

**Chapter 5**  
**Single-Phase Systems**

Name: \_\_\_\_\_

Date: \_\_\_\_\_

The goal of Chapter 5 is to introduce students to calculations of physical properties of the process materials and the derivation of additional relations between the process variables from these properties. The following problems build upon the fundamentals covered in your text as applied to hydrogen processing, hydrogen as an energy carrier, and the use of hydrogen in fuel cells.

- 5.1-1 Determination of a Solution Density
- 5.2-1 The Ideal Gas Equation of State
- 5.2-2 Conversion from Standard Conditions
- 5.2-3 Effect of Temperature and Pressure on Volumetric Flow Rates
- 5.2-4 Standard and True Volumetric Flow Rates
- 5.2-5 Material Balances on an Evaporator-Compressor
- 5.3-1 The Truncated Virial Equation of State
- 5.3-2 The SRK Equation of State
- 5.3-3 Estimation of Volumes using the SRK Equation of State
- 5.4-1 Tabulated Compressibility Factors
- 5.4-2 The Generalized Compressibility Chart
- 5.4-3 Kay's Rule

**Example 5.1-1 Determination of a Solution Density**

(a) A Direct-Methanol Fuel Cell is being fed with a liquid mixture of 90 wt % methanol and 10 wt % water at a temperature of 20 °C. Determine the density of this mixture by looking up a tabulated value and compare it with the calculated value, assuming volume additivity of the solution components.

**Strategy**

To calculate the density of the methanol and water mixture, we will need the values of the densities of the pure components of the liquid mixture entering the fuel cell.

**Solution**

The density of the methanol/water mixture can be found in *Perry's Chemical Engineers' Handbook*, 8<sup>th</sup> edition, p. 2-116, to be:

$$\rho (90 \text{ wt. \% CH}_3\text{OH, } 20 \text{ }^\circ\text{C}) = \text{_____ g/cm}^3$$

If we assume volume additivity for this mixture, its density can be calculated from the individual density values for each of the components, using the following equation:

$$\frac{1}{\bar{\rho}} = \frac{X_{\text{CH}_3\text{OH}}}{\rho_{\text{CH}_3\text{OH}}} + \frac{X_{\text{H}_2\text{O}}}{\rho_{\text{H}_2\text{O}}}$$

The density of each component can be found in the literature to be:

$$\rho (\text{H}_2\text{O, } 20 \text{ }^\circ\text{C}) = 0.9982 \text{ g/cm}^3 \text{ (CRC Handbook of Chemistry and Physics, 70}^{\text{th}} \text{ edition)}$$

$$\rho (\text{CH}_3\text{OH, } 20 \text{ }^\circ\text{C}) = \text{_____ g/cm}^3 \text{ (Lange's Handbook of Chemistry, 10}^{\text{th}} \text{ edition)}$$

Substituting these values:

$$\frac{1}{\bar{\rho}} = \frac{0.9 \frac{\text{g CH}_3\text{OH}}{\text{cm}^3}}{\text{_____ g CH}_3\text{OH}} + \frac{0.1 \frac{\text{g H}_2\text{O}}{\text{cm}^3}}{0.9982 \frac{\text{g H}_2\text{O}}{\text{cm}^3}}$$

$$\frac{1}{\bar{\rho}} = 1.237 \frac{\text{cm}^3}{\text{g}}$$

Taking the reciprocal of this value, yields the density of the mixture:

$$\bar{\rho} = \text{_____ } \frac{\text{g}}{\text{cm}^3}$$

The error between the theoretical and calculated values can be estimated as follows:

$$\% \text{ error} = \frac{\rho_{\text{calculated}} - \rho_{\text{tabulated}}}{\rho_{\text{tabulated}}} \times 100$$

$$\% \text{ error} = \frac{\frac{\text{g}}{\text{cm}^3} - 0.8202 \frac{\text{g}}{\text{cm}^3}}{0.8202 \frac{\text{g}}{\text{cm}^3}} \times 100$$

$\% \text{ error} = \underline{\hspace{2cm}} \%$
--

As it can be seen, there is a good agreement between the calculated and tabulated data for the density of this mixture.

(b) Estimate the density of a mixture containing 80 wt % methanol and 20 wt. % ethanol at 20 °C.

### Strategy

Similarly to the problem solved in part (a), we will require the values of the density of each component of the mixture and use the formula that assumes volume additivity of the components.

### Solution

The density of the methanol/ethanol mixture can be obtained from the following equation:

$$\frac{1}{\bar{\rho}} = \frac{X_{\text{CH}_3\text{OH}}}{\rho_{\text{CH}_3\text{OH}}} + \frac{X_{\text{C}_2\text{H}_5\text{OH}}}{\rho_{\text{C}_2\text{H}_5\text{OH}}}$$

The density of each component can be found in the literature to be:

$$\rho(\text{CH}_3\text{OH}, 20\text{ }^\circ\text{C}) = 0.7917 \text{ g/cm}^3 \text{ (Lange's Handbook of Chemistry, 10}^{\text{th}} \text{ edition)}$$

$$\rho(\text{C}_2\text{H}_5\text{OH}, 20\text{ }^\circ\text{C}) = 0.7907 \text{ g/cm}^3 \text{ (Lange's Handbook of Chemistry, 10}^{\text{th}} \text{ edition)}$$

Substituting these values:

$$\frac{1}{\bar{\rho}} = \frac{\frac{\text{g CH}_3\text{OH}}{\text{g CH}_3\text{OH}}}{0.7917 \frac{\text{g CH}_3\text{OH}}{\text{cm}^3}} + \frac{\frac{\text{g C}_2\text{H}_5\text{OH}}{\text{g C}_2\text{H}_5\text{OH}}}{\frac{\text{g C}_2\text{H}_5\text{OH}}{\text{cm}^3}}$$

$$\frac{1}{\bar{\rho}} = 1.263 \frac{\text{cm}^3}{\text{g}}$$

Supplemental Material for Elementary Principles of Chemical Processes

$$\bar{\rho} = \frac{\text{g}}{\text{cm}^3}$$

### Example 5.2-1 The Ideal-Gas Equation of State

A metal hydride tank must be designed to store hydrogen gas, which will be used as fuel in Proton Exchange Membrane Fuel Cells. The tank will contain 40 g of H<sub>2</sub> at a pressure of 10 psig. The temperature inside the tank must be 20 °C.

(a) Calculate the container volume in liters.

#### Strategy

For this problem, we will assume ideal behavior of hydrogen. Hence, we can use the ideal gas equation of state to determine the volume of the gas.

