pure CO₂ injection. The second part of the comparison study will be for CO₂ storage in coalbed with flue gas injection. Proposed problem sets are presented along with preliminary simulation results obtained from various numerical

simulators. The problems selected for comparison are intended to exercise many of the CBM related features of the simulators that are of practical and theoretical interest.

Introduction

The injection of carbon dioxide (CO₂), a greenhouse gas (GHG), in coalbeds is probably the most attractive option of all underground CO₂ storage possibilities: the CO₂ is stored and at the same time the recovery of coalbed methane (CBM) is enhanced (Gunter et al., 1997). The revenue of methane (CH₄) production can offset the expenditures of the storage operation (Wong et al., 2000a and 2000b).

Coalbeds are characterized by their dual porosity: they contain both primary (micropore and mesopore) and secondary (macropore and natural fracture) porosity systems. The primary porosity system contains the vast majority of the gas-in-place volume while the secondary porosity system provides the conduit for mass transfer to the wellbore. Primary porosity gas storage is dominated by adsorption. The primary porosity system is relatively impermeable due to the small pore size. Mass transfer for each gas molecular species is dominated by diffusion that is driven by the concentration gradient. Flow through the secondary porosity system is dominated by Darcy flow that relates flow rate to permeability and pressure gradient.

Figure 1 illustrates the overall process of gas storage and the movement through coalbeds. The conventional primary CBM recovery process begins with a production well that is often stimulated by hydraulic fracturing to connect the wellbore to the coal natural fracture system via an induced fracture. When the pressure in the well is reduced by opening the well on the surface or by pumping water from the well, the pressure in the induced fracture is reduced which in turn reduces the pressure in the coal natural fracture system. Gas and water begin moving through the natural and induced fractures in the direction of decreasing pressure. When the natural fracture system pressure drops, gas molecules desorb from the primary-secondary porosity interface and are released into the secondary porosity system. 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 mesoporosity. Adsorbed gas continues to be released as the pressure is reduced.

When CO₂ (which is more strongly adsorbable than CH₄) is injected into the coal natural fracture system during the CO₂ storage process, it is preferentially adsorbed into the primary porosity system. Upon adsorption, the CO₂ drives CH₄ from the primary porosity into the secondary porosity system. The secondary porosity pressure is increased due to CO₂ injection and the CH₄ flows to production wells. The CO₂ is stored in-situ and is not produced unless the injected gas front reaches the production wells. The process, in general, is terminated at CO₂ breakthrough. A full understanding of all the complex mechanisms involved in the CO₂ storage process is essential to have more confidence in the numerical modeling of the process.

The objective of this study of comparison of numerical simulators is to provide the incentive to improve existing CBM simulators for capability and performance assessment of CO₂ storage in deep, unminable coalbeds.

Descriptions of Numerical Simulators

Seidle and Arri, 1990 have demonstrated that conventional oil and gas numerical models can be used for primary CBM recovery process, provided that the diffusion of CH₄ from the primary porosity system into the natural fracture system of the coal is much faster than Darcy flow through the natural fractures into the production well. In this way, numerical models with only a single porosity approach can be used. Since then, many commercial and research numerical models have been developed to model primary CBM recovery process taken into account of many important features such as:

- dual porosity nature of coalbed;
- Darcy flows of gas and water (i.e., multiphase flow) in the natural fracture system in coal;
- diffusion of a single gas component (i.e., pure gas) from the coal matrix to the natural fracture system;
- adsorption/desorption of a single gas component (i.e., pure gas) at the coal surface; and
- coal matrix shrinkage due to gas desorption.

A general description of the two types of CBM numerical simulators is given in Table 1.

