Reservoir Screening for CO₂ Sequestration

Course No: P05-002
Credit: 5 PDH

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Introduction

Due to the concern over the amount of carbon dioxide (CO$_2$) being emitted into the atmosphere by industry, enterprises have been created to capture and store (known as sequestration) CO$_2$ in subsurface reservoirs. This is typically referred to as CCS, or Carbon Capture and Storage. Any potential reservoir of interest must be screened for viability and CO$_2$ storage volume. The purpose of this course is to educate one on how to estimate the volume of CO$_2$ that can be sequestered in particular reservoirs. This is a necessary step to determine whether a reservoir, or reservoirs are capable of sequestering a given amount of CO$_2$.

The course will not discuss the subjects of injection rates, well placement, or timing of injection. It is assumed, because of the enormity of such projects that once a reservoir is chosen it will be modeled to determine well placement and injection rates.

There are three types of reservoirs that are potential candidates for the sequestration of CO$_2$. Reservoirs are defined as rock formations which contain pores or pore space where fluids can exist. The reservoirs available for CO$_2$ sequestration are:
- Aquifers
- Abandoned natural gas reservoirs
- Oil reservoirs

This course will discuss storage in aquifers and abandoned natural gas reservoirs. The injection of CO$_2$ into oil reservoirs is a tertiary recovery process. Additional oil is recovered as CO$_2$ is absorbed by the oil (known as miscibility) and reduces the surface tension and viscosity of the oil. Due to the complexity of the process and the fact that there are texts and courses covering this subject, we will eliminate oil reservoirs from discussion in this course.

An aquifer is a reservoir where the pore space is entirely filled with water. In particular, salt-water aquifers are the ones of choice because they are not used for drinking water. CO$_2$ has the ability to dissolve in water (i.e., club soda) and therefore has the potential to be stored there. It should be mentioned that the ability of water to store CO$_2$ decreases with salt content.

Some of the best candidates for CO$_2$ sequestration are abandoned natural gas reservoirs. The pore space in these reservoirs contain a percentage of water (known as water saturation) and a percentage of space taken up by gas known as hydrocarbon pore volume (HCPV). This allows CO$_2$ to be compressed into the HCPV and also some of the CO$_2$ to dissolve into the water in the reservoir.

Definitions and Units

This course will involve the use of several terms, abbreviated symbols, and various units of measurement. The tables below define certain terms, abbreviated symbols and their associated units of measurement.

Terms, Definitions, Units, and Symbols			
Term	**Definition**	**Units**	**Symbol**
Abandonment Pressure	The pressure at which a reservoir ceases production.	psia	P_{ab}
CO_2 Sequestration	The storage of CO2 in subsurface reservoirs		
CO_2 Solubiity in Water	The amount of CO2 that can be disolved in water.	lb	
Cubic Feet	A measurement of volume.	ft^3 or cf	
Cumulative Gas	The gas produced from initial conditions to the current date.	MMscf	G
Density	The mass of a substance per unit volume.	lb/ft^3	r
Gas Deviation Factor	A factor used to adust the Ideal Gas Law for the molecular interactions of hydrocarbon gases.	No Units	z
Gas Formation Volume Factor	The volume of 1 standard cubic foot of gas at reservoir conditions.	ft^3/scf	B_g
Hydrocarbon Pore Volume	The volume of the reservoir capable of containing fluids minus water.	ft^3	HCPV
Initial Pressure	The pressure in a reservoir at initial conditions.	psia	P_i
Million Cubic Feet	A measurement of volume.	MMcf	
Natural Gas	A natural gaseous substance primarily composed of hydrocarbons.		
Original gas-in-place	The gas volume contained in the reservoir at initial conditions.	MMscf	OGIP
Pore Volume	The volume of the reservoir capable of containing fluids.	ft^3	PV
Porosity	The non-solid portion of a rock capable of holding fluids.	% or decimal	Φ
Pound	A measurement of weight or mass.	lb	
Reservoir	A rock unit containing pore space capable of holding fluids.		
Reservoir Area	The areal extent of a reservoir.	acres	
Reservoir Height	The vertical height of a reservoir.	ft	
Reservoir Volume	The reservoir area multiplied by the reservoir height.	acre-ft or ft^3	V_r
Residual Gas	The gas remaining in the reservoir at abandonment.	MMscf	G_{res}
Sequestration Pressure	The pressure at which CO2 will be stored in a reservoir.	psia	P_s
Standard Conditions	The state of a fluid at standard pressure and temperature.		
Standard Cubic Feet	A measurement of volume at standard conditions.	scf	
Standard Pressure	The pressure at which fluids are measured. Each state has its own standard pressure. A list of standard pressured for each state is located under the tab "State Pressure Bases" in the accompanying Excel workbook.	psia	
Standard Temperature	The temperature at which fluids are measured. The standard temperature is 60°F.	°F	
Thousand Cubic Feet	A measurement of volume.	Mcf	
Water Saturation	The portion of the porosity filled with water.	% or decimal	Sw

There is sometimes confusion using the terms for cubic feet as ft^3 and cf. These unit symbols have identical meanings. Reservoir volumes are large and the units used are typically thousands or millions of cubic feet. The symbols for these, respectively are Mcf and MMcf rather than Mft^3 and $MMft^3$. When referring to thousand and millions of standard cubic feet the symbols Mscf and MMscf are used.

Properties of CO₂

When one thinks of CO_2, one normally thinks of it as a gas at atmospheric conditions. One may also be familiar with a solid form of CO_2 known as "dry ice" used as a coolant for packaged goods. Dry ice is so named because it does not melt, but immediately turns to CO_2 gas. This is known as sublimation. One never observes CO_2 as a liquid because it doesn't exist at atmospheric conditions.

Shown below is a phase diagram of CO_2. A phase diagram shows the various phases of a substance (solid, liquid, gas) at various temperatures and pressures.
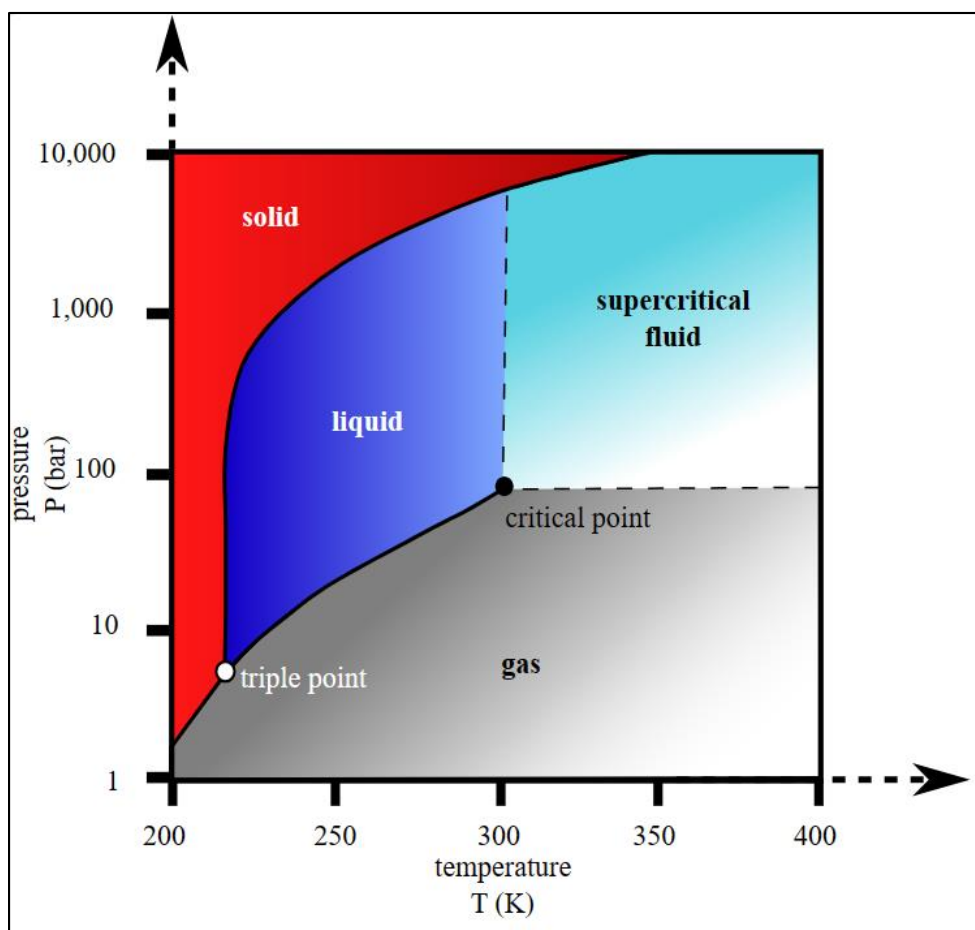
As we will soon see, CO_2 will exist as a supercritical fluid under most subsurface reservoir conditions.

The table below lists some of the important properties of CO_2.

Properties of Carbon Dioxide	
Chemical Formula	CO_2
Molecular Weight (g/mol)	44.01
Critical Pressure (psia)	1,070
Critical Temperature (^{o}F)	87
Phase at Standard Conditions	Gas
Specific Gravity at Standard Conditions	1.52
Density at Standard Conditions (lb/scf)	0.115

There are two properties of CO_2 that are most important when calculating the amount of CO_2 that can be sequestered in a reservoir. These are CO_2 density and CO_2 solubility in water.

As with other substances, the density of CO_2 changes as its phase changes. Density is defined as mass per unit of volume. For this course we will use pounds per cubic foot (lb/ft^3). CO_2 density can be found in several sources. The one we will use for this course is a website from the National Institute of Standards and Technology of the US Department of Commerce. The website is:

[Thermophysical Properties of Fluid Systems (nist.gov)](nist.gov)

Opening the page gives this menu:

From the drop-down box I have chosen "carbon dioxide" and the following units for each of the items:

- Temperature – Fahrenheit
- Pressure – psia
- Density – lbm/ft^3
- Energy – Bru/lbm
- Velocity – ft/s
- Viscosity – cp
- Surface tension – lb/in
- Data type – Isothermal properties
- Standard state convention – Default for fluid

Clicking on the "Press to Continue" button, the following screen comes up:

Isothermal Properties for Carbon dioxide

This option will supply data on a constant temperature curve over the specified pressure range. Values should not extend ex

1. Enter temperature in selected units:

   120   (Acceptable range: -69.804 to 3140.3 F)

2. Enter pressure range and increment in selected units:

   P$_{Low}$ 100   (min value: 0.0 psia)

   P$_{High}$*   2500

   P$_{Increment}$ 100

   * The maximum pressure limit is the lowest of the following values:

   o 116030.2 psia

   o The pressure at which a density of 73.568 lbm/ft3 is reached.

3. Check here if you want to use the intereactive display (requires JavaScript and HTML 5 canvas capable browser) ☐
4. Number of digits to be displayed in tables (does not effect accuracy of computations): 5 ▾
5.   **Press for Data**

For a given reservoir of interest, you will know the reservoir pressure and temperature. For this example, I chose a temperature of 120 °F, low pressure of 100 psia, a high pressure of 2,500 psia and a pressure increment of 100 psia. Clicking on the "Press for Data" button will give the chart shown on the following page.