#### Solution

The ideal gas equation of state is shown below:

$$PV = nRT$$

From this equation, we can solve for the volume, to yield:

$$V = \frac{nRT}{P}$$

First we need to determine the number of moles of hydrogen  $n$ , by dividing the mass of hydrogen by its molecular weight:

$$n = \frac{m_{\text{H}_2}}{M_{\text{H}_2}} = \frac{40 \text{ g}}{2 \frac{\text{g}}{\text{mol}}} = \text{_____ moles}$$

The value of  $R$  is the gas constant, whose value will depend on the units of  $P$ ,  $V$ ,  $n$  and  $T$ . For this problem, we will use:

$$R = 0.08205 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}$$

Also, since the temperature is given in °C, it must be converted to degrees Kelvin:

$$T(\text{K}) = T(^{\circ}\text{C}) + 273 = 20 \text{ }^{\circ}\text{C} + 273$$

$$T(\text{K}) = \text{_____ K}$$

Now, since we know all the values on the right hand side of this equation, we can substitute them to calculate the volume of hydrogen inside the tank. The variable  $P$  represents the absolute pressure of the gas, therefore we need to add the atmospheric pressure of 14.7 psi to the value of the manometric pressure given in the problem statement:

$$V = \frac{(20 \text{ moles}) \left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) ( \text{ \_\_\_\_\_\_ } \text{ K} )}{( \text{ \_\_\_\_\_\_ } \text{ psi} )}$$

In this equation it can be seen that the gas constant has units of *atm* and the pressure has units of *psi*. Hence, the pressure must be multiplied by a conversion factor:

$$V = \frac{(20 \text{ moles}) \left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) ( \text{ \_\_\_\_\_\_ } \text{ K} )}{( \text{ \_\_\_\_\_\_ } \text{ psi} ) \left( \frac{1 \text{ atm}}{14.7 \text{ psi}} \right)}$$

$$\boxed{V = \text{ \_\_\_\_\_\_ } \text{ L}}$$

(b) Determine if the ideal gas assumption is correct for this problem.

### Strategy

We need to verify if the molar volume of hydrogen satisfies the following criterion:

$$\frac{RT}{P} > 5 \frac{\text{L}}{\text{mol}} \quad (\text{diatomic gases})$$

### Solution

If the criterion for the result of  $\frac{RT}{P} > 5 \frac{\text{L}}{\text{mol}}$  is satisfied, the percent error between the real volume of the gas and the volume of the gas if considered ideal, is expected to be less than 1%. After substituting the properties given for the gas in this problem into this equation, we get:

$$\frac{RT}{P} = \frac{\left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) ( \text{ \_\_\_\_\_\_ } \text{ K} )}{( \text{ \_\_\_\_\_\_ } \text{ psi} ) \left( \frac{1 \text{ atm}}{14.7 \text{ psi}} \right)}$$

$$\boxed{\frac{RT}{P} = \text{ \_\_\_\_\_\_ } \frac{\text{L}}{\text{mol}}}$$

Thus, the gas in this problem can be considered ideal.

### Example 5.2-2 Conversion from Standard Conditions

Hydrogen is entering a fuel cell stack at a rate of  $1 \frac{\text{g}}{\text{s}}$  and at a temperature and pressure of  $40^\circ\text{C}$  and  $2.5 \text{ atm}$ , respectively. Determine the volumetric flow rate of hydrogen in  $\frac{\text{m}^3}{\text{h}}$  by converting it from standard conditions.

#### Strategy

It is known that the ideal gas equation of state for any temperature and pressure is given by:

$$PV = nRT$$

For standard conditions, this equation can be written as follows:

$$P_{\text{std}} \hat{V}_{\text{std}} = RT_{\text{std}}$$

where  $\hat{V}_{\text{std}}$  represents the molar volume at standard conditions.

The volumetric flow rate at the process conditions can be determined if we divide these two equations to yield:

$$\frac{PV}{P_{\text{std}} \hat{V}_{\text{std}}} = \frac{nRT}{T_{\text{std}}}$$

#### Solution

First we need to convert the mass flow rate to molar flow rate, using the molecular weight of hydrogen:

$$\dot{n} = \frac{1 \frac{\text{g}}{\text{s}} \left( \frac{3600 \text{ s}}{1 \text{ h}} \right)}{2 \frac{\text{g}}{\text{mol}}} = \frac{\text{mol}}{\text{h}}$$

Now we can use the equation which relates the gas conditions at any temperature and pressure with the standard conditions:

$$\frac{PV}{P_{\text{std}} \hat{V}_{\text{std}}} = \frac{nT}{T_{\text{std}}}$$

The standard conditions are:

Daniel López Gaxiola  
Jason M. Keith

Student View

Supplemental Material for Elementary Principles of Chemical Processes

$$P_{\text{std}} = 1 \text{ atm}$$

$$\hat{V}_{\text{std}} = 22.4 \frac{\text{L}}{\text{mol}}$$

$$T_{\text{std}} = 273 \text{ K}$$

Since we are using molar flow rate instead of number of moles, the previous equation can be solved for  $\dot{V}$  and written as:

$$\dot{V} = \dot{n} \frac{T}{T_{\text{std}}} \frac{P_{\text{std}}}{P} \hat{V}_{\text{std}}$$

We can substitute the known values to yield:

$$\dot{V} = \frac{\left( \frac{\text{mol}}{\text{h}} \right) ( \text{K} ) (1 \text{ atm}) (22.4 \frac{\text{L}}{\text{mol}})}{( \text{atm} ) (273 \text{ K})}$$

$$\dot{V} = \frac{\text{L}}{\text{h}}$$

Converting to  $\frac{\text{m}^3}{\text{h}}$ :

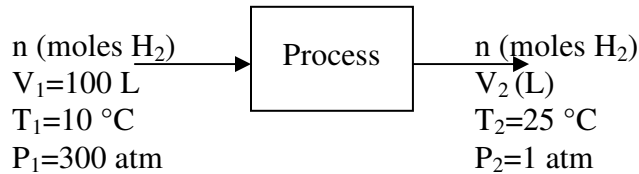
$$\dot{V} = \frac{\text{L}}{\text{h}} \left( \frac{1 \text{ m}^3}{1000 \text{ L}} \right)$$

$$\dot{V} = \frac{\text{m}^3}{\text{h}}$$



**Example 5.2-3 Effect of Temperature and Pressure on Volumetric Flow Rates**

100 L of hydrogen gas are being stored in a tank at a pressure of 300 atm and a temperature of 10 °C. Before hydrogen enters through the channels of the bipolar plate in a proton exchange membrane fuel cell, the gas is heated to a temperature of 25 °C and its pressure is reduced to 1 atm. Determine the volume occupied by the gas in its final conditions. A diagram describing this process is shown below:

**Strategy**

For this problem we will assume that the hydrogen behavior is described by the ideal gas equation of state. This equation will have to be applied for both initial and final conditions.