Five numerical simulators are being compared at the Alberta Research Council (ARC) Inc. and the Netherlands Institute of Applied Geoscience TNO for their capability to model CO₂ storage process based on valuable field test data which have been collected in the ARC's CO₂ storage project through performing micro-pilot tests by CO₂/flue gas injection into coal seams in Alberta, Canada (Wong and Gunter, 1999): (1) STARS, Computer Modelling Group (CMG) Ltd., Calgary, Alberta, Canada; (2) GEM, Computer Modelling Group (CMG) Ltd., Calgary, Alberta, Canada; (3) ECLIPSE, Schlumberger GeoQuest, Abingdon, Oxon, United Kingdom; (4) GCOMP, BP-Amoco, Houston, Texas, U.S.A.; and (5) SIMED II, Commonwealth Scientific and Industrial Research Organization (CSIRO), Sydney, New South Wales, Australia. The numerical simulators, STARS and GCOMP, are conventional oil and gas simulators converted to model the CO₂ storage process. While the other three numerical simulators are developed with CBM features.

We believe that in order for a numerical simulator to successfully history match the ARC's field test data, the simulator should have the capability to handle the more complicated mechanisms involved in the CO₂ storage process (Law et al., 2000), such as:

- coal matrix swelling due to CO₂ adsorption on the coal surface;
- compaction and dilation of the natural fracture system due to stresses;
- diffusion of multiple gas components (i.e., mixed gas) from the coal matrix to the natural fracture system;
- movement of water between the coal matrix and the natural fracture system;

- adsorption/desorption of multiple gas components (i.e., mixed gas) at the coal surface; and
- non-isothermal adsorption due to difference in temperatures between the coalbed and the injected CO₂.

Unfortunately, not all these features are available in the existing CBM numerical simulators. Better understanding of these process mechanisms in both the field and in the laboratory will lead to the improvement of the numerical simulators.

Approach

We propose an approach (Pruess et al., 2001) to organize and manage the simulator comparison study; facilitate the development and selection of appropriate test problems; distribute them to interested groups of scientists and engineers who want to participate in this exercise; and solicit, collect, reconcile, and document solutions. Development and selection of sample test problems is made on the basis of major mechanisms expected to occur in the CO₂ storage process into coalbeds, taking into account the existing simulation capabilities and future needs.

The initial test problems emphasize the comparison of the performance of existing CBM simulators, which may not have all the features to properly model the CO₂ storage process. At a later stage, test problems will be developed that address more complicated process mechanisms. At this stage, improvement on existing numerical simulators may be necessary. Finally, performance of numerical simulators will be compared for their capability to history match available field test data of CO₂ storage into coalbeds with production of CBM.

Two sets of test problems have been assembled, which are intended to initiate the study. At the present time, ARC and TNO are working very closely with various simulator developers to compare their numerical simulators and identify/recommend improvements in future model development. However, this study is opened to other interested technical groups worldwide who are invited to model and study the test problems using their own simulators and funding.

Descriptions of Test Problem Sets

The first problem set deals with a single well test with pure CO₂ injection and the second problem set deals with CO₂ injection/CBM production in an inverted five-spot pattern. These two problem sets compare the basic features of the numerical simulators for CBM modeling which allows most CBM simulators to be used in the early stage of this study.

- Darcy flows of gas and water in the natural fracture system in coal;
- adsorption/desorption of two different gas components (i.e., CH₄ + CO₂) at the coal surface;
- instantaneously gas flow (i.e., diffusion) between the primary/secondary porosity system;
- no coal matrix shrinkage/swelling due to gas desorption/adsorption;

- no compaction and dilation of natural fracture system due to stresses; and
- no non-isothermal adsorption due to difference in temperatures between the coalbed and the injected CO₂.

The problem sets have as many common features as possible (e.g., coalbed characteristics, well radius, etc.).

Coalbed Characteristics

Coalbed Properties

Coal seam thickness = 9 m [29.527 ft]
 Top of coal seam = 1253.6 m [4112.8 ft]
 Absolute permeability of natural fracture = 3.65 md
 Porosity of natural fracture = 0.001
 Effective coalbed compressibility = 1.45×10^{-7} /kPa [1 x 10⁻⁶ /psia]

Initial Reservoir Conditions

Temperature = 45°C [113°F]
 Pressure (assumed uniform from top to bottom) = 7650 kPa [1109.5 psia]
 Gas saturation = 0.408
 Water saturation = 0.592

Water Properties at 45°C (113°F)