Fluid Data

Isothermal Data for T = 120.00 F

Temperature (F)	Pressure (psia)	Density (lbm/ft3)	Volume (ft3/lbm)	Internal Energy (Btu/lbm)	Enthalpy (Btu/lbm)	Entropy (Btu/lbm*R)	Cv (Btu/lbm*R)	Cp (Btu/lbm*R)	Sound Spd. (ft/s)	Joule-Thomson (F/psia)	Viscosity (cP)	Therm. Cond. (W/m*K)	Phase
120.00	100.00	0.72704	1.3754	198.98	224.45	0.58094	0.16532	0.21657	901.09	0.11181	0.016125	0.018809	vapor
120.00	200.00	1.4969	0.66804	197.23	221.97	0.54659	0.16847	0.22696	886.98	0.11189	0.016230	0.019246	vapor
120.00	300.00	2.3162	0.43174	195.38	219.37	0.52504	0.17183	0.23902	872.53	0.11186	0.016359	0.019753	vapor
120.00	400.00	3.1931	0.31317	193.42	216.62	0.50858	0.17543	0.25321	857.70	0.11171	0.016517	0.020349	vapor
120.00	500.00	4.1383	0.24165	191.33	213.70	0.49477	0.17932	0.27019	842.47	0.11139	0.016712	0.021057	vapor
120.00	600.00	5.1655	0.19359	189.08	210.59	0.48249	0.18357	0.29089	826.81	0.11085	0.016953	0.021911	vapor
120.00	700.00	6.2934	0.15890	186.64	207.24	0.47110	0.18825	0.31675	810.70	0.11002	0.017254	0.022962	vapor
120.00	800.00	7.5479	0.13249	183.97	203.60	0.46019	0.19347	0.34998	794.13	0.10877	0.017633	0.024284	vapor
120.00	900.00	8.9663	0.11153	181.01	199.60	0.44940	0.19940	0.39429	777.12	0.10697	0.018122	0.025993	vapor
120.00	1000.0	10.605	0.094294	177.66	195.12	0.43840	0.20624	0.45615	759.75	0.10437	0.018768	0.028272	vapor
120.00	1100.0	12.555	0.079649	173.78	190.00	0.42680	0.21431	0.54782	742.21	0.10063	0.019654	0.031423	vapor
120.00	1100.0	12.555	0.079649	173.78	190.00	0.42680	0.21431	0.54782	742.21	0.10063	0.019654	0.031423	supercritical
120.00	1100.0	12.555	0.079649	173.78	190.00	0.42680	0.21431	0.54782	742.21	0.10063	0.019654	0.031423	supercritical
120.00	1200.0	14.973	0.066788	169.14	183.98	0.41408	0.22392	0.69407	725.14	0.095152	0.020939	0.035950	supercritical
120.00	1300.0	18.141	0.055124	163.35	176.62	0.39943	0.23502	0.94397	710.71	0.086964	0.022952	0.042620	supercritical
120.00	1400.0	22.497	0.044451	155.95	167.47	0.38206	0.24553	1.3399	706.55	0.074774	0.026372	0.051796	supercritical
120.00	1500.0	28.018	0.035691	147.40	157.31	0.36326	0.24887	1.6234	733.94	0.059183	0.031899	0.060462	supercritical
120.00	1600.0	32.998	0.030305	140.28	149.25	0.34832	0.24379	1.4316	803.85	0.045127	0.038162	0.064556	supercritical
120.00	1700.0	36.493	0.027402	135.44	144.06	0.33844	0.23791	1.1703	889.30	0.035429	0.043384	0.066902	supercritical
120.00	1800.0	38.948	0.025676	132.05	140.61	0.33164	0.23355	0.99594	970.15	0.029015	0.047511	0.069123	supercritical
120.00	1900.0	40.795	0.024513	129.48	138.11	0.32652	0.23045	0.88394	1043.3	0.024543	0.050896	0.071299	supercritical
120.00	2000.0	42.268	0.023659	127.42	136.18	0.32243	0.22814	0.80700	1109.3	0.021240	0.053780	0.073356	supercritical
120.00	2100.0	43.489	0.022994	125.69	134.63	0.31901	0.22635	0.75090	1169.5	0.018688	0.056310	0.075277	supercritical
120.00	2200.0	44.534	0.022455	124.20	133.35	0.31607	0.22490	0.70818	1224.9	0.016649	0.058578	0.077070	supercritical
120.00	2300.0	45.446	0.022004	122.88	132.26	0.31348	0.22371	0.67454	1276.2	0.014976	0.060642	0.078747	supercritical
120.00	2400.0	46.258	0.021618	121.71	131.31	0.31116	0.22271	0.64735	1324.2	0.013575	0.062547	0.080323	supercritical
120.00	2500.0	46.988	0.021282	120.64	130.49	0.30905	0.22186	0.62488	1369.2	0.012381	0.064322	0.081811	supercritical

Auxiliary Data

Reference States, IIR Convention

Enthalpy	H = 200 kJ/kg at 0°C for saturated liquid.
Entropy	S = 1 J/g*K at 0°C for saturated liquid.

Additional fluid properties

Critical temperature (T$_c$)	87.7608 F
Critical pressure (P$_c$)	1070.0 psia
Critical density (D$_c$)	29.1913 lbm/ft3
Acentric factor	0.22394
Normal boiling point	-109.24 F
Dipole moment	0.0 Debye

Although the chart is small here in the text, the temperature is listed in column 1, the pressure in column 2, and the density in column 3. The column at the far right lists the phase of CO_2 as it exists at each temperature and pressure.

The example below will allow you to use the website to find the density of CO_2.

Example Problem:

Find the density of CO_2 at a temperature of 125 °F and a pressure of 2,700 psia.

Answer:

Using the NIST website, the density is 47.164 lbm/ft^3 as shown in the table below:

Isothermal Data for T = 125.00 F

Temperature (F)	Pressure (psia)	Density (lbm/ft3)
125.00	2500.0	45.765
125.00	2600.0	46.496
125.00	2700.0	47.164

Data for CO_2 solubility in water is extremely difficult to find. Even when found, almost all solubilities are for CO_2 dissolved in fresh water. Additionally, the units are typically moles of CO_2 per liter and require conversions to field units. A reference that contains a graph of solubility data is a publication by the Interstate Oil Compact Commission in 1983 titled *Improved Oil Recovery*. Shown below is a graph of CO_2 solubility in distilled water at various temperatures and pressures.
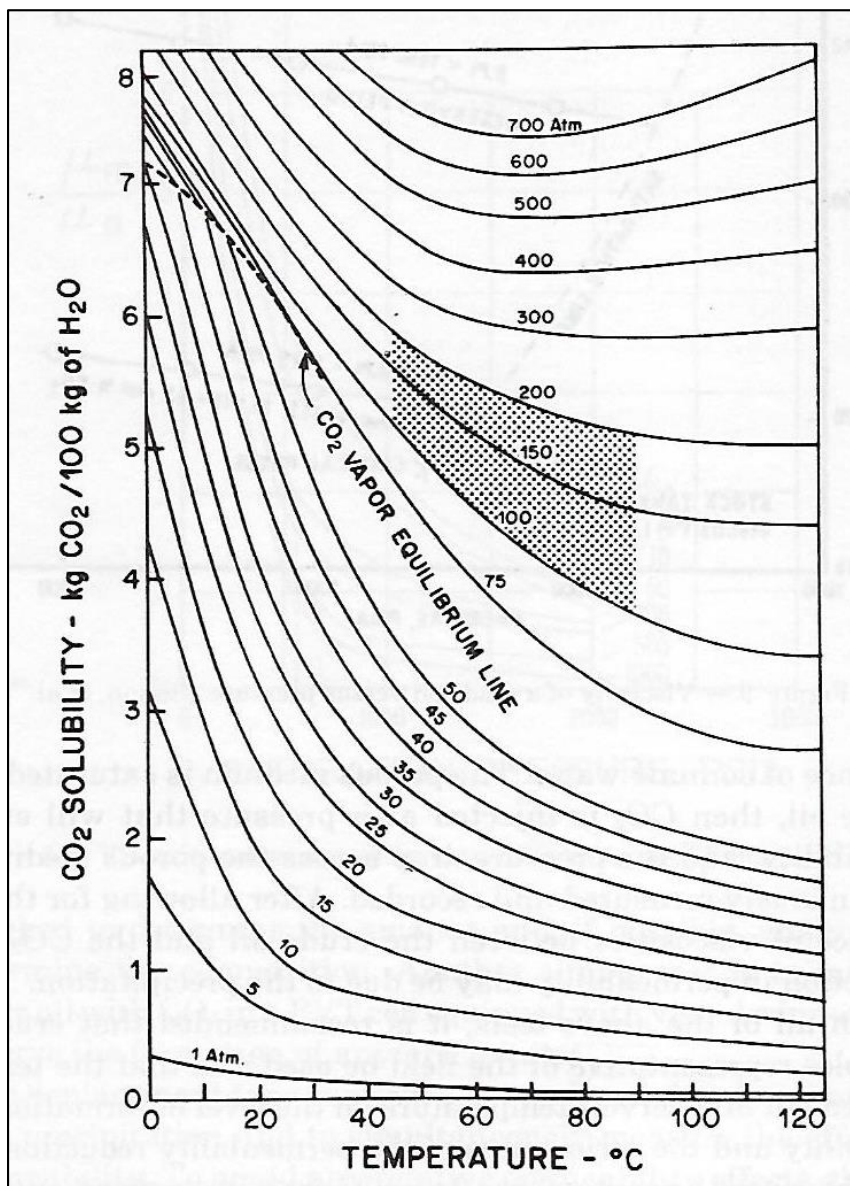
From *Improved Oil Recovery*, Interstate Oil Compact Commission, 1983

Note that the solubility (listed on the y-axis) is given in kg CO_2 per 100 kg of H_2O. This is the same as lb CO_2 per 100 lb of H_2O. Also notice that the pressure is given in atmospheres and the temperature in ºC. A copy of this chart is in the workbook under the tab labeled "**CO₂ Solubility in Water Chart**".

It will be necessary to convert pressure from psia to bars and temperature from °F to °C to use this chart. The equations below can be used for the conversion:

$$T_{oC} = \frac{(T_{oF} - 32)}{1.8}$$

$$P_{bar} = \frac{P_{psia}}{14.696}$$

where,

T_{oC} = temperature in °C
T_{oF} = temperature in °F
P_{bar} = pressure in bars
P_{psia} = pressure in psia

To understand the use of this graph, perform the following example.

Example Problem:

Find the solubility of CO_2 in water at a reservoir temperature of 122 °F and pressure of 2,400 psia.
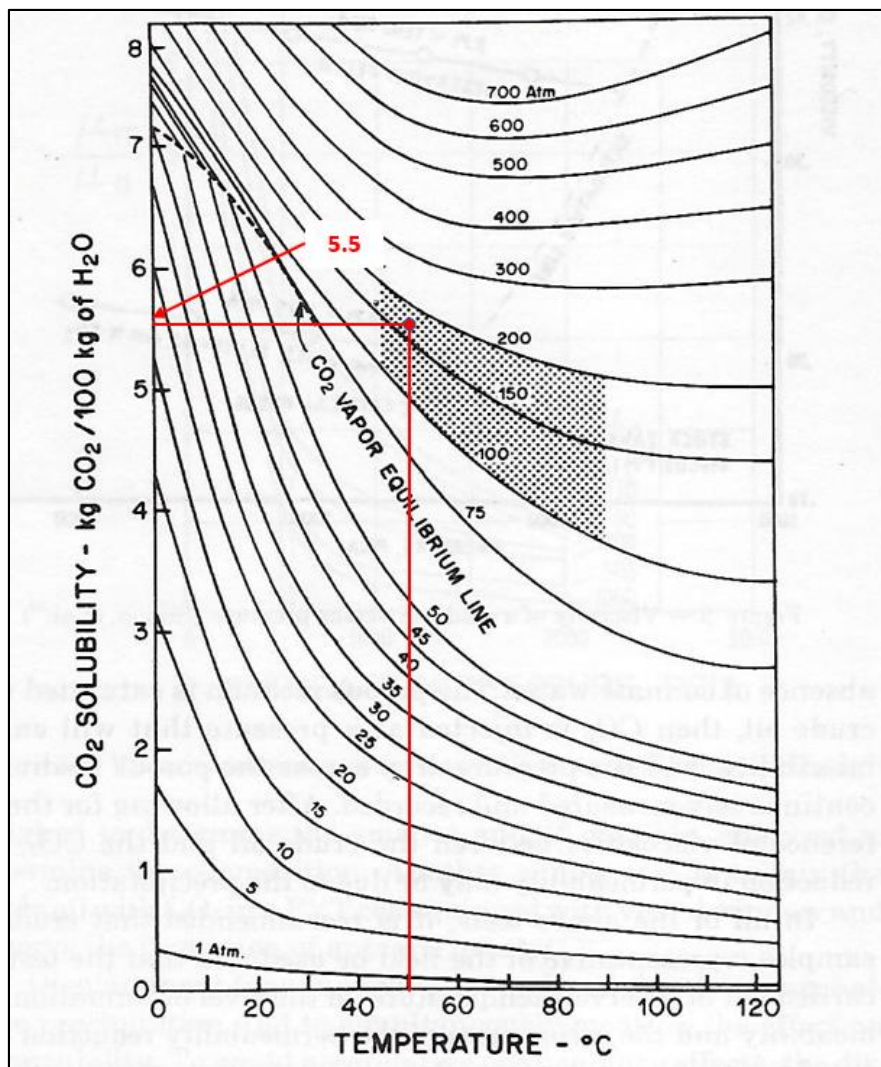
Answer:

The first thing to do is to convert the reservoir temperature and pressure to units of the solubility graph. This is done as:

$$T_{oC} = \frac{(T_{oF} - 32)}{1.8} = \frac{(122 - 32)}{1.8} = 50 \; C$$

$$P_{bar} = \frac{P_{psia}}{14.504} = \frac{2,400}{14.696} = 163 \; atm$$

Entering the graph with the above values gives 5.5 lbm CO_2 per 100 lbm H_2O as shown below.

As mentioned in the introduction, CO_2 solubility decreases with an increase in salinity. If an aquifer is being considered for CO_2 sequestration, it is recommended that laboratory tests be done on a water sample to determine CO_2 solubility. The graph on the following page (different units than the graph above) shows the effects of 10% salinity compared to distilled water. At 1,000 psi the difference is a 40% loss in solubility at 75 °F and a 25% reduction at 122 °F.

For all calculations in this course, we will use CO_2 solubility data for distilled water.