**Solution**

For the hydrogen at the initial conditions, the ideal gas equation can be written as follows:

$$P_1 V_1 = n_1 R T_1$$

When the hydrogen exits the storage tank, its properties will be described by the following equation:

$$P_2 V_2 = n_2 R T_2$$

If we divide these two equations, we get:

$$\frac{P_1 V_1}{P_2 V_2} = \frac{n_1 R T_1}{\text{—————}}$$

In the process described on the problem statement, there are no additional streams feeding or removing hydrogen. Thus:

$$n_1 = n_2$$

## Supplemental Material for Elementary Principles of Chemical Processes

With this consideration, the ratio of the two equations can be reduced to:

$$\frac{P_1 V_1}{P_2 V_2} = \frac{T_1}{T_2}$$

After solving for  $V_2$  and substituting all the known values into this equation, we get:

$$V_2 = \frac{P_1}{P_2} \frac{T_2}{T_1} V_1 = \frac{(\text{_____ atm})}{(1 \text{ atm})} \frac{(298 \text{ K})}{(\text{_____ K})} (\text{_____ L})$$

$V_2 = \text{_____ L}$
------------------------

**Example 5.2-4 Standard and True Volumetric Flow Rates**

A large-scale steam-methane reforming plant is consuming methane at a rate of  $5.39 \times 10^6$  SCFH. The pressure of methane in the feed stream was measured to be 16 bar and the gas enters the process at a temperature of 723 K.

(a) Determine the molar flow rate of methane at standard conditions in  $\frac{\text{kmol}}{\text{h}}$ .

**Strategy**

To determine the molar flow rate, we will use the ideal gas equation of state at standard conditions.

**Solution**

The molar flow rate can be obtained using the molar volume of an ideal gas at standard temperature and pressure:

$$\hat{V}_{\text{std}} = \frac{\text{L (STP)}}{\text{kmol}}$$

The volumetric flow rate given in the problem statement must be converted to the units of  $\frac{\text{L}}{\text{h}}$ . The units of SCFH can be also written as  $\text{ft}^3(\text{STP})$  for conditions of standard temperature and pressure.

$$\dot{V}_{\text{std}} = 5.39 \times 10^6 \frac{\text{ft}^3(\text{STP})}{\text{h}} \left( \frac{28.32 \text{ L}}{1 \text{ ft}^3} \right) = \frac{\text{L(STP)}}{\text{h}}$$

Now the molar flow rate can be determined from the following equation:

$$\dot{n} = \frac{\dot{V}_{\text{std}}}{\hat{V}_{\text{std}}}$$

Substituting the variables on the right hand side of this equation:

$$\dot{n} = \frac{\text{L(STP)}}{\text{h}} \left( \frac{1 \text{ kmol}}{\text{L (STP)}} \right)$$

$$\boxed{\dot{n} = 6815 \frac{\text{kmol}}{\text{h}}}$$

(b) Calculate the volumetric flow rate of methane at the process conditions.

### Strategy

For this problem, the ideal equation of state can be applied at two different process conditions, similar to example 5.2-3, with the difference that the initial conditions of the gas will be standard temperature and pressure.

### Solution

The equation that relates the properties of an ideal gas at two different conditions, is given by:

$$\frac{P_1 V_1}{P_2 V_2} = \frac{T_1}{T_2}$$

For the operation conditions in this process, this equation can be rewritten as:

$$\frac{P_{\text{std}} \dot{V}_{\text{std}}}{P_2 \dot{V}_2} = \frac{T_2}{T_{\text{std}}}$$

We can solve for the volumetric flow rate of the methane that will be entering the steam-methane reforming plant, to get:

$$\dot{V}_2 = \frac{T_2}{T_{\text{std}}} \dot{V}_{\text{std}}$$

Substituting the known values for pressure, temperature and volumetric flow rate:

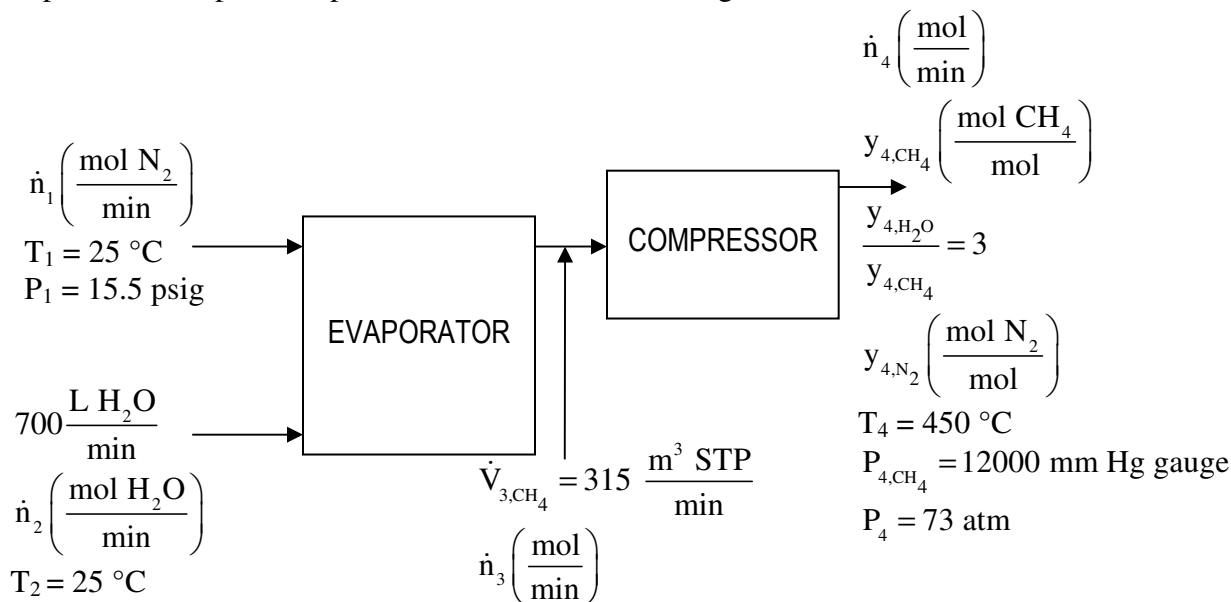
$$\dot{V}_2 = \frac{(1 \text{ atm})}{(\text{--- bar}) \left( \frac{1 \text{ atm}}{1.01325 \text{ bar}} \right)} \frac{(\text{--- K})}{(273 \text{ K})} \left( \text{---} \frac{\text{L}}{\text{h}} \right)$$

$$\boxed{\dot{V}_2 = \text{---} \frac{\text{L}}{\text{h}}}$$

**Example 5.2-5 Material Balances on an Evaporator - Compressor**

In the following process, liquid water is being evaporated for use in a large-scale steam-methane reforming plant. The steam exiting the evaporator will be mixed with a methane stream. The methane must enter the steam-methane reforming process at a pressure of 12 000 mm Hg gauge. In order to bring methane to these conditions, the steam-methane mixture will enter a compressor before being fed into the steam-reforming process.