Density = 990 kg/m³ [61.8 lb/ft³]
 Viscosity = 0.607 cp
 Compressibility = 5.8×10^{-7} /kPa [4 x 10⁻⁶ /psia]

Pure Gas Adsorption Isotherms at 45°C (113°F)

Average in-situ coal density = 1434 kg/m³ [89.5 lb/ft³]
 Average in-situ moisture content (by wt.), $w_{we} = 0.0672$
 Average in-situ ash content (by wt.), $w_a = 0.156$

The dry, ash-free isotherm parameters shown in Table 2 will be used to estimate the in-situ storage capacity as a function of pressure, ash content, and in-situ moisture content using the Langmuir relationship (Langmuir, 1918):

$$G_s = G_{sL} \left[1 - (w_a + w_{we}) \right] \frac{p}{p + p_L}$$

where:

G_s gas storage capacity
 G_{sL} dry, ash-free Langmuir storage capacity
 w_a ash content, weight fraction
 w_{we} equilibrium moisture content, weight fraction
 p pressure
 p_L Langmuir pressure

The individual component isotherm parameters are used to compute storage capacity when multiple gas species are present. The computation is based upon extended Langmuir isotherm theory (Arri et al., 1992). The extended Langmuir isotherm relationship is listed as following:

$$G_{si} = G_{sLi} \left[1 - (w_a + w_{we}) \right] \frac{\frac{p y_i}{p_{Li}}}{1 + p \sum_{j=1}^{nc} \frac{y_j}{p_{Lj}}}$$

where:

G_{si}	multicomponent storage capacity of component i, in-situ basis
G_{sLi}	single component Langmuir storage capacity of component i, dry, ash-free basis
p_{Li} or p_{Lj}	single component Langmuir pressure of component i or j
y_i or y_j	mole fraction of component i or j in the free gas (vapor) phase
nc	number of components
p	pressure of the free gas phase

Relative Permeability Data

The relative permeability relationship shown in Table 3 is based upon the relationship published by Gash, 1991. No effect of temperature or hysteresis on the relative permeability is considered and the capillary pressures are assumed to be zero.

Problem Set 1

Problem 1: Single well CO₂ injection test.

Grid System

Cylindrical (r-θ-z) grid system: 29 x 1 x 1 (see Figure 2)

Area = 160 acres

Radius = 454 m [1489.5 ft]

r-direction: see Table 4

θ-direction: Δθ = 360°

z-direction: Δz = 9 m [29.5 ft]

Operating Conditions

Well location: (i = 1, j = 1, k = 1)

Well radius (2 7/8" well): 0.0365 m [0.11975 ft]

Well skin factor = 0

15-day CO₂ injection period (0 – 15 days):

CO₂ injection rate (full well) = 28316.82 sm³/d [1 x 10⁶ scf/d]

Maximum bottom-hole pressure = 15000 kPa [2175.6 psia]
 45-day shut-in period (15 – 60 days)
 Well shut-in for pressure falloff
 60-day production period (60 – 120 days)
 Max. gas production rate (full well) = 100000 m³/d [3.5315 x 10⁶ scf/d]
 Minimum bottom-hole pressure = 275 kPa [39.885 psia]
 62.5-day shut-in period (120 – 182.5 days)
 Well shut-in for pressure buildup

Numerical Results

Injection/production histories (results presented in full well):
 Cumulative CO₂/CH₄ production in [sm³]
 CO₂/CH₄ production rates in [sm³/day]
 Production gas composition in [mole fraction]
 Cumulative water production in [sm³]
 Water production rates in [sm³/day]
 Well bottom-hole pressure in [kPa]
 Contours at 5, 15, 30, 45, 60, 75, 90, 105, 120, 150 and 182.5 days:
 Mole fractions of CO₂ in gas phase
 Pressure in [kPa]

Problem Set 2

Problem 2: 5-spot CO₂ injection process.