SOLUBILITY OF CO₂ IN WATER AND BRINE
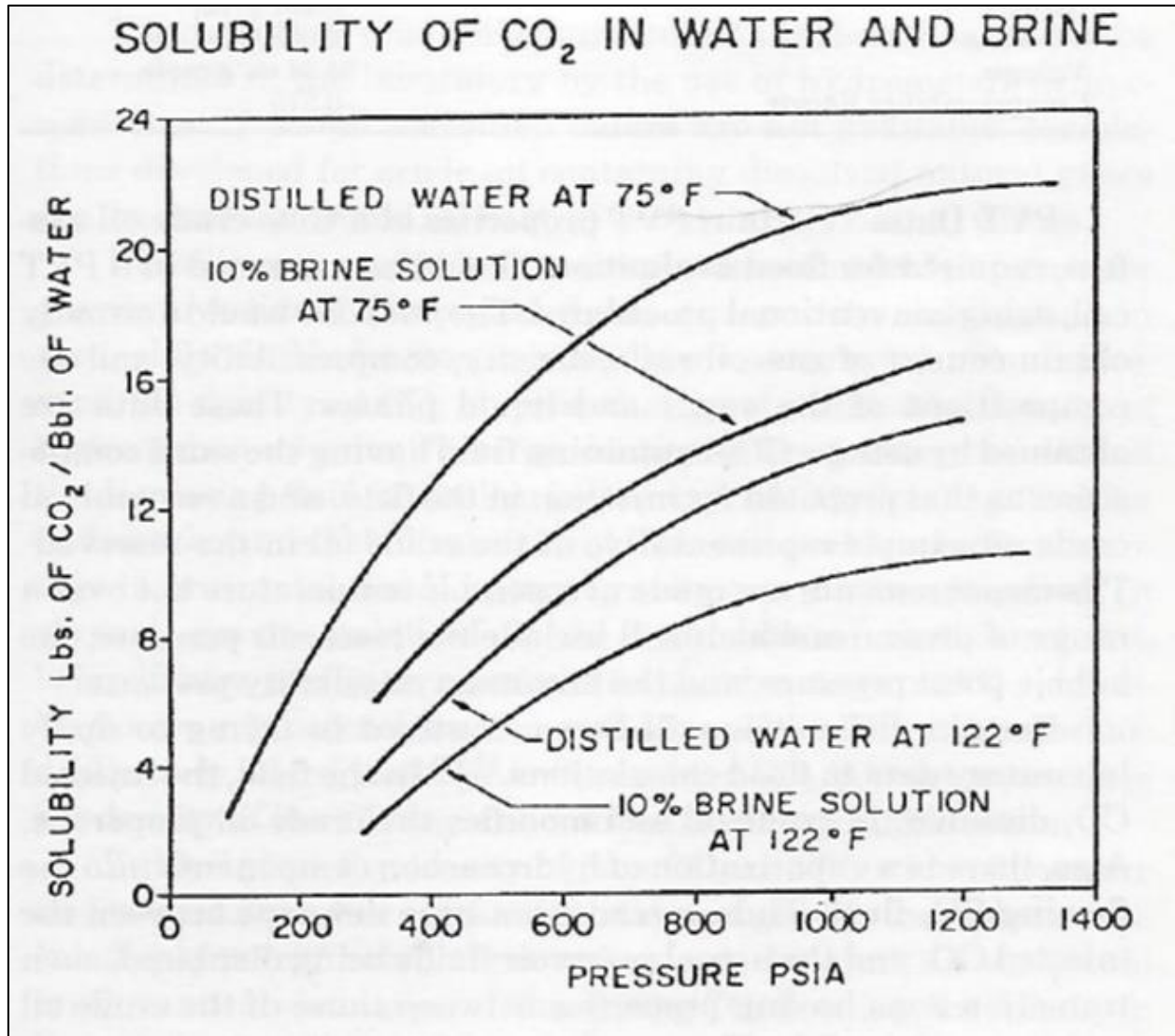
From *Improved Oil Recovery*, Interstate Oil Compact Commission, 1983

CO$_2$ Sequestration in Aquifers

As mentioned above, CO$_2$ can be sequestered in salt-water aquifers. Aquifers exist predominantly at hydrostatic pressure. Hydrostatic pressure is the pressure created by the height of water above the reservoir. For pure water (no salt), the hydrostatic pressure at a given depth can be calculated as:

$$P = 0.433 * H$$

where,

P = reservoir pressure in psia
H = vertical depth from the surface to the reservoir in feet

Salt will increase the weight of water and also the pressure at any given depth. The graph below shows the relationship between water salinity, temperature, and pressure. Sea water contains about 35,000 ppm salt and has a density of 63.96 lbm/ft^3 (1.025 g/cc), which is a pressure gradient of 0.444 psi/ft of depth. For any aquifer of interest, the pressure at depth will most likely be known.
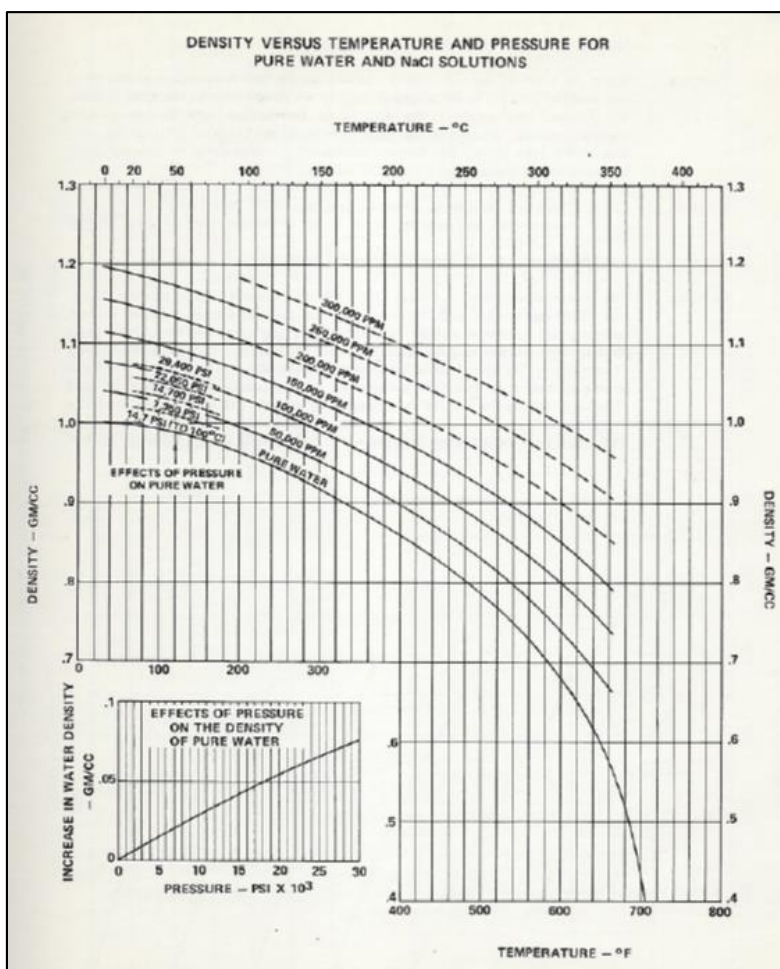
From Gearhart Owens, 1978

It will be assumed throughout this course that the sequestration pressure (the pressure under which CO$_2$ will be stored in the reservoir) will not exceed the original pressures of either an aquifer or abandoned natural gas reservoir. The reason for this is the fact that the original fluids in the reservoir did not leak at original conditions. This is good evidence that CO$_2$ will likely not leak when the reservoir is maintained at its original pressure.

Since aquifers are at or close to the original pressure when CO$_2$ injection is commenced, the injection pressure must be closely monitored to prevent injecting above the fracture pressure. The fracture pressure is the pressure at which a hydraulic fracture is created in the reservoir. Most CO$_2$ injection wells will likely be hydraulically fractured to allow for higher injection rates, so the fracture pressure will be known. Hydraulic fracture treatments will be designed such that no fractures leave the reservoir where they could create leaks above or below.

In an aquifer, the pore space is totally filled with water. The water is essentially a warehouse where CO$_2$ will be stored. The diagrams below illustrate the pore space in the reservoir before and after CO$_2$ sequestration.

100%
Water

Water
+
Dissolved
CO2

Before
Sequestration

After
Sequestration
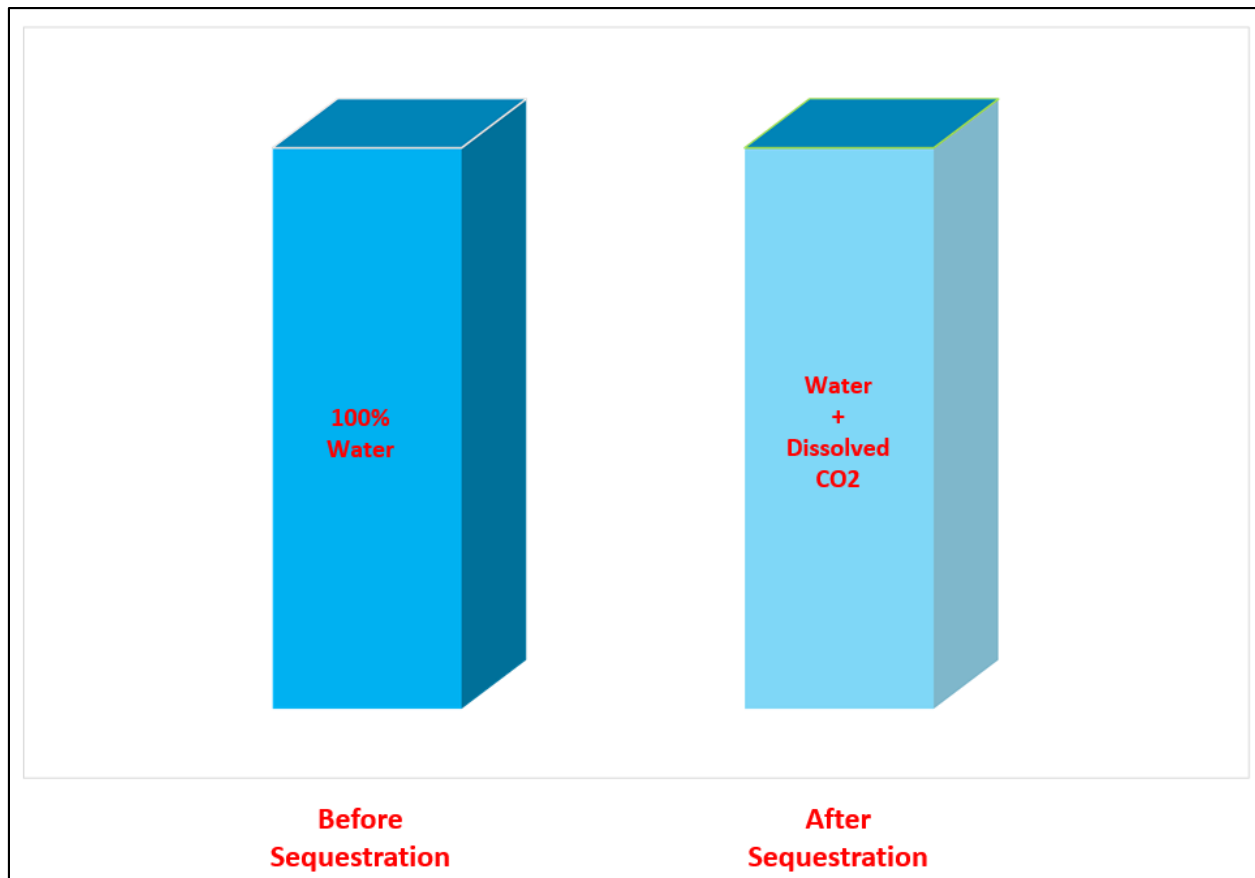
The estimation of how much CO₂ can be sequestered in an aquifer will follow these steps:
1) Determine the reservoir area, height, porosity, reservoir pressure, reservoir temperature, standard pressure and standard temperature. (This course will not go into detail on how to find or calculate these parameters, but they will be provided in examples and quiz questions).
2) Calculate the volume and weight of water in the reservoir
3) Estimate the solubility of CO₂ in water at reservoir (sequestration) pressure and temperature.
4) Calculate how many pounds of CO₂ that can be sequestered.
5) Calculate the volume of CO₂ that can be sequestered in standard cubic feet.

As can be seen from the steps listed above, the estimation of how much CO₂ that can be sequestered in an aquifer is fairly straight forward and is accomplished in just a few steps.

Step 5 is a conversion of CO₂ sequestered to standard conditions. This is necessary since the CO₂ being sequestered is produced and measured at atmospheric conditions. It also provides a standardized way of measuring CO₂ volumes. The density of CO₂ at standard conditions of 60ºF and 14.65 psia is 0.115 lb/ft³ ($\rho CO2_{std}$). The density of water at standard conditions is 62.4 lb/ft³.