Nitrogen will be fed into this process, to avoid combustion of methane. A diagram of this evaporation-compression process is shown in the next figure:



Determine all the unknown flow rates in this process, and the molar fractions of methane, water and nitrogen in the stream exiting the compressor.

**Strategy**

The unknown flow rates of this process can be calculated using mass balances and the ideal gas equation of state. If either the molar or volumetric flow rates are known, we can use density data to determine the unknown value.

**Solution**

We can start solving this problem by calculating the molar flow rate  $\dot{n}_2$ . As it can be seen, the volumetric flow rate is already given, hence we can look up the tabulated density of liquid water at  $T = 25 \text{ }^\circ\text{C}$ .

$$\dot{n}_2 = \dot{V}_2 \rho_2 M_{\text{H}_2\text{O}}$$

## Supplemental Material for Elementary Principles of Chemical Processes

The density of water at this conditions was found to be  $\rho = \text{_____ g/cm}^3$  (*Perry's Chemical Engineers' Handbook*, 8<sup>th</sup> edition, p. 2-96). Substituting the known values into the equation for the molar flow rate  $\dot{n}_2$ :

$$\dot{n}_2 = 700 \frac{\text{L}}{\text{min}} \left( \text{_____} \frac{\text{g}}{\text{L}} \right) \left( \frac{1 \text{ mol}}{18 \text{ g}} \right)$$

$$\dot{n}_2 = \text{_____} \frac{\text{mol}}{\text{min}}$$

The molar fraction of the methane exiting the compressor can be determined from the definition of partial pressure of a gas, given by:

$$P_{4,\text{CH}_4} = y_{4,\text{CH}_4} P_4$$

solving for the molar fraction  $y_{4,\text{CH}_4}$  and substituting the values for the partial and total pressures.

$$y_{4,\text{CH}_4} = \frac{P_{4,\text{CH}_4}}{P_4} = \frac{(12000 \text{ mm Hg gauge} + \text{_____ mm Hg}) \left( \frac{1 \text{ atm}}{\text{_____ mm Hg}} \right)}{73 \text{ atm}}$$

$$y_{4,\text{CH}_4} = \text{_____} \frac{\text{mol CH}_4}{\text{mol}}$$

Since the partial pressure of methane was given in mm Hg gauge, we had to add the atmospheric pressure to that value, in order to get the absolute partial pressure of methane.

The ratio of the moles of water to the moles of methane required for the steam-methane reforming reaction is 3. This ratio can be used to determine the molar fraction of water  $y_{4,\text{H}_2\text{O}}$ :

$$y_{4,\text{H}_2\text{O}} = 3y_{4,\text{CH}_4}$$

$$y_{4,\text{H}_2\text{O}} = 3( \text{_____} )$$

$$y_{4,\text{H}_2\text{O}} = \text{_____} \frac{\text{mol H}_2\text{O}}{\text{mol}}$$

The only species exiting the compressor are nitrogen, steam and methane, so the sum of the molar fractions of these three species must be equal to 1:

$$y_{4,\text{CH}_4} + y_{4,\text{H}_2\text{O}} + y_{4,\text{N}_2} = 1$$

From this equation we can solve for the molar fraction of nitrogen, and substitute the molar fractions of steam and methane into the equation to get:

Supplemental Material for Elementary Principles of Chemical Processes

$$y_{4,N_2} = 1 - y_{4,CH_4} - y_{4,H_2O} = 1 - 0.23 - \underline{\hspace{2cm}}$$

$$y_{4,N_2} = \frac{\text{mol } N_2}{\text{mol}}$$

The volumetric flow rate of methane at standard conditions entering the compressor can be used to determine the molar flow rate  $n_3$ . For this, the ideal gas equation of state can be used:

$$P_{\text{std}} \dot{V}_3 = \dot{n}_3 RT_{\text{std}}$$

solving for  $n_3$  and entering the known values in this equation we get:

$$\dot{n}_3 = \frac{\dot{V}_3 P_{\text{std}}}{RT_{\text{std}}} = \frac{(1 \text{ atm}) \left( \underline{\hspace{2cm}} \frac{\text{m}^3}{\text{min}} \right) \left( \frac{1000 \text{ L}}{\text{m}^3} \right)}{\left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) (273 \text{ K})}$$

$$\dot{n}_3 = \underline{\hspace{2cm}} \frac{\text{mol}}{\text{min}}$$

Now that the molar fraction of water exiting the compressor is known, it can be used to determine the molar flow rate of liquid water by doing an overall mol balance on water:

$$\text{Input} = \text{Output}$$

$$\dot{n}_2 = y_{4,H_2O} \dot{n}_4$$

Solving for  $n_4$  and substituting the values for  $n_2$  and  $y_{4,H_2O}$ :

$$\dot{n}_4 = \frac{\dot{n}_2}{y_{4,H_2O}} = \frac{\underline{\hspace{2cm}} \frac{\text{mol}}{\text{min}}}{\underline{\hspace{2cm}}}$$

$$\dot{n}_4 = \underline{\hspace{2cm}} \frac{\text{mol}}{\text{min}}$$

Finally, the molar flow rate of the inert gas used in this process can be calculated by performing an overall molar balance on the process:

$$\text{Input} = \text{Output}$$

$$\dot{n}_1 + \dot{n}_2 + \dot{n}_3 = \dot{n}_4$$

Supplemental Material for Elementary Principles of Chemical Processes

Solving for  $n_1$  and substituting the calculated values for the molar flow rates  $n_2$ ,  $n_3$  and  $n_4$ :

$$\dot{n}_1 = \dot{n}_4 - \dot{n}_2 - \dot{n}_3 = \left( \text{—————} \frac{\text{mol}}{\text{min}} \right) - \left( \text{—————} \frac{\text{mol}}{\text{min}} \right) - \left( \text{—————} \frac{\text{mol}}{\text{min}} \right)$$

$$\boxed{\dot{n}_1 = 3 \times 10^3 \frac{\text{mol}}{\text{min}}}$$



**Example 5.3-1 The Truncated Virial Equation of State**

A process to obtain hydrogen is by gasification of biomass, which consists of the combination of biomass with steam and oxygen at high temperature and pressure to produce synthesis gas. The hydrogen in the product stream is purified using adsorbers or membranes. In this process, hydrogen is produced at a rate of 300 kg/day and placed in a 30-m<sup>3</sup> tank at a temperature of 27 °C.