Grid System

Rectangular (x-y-z) grid system: 11 x 11 x 1 (see Figure 3)

Area = ¼ of a 2.5 acres pattern
 Pattern half width = 50.294 m [165 ft]
 x and y-directions: see Table 5
 z-direction: Δz = 9 m [29.5 ft]

Operating Conditions

Well locations:
 Injection well: (i = 1, j = 1, k = 1)
 Production well: (i = 11, j = 11, k = 1)
 Well radius (2 7/8" well): 0.0365 m [0.11975 ft]
 Well skin factor = 0

182.5-day continuous CO₂ injection/production period (0 – 182.5 days):
 CO₂ injection rate (full well) = 28316.82 sm³/d [1 x 10⁶ scf/d]
 Maximum bottom-hole pressure = 15000 kPa [2175.6 psia]
 Max. gas production rate (full well) = 100000 m³/d [3.5315 x 10⁶ scf/d]
 Minimum bottom-hole pressure = 275 kPa [39.885 psia]

Numerical Results

Injection/production histories (results presented as full 5-spot pattern- one injector and one producer):
 Cumulative CO₂/CH₄ production in [sm³]

CO₂/CH₄ production rates in [sm³/day]
Production gas composition in [mole fraction]
Cumulative CO₂ injection in [sm³]
CO₂ injection rate in [sm³/day]
Cumulative water production in [sm³]
Water production rates in [sm³/day]
Injection/production well bottomhole pressures
Contours at 5, 15, 30, 45, 60, 75, 90, 105, 120, 150 and 182.5 days:
Mole fractions of CO₂ in gas phase
Pressure in [kPa]

Problem 2P: 5-spot primary production process.

Grid System

Same as Problem 2

Operating Conditions

Well locations:

Production well: (i = 11, j = 11, k = 1)

Well radius (2 7/8" well): 0.0365 m [0.11975 ft]

Well skin factor = 0

182.5-day continuous gas production period (0 – 182.5 days):

Max. gas production rate (full well) = 100000 m³/d [3.5315 x 10⁶ scf/d]

Minimum bottom-hole pressure = 275 kPa [39.885 psia]

Numerical Results

Production histories (results presented as full 5-spot pattern – one producer):

Cumulative CH₄ production in [sm³]

CH₄ production rate in [sm³/day]

Cumulative water production in [sm³]

Water production rates in [sm³/day]

Production well bottom-hole pressure in [kPa]

Contours at 5, 15, 30, 45, 60, 75, 90, 105, 120, 150 and 182.5 days:

Pressure in [kPa]

Proposed Future Problem Sets

Problem Set 3: 5-spot CO₂ injection test

Dual porosity approach with mixed gas diffusion from coal matrix to natural fracture system.

Problem Set 4: 5-spot CO₂ injection test

Natural fracture permeability/porosity as functions of natural fracture pressure.

Problem Set 5: 5-spot CO₂ injection test

Natural fracture permeability/porosity as functions of pressure and adsorbed gas content (i.e. coal shrinkage and swelling effects).

Problem Set 6: History matching of available field data

Preliminary Numerical Results

Since the comparison is still ongoing, it will not be appropriate to publish all of the numerical results from various numerical simulators at this stage. Examples for the prediction by the numerical simulators, GEM and GCOMP, are presented to demonstrate the capability of the existing numerical simulators to model the CO₂ storage process.

Figure 4 shows well bottom-hole pressures for the Problem Set 1 indicating the four operating stages; (1) CO₂ injection stage; (2) pressure fall-off stage; (3) gas production stage; and (4) pressure buildup stage. Figure 5 shows CH₄ production rate for the Problem Set 2 indicating the enhancement of CH₄ production due to CO₂ injection. It is found that the prediction by GEM (curves in figures) and GCOMP (symbols in figures) are in general agreement. This indicates that existing numerical simulators have very similar performance even though they use two very different modeling approaches as shown in Table 1.

Readers are encouraged to submit comments, suggestions, and solutions to us via e-mail.