Since water entirely fills the porosity of the reservoir, the volume of water in the aquifer is simply the pore volume of the reservoir. The pore volume can be calculated by the following equation:

$$PV = 0.04356 * A * h * \emptyset$$

where,
PV = pore volume of reservoir in MMcf
A = reservoir area in acres
H = reservoir height in feet
∅ = reservoir porosity as a decimal

The Excel workbook has a tab labeled "**Sequestration in Aquifer**" which can be used to estimate CO₂ sequestration in aquifers. The spreadsheet can be used to solve any of the examples for aquifer sequestration in the text and the quiz. The spreadsheet has 50 rows for use when screening reservoirs for a CO₂ sequestration project. Data is entered into the highlighted cells.

The example below will demonstrate how to estimate CO₂ sequestration in an aquifer. This example is listed on Row 4 on the spreadsheet.

Example Problem:

Estimate how much CO_2 can be sequestered in an aquifer with the following properties. Express the answer in both pounds of CO_2 and standard cubic feet of CO_2 that can be sequestered.

Reservoir depth = 5,400 ft   Reservoir area = 3,200 acres   Reservoir height = 50 ft
Reservoir porosity = 24.1%   Reservoir temp = 118°F   Reservoir pressure = 2,350 psia
Standard pressure = 14.65 psia   Standard temp = 60°F

Answer:

Step 1) This is just the given data.

Step 2) Since the pore space of the reservoir is totally filled with water, the volume of water is simply the pore volume of the reservoir. The pore space of the reservoir is calculated from the formula below.

$$PV = 0.04356 * A * h * \emptyset$$

where,

   PV = pore volume of reservoir in MMcf
   A = reservoir area in acres
   H = reservoir height in feet
   $\emptyset$ = reservoir porosity as a decimal

For this reservoir, the pore volume, or water volume is:

$$PV = 0.04356 * 3,200 * 50 * 0.241 = 1679.7 \, MMcf$$

The weight of water in pounds is simply the volume multiplied by the water density of 62.4 lb/ft³ as follows:
$$W = PV * \rho_w$$

where,

   W = weight of water in million lb
   PV = pore volume in MMcf
   ρ_w = density of water in lb/ft³

So, the amount of water in the aquifer, expressed in millions of pounds is:

$$W = PV * \rho_w = 1679.7 * 62.4 = 104,811 \, million \, lb$$

Step 3) Calculate the pressure in bars and the temperature in ℃, find water solubility from the chart.

$$T_{oC} = \frac{(T_{oF} - 32)}{1.8} = \frac{(118 - 32)}{1.8} = 48\ C$$

$$P_{bar} = \frac{P_{psia}}{14.504} = \frac{2,350}{14.696} = 160\ atm$$
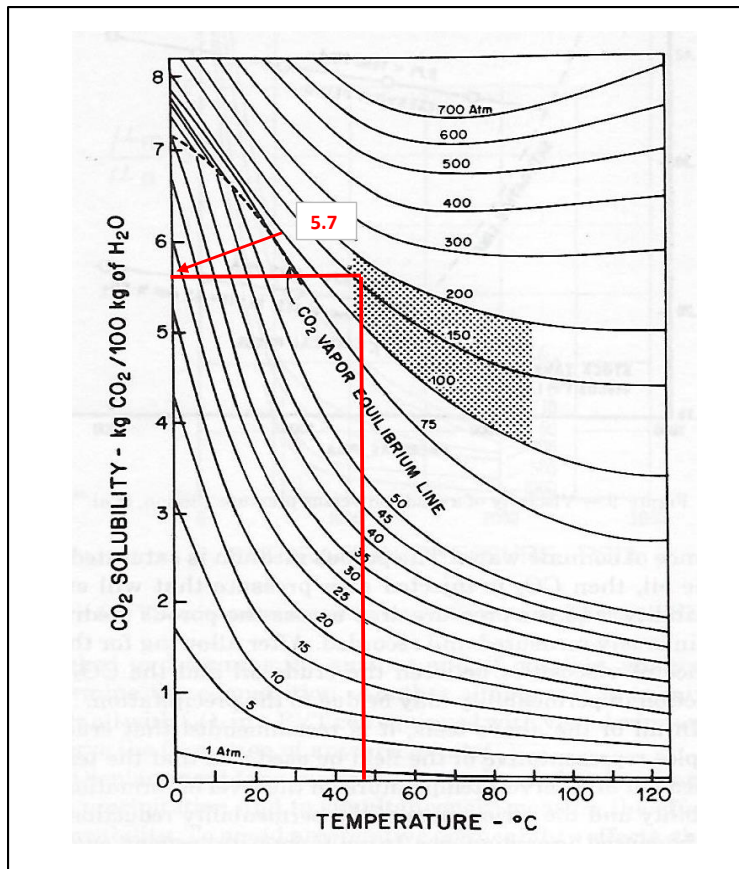
The solubility is 5.7 lb CO₂/100 lb H₂O.

Step 4) Calculate the lb of CO₂ that can be sequestered in the aquifer. This will be the CO₂ solubility multiplied by the amount of water in the reservoir as:

$$Sequestered\ CO_2 = Water\ Mass\ x\ CO_2\ Solubility = 104,811 * \frac{5.7}{100} = 5,974\ million\ lb$$

Step 5) Calculating the standard cubic feet of CO_2 that can be sequestered is done by dividing the pounds of CO_2 sequestered in the aquifer by the density of CO_2 at standard conditions. The density of CO_2 at standard conditions is 0.115 lb/ft^3. Here is the calculation:

$$Sequestered\ CO2\ at\ Std\ Conditions = \frac{Sequestered\ CO_2\ in\ lbs}{\rho CO2_{std}} = \frac{5,974}{0.115} = 51,948\ MMscf$$

This problem has been input into the Excel workbook under the tab "**Sequestration in Aquifer**" on row 4.

Natural Gas and Natural Gas Reservoirs

Before one can estimate how much CO$_2$ can be sequestered in an abandoned natural gas reservoir, one must understand how natural gas and natural gas reservoirs behave. The following sections will discuss the ideal gas law, natural gas properties, how the gas deviation factor is determined and the gas formation volume factor is calculated.

Ideal Gas Law

In order to understand gas properties, one must understand how gases behave. Gas molecules, unlike the other phases of matter – liquids and solids, are not bound together by intermolecular and viscous forces. As such, gases completely fill whatever container in which they reside. This property is very important and can be used to determine how gases behave under the effects of pressure, temperature, and volume.

The Ideal Gas Law is an equation of state that relates pressure, temperature, and volume. This equation is the results of combining Boyle's law, Charles' law, Avogadro's law, and Gay-Lussac's law. Shown below is the Ideal Gas Law equation of state:

$$PV = nRT$$

where,

P = pressure (psia – pounds per square inch absolute)
V = volume (scf – standard cubic feet)
T = temperature (°R - degrees Rankine)
n = number of moles of gas (moles)
R = ideal gas constant (10.73 scf-psia/mole-°R)

The purpose of R, the ideal gas constant is to convert to consistent units. Depending on the units used, R will change. It should always be remembered that when dealing with gases, temperature is always in absolute units (i.e., Kelvin or Rankine). In the USA, we use units of Rankine (Fahrenheit plus 459.67 degrees).

Based on the Ideal Gas Law, one can derive a very important relationship. If a gas is composed of different types of molecules (i.e., nitrogen, oxygen, etc.), the volume percentage of each gas is equal to the molar percentage of that gas. This can be shown as follows:

Let *V* be the total gas volume and N be the total number of moles. The Ideal Gas Law equation is then:

$$PV = NRT$$

Let *v* be the volume of a single gas component and n be the moles of that component. The Ideal Gas Law for that component is then:

$$Pv = nRT$$

Taking a ratio of the individual gas component to the total gas gives the following:

$$\frac{Pv}{PV} = \frac{nRT}{NRT}$$

Since P, R, and T are all equal, this equation can be simplified as:

$$\frac{v}{V} = \frac{n}{N}$$

This clearly shows that the ratio of an individual component to the total volume is the same as the number of moles of a component to the total number of moles of gas. This is very important because gas samples are analyzed in the laboratory and the results presented as mole percentages, which in effect are volume percentages.

This equation of state works well under normal ranges of pressure and temperature when the interaction between molecules is relatively small. In the case of hydrocarbon gases, however, the molecular interactions are not small and must be taken into account. For that purpose, the Ideal Gas Law is modified to account for these interactions. Shown below is the Ideal Gas Law equation modified for hydrocarbon gases:

$$PV = nRTz$$

where,

z = gas deviation factor

This course will discuss how to determine z based on the reduced pressure and temperatures. The value for z does depend on the constituents that make up the natural gas. Specifically, the value of z depends on the gas specific gravity and the reduced pressure and reduced temperature. The reduced pressure is the measured pressure divided by the critical pressure and the reduced temperature is the measured temperature divided by the critical temperature. The determination of the critical pressure and temperature will be discussed in a later section of this course. However, shown below are the equations for the reduced pressure and temperature.

$$Pr = P/Pc$$

$$Tr = T/Tc$$

where,

Pr = reduced pressure
P = measured pressure (psia)
Pc = critical pressure (psia)
Tr = reduced temperature
T = measured temperature (ºR)
Tc = critical temperature (ºR)

Example Problem:

How many moles of gas are there in the container given the following data:

Container volume = 2 scf
Temperature = 80 ºF
Pressure = 500 psia

Answer:

The first thing to do is calculate the temperatures in absolute temperature degrees, so the temperature is:

T = 80 + 459.67 = 539.67 ºR

Rearrange the Ideal Gas Law equation to solve for "n" as shown below:

$$n = \frac{PV}{RT} = \frac{(500)*(2)}{(10.73)*(539.67)} = 0.17 \; moles$$

What is Natural Gas

Most of us think of natural gas as something we use in our homes for heating or cooking. It is true that we tend to call gas delivered to our homes as "natural gas", but in reality, it is a nearly single component called "methane" that is derived from natural gas. So, what is natural gas and what is it composed of?

Webster's Dictionary defines natural gas as
> *"gas issuing from the earth's crust through natural openings or bored wells, especially a combustible mixture of methane and other hydrocarbons used chiefly as a fuel and raw material"*

Natural gas is created in the earth's crust by the decay and reduction of organic material. As organic material is deposited on the earth's surface and subsequently buried, it is subjected to increased pressure and temperature. As this process continues, the organic material is reduced to petroleum. Depending on the composition of the original organic matter, the temperature, and pressure, the petroleum is either gaseous or liquid. As this petroleum forms, it begins to seep and being lighter than water, begins to move toward the earth's surface. This seeping petroleum moves along faults or through porous rocks and either makes it to the surface or is trapped along the way. There are various ways petroleum can be trapped, but most commonly with some type of seal like an impervious rock layer that prevents its further upward movement. The trapped petroleum exists in porous rocks known as reservoirs. Natural gas can exist in reservoirs as a gas or can be liberated from oil as it is produced. Natural gas can also exist in coal seams and is referred to as coalbed methane or coal seam gas. In the case of gas existing in coal seams, the coal is both the source rock and reservoir and the gas is actually attached to the surface of the coal.

Although there are gases emanating from the earth that do not contain hydrocarbons (i.e., nitrogen and carbon dioxide), the discussions in this course will be concerned only with hydrocarbon natural gases. Unlike non-hydrocarbon gases, hydrocarbon gases behave quite differently to pressure and temperature. With the exception of very high pressures and temperatures, non-hydrocarbon gases closely follow the Ideal Gas Law. The Ideal Gas Law is an equation of state that relates pressure, temperature and volume. Due to the interaction of hydrocarbon molecules, hydrocarbon gases deviate from the Ideal Gas Law. By analyzing the composition of natural gas, one can adjust the Ideal Gas Law to account for these interactions and properly calculate the relationship between pressure, temperature and volume.

Components of Natural Gas

The most common hydrocarbon constituents of natural gas are known as alkanes or paraffins. An alkane is a molecule composed of carbon and hydrogen with single bonds between the atoms and
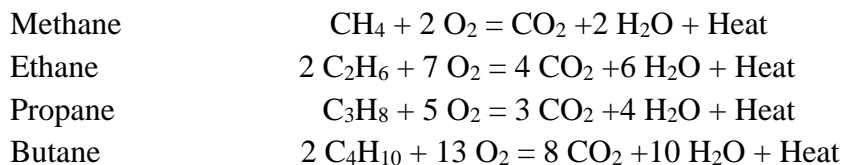
forming a chain-like structure. The simplest alkane is methane, which consists of a single carbon atom connected to four hydrogen atoms. Alkanes are named by the number of carbon atoms that make up the molecule. After methane, the next molecule containing two carbon atoms is called ethane. An alkane containing three carbon atoms is propane. Shown below are diagrams of the first four alkanes.
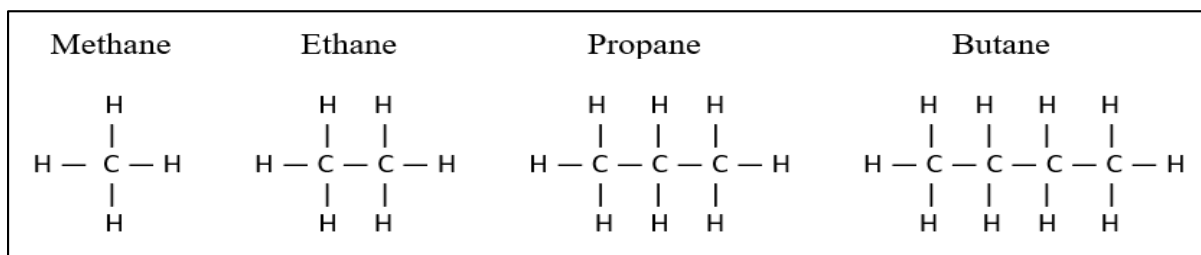
The first thing to notice is that there is a relationship between the number of hydrogen atoms and the number of carbon atoms. If n is the number of carbon atoms, then the number of hydrogen atoms is 2n+2. Since there is a direct relationship between the carbon and hydrogen atoms that comprise alkane molecules, there is also a direct relationship between the molecular weight and heating content of the alkanes.