Determine the tank pressure after a day of operation using the ideal equation of state and the virial equation of state truncated after the second term. Using these results, estimate the percentage error obtained if the ideal gas equation is used.

**Strategy**

To use the virial equation of state, certain parameters need to be looked up in tables to determine the coefficient B of the second term of this equation.

**Solution**

The molar volume of the hydrogen obtained by biomass gasification can be obtained by dividing the volume of the tank by the number of moles of hydrogen produced:

$$\hat{V} = \frac{V}{n} = \frac{\text{_____ m}^3 \left( \frac{1000\text{L}}{1 \text{ m}^3} \right)}{\text{_____ kg} \left( \frac{1000\text{g}}{1 \text{ kg}} \right) \left( \frac{1 \text{ mol H}_2}{\text{_____ g}} \right)}$$

$$\hat{V} = \text{_____} \frac{\text{L}}{\text{mol}}$$

Now we have all the information and we can substitute these values into the ideal equation of state to calculate the pressure:

$$P_{\text{ideal}} = \frac{RT}{\hat{V}} = \frac{\left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) \left( \text{_____ K} \right)}{\text{_____} \frac{\text{L}}{\text{mol}}}$$

$$P_{\text{ideal}} = \text{_____ atm}$$

The virial equation of state is shown below:

$$\frac{PV}{RT} = 1 + \frac{B}{RT} P$$

Solving for the pressure  $P$ , this equation can be written as:

$$P = \frac{RT}{V - B}$$

Because of the small mass of hydrogen, an alternative procedure to determine the coefficient  $B$  for this gas is described by Prausnitz et al. in the Appendix C of the book *Molecular Thermodynamics of Fluid-Phase Equilibria*, 3<sup>rd</sup> Edition. Looking at the values summarized in Table C-1 of this book, for  $T=300$  K, the coefficient  $B$  will be:

$$B = 14.8 \frac{\text{cm}^3}{\text{mol}}$$

Substituting the known quantities into the virial equation of state, we get:

$$P = \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}\right) (\text{---} \text{ K})}{\text{---} \frac{\text{L}}{\text{mol}} - \left[ \left(14.8 \frac{\text{cm}^3}{\text{mol}}\right) \left(\frac{1 \text{ L}}{\text{---} \text{ cm}^3}\right) \right]}$$

$P = \text{---} \text{ atm}$

The error between using the ideal equation of state and the truncated virial equation can be estimated using the following equation:

$$\epsilon = \frac{P - P_{\text{ideal}}}{P_{\text{ideal}}} \times 100\%$$

Substituting the pressure values found yields:

$$\epsilon = \frac{\text{---} - 123.1 \text{ atm}}{123.1 \text{ atm}} \times 100\%$$

$\epsilon = \text{---} \% \text{ overprediction}$

**Example 5.3-2 The SRK Equation of State**

500 g of hydrogen are being stored in a vehicle tank with a volume of 0.3 m<sup>3</sup> and at a temperature of 40 °C. Determine the hydrogen pressure in the tank using the Soave-Redlich-Kwong (SRK) equation. Using these results, estimate the percentage error obtained if the ideal gas equation is used.

**Strategy**

In order to use the SRK equation we have to look for tabulated values for the critical properties of hydrogen, as well as the Pitzer acentric factor, which is a function of the geometry and polarity of a molecule.

**Solution**

The SRK equation of state is:

$$P = \frac{RT}{\hat{V} - b} - \frac{\alpha a}{\hat{V}(\hat{V} + b)}$$

To solve for the pressure from this equation, first we need to find the unknown parameters  $\alpha$ ,  $a$  and  $b$ , and determine the molar volume  $\hat{V}$  of the hydrogen inside the tank.

The molar volume can be determined from the mass of hydrogen and the volume of the tank. After substituting the values, we find the molar volume of hydrogen to be:

$$\hat{V} = \frac{V}{n} = \frac{\text{_____ m}^3 \left( \frac{1000 \text{ L}}{1 \text{ m}^3} \right)}{\text{_____ g} \left( \frac{1 \text{ mol}}{2 \text{ g}} \right)}$$

$$\hat{V} = \text{_____} \frac{\text{L}}{\text{mol}}$$

The values of the critical properties for different substances can be found in Table B.1 of the book *Elementary Principles of Chemical Processes*, 3<sup>rd</sup> Edition, by Felder and Rousseau. For hydrogen:

$$T_c = \text{_____ K}$$

$$P_c = \text{_____ atm}$$

With these values, the parameters a and b can now be calculated using equations 5.3-8 and 5.3-9 from the book. After entering the critical properties into these equations, we get:

$$a = 0.42747 \frac{(RT_c)^2}{P_c} = 0.42747 \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \times \text{_____ K}\right)^2}{\text{_____ atm}}$$

$$a = \text{_____} \frac{\text{L}^2 \cdot \text{atm}}{\text{mol}^2}$$

$$b = 0.08664 \frac{RT_c}{P_c} = 0.08664 \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \times \text{_____ K}\right)}{\text{_____ atm}}$$

$$b = \text{_____} \frac{\text{L}}{\text{mol}}$$

The following equation was found by M. S. Graboski and T. E. Daubert (1979) for calculating the parameter  $\alpha$  for hydrogen gas:

$$\alpha = 1.202e^{-0.30228T_r}$$

where:

$$T_r = \frac{T}{T_c}$$

We can substitute the operation and critical temperatures into the equation for the reduced temperature  $T_r$ :

$$T_r = \frac{313.15 \text{ K}}{\text{_____ K}} = \text{_____}$$

Now we can proceed to solve for the parameter  $\alpha$ , by entering the values of  $T_r$  to get:

$$\alpha = 1.202e^{-0.30228(\text{_____})}$$

$$\alpha = \text{_____}$$

After calculating all the required parameters for the SRK equation of state, the values we found can be substituted into this equation to yield:

Supplemental Material for Elementary Principles of Chemical Processes

$$P = \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}\right) (\text{ } \text{K})}{\frac{\text{L}}{\text{mol}} - 0.018 \frac{\text{L}}{\text{mol}}} - \frac{\left(\frac{\text{L}^2 \cdot \text{atm}}{\text{mol}^2}\right)}{\frac{\text{L}}{\text{mol}} \left(\frac{\text{L}}{\text{mol}} + 0.018 \frac{\text{L}}{\text{mol}}\right)}$$

$$\boxed{P = 21.7 \text{ atm}}$$

For comparison, we can calculate the pressure using the ideal gas equation of state:

$$P = \frac{RT}{\hat{V}} = \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}\right) (\text{ } \text{K})}{\frac{\text{L}}{\text{mol}}}$$

$$P = \text{ } \text{ atm}$$

The difference between using the ideal and the SRK equations of state can be evaluated with an error term  $\epsilon$ , defined as:

$$\epsilon = \frac{P_{\text{SRK}} - P_{\text{ideal}}}{P_{\text{ideal}}} \times 100\%$$

By substituting the values for the pressure obtained from both equations we get:

$$\epsilon = \frac{21.7 \text{ atm} - \text{ } \text{ atm}}{\text{ } \text{ atm}} \times 100\%$$

$$\boxed{\epsilon = \text{ } \%}$$

**Example 5.3-3 Estimation of Volumes using the SRK Equation of State**

A stream of methane is entering to a steam-methane reforming plant at a temperature of 723 K and at a molar flow rate of 350 kmol/h. Using the SRK equation of state, determine the volumetric flow rate of methane in m<sup>3</sup>/h at pressures of 0.1 bar, 1 bar, 10 bar, 20 bar and 50 bar.

**Strategy**

The molar volume of methane at different pressures can be obtained from the SRK equation of state using trial and error. This will have to be done at the different pressures given in the problem statement.

**Solution**

The SRK equation of state is given by:

$$P = \frac{RT}{\hat{V} - b} - \frac{\alpha a}{\hat{V}(\hat{V} + b)}$$

This equation can be rewritten as follows:

$$P - \frac{RT}{\hat{V} - b} + \frac{\alpha a}{\hat{V}(\hat{V} + b)} = 0$$

The values of the critical properties of methane can be found in Table B.1 of the book *Elementary Principles of Chemical Processes*, 3<sup>rd</sup> Edition, by Felder and Rousseau:

$$T_c = \text{_____ K}$$

$$P_c = \text{_____ atm}$$

With these values, the parameters a and b can now be calculated:

$$a = 0.42747 \frac{(RT_c)^2}{P_c} = 0.42747 \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \times \text{_____ K}\right)^2}{\text{_____ atm}}$$

$$a = \text{_____} \frac{\text{L}^2 \cdot \text{atm}}{\text{mol}^2}$$

$$b = 0.08664 \frac{RT_c}{P_c} = 0.08664 \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \times \text{_____ K}\right)}{\text{_____ atm}}$$

Supplemental Material for Elementary Principles of Chemical Processes

$$b = \frac{\text{L}}{\text{mol}}$$

To determine the parameter  $\alpha$ , we need to calculate the reduced temperature and the parameter  $m$  as a function of the acentric factor  $\omega$ . We can look for the value of  $\omega$  in Table 5.3-1 of the book *Elementary Principles of Chemical Processes*, 3<sup>rd</sup> Edition, by Felder and Rousseau :

$$\omega = 0.008$$

The reduced temperature and the parameter  $m$  can be now determined as follows:

$$T_r = \frac{T}{T_c} = \frac{\text{K}}{\text{K}} = 3.8$$

$$m = 0.48508 + 1.55171\omega - 0.1561\omega^2$$

$$m = 0.48508 + [1.55171 \times (0.008)] - [0.1561 \times (0.008)^2]$$

$$m = \text{_____}$$

Substituting the values we found for  $m$  and  $T_r$ , we can estimate the value of  $\alpha$  to be:

$$\alpha = [1 + m(1 - \sqrt{T_r})]^2 = [1 + \text{_____}(1 - \sqrt{3.8})]^2$$

$$\alpha = \text{_____}$$

Now the SRK equation of state can be written as follows:

$$P - \frac{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}\right) \left(\text{_____ K}\right)}{\hat{V} - \frac{\text{L}}{\text{mol}}} + \frac{\text{_____} \left(\frac{\text{L}^2 \cdot \text{atm}}{\text{mol}^2}\right)}{\hat{V}(\hat{V} + \frac{\text{L}}{\text{mol}})} = 0$$

This equation can be reduced to yield:

$$P - \frac{59.3}{\hat{V} - \text{_____}} + \frac{\text{_____}}{(\hat{V}^2 + \text{_____} \hat{V})} = 0$$

where the molar volume  $\hat{V}$  has units of  $\frac{\text{L}}{\text{mol}}$  and the pressure  $P$  has units of atm.

The following table is showing the results for the molar volume obtained from this equation at different pressure values.

<b>P</b>	$\hat{V} \left( \frac{\text{L}}{\text{mol}} \right)$
0.1 bar	_____
1 bar	60.1
10 bar	_____
20 bar	_____
50 bar	_____

The volumetric flow rates of methane into the process can be now calculated with the following equation:

$$\dot{V} = \dot{n} \hat{V}$$

Substituting the molar flow rate of 350 kmol/h given in the problem statement, and the different molar volumes obtained for different pressure conditions, we can calculate the molar flow rate as follows:

$$\dot{V} = \left( \text{_____} \frac{\text{kmol}}{\text{h}} \right) \left( \frac{1000 \text{ mol}}{1 \text{ kmol}} \right) \left( \frac{1 \text{ m}^3}{1000 \text{ L}} \right) \hat{V} \left( \frac{\text{L}}{\text{mol}} \right)$$

reducing this equation yields:

$$\dot{V} \left( \frac{\text{m}^3}{\text{h}} \right) = \text{_____} \hat{V} \left( \frac{\text{L}}{\text{mol}} \right)$$

The results obtained for  $\dot{V}$  are summarized in the following table:

<b>P</b>	$\hat{V} \left( \frac{\text{L}}{\text{mol}} \right)$	$\dot{V} \left( \frac{\text{m}^3}{\text{h}} \right)$
0.1 bar	_____	$2.1 \times 10^5$
1 bar	60.1	_____
10 bar	_____	_____
20 bar	_____	_____
50 bar	_____	427



**Example 5.4-1 Tabulated Compressibility Factors**

A large-scale coal gasification facility produces  $1.2 \times 10^6$  kg of hydrogen each day, which can be used as fuel in proton exchange membrane fuel cells. This gas is being produced at a pressure of 6300 kPa and a temperature of 650 K. Determine the volumetric flow rate of hydrogen production using the compressibility factor  $z$ .