Acknowledgement

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Table 1: Types of CBM numerical simulators

Parameters	Convention Oil & Gas Numerical Simulators	Coalbed Methane Numerical Simulators
Naturally fractured reservoir	Single porosity approach	Dual porosity approach
Physics of gas flow in natural fracture system	Darcy flow (Multiple gas components)	Darcy flow (Limited gas components)
Physics of gas flow between primary/secondary porosity systems	Gas flow instantaneously	Fick's law gas diffusion
Gas adsorption	Adsorption described by gas/oil equilibrium K-values (coal as immobile oil)	Adsorption described by Langmuir isotherms

Table 2: Dry, ash-free Langmuir isotherm parameters

	Methane		Carbon Dioxide		Nitrogen	
	kPa	psia	kPa	psia	kPa	psia
Langmuir Pressure, P_L	4688.5	680	1903	276	27241	3951
Dry, Ash-Free Langmuir Volume, G_{sL}	m ³ /kg	scf/ton	m ³ /kg	scf/ton	m ³ /kg	scf/ton
	0.0152	486.0	0.0310	993.8	0.0150	482.0

Table 3: Relative permeability relationship

Water Saturation, S_w	Rel. Perm. to Water, k_{rw}	Rel. Perm. to Gas, k_{rg}
1.00	1.000	0.000
0.975	0.814	0.0035
0.950	0.731	0.007
0.90	0.601	0.018
0.85	0.490	0.033
0.80	0.392	0.051
0.75	0.312	0.070
0.70	0.251	0.090
0.65	0.200	0.118
0.60	0.154	0.147
0.55	0.116	0.180
0.50	0.088	0.216
0.45	0.067	0.253
0.40	0.049	0.295
0.35	0.035	0.342
0.30	0.024	0.401
0.25	0.015	0.466
0.20	0.007	0.537
0.15	0.002	0.627
0.10	0.0013	0.720
0.05	0.0006	0.835
0.00	0.000	1.000

Table 4: Radial grid system used for Problem Set 1

i	Δr		r	
	(m)	(ft)	(m)	(ft)
1	0.9110	2.9888	0.9110	2.9888
2	1.1600	3.8058	2.0710	6.7946
3	1.3456	4.4147	3.4166	11.2093
4	1.5609	5.1211	4.9775	16.3303
5	1.8106	5.9403	6.7881	22.2706
6	2.1003	6.8907	8.8884	29.1614
7	2.4364	7.9934	11.3248	37.1548
8	2.8262	9.2723	14.1510	46.4271
9	3.2784	10.7559	17.4294	57.1830
10	3.8030	12.4770	21.2324	69.6601
11	4.4114	14.4731	25.6438	84.1332
12	5.1173	16.7890	30.7611	100.9222
13	5.9360	19.4751	36.6971	120.3973
14	6.8858	22.5912	43.5829	142.9885
15	7.9875	26.2057	51.5704	169.1942
16	9.2655	30.3986	60.8359	199.5928
17	10.7480	35.2625	71.5839	234.8553
18	12.4677	40.9045	84.0516	275.7598
19	14.4625	47.4491	98.5141	323.2090
20	16.7765	55.0410	115.2906	378.2500
21	19.4608	63.8478	134.7514	442.0977
22	22.5745	74.0633	157.3259	516.1611
23	26.1864	85.9134	183.5123	602.0744
24	30.3763	99.6598	213.8886	701.7342
25	35.2364	115.6050	249.1250	817.3392
26	40.8742	134.1017	289.9992	951.4409
27	47.4141	155.5581	337.4133	1106.9990
28	55.0005	180.4478	392.4138	1287.4468
29	61.4972	201.7625	453.9110	1489.2093

Table 5: Rectangular grid system used for Problem Set 2

i or j	Δx or Δy		x or y	
	(m)	(ft)	(m)	(ft)
1	2.5	8.2	2.5	8.2
2	5.0	16.4	7.5	24.6
3	5.0	16.4	12.5	41.0
4	5.0	16.4	17.5	57.4
5	5.0	16.4	22.5	73.8
6	5.294	17.37	27.794	91.17
7	5.0	16.4	32.794	107.57
8	5.0	16.4	37.794	123.97
9	5.0	16.4	42.794	140.37
10	5.0	16.4	47.794	156.77
11	2.5	8.2	50.294	164.97