The molecular weight of carbon is approximately 12 pounds per pound-mole and the molecular weight of hydrogen is approximately 1 pound per pound-mole. Using the formula for the relationship between the number of carbon and hydrogen atoms gives an increase of 14 pounds per pound-mole for each increment in alkanes.

Hydrocarbons create energy by reacting with oxygen (i.e., burning or combustion). If one combines a hydrocarbon with oxygen, the result is carbon dioxide (CO_2), water (H_2O), and heat. The amount of heat is directly proportional to the amount of carbon, hydrogen, and oxygen consumed in the process. Shown below are the equations for combustion for the first four alkanes.

Methane	$CH_4 + 2\ O_2 = CO_2 + 2\ H_2O + Heat$
Ethane	$2\ C_2H_6 + 7\ O_2 = 4\ CO_2 + 6\ H_2O + Heat$
Propane	$C_3H_8 + 5\ O_2 = 3\ CO_2 + 4\ H_2O + Heat$
Butane	$2\ C_4H_{10} + 13\ O_2 = 8\ CO_2 + 10\ H_2O + Heat$

Example Problem:

a) How many hydrogen atoms are in a molecule of octane (8 carbons atoms)?
b) What is the estimated molecular weight?

Answer:

a) Using the equation that hydrogen atoms are 2n+2 carbon atoms:

2 x 8 + 2 = 18 hydrogen atoms in octane

b) The estimated molecular weight is 12 times the number of carbon atoms plus 1 times the number of hydrogen atoms as:

Estimated molecular weight of octane = 12 x 8 + 1 x 18 = 114 pound per pound-mole

Besides the major alkane hydrocarbons, there are other constituents of natural gas that occur. The most common of these are:

> Air
> Nitrogen (N_2)
> Oxygen (O_2)
> Carbon Dioxide (CO_2)
> Hydrogen Sulfide (H_2S)
> Hydrogen (H_2)
> Argon (Ar)
> Helium (He)

When computing properties of natural gas, these constituents must be taken into account as they affect the overall properties of the gas. As a rule, most of these constituents occur in minor amounts. The exception to this rule are carbon dioxide (CO_2) and nitrogen (N_2) which can sometimes occur in large amounts. Although some gas contracts allow for small amounts of non-hydrocarbons in the gas stream, prior to sale or use for commercial purposes, the major portion of these constituents must be removed. In gases containing hydrogen sulfide (H_2S), this constituent is extremely toxic and must always be removed prior to transmission or sale.

Table 1 shown on the next page lists the most common constituents of natural gas along with their molecular formula, molecular weight, critical pressure, and critical temperature. Occasionally, a natural gas contains other gases such as benzene or toluene. If these are present, their properties can be added to the table and used to calculate overall properties of the gas. The footnote on Table 1 gives the source of the gas property data and can be referenced for additional constituents.

Table 1				
Common Constituents of Natual Gases				
Component	**Molecular Formula**	**[1,2]Molecular Weight**	**[1,2]Critical Pressure (psia)**	**[1,2,3]Critical Temperature (°R)**
Methane	CH_4	16.042	667.00	343.01
Ethane	C_2H_6	30.069	706.60	549.59
Propane	C_3H_8	44.096	615.50	665.59
Iso-Butane	C_4H_{10}	58.122	527.90	734.08
N-Butane	C_4H_{10}	58.122	550.90	765.22
Iso-Pentane	C_5H_{12}	72.149	490.40	828.67
N-Pentane	C_5H_{12}	72.149	488.80	845.47
Hexane	C_6H_{14}	86.175	436.90	913.47
Heptane	C_7H_{16}	100.202	396.80	972.57
Octane	C_8H_{18}	114.229	360.70	1,023.87
Nonane	C_9H_{20}	128.255	330.70	1,070.47
Decane	$C_{10}H_{22}$	142.282	304.60	1,111.87
Air		28.959	551.90	238.70
Nitrogen	N_2	28.014	492.50	227.14
Oxygen	O_2	31.999	731.40	278.24
Carbon Dioxide	CO_2	44.010	1,070.00	547.45
Hydrogen Sulfide	H_2S	34.082	1,306.50	672.48
Hydrogen	H_2	2.016	190.70	59.77
Argon	Ar	39.948	705.32	271.24
Helium	He	4.003	33.00	9.35

Notes:

 1 - From Gas Processors Suppliers Association Engineering Data Book, Twelfth Edition, 2004

 2 - From NIST Chemistry WebBook, SRD 69 https://webbook.nist.gov/chemistry/fluid/

 3 - Degrees Rankine = Degrees Fahrenheit + 459.67

Calculation of Natural Gas Properties from Gas Composition

The composition of a natural gas is made by analyzing a sample of the gas. The sample can be taken directly form the reservoir using a special device or can be taken at the surface from the production facilities. Once the sample is taken it is sent to a laboratory where measurements of the components and their proportion of the total gas are made.

The amount of each component of the gas sample is reported as "Mole %" which is the percentage of the number of molecules of the component divided by the total number of gas molecules. For a gas, the Mole % is the same as the volume percent.

Shown below in Table 2 is an example of a gas sample.

Table 2 Example Gas Sample	
Component	**Measured Mole %**
Methane	79.28
Ethane	3.55
Propane	3.43
I-C4	1.80
N-C4	1.54
I-C5	1.66
N-C5	1.30
C6	1.92
C7	0.88
C8	0.75
C9	0.00
C10	0.00
O2	0.00
N2	2.44
CO2	1.30
H2S	0.00
Ar	0.15
Total	100.00

Notice that many of the components are simply listed as the number of carbon atoms in the molecule. This is common practice in some labs. It is fortunate that for this gas sample the total of the constituents add up to 100 percent. In some cases, the total is not 100% and must be adjusted so the total is equal to 100 percent. Due to the methods used and the percision of the instruments making the measurements, the totals do not always add to 100 percent. In those cases, an adjustment to the percentage of each component must be made. Table 3 shows a gas sample where the components do not add up to 100 percent and the method used to correct the tabel values.

Table 3 Example Gas Sample Adjustment		
Component	**Measured Mole %**	**Adjusted Mole %**
Methane	78.20	78.61
Ethane	3.66	3.68
Propane	3.40	3.42
I-C4	1.84	1.85
N-C4	1.62	1.63
I-C5	1.65	1.66
N-C5	1.22	1.23
C6	1.88	1.89
C7	0.91	0.91
C8	0.82	0.82
C9	0.25	0.25
C10	0.14	0.14
O2	0.00	0.00
N2	2.44	2.45
CO2	1.30	1.31
H2S	0.00	0.00
Ar	0.15	0.15
Total	99.48	100.00

Notes:
  Adjusted Mole% = Measured Mole % / Total Measured Mole %

The adjusted mole percentages are just the measured mole percentages divided by the total of the measured mole percentages. When the total of the measured mole % is 98 percent or greater, this method can be used with fair accuracy. If the sum is less than 98 percent, the accuracy of this method decreases and might warrant an new gas sample.

Calculating the gas properties of the sampled gas is done by combining the results of the gas sample with the properties shown in Table 1. For the purpose of showing how to calculate gas properties of a gas sample, we will use the gas sample shown in Table 2. Table 4 on the next page combines the mole percentages of the gas sample in Table 2 and the properties of each component from Table 1 into a single table.

Table 4
Gas Composition from Table 2 and Gas Properties from Table 1

Component	Molecular Formula	Mole Fraction (%)	Molecular Weight	Critical Pressure (psia)	Critical Temperature (^{o}R)
Methane	CH_4	79.28	16.042	667.00	343.01
Ethane	C_2H_6	3.55	30.069	706.60	549.59
Propane	C_3H_8	3.43	44.096	615.50	665.59
Iso-Butane	C_4H_{10}	1.80	58.122	527.90	734.08
N-Butane	C_4H_{10}	1.54	58.122	550.90	765.22
Iso-Pentane	C_5H_{12}	1.66	72.149	490.40	828.67
N-Pentane	C_5H_{12}	1.30	72.149	488.80	845.47
Hexane	C_6H_{14}	1.92	86.175	436.90	913.47
Heptane	C_7H_{16}	0.88	100.202	396.80	972.57
Octane	C_8H_{18}	0.75	114.229	360.70	1,023.87
Nonane	C_9H_{20}	0.00	128.255	330.70	1,070.47
Decane	$C_{10}H_{22}$	0.00	142.282	304.60	1,111.87
Air		0.00	28.959	551.90	238.70
Nitrogen	N_2	2.44	28.014	492.50	227.14
Oxygen	O_2	0.00	31.999	731.40	278.24
Carbon Dioxide	CO_2	1.30	44.010	1,070.00	547.45
Hydrogen Sulfide	H_2S	0.00	34.082	1,306.50	672.48
Hydrogen	H_2	0.00	2.016	190.70	59.77
Argon	Ar	0.15	39.948	705.32	271.24
Helium	He	0.00	4.003	33.00	9.35
Total		**100.00**			

To determine the properties of the gas sample, we will now add some columns to Table 4 so we can calculate the mole percentage weighted properties of each component. Table 5 shows the additional columns where the weighted values are tabulated and accumulated. To calculate the mole weighted value of each property, multiply the value for that property by the mole percentage for the given component. This table can be created manually, or it can be created using a spreadsheet program.

In this example, the mole percentage for ethane is 3.55%. The value for the critical pressure of ethane is 706.6 psia. Multiplying 706.6 psia by 3.55% give a mole weighted value of 25 psia as shown in mole weighted critical pressure column for ethane. Once we have calculated the mole weighted values for each component in the gas sample, the values are summed to arrive at the properties for the gas sample.

| | | | | | Mole Fraction Weighted | | |
Component	Molecular Formula	Mole Fraction (%)	Molecular Weight	Critical Pressure (psia)	Critical Temperature (°R)	Molecular Weight	Critical Pressure (psia)	Critical Temperature (°R)
Methane	CH_4	79.28	16.042	667.00	343.01	12.72	529	272
Ethane	C_2H_6	3.55	30.069	706.60	549.59	1.07	25	20
Propane	C_3H_8	3.43	44.096	615.50	665.59	1.51	21	23
Iso-Butane	C_4H_{10}	1.80	58.122	527.90	734.08	1.05	10	13
N-Butane	C_4H_{10}	1.54	58.122	550.90	765.22	0.90	8	12
Iso-Pentane	C_5H_{12}	1.66	72.149	490.40	828.67	1.20	8	14
N-Pentane	C_5H_{12}	1.30	72.149	488.80	845.47	0.94	6	11
Hexane	C_6H_{14}	1.92	86.175	436.90	913.47	1.65	8	18
Heptane	C_7H_{16}	0.88	100.202	396.80	972.57	0.88	3	9
Octane	C_8H_{18}	0.75	114.229	360.70	1,023.87	0.86	3	8
Nonane	C_9H_{20}	0.00	128.255	330.70	1,070.47	0.00	0	0
Decane	$C_{10}H_{22}$	0.00	142.282	304.60	1,111.87	0.00	0	0
Air		0.00	28.959	551.90	238.70	0.00	0	0
Nitrogen	N_2	2.44	28.014	492.50	227.14	0.68	12	6
Oxygen	O_2	0.00	31.999	731.40	278.24	0.00	0	0
Carbon Dioxide	CO_2	1.30	44.010	1,070.00	547.45	0.57	14	7
Hydrogen Sulfide	H_2S	0.00	34.082	1,306.50	672.48	0.00	0	0
Hydrogen	H_2	0.00	2.016	190.70	59.77	0.00	0	0
Argon	Ar	0.15	39.948	705.32	271.24	0.06	1	0
Helium	He	0.00	4.003	33.00	9.35	0.00	0	0
Total		**100.00**				**24.08**	**649**	**411**
Sp. Gravity =		**0.832**						

Table 5
Calculation of Mole Fraction Weighted Properties

For this sample, the gas sample molecular weight is 24.08, the critical pressure is 649 psia, and the critical temperature is 411 °R. Now that the properties for the gas sample have been calculated, we can use these values to determine gas deviation factor and gas formation volume factor.