**Strategy**

For this problem we need to look up for tabulated values of the compressibility factor at the process condition and use its definition to determine the volumetric flow rate.

**Solution**

The compressibility factor at different temperature and pressures can be found in *Perry's Chemical Engineers' Handbook*, 7<sup>th</sup> Edition, p. 2-142.

Since there is no data for the exact temperature and pressure conditions given for this problem, we can use linear interpolation to estimate the compressibility factor at  $P = 6300$  kPa and  $T = 650$  K. The data given in the book is shown below:

		Pressure (bar)		
		60	63	80
Temperature (K)	600	1.0204	Z @ 63 bar,600 K	1.0272
	650	Z @ 60 bar,650 K	Z @ 63 bar,650 K	Z @ 80 bar,650 K
	800	1.0156	Z @ 63 bar,800 K	1.0208

We have two choices to solve this problem. We can interpolate down at constant pressure, then across at constant temperature. The second alternative is to interpolate across at constant temperature and then down at constant pressure.

From the table shown above, we need to calculate first the values of the compressibility factor at a constant temperature of 650 K at a pressure of 60 bar. We setup the linear interpolation as:

$$\frac{T_{\text{mid}} - T_{\text{low}}}{T_{\text{high}} - T_{\text{low}}} = \frac{Z_{@ T_{\text{mid}}} - Z_{@ T_{\text{low}}}}{Z_{@ T_{\text{high}}} - Z_{@ T_{\text{low}}}}$$

Supplemental Material for Elementary Principles of Chemical Processes

Inserting the numbers from the table, we have:

$$\frac{650 \text{ K} - 600 \text{ K}}{\text{_____ K} - 600 \text{ K}} = \frac{z_{@ 60 \text{ bar}, 650 \text{ K}} - 1.0204}{1.0156 - \text{_____}}$$

Solving for  $z_{@ 60 \text{ bar}, 650 \text{ K}}$ :

$$z_{@ 60 \text{ bar}, 650 \text{ K}} = \left[ \frac{650 \text{ K} - 600 \text{ K}}{\text{_____ K} - 600 \text{ K}} (1.0156 - \text{_____}) \right] + 1.0204 = \text{_____}$$

Repeating this procedure for the compressibility factors at a pressure of 80 bar we have:

$$z_{@ 80 \text{ bar}, 650 \text{ K}} = \left[ \frac{650 \text{ K} - 600 \text{ K}}{\text{_____ K} - 600 \text{ K}} (1.0208 - \text{_____}) \right] + 1.0274 = \text{_____}$$

After substituting the calculated values for the compressibility factors at  $T=650 \text{ K}$  in the table, we get:

		Pressure (bar)		
		60	63	80
Temperature (K)	600	1.0204	$z_{@ 63 \text{ bar}, 600 \text{ K}}$	1.0272
	650	_____	$z_{@ 63 \text{ bar}, 650 \text{ K}}$	_____
	800	1.0156	$z_{@ 63 \text{ bar}, 800 \text{ K}}$	1.0208

At this point, we can solve for the compressibility factor at the operation conditions in the process described in this problem.

Interpolating across at a constant temperature and solving for  $z_{@ 63 \text{ bar}, 650 \text{ K}}$  yields:

$$z_{@ 63 \text{ bar}, 650 \text{ K}} = \left[ \frac{\text{_____ bar} - 60 \text{ bar}}{80 \text{ bar} - 60 \text{ bar}} (\text{_____} - \text{_____}) \right] + 1.0192$$

Thus, the compressibility factor is estimated to be:

$$z_{@ 63 \text{ bar}, 650 \text{ K}} \approx \text{_____}$$

Alternatively, the interpolation can also be performed first determining the values of the compressibility factor at a constant pressure of 63 bar, and at both temperatures of 600 K and 800 K. For this case, the interpolation can be done using the following equation:

$$\frac{P_{\text{mid}} - P_{\text{low}}}{P_{\text{high}} - P_{\text{low}}} = \frac{Z_{@ P_{\text{mid}}} - Z_{@ P_{\text{low}}}}{Z_{@ P_{\text{high}}} - Z_{@ P_{\text{low}}}}$$

Substituting the values from the table yields:

$$Z_{@ 63 \text{ bar}, 600 \text{ K}} = \left[ \frac{\text{_____ bar} - 60 \text{ bar}}{80 \text{ bar} - 60 \text{ bar}} \left( \text{_____} - 1.0204 \right) \right] + \text{_____} = 1.0214$$

$$Z_{@ 63 \text{ bar}, 800 \text{ K}} = \left[ \frac{\text{_____ bar} - 60 \text{ bar}}{80 \text{ bar} - 60 \text{ bar}} \left( \text{_____} - 1.0156 \right) \right] + \text{_____} = 1.0164$$

If we enter the calculated compressibility factors into the previous table, we get:

		Pressure (bar)		
		60	63	80
Temperature (K)	600	1.0204	1.0214	1.0272
	650	_____	Z @ 63 bar, 650 K	_____
	800	1.0156	1.0164	1.0208

Now the only unknown value is the compressibility factor at the operation conditions in the process, which can be calculated using interpolation as follows:

$$\frac{650 \text{ K} - 600 \text{ K}}{800 \text{ K} - 600 \text{ K}} = \frac{Z_{@ 63 \text{ bar}, 650 \text{ K}} - \text{_____}}{\text{_____} - \text{_____}}$$

Solving for Z @ 63 bar, 650 K yields:

$$Z_{@ 63 \text{ bar}, 650 \text{ K}} = \left[ \frac{650 \text{ K} - 600 \text{ K}}{800 \text{ K} - 600 \text{ K}} \left( \text{_____} - \text{_____} \right) \right] + \text{_____}$$