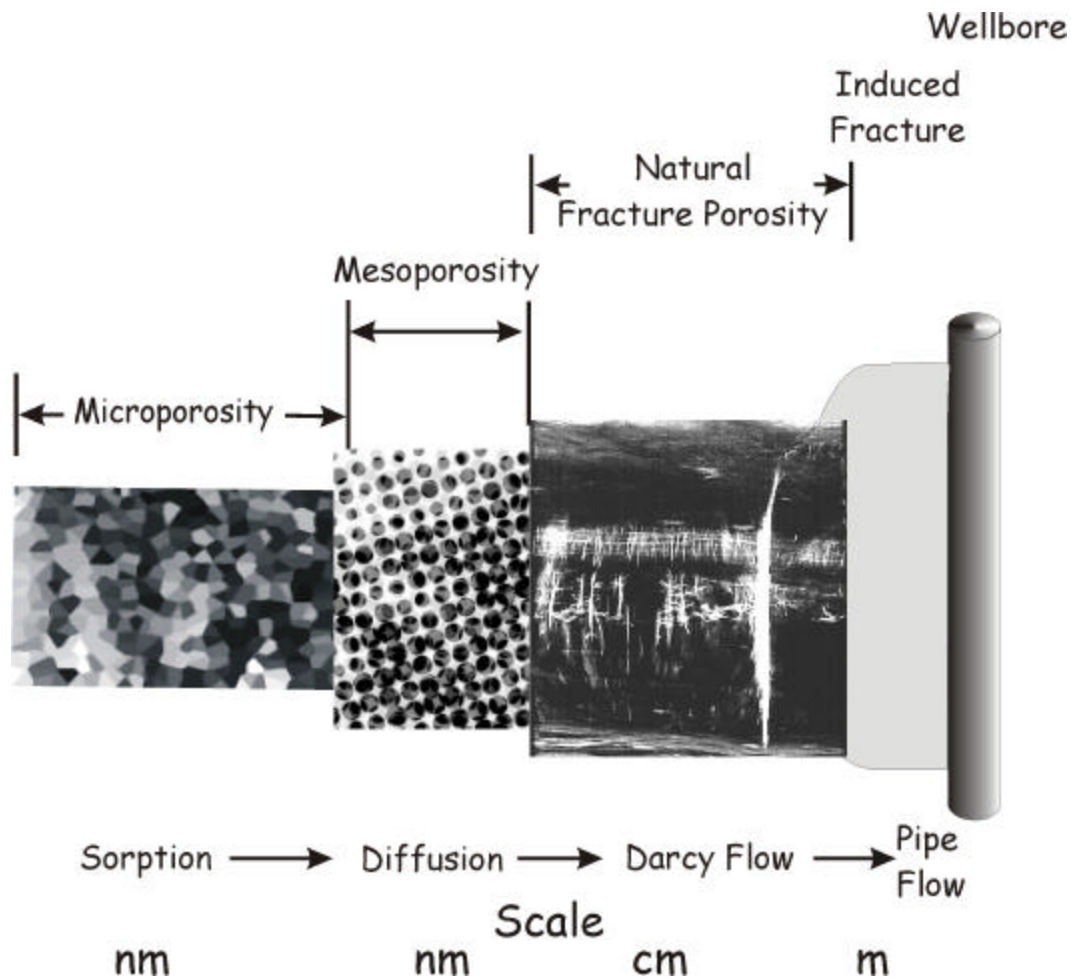


Figure 1: Coal storage and flow mechanisms

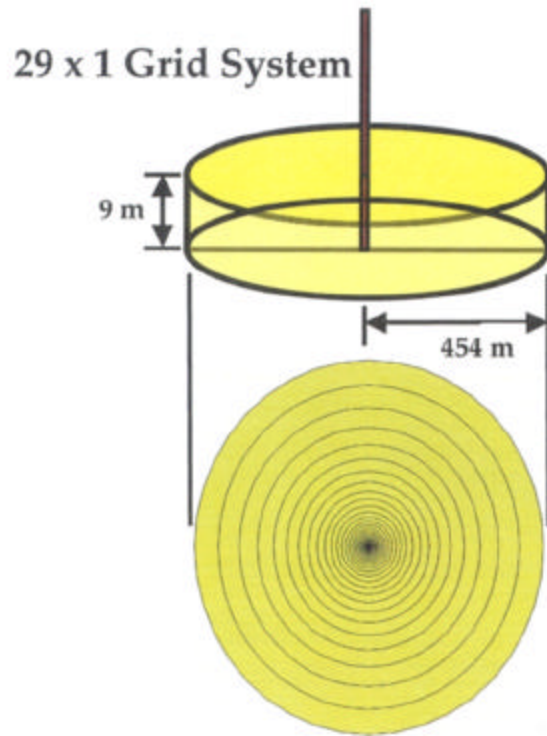


Figure 2: Schematic diagram of radial grid system used in Problem Set 1