The specific gravity of gas is the weight of the gas relative to the weight of air. Once the molecular weight of the gas sample is known, we can simply divide it by the molecular weight of air to obtain its specific gravity. The specific gravity is calculated as follows.

$$Specific\ Gravity = \frac{Molecular\ Weight\ of\ Gas\ Sample}{28.595}$$

The Excel workbook that is part of the course material has a tab labeled **"Gas Composition"**. The gas sample shown in Table 5 has been input into that spreadsheet. The area of the spreadsheet highlighted in yellow is available for input. The remainder of the spreadsheet is calculated.

Determination of the Gas Deviation Factor

As mentioned in the previous sections, due to the molecular interactions of hydrocarbon molecules, hydrocarbon gases deviate from the ideal gas law. To account for this deviation, the gas deviation factor, z is used in the Ideal Gas Law. The relationship between pressure, volume, temperature and moles of gas then becomes:

$$PV = nRTz$$

where,

P = pressure (psia – pounds per square inch absolute)

V = volume (scf – standard cubic feet)

T = temperature (°R - degrees Rankine)

n = number of moles of gas (moles)

R = ideal gas constant (10.73 scf-psia/mole-°R)

z = gas deviation factor

The determination of z is based on a chart created from the results of experiments with hydrocarbon gases and first published by Katz and Standing in 1942. A copy of the gas deviation factor chart is shown below.
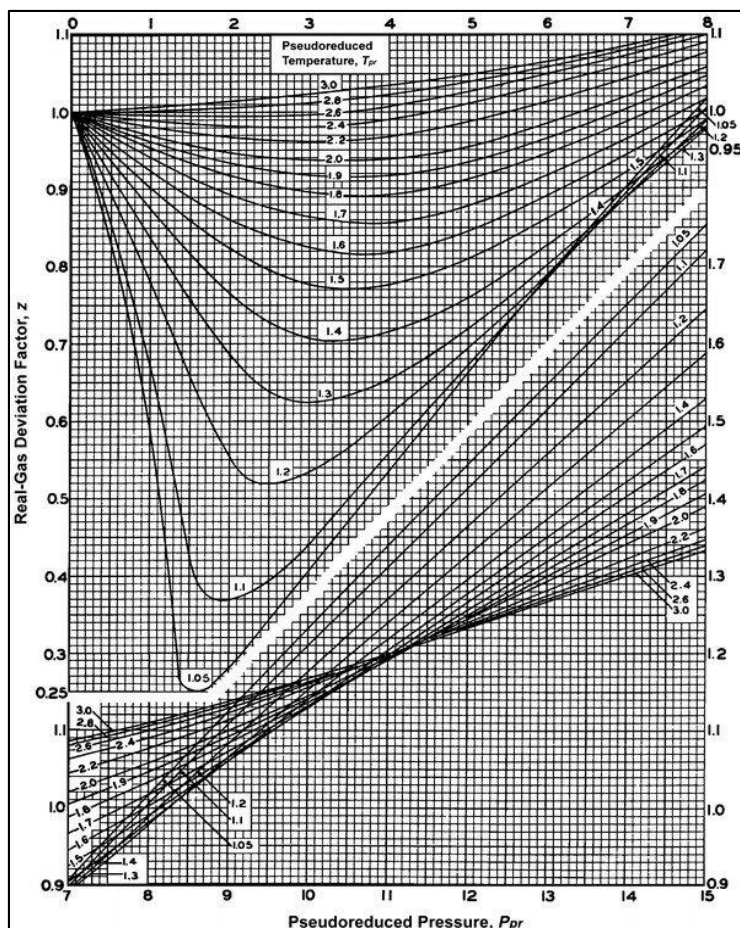
The axes of the chart are Pseudoreduced Pressure (Pr) and Gas Deviation Factor (z). There are various lines on the chart for the Pseudoreduced Temperature (Tr). The term "pseudo" is used to denote that the values of Critical Pressure and Critical Temperature are derived from gas composition data, as shown in Table 5, for example. From here on we will use the terms Reduced Pressure and Reduced Temperature.

To use this chart to find z, we must first calculate the reduced pressure and temperature using the following equations:

$$P_r = P/P_c$$

$$T_r = T/T_c$$

where,

P_r = reduced pressure
P = measured pressure (psia)
P_c = critical pressure (psia)
T_r = reduced temperature
T = measured temperature (°R)
T_c = critical temperature (°R)

The most efficient method to show how to determine the z, the gas deviation factor is to use an example.

Example Problem:

A reservoir contains the gas whose composition is given in Table 5. The reservoir pressure is 1,950 psia and the temperature is 106 °F. What is the gas deviation factor of the reservoir?

Answer:

The reservoir temperature is given in °F and must be converted to °R as follows:

$$T = 460 + 106 = 566 \text{ R}$$

From Table 5, the critical pressure is 649 psia and the critical temperature is 411 °R.
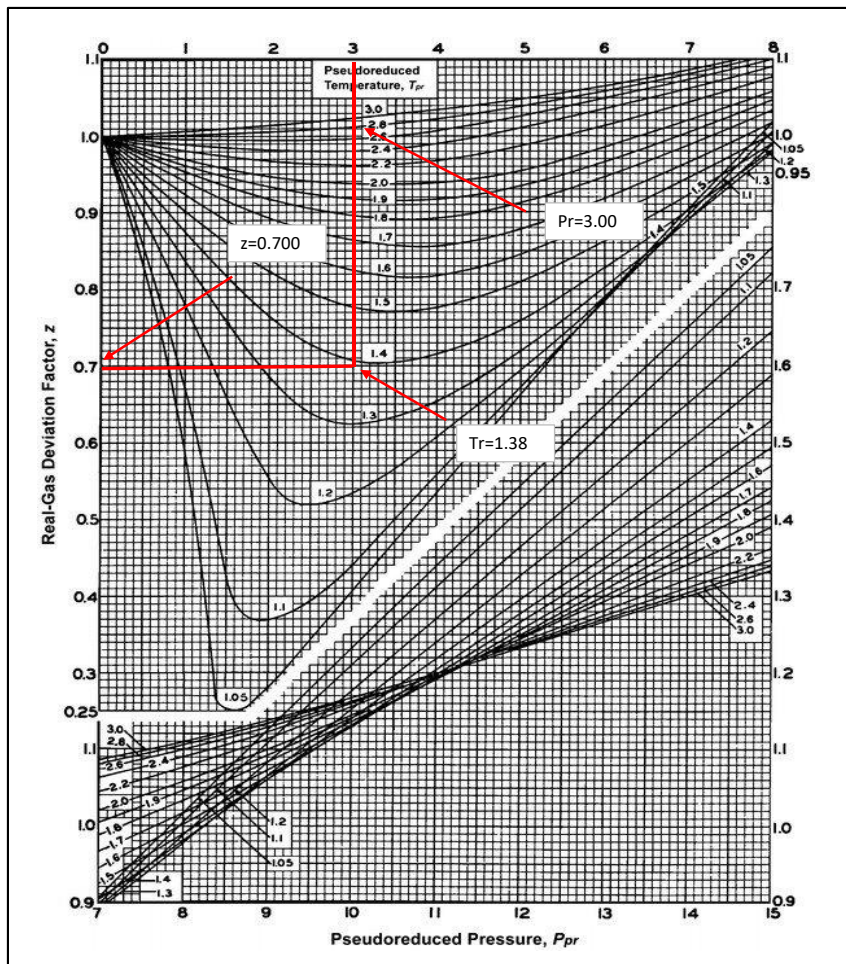
The reduced pressure is:

$$P_r = \frac{1950}{649} = 3.00$$

and the reduced temperature is:

$$T_r = \frac{566}{411} = 1.38$$

Entering the chart as shown below with a reduced pressure of 3.00 and moving downward to an interpolated reduced temperature of 1.38 gives a gas deviation factor, z of 0.70.

This method indeed works to determine the gas deviation factor. However, the method is time consuming and it is sometimes difficult to see details on the chart. Subsequent to the development of this chart, several digital calculation methods have been developed. The method created by Brill and Beggs in 1973 is accurate and only uses reduced pressure, reduced temperature, and gas gravity. A gas deviation factor calculator using this method is located in the Excel workbook under

the tab labeled "**z Factor Calculator**". The values for this example are entered into the worksheet. For the remainder of this course, we will be using the worksheet to determine gas deviation factors.

Calculation of the Gas Formation Volume Factor

As gas is produced from a reservoir under pressure and temperature higher than those at the surface, gas expands. In layman's terms, a given number of molecules of gas take up less space in the reservoir than they do at the surface. To account for the change in gas volume from the surface to the reservoir, one uses the gas formation volume factor B_g.

The units for B_g are reservoir cubic feet per standard cubic feet, of ft^3/scf. The gas formation volume factor is the number of cubic feet in the reservoir taken up by 1 standard cubic foot.

The denominator uses the units of "standard cubic feet". A standard cubic foot is defined by both a standard gas pressure and a standard gas temperature. In the United States, the standard temperature is 60 °F (520 °R). The standard pressure, however, changes with each state. For example, in Oklahoma, the standard pressure is 14.65 psia and in Louisiana it is 15.025 psia. A table of standard pressures for each state is provided in the Excel workbook under the tab "State Pressure Bases". For the purpose of this course, we will always use a pressure base of 14.65 psia unless otherwise stated.

The gas formation volume factor, B_g as,

$$B_g = \frac{P_{sc}}{T_{sc}} * \frac{zT}{P}$$

where,

        T_{sc} = standard temperature (°R)
        P_{sc} = standard pressure (psia)
        z = gas deviation factor
        T = reservoir temperature (°R)
        P = reservoir pressure (psia)

The gas deviation factor can be calculated using the spreadsheet labeled "**z Factor Calculator**" and is seen in column "E" in the spreadsheet.

Example Problem:

A reservoir contains the gas whose composition is given in Table 5. The reservoir pressure is 1,950 psia and the temperature is 106 ºF. The standard pressure is 14.65 psia and standard temperature is 60ºF (520ºR). What is the gas formation volume factor?

Answer:

The gas deviation factor can be found using the spreadsheet labeled "**z Factor Calculator**" and is equal to 0.705.

The gas formation volume factor is:

$$B_g = \frac{P_{sc}}{T_{sc}} * \frac{zT}{P} = \frac{14.65}{520} * \frac{(0.705)*(460+106)}{1,950} = 0.0058 \; ft^3/scf$$

Notice that in column "E" of the spreadsheet is the value of B_g.

Discussion of Reservoir Area and Thickness

This course will not discuss how to determine the reservoir area or thickness. We will, however, discuss some of the methods used to obtain those values.

The area of the reservoir is defined as the areal extent of the reservoir known to contain gas. The thickness is defined as the vertical thickness of the reservoir containing gas. Multiplied together, the area times the thickness is the total rock volume of the reservoir. In the United States, areas are measured in acres and thickness in feet.

The reservoir area can be determined or estimated using information from wells drilled into the reservoir. The reservoir area can also be found using seismic methods. The data from either wells or seismic, or both, is mapped and the extent of the reservoir is found by extrapolating contours. The area of the reservoir can be determined using a planimeter or other method. Most 3-D geologic modeling software can calculate the area within given contour intervals.

The thickness of the reservoir can be determined in a similar manner to area, using well data and/or seismic data. The common method is to contour the thickness at each data point (either well or seismic) and overlay it on the reservoir contour map. To arrive at an average thickness, the area of each thickness interval is calculated and summed for the entire reservoir. The result of this is the rock volume of the reservoir, typically calculated as acre-feet. In the volumetric formula for OGIP,

these are the parameters A x h. If one desires to calculate the volume of the reservoir in cubic feet, use the following formula:

$$V_r = 43,560 * A * h$$

where,

      V_r = reservoir volume in ft3
      A = reservoir area in acres
      H = reservoir thickness in feet

Since reservoirs are usually quite large, it is more convenient to calculate the reservoir volume (V_r) in millions of cubic feet as follows:

$$V_r = 0.04356 * A * h$$

Discussion of Porosity and Water Saturation

Porosity is defined as the portion of the reservoir void of rock expressed as a percentage of the rock volume. It is essentially the percentage of "holes" in the rock. If the porosity of a rock is 15%, it means that 15% of the rock is void space and 85% of the rock is solid material. Porosity is the portion of the rock where all fluids exist. Porosity is given the symbol phi and can be in the units of decimal or percent.

Water saturation is the percentage of the pore space that is taken up by water. The remainder, or 100% less the water saturation, is the portion of the pore space that contains gas (typically referred to as hydrocarbon saturation). Water saturation, rather than hydrocarbon saturation has become a standard because it is typically derived from well logs which detect the presence of water, not hydrocarbons.

The most common method of obtaining porosity and water saturation is from well logs. Occasionally, cores are taken while drilling and sent to a lab where porosity and water saturations are determined. Well logs are obtained by running an electrical device on a cable to the bottom of a newly drilled well and pulling it up to the surface. During the pull to the surface, various rock properties are measured by the different types of devices connected to the cable. Typically measured are the natural radioactivity of the rock, the density of the rock, the electrical conductivity of the rock, hydrogen in the rock, travel of sound through the rock, etc. Based on these measurements, porosity and water saturation of the various rock layers can be calculated.

Both porosity and water saturations can vary throughout the thickness of the rock. They can also vary across the area of the reservoir. As such, the estimation of porosity and water saturation in a reservoir can be a very complicated process.

The most common way to account for the variations in porosity and water saturation is to create data points for each well of porosity times feet (porosity-feet) and porosity times feet times hydrocarbon saturation. These values are then contour mapped and the volumes measured and summarized. This results in the value of A x h x Ø x (1-Sw) in the volumetric equation. Table 6 below gives an example for a particular well of the calculation of porosity-feet and porosity x hydrocarbon-feet. The values are calculated as decimals, rather than percents.

Table 6
Calculation of Porosity-Feet and Water Saturation-Feet

Depth (ft)	h (ft)	Porosity (%)	S$_w$ (%)	S$_{hc}$ (%)	Porosity Feet	Por x S$_{hc}$ Feet
3614	2	20.5	19.9	80.1	0.410	0.328
3616	4	14.0	24.1	75.9	0.560	0.425
3620	6	11.4	25.3	74.7	0.684	0.511
3626	4	16.2	27.0	73.0	0.648	0.473
3630	2	17.9	26.7	73.3	0.358	0.262
3632	6	15.2	28.4	71.6	0.912	0.653
3638	5	13.8	26.7	73.3	0.690	0.506
3643	2	13.4	33.4	66.6	0.268	0.178
3645	3	12.8	36.8	63.2	0.384	0.243
TOTAL	**34**				**4.914**	**3.580**

Notes:
S$_{hc}$ = Hydrocarbon saturation

For this well, the average porosity and hydrocarbon saturation can be calculated as:

$$\emptyset = \frac{\emptyset * h}{h} = \frac{4.914}{34} = 0.144 = 14.4\%$$

In a similar fashion, the hydrocarbon saturation can be calculated by the following:

$$S_{hc} = \frac{\emptyset * h * S_{hc}}{\emptyset * h} = \frac{3.580}{4.914} = 0.729 = 72.9\%$$

Therefore, water saturation for this well is:

$$S_w = 100 - S_{hc} = 100 - 72.9 = 27.1\%$$

Notice that an arithmetic average of porosity that ignores the number of feet gives an incorrect value. Similarly, since water saturation and therefore hydrocarbon saturation are percentages of a given porosity, calculating the average value must take into account both the porosity and the number of feet of porosity. I will leave it to you to verify, but the arithmetic averages of porosity and water saturation from Table 6 are 15.0% and 27.6%, respectively. Although the values appear to be fairly close to the weighted values (the correct ones) in this instance, they can be quite different in some cases.

Calculation of Pore Volume, Hydrocarbon Pore Volume, and Water Volume

The pore volume of a reservoir is the total rock volume multiplied by the porosity as shown here:

$$PV = 0.04356 * A * h * \emptyset$$

where,

PV = reservoir pore volume in MMcf

A = reservoir area in acres

h = reservoir thickness in feet

$\emptyset$ = reservoir porosity in decimal

The hydrocarbon pore volume is calculated as:

$$HCPV = 0.04356 * A * h * \emptyset * (1 - S_w)$$

where,

HCPV = hydrocarbon pore volume in MMcf

A = reservoir area in acres

h = reservoir thickness in feet

$\emptyset$ = reservoir porosity in decimal

S_w = water saturation in decimal

The water volume in the reservoir expressed in millions of cubic feet is then obviously the difference between the two, or:

$$PV - HCPV = 0.04356 * A * h * \emptyset * S_w$$

The HCPV is the reservoir volume available for gas in the reservoir. Since gas is measured and sold at standard conditions, it is necessary to convert the volume from reservoir conditions to surface conditions. This is done using the gas formation volume factor. When the gas formation volume factor at initial conditions is used, the subscript "i" is added. OGIP is calculated as follows:

$$OGIP = \frac{0.04356 * A * h * \emptyset * (1 - S_w)}{B_{gi}}$$

where,

OGIP = original gas-in-place in MMscf (millions of standard cubic feet)
A = reservoir area in acres
h = reservoir thickness in feet
$\emptyset$ = reservoir porosity in decimal
S_w = water saturation in decimal
B_{gi} = initial gas formation volume factor in ft^3/scf

Calculation of Residual Gas Volume

Residual gas is the gas remaining in the reservoir at abandonment. If one calculates the original gas-in-place and has the cumulative gas production information, the residual gas is simply the difference between the two as:

$$G_{res} = OGIP - G$$

where,

G_{res} = residual gas in MMscf
OGIP = OGIP = original gas-in-place in MMscf
G = cumulative gas production in MMscf

We will term the volume in the reservoir taken up by the residual gas as HCPV$_{res}$. As CO₂ is injected and the reservoir pressure reaches the sequestration pressure (initial reservoir pressure), this is the amount of reservoir volume that will contain the residual gas. The HCPV$_{res}$ is calculated as:

$$HCPV_{res} = G_{res} * B_{gi}$$

where,

HCPV$_{res}$ = residual hydrocarbon pore volume in MMcf

Example Problem:

A reservoir contains the gas whose composition is given in Table 5. The average reservoir depth is 4,500 feet. The reservoir covers an area of 2,860 acres at a thickness of 28 feet. The porosity of the reservoir is 18.6% and the average water saturation is 32%. The reservoir pressure is 1,950 psia and the temperature is 106 °F. The standard conditions are 14.65 psia and 60 °F. The cumulative production is 71,048 MMscf.

   a) What is the hydrocarbon pore volume?
   b) What is the water volume?
   c) What is the OGIP?
   d) What is the residual gas volume at standard conditions in MMscf?
   e) What is the residual hydrocarbon pore volume in the reservoir?

Feel free to use the worksheet to perform the calculations.

Answer:

   a) From prior calculations and determinations from the examples above, we already know the following:

$$z = 0.705$$
$$B_g = 0.0058 \text{ ft}^3/\text{scf}$$

$$HCPV = 0.04356 * A * h * \emptyset = 0.04356 * 2860 * 28 * .186 = 648.8 \; MMcf$$

   b) The water volume is:

$$Water\ Volume = 0.04356 * A * h * \emptyset * S_w = 0.04356 * 2860 * 28 * .186 * 0.32$$

$$= 207.6 \; MMcf$$

   c) From prior calculations and determinations from examples above, we already know the following:

$$z = 0.705$$
$$B_{gi} = 0.0058 \text{ ft}^3/\text{scf}$$

   The OGIP is:

$$OGIP = \frac{0.04356 * A * h * \emptyset * (1 - S_w)}{B_{gi}} = \frac{0.04356 * 2860 * 28 * .186 * (1 - .32)}{0.0058}$$

$$= 76,068 \; MMscf$$

d) The residual gas volume is calculated as:

$$G_{res} = OGIP - G = 76{,}068 - 71{,}048 = 5{,}020 \ MMscf$$

e) The residual hydrocarbon pore volume in the reservoir is:

$$HCPV_{res} = G_{res} * B_{gi} = 5{,}020 * .0058 = 29 \ MMcf$$

CO_2 Sequestration in Abandoned Gas Reservoirs

The estimation of the amount of CO_2 that can be sequestered in abandoned gas reservoirs is a bit more complicated than that of an aquifer. The reason is because we have both water-filled porosity and gas-filled porosity in the reservoir. At abandonment, the gas in the reservoir has expanded to fill all the pore space in the reservoir that is not filled by water. This is known as the hydrocarbon pore volume (HCPV). When CO_2 is injected into the reservoir and pressure increases, this remaining gas (termed residual gas) will be compressed and take up some of the HCPV. Because of this, a portion of the HCPV will not be available for CO_2 sequestration.

The diagrams below show the fluid distributions in an abandoned gas reservoir before and after CO_2 sequestration.

As can be seen, CO_2 will be sequestered in both the hydrocarbon pore space and dissolved in reservoir water. It is assumed that the sequestration pressure will be equal to the initial reservoir pressure.

The estimation of CO_2 sequestration in abandoned gas reservoirs involves several steps. The assumption for this method is that there is sufficient information available for the calculations. The following data are needed for these calculations:
- Reservoir area
- Reservoir height
- Average porosity
- Average water saturation
- Gas composition or gas gravity and critical pressure and temperature
- Initial reservoir pressure
- Reservoir temperature
- Cumulative gas production

An additional assumption is that the CO_2 sequestration pressure will be equal to the original reservoir pressure.

The estimation of CO_2 sequestration in abandoned gas reservoirs involves the following steps:
1) Obtain the data listed above
2) Calculate the hydrocarbon pore volume (HCPV) and the water volume in the reservoir
3) Calculate the gas formation volume factor (B_g) at the initial reservoir pressure
4) Calculate the residual gas volume at standard conditions and at CO_2 sequestration pressure (the initial reservoir pressure)
5) Calculate the HCPV available for CO_2 sequestration
6) Using the NIST website, find the CO_2 density at the CO_2 sequestration pressure and reservoir temperature
7) Calculate the lb of CO_2 that can be sequestered in the HCPV
8) Determine CO_2 solubility at the CO_2 sequestration pressure
9) Calculate the lb of CO_2 that can be sequestered in the reservoir water
10) Sum the lb of CO_2 sequestered in the HCPV and the reservoir water
11) Calculate at standard conditions the total CO_2 that can be sequestered in the reservoir

To show each of these steps, we will use an example. The reservoir chosen will be identical to the example used for the aquifer, except the water saturation in this example will be 32% (not 100% as in the aquifer example). By using the same example reservoir, one will be able to compare the amount of CO_2 sequestered in an aquifer with the amount sequestered in an abandoned gas reservoir.

This example problem is solved in the spreadsheet in the Excel workbook titled "**Sequestration Gas Res**" on row 4.

Example Problem:

Estimate how much CO_2 can be sequestered in an abandoned gas reservoir with the following properties. Express the answer in both pounds of CO_2 and standard cubic feet of CO_2 that can be sequestered.

Reservoir depth = 5,400 ft   Reservoir area = 3,200 acres   Reservoir height = 50 ft
Reservoir porosity = 24.1%   Reservoir temp = 118ºF   Reservoir pressure = 2,350 psia
Reservoir water saturation = 32%   Cumulative Gas = 204,420 MMscf
Critical Pressure = 649 psia   Critical Temperature = 411ºR
Standard pressure = 14.65 psia   Standard temp = 60ºF

Answer:

Step 1) This is just the given data.

Step 2) The hydrocarbon pore volume is given by:

$$HCPV = 0.04356 * A * h * \emptyset * (1 - S_w) = 0.04356 * 3200 * 50 * .241 * (1 - .32)$$

$$= 1,142.2 \ MMcf$$

The water volume is given by:

$$Water\ Volume = 0.04356 * A * h * \emptyset * S_w = 0.04356 * 3200 * 50 * .241 * 0.32$$

$$= 537.5 MMcf$$

Step 3) The gas deviation factor must first be determined to use in the calculation of Bg. The reduced pressure and temperature are:

$$P_r = \frac{2350}{649} = 3.62$$

$$T_r = \frac{(460 + 118)}{411} = 1.41$$

The gas deviation factor, z, from the "z Factor Calculator" worksheet is 0.718.

The gas formation volume factor, Bg, is calculated as:

$$B_g = \frac{P_{sc}}{T_{sc}} * \frac{zT}{P} = \frac{14.65}{520} * \frac{(0.718) * (460 + 118)}{2,350} = 0.0050 \, ft^3/scf$$

Step 4) The residual hydrocarbon volume at standard conditions is the OGIP minus the cumulative gas production. The OGIP is calculated as:

$$OGIP = \frac{0.04356 * A * h * \emptyset * (1 - S_w)}{B_{gi}} = \frac{0.04356 * 3200 * 50 * .241 * (1 - .32)}{0.0050}$$

$$= 228,436 \, MMscf$$

The residual gas is then determined by:

$$G_{res} = OGIP - G = 228,436 - 204,420 = 24,016 \, MMscf$$

The reservoir volume at sequestration pressure taken up by the residual gas is:

$$HCPV_{res} = G_{res} * B_g = 24,016 * 0.0050 = 120.1 \, MMcf$$

Step 5) The hydrocarbon pore volume available for sequestration is:

$$HCPV_{seq} = HCPV - HCPV_{res} = 1,142.2 - 120.1 = 1,022.1 \, MMcf$$

Another way to solve for this is to assume (correctly) that the volume available is the cumulative gas volume at original reservoir conditions. This is indeed equal to the available sequestration volume as calculated below:

$$HCPV_{seq} = G * B_g = 204,420 * 0.0050 = 1,022.1 \, MMcf$$

Step 6) Using the NIST website link given below, the density of CO_2 at a pressure of 2,350 psia and a temperature of 118oF is 46.385 lb/ft3.