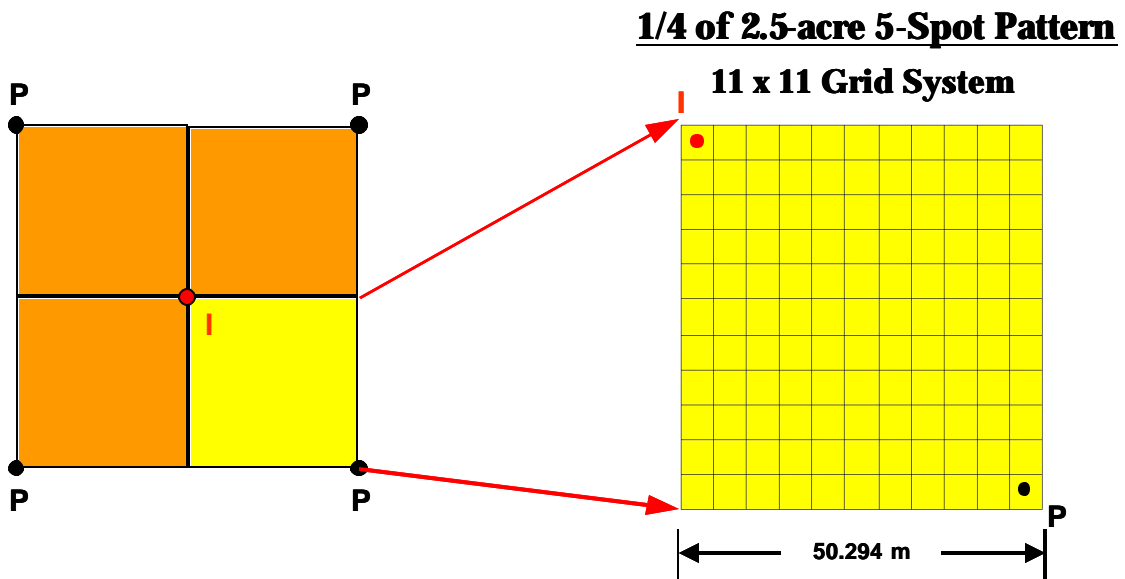


Figure 3: Schematic diagram of rectangular grid system used in Problem Set 2

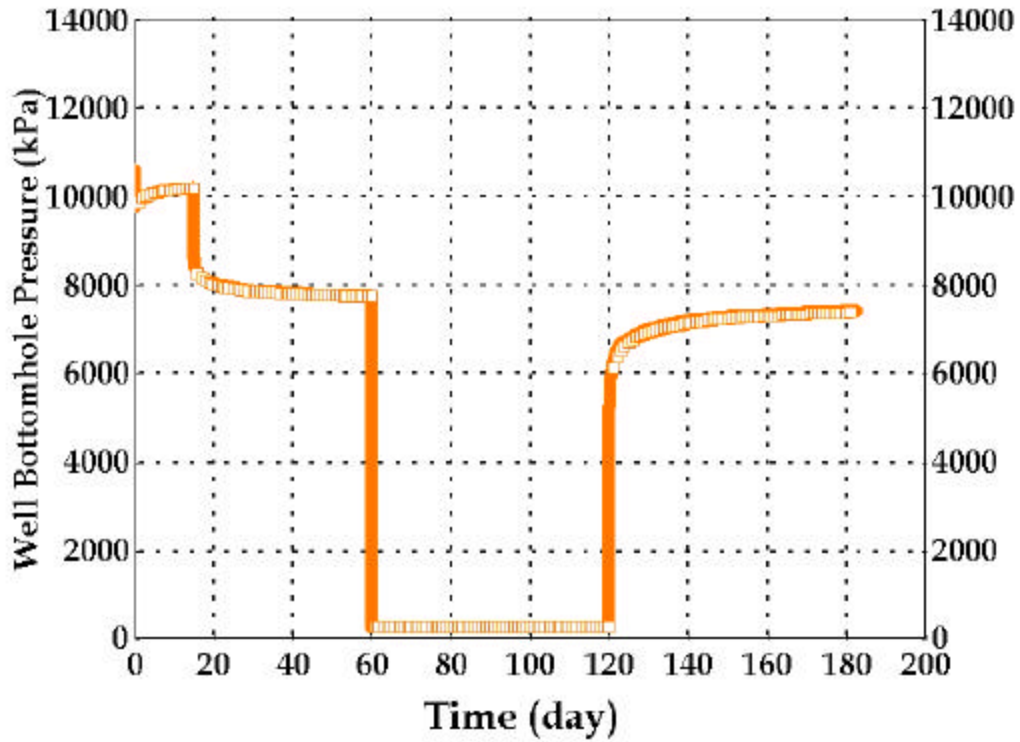