[Thermophysical Properties of Fluid Systems (nist.gov)](#)

Step 7) From Step 5 above, the available sequestration volume in the reservoir is 1,022.1 MMcf. The amount of CO_2 that can be stored is:

$$CO_2 Sequestered\ in\ HCPV = HCPV_{seq} * \rho_{CO2} = 1,022.1 * 46.385 = 47,410\ million\ lb\ CO_2$$

Step 8) To use the chart, the temperature and pressure must be converted to °C and bars, respectively as shown below:

$$T_{oC} = \frac{(T_{oF} - 32)}{1.8} = \frac{(118 - 32)}{1.8} = 48\ C$$

$$P_{bar} = \frac{P_{psia}}{14.504} = \frac{2,350}{14.696} = 160\ atm$$
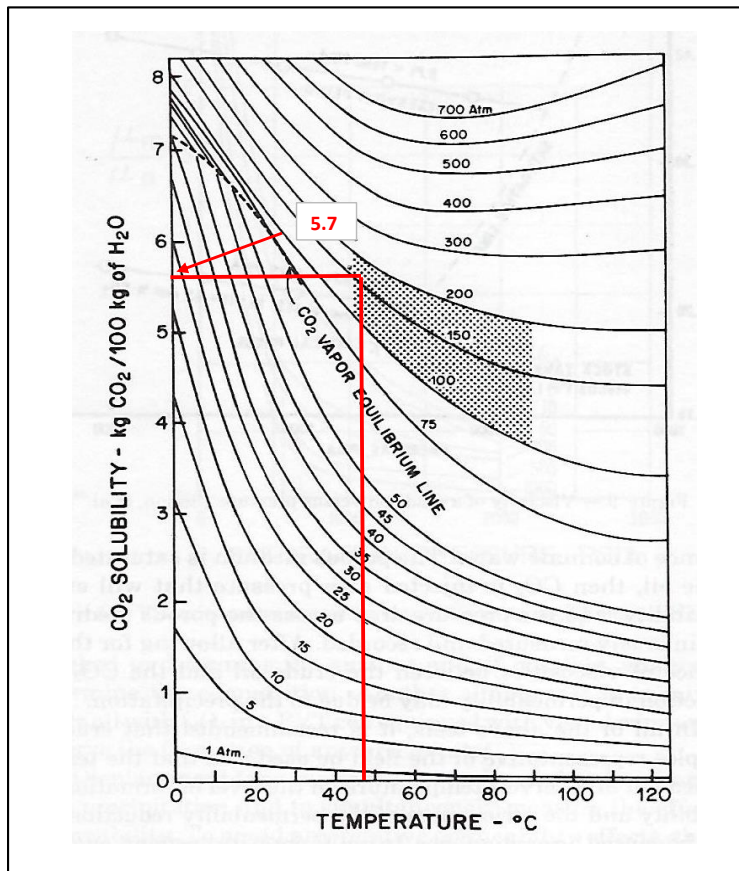
The solubility is 5.7 lb CO_2/100 lb H_2O.

Step 9) The weight of water in pounds is simply the volume multiplied by the water density of 62.4 lb/ft^3 as follows:

$$W = PV * \rho_w = 537.5 * 62.4 = 33,540 \; million \; lb \; of \; water$$

The volume of CO₂ that can be sequestered in reservoir water is:

$$Sequestered \; CO_2 = Water \; Mass \; x \; CO_2 \; Solubility = 33,540 * \frac{5.7}{100} = 1,912 \; million \; lb \; CO_2$$

Step 10) The total amount of CO₂ that can be sequestered in the reservoir is the sum of the amount sequestered in the pore volume and dissolved in the reservoir water as follows:

$$Total \; CO_2 Sequestered = 47,410 + 1,912 = 49,322 \; million \; lb \; CO_2$$

Step 11) The amount of CO₂ at standard conditions that can be sequestered is:

$$Sequestered \; CO_2 \; at \; Std \; Conditions = \frac{Sequestered \; CO_2 \; in \; lbs}{\rho CO2_{std}} = \frac{49,322}{0.115}$$

$$= 428,887 MMscf$$

There has been much talk about sequestering CO₂ in aquifers. However, as seen from the calculations above, much more CO₂ can be sequestered in abandoned gas reservoirs. Of the CO₂ sequestered in the above example, the amount sequestered in the HCPV as a percentage of the total sequestered is:

$$Percent \; Sequestered \; in \; Pore \; Space = 100 * \frac{47,410}{49,322} = 96\%$$

So, in this example, even with a water saturation of 32% (about a third of the porosity), the amount of CO₂ sequestered in the reservoir is less than 5% of the total.

When we compare the amount of CO₂ sequestered in this example of an abandoned gas reservoir to that of an aquifer of the same size and pore volume (original example) we see it is much larger. Using CO₂ sequestered at standard conditions for comparison, the ratio of CO₂ sequestered in the abandoned gas reservoir to aquifer is:

$$Ratio \; Gas \; Reservoir \; to \; Acquifer = \frac{428,887}{51,948} = 8.3$$

So, there is over 8 times more CO₂ sequestered in the abandoned gas reservoir as aquifer.

CO₂ Sequestration in Abandoned Gas Reservoirs – Limited Information

The previous section gives detailed instructions on calculating CO_2 sequestration volumes when significant reservoir information is available. This may be the case when a particular reservoir is being offered by the operator for CO_2 sequestration or personnel at the operating company are evaluating the reservoir internally for use as storage. However, if one is using public data, limited information may only be available for a cursory evaluation.

The method outlined here enables one to estimate the amount of CO_2 that may be sequestered in the pore space of an abandoned gas reservoir. Since water saturation will not be considered (it is usually not available as part of the limited information), only the amount of CO_2 sequestered in the pore space can be calculated. However, as shown in previous examples, the amount that could be sequestered in the reservoir water is likely small and on the order of 5% or less of the total sequestered CO_2.

In some cases, reservoir information may be available from state agencies (i.e., oil and gas commissions) or geologic society publications. Some state agencies keep very good field records while others only collect basic information.

The mere basic information needed to estimate CO_2 sequestration volumes is:
- Initial reservoir pressure
- Reservoir temperature
- Cumulative gas production
- Gas analysis or at least the gas gravity

Probably the most difficult item to find on the above list is the gas composition or gas gravity. If gas analysis or gas gravity is not available, there are some resources available in the public domain. The US Bureau of Mines (no longer in existence) used to maintain books that contained reported gas analyses on wells whose gas was analyzed. A book containing gas analyses for the years 1917-1958 titled *Analysis of Natural Gases 1917-1985* can be found in pdf format from the National Technical Reports Library (US Department of Commerce) at this internet address:

[Analyses of Natural Gases, 1917-85. | National Technical Reports Library - NTIS](#)

A good deal of this information is in digital form and can be found as a downloadable .csv file. Once imported into Excel, filters can be set up to hopefully find a gas analysis in or near the field and in the reservoir of study. That file can be downloaded from the US Geological Survey at this site:

[Natural Gas Compositional Analyses Dataset of Gases from United States Wells - ScienceBase-Catalog](#)

The data from these sources can be easily input into the "Gas Composition" worksheet to find the critical pressure and temperature needed to determine the gas deviation factor.

In cases where only the gas gravity is known, there are some correlations that enable one to find the associated critical temperature and pressure. A table of gas gravity versus critical pressure and critical temperature was prepared by the California Natural Gasoline Association in 1941. This table can be found in several publications and is still a good source of data.

A table of the data has been placed in the Excel workbook under the tab "Sp Gr vs Pc Tc".

Gas Specific Gravity vs P_c and T_c

Sp. Gr.	P_c (psia)	T_c (°R)	Sp. Gr.	P_c (psia)	T_c (°R)	Sp. Gr.	P_c (psia)	T_c (°R)
0.55	673	336	0.75	667	408	0.95	660	474
0.56	673	341	0.76	667	411	0.96	660	477
0.57	672	346	0.77	666	415	0.97	659	481
0.58	672	350	0.78	666	418	0.98	659	484
0.59	672	354	0.79	666	421	0.99	659	487
0.60	671	358	0.80	665	424	1.00	658	491
0.61	671	362	0.81	665	428	1.01	658	494
0.62	671	365	0.82	665	431	1.02	657	497
0.63	670	368	0.83	665	434	1.03	656	500
0.64	670	372	0.84	664	438	1.04	656	504
0.65	670	375	0.85	664	441	1.05	655	507
0.66	670	378	0.86	664	444	1.06	655	510
0.67	669	382	0.87	663	448	1.07	654	514
0.68	669	385	0.88	663	451	1.08	654	517
0.69	669	388	0.89	662	454	1.09	653	520
0.70	668	392	0.90	662	457	1.10	652	524
0.71	668	395	0.91	662	461	1.11	652	527
0.72	668	398	0.92	662	464	1.12	651	530
0.73	668	401	0.93	661	467	1.13	651	534
0.74	667	405	0.94	661	471	1.14	650	537

from Caifornia Natural Gas Association, *Bulletin TS-461*, 1941

To use the table, simply start with the gas gravity and look to the right to find the critical pressure and temperature. Now one can find the gas deviation factor and with the reservoir pressure and temperature, the gas formation volume factor from the spreadsheet "z Factor Calculator".

The following steps should be followed to estimate CO_2 sequestration in an abandoned gas reservoir with limited information:

1) Obtain reservoir pressure, temperature, cumulative gas production, and gas gravity or gas composition
2) Calculate the gas formation volume factor
3) Calculate the available pore volume for CO_2 using cumulative gas production
4) Calculate the CO_2 density at initial reservoir pressure
5) Calculate the lb of CO_2 that can be sequestered in the reservoir
6) Calculate the amount of CO_2 at standard conditions that can be sequestered

All of the above can be done using the spreadsheet under the tab "Seq Limited Info".

We will now follow an example using the same reservoir as the last two examples. We should find that we are able to store the same amount of CO_2 in the pore space as the last example.

Example Problem:

Estimate how much CO_2 can be sequestered in an abandoned gas reservoir with the following properties. Express the answer in both pounds of CO_2 and standard cubic feet of CO_2 that can be sequestered.

Reservoir depth = 5,400 ft   Reservoir temp = 118ºF   Reservoir pressure = 2,350 psia
Cumulative Gas = 204,420 MMscf
Critical Pressure = 649 psia   Critical Temperature = 411ºR
Standard pressure = 14.65 psia   Standard temp = 60ºF

Answer:

Step 1) This is the given data.

Step 2) The gas deviation factor must first be determined to use in the calculation of Bg. The reduced pressure and temperature are:

$$P_r = \frac{2350}{649} = 3.62$$

$$T_r = \frac{(460 + 118)}{411} = 1.41$$

The gas deviation factor, z, from the "z Factor Calculator" worksheet is 0.718.

The gas formation volume factor, Bg, is calculated as:

$$B_g = \frac{P_{sc}}{T_{sc}} * \frac{zT}{P} = \frac{14.65}{520} * \frac{(0.718) * (460 + 118)}{2{,}350} = 0.0050 \ ft^3/scf$$

Step 3) The volume available is the cumulative gas volume at original reservoir conditions. This is calculated below:

$$HCPV_{seq} = G * B_g = 204{,}420 * 0.0050 = 1{,}022 \ MMcf$$

Step 4) Using the NIST website link given below, the density of CO_2 at a pressure of 2,350 psia and a temperature of 118ºF is 46.385 lb/ft3.

[Thermophysical Properties of Fluid Systems (nist.gov)](nist.gov)

Step 5) From Step 3 above, the available sequestration volume in the reservoir is 1,022 MMcf. The amount of CO_2 that can be stored is:

$$CO_2 Sequestered \ in \ HCPV = HCPV_{seq} * \rho_{CO2} = 1{,}022 * 46.385 = 47{,}405 \ million \ lb \ CO_2$$

Step 6) The amount of CO_2 at standard conditions that can be sequestered is:

$$Sequestered \ CO_2 \ at \ Std \ Conditions = \frac{Sequestered \ CO_2 \ in \ lbs}{\rho CO2_{std}} = \frac{47{,}405}{0.115}$$
$$= 412{,}217 \ MMscf$$

In comparing the CO_2 sequestered of 17,410 million lb CO_2 with Step 7 of the previous example, they are indeed the same value.

This example is found on the spreadsheet "**Seq Limited Info**" on row 4.

As seen, this method is an excellent way to review a large volume of reservoirs using very few steps.

Conclusion

Hopefully, after taking this course you will feel confident to screen potential reservoirs by sequestration volume. When undertaking a CO$_2$ sequestration project, estimating the sequestration volume of a potential reservoir is likely the most important consideration. This is especially true when the volume from the CO$_2$ source requiring sequestration is known.

It is important to estimate CO$_2$ sequestration for several reservoirs as other considerations can affect the determination of the final selection for sequestration. Knowing the reservoir volume is sufficient for sequestration will eliminate that as a concern for project success.

Although it wasn't covered in this course, one must keep in mind other factors that can eliminate a reservoir as a sequestration candidate. These include:
- Lack of access to the reservoir
- Inability to purchase or obtain rights to the reservoir
- High injection rates
- Proximity to the source of CO$_2$
- Economics of the project

Some of the above items may be discovered during the sequestration volume estimation process (i.e., lack of access), while others may not be known until later in the planning stage (economics of the project). The estimation of sequestration volumes can be performed regardless of what stage of planning one is in.

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