Figure 4: Well bottom-hole pressure for Problem Set 1
(Curve – GEM; Symbols – GCOMP)

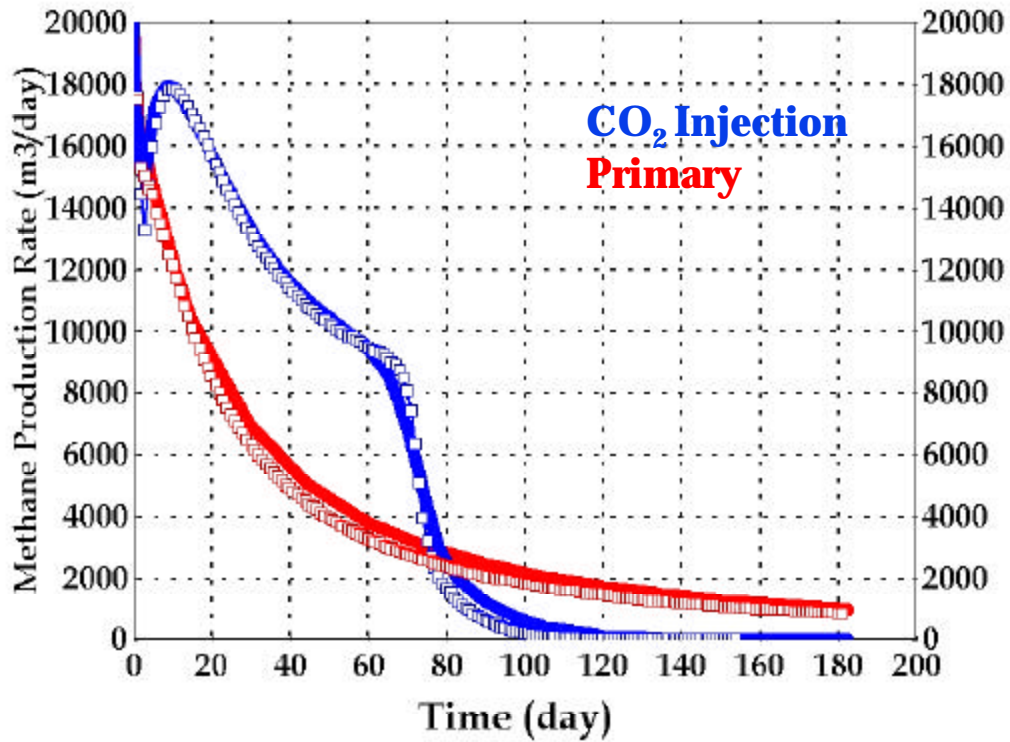


Figure 5: Methane production rate for Problem Set 2
(Curves – GEM; Symbols – GCOMP)