And the result obtained from the interpolation will be:

$$z_{@ 63 \text{ bar}, 650 \text{ K}} \approx \underline{\hspace{2cm}}$$

Recalling the definition of the compressibility factor z:

$$z = \frac{P\dot{V}}{nRT}$$

The molar flow rate can be obtained dividing the mass flow rate by the molecular weight of the gas. After substituting the values, we get:

$$\dot{n} = \frac{\dot{m}}{M_{\text{H}_2}} = \frac{\underline{\hspace{2cm}} \frac{\text{kg} \left( \frac{1000 \text{ g}}{1 \text{ kg}} \right)}{\text{h}}}{\left( \frac{2 \text{ g}}{1 \text{ mol H}_2} \right)}$$

$$\dot{n} = \underline{\hspace{2cm}} \frac{\text{mol}}{\text{h}}$$

Now we can solve for the volumetric flow rate from the compressibility factor definition and substitute the operation conditions for this process to get:

$$\dot{V} = \frac{znRT}{P} = \frac{\left( \underline{\hspace{2cm}} \right) \left( \underline{\hspace{2cm}} \frac{\text{mol}}{\text{h}} \right) \left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) \left( \underline{\hspace{2cm}} \text{ K} \right)}{6300 \text{ kPa} \left( \frac{1 \text{ atm}}{\underline{\hspace{2cm}} \text{ kPa}} \right)}$$

$$\dot{V} = \underline{\hspace{2cm}} \frac{\text{L}}{\text{h}}$$

**Example 5.4-2 The Generalized Compressibility Chart**

A midsize steam-methane reforming plant is consuming methane at a rate of 125 000 mol/h and converting it into synthesis gas, which is a mixture of H<sub>2</sub> and CO. The methane is being fed into the process at an absolute pressure of 233 psi and a temperature of 723 K. Using the generalized compressibility chart estimate the volumetric flow rate of methane entering the steam-methane reforming facility in  $\frac{\text{m}^3}{\text{h}}$ .

**Strategy**

The generalized compressibility chart is showing the compressibility factor  $z$  as a function of reduced properties of the gas. In order to determine the volumetric flow rate, these reduced properties must be calculated for the methane used in this process.

**Solution**

The critical properties of methane can be obtained from table B.1 in the book *Elementary Principles of Chemical Processes*, 3<sup>rd</sup> Edition, by Felder and Rousseau.

$$T_c = \text{_____ K}$$

$$P_c = \text{_____ atm}$$

With these critical properties, the reduced pressure and temperature can be calculated for methane. The reduced properties can be calculated using the following equations:

$$T_r = \frac{T}{T_c} \qquad P_r = \frac{P}{P_c}$$

Substituting the critical properties and the operation conditions for the steam-methane reforming process described in this problem, the reduced properties can be calculated to get:

$$T_r = \frac{\text{_____ K}}{\text{_____ K}}$$

$$T_r = \text{_____}$$

$$P_r = \frac{\text{_____ psi} \left( \frac{1 \text{ atm}}{\text{_____}} \right)}{\text{_____ atm}}$$

$$P_r = \text{_____}$$

Supplemental Material for Elementary Principles of Chemical Processes

The generalized compressibility chart (Figure 5.4-2 in the Felder & Rousseau book) can be used to read the value of  $V_{r,ideal}$ . The value read from the graph at  $P_r = \underline{\hspace{2cm}}$  and  $T_r = \underline{\hspace{2cm}}$  was estimated to be:

$$V_{r,ideal} \approx \underline{\hspace{2cm}}$$

The ideal reduced volume is defined by the following equation:

$$V_{r,ideal} = \frac{P_C \hat{V}}{RT_C}$$

Substituting the values of  $P_C, T_C$  and  $R$  into this equation yields:

$$V_{r,ideal} = \frac{(\underline{\hspace{2cm}} \text{ atm}) \hat{V}}{\left(0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}}\right) (\underline{\hspace{2cm}} \text{ K})} = 2.93 \hat{V}$$

Where the molar volume  $\hat{V}$  has units of  $\frac{\text{L}}{\text{mol}}$ .

We can solve for the molar volume  $\hat{V}$  and substitute the value of  $V_{r,ideal}$  to get:

$$\hat{V} = \frac{V_{r,ideal}}{2.93} = \frac{\underline{\hspace{2cm}}}{2.93}$$

$$\hat{V} = \underline{\hspace{2cm}} \frac{\text{L}}{\text{mol}}$$

This value can now be multiplied by the molar flow rate of methane in the feed stream of this process, to calculate the volumetric flow rate:

$$\dot{V} = \dot{n} \hat{V} = \underline{\hspace{2cm}} \frac{\text{mol}}{\text{h}} \left( \underline{\hspace{2cm}} \frac{\text{L}}{\text{mol}} \right) \left( \frac{1 \text{ m}^3}{1000 \text{ L}} \right)$$

$$\dot{V} = \underline{\hspace{2cm}} \frac{\text{m}^3}{\text{h}}$$

**Example 5.4-3 Kay's Rule**

Synthesis gas can be produced by partial oxidation of coal with oxygen and steam at high temperatures and pressures. The synthesis gas being produced by this process consists of 67 mol % of hydrogen and 33 mol % of carbon monoxide. The syngas is exiting the process at a temperature of 750 °C and a pressure of 30 bar. Determine the molar volume of this mixture using Kay's Rule.

**Strategy**

To use Kay's Rule, the pseudocritical properties of the mixture must be calculated. These properties are averages of the critical properties of the pure components of the mixture.

**Solution**

The critical properties of the pure components CO and H<sub>2</sub> can be obtained from table B.1 in the book by Felder and Rousseau.

$$\begin{aligned} T_{C,H_2} &= \text{_____ K} & T_{C,CO} &= \text{_____ K} \\ P_{C,H_2} &= 12.8 \text{ atm} & P_{C,CO} &= \text{_____ atm} \end{aligned}$$

When using compressibility factors, if the gas is either hydrogen or helium, the critical properties must be adjusted using Newton's corrections, shown in the following equations:

$$\begin{aligned} T_c^a &= T_c + 8 \text{ K} \\ P_c^a &= P_c + 8 \text{ atm} \end{aligned}$$

Thus, for hydrogen we get:

$$\begin{aligned} T_c^a &= \text{_____ K} + 8 \text{ K} = \text{_____ K} \\ P_c^a &= 12.8 \text{ atm} + 8 \text{ atm} = \text{_____ atm} \end{aligned}$$

Now that the critical properties of the pure constituents of the syngas are known, we can take weighted averages of these values to determine the pseudocritical properties:

$$\begin{aligned} T'_c &= y_{H_2} T_{C,H_2}^a + y_{CO} T_{C,CO} = \text{_____} ( \text{_____ K} ) + \text{_____} ( \text{_____ K} ) \\ T'_c &= \text{_____ K} \\ P'_c &= y_{H_2} P_{C,H_2}^a + y_{CO} P_{C,CO} = \text{_____} ( \text{_____ atm} ) + \text{_____} ( \text{_____ atm} ) \\ P'_c &= \text{_____ atm} \end{aligned}$$

These pseudocritical properties of the H<sub>2</sub>-CO mixture can be now used to calculate the pseudoreduced temperature and pressure. After substituting the known values for operation and pseudocritical conditions we get:

$$T'_r = \frac{T}{T'_c} = \frac{\text{_____ K}}{\text{_____ K}}$$

$$T'_r = \text{_____}$$

$$P'_r = \frac{P}{P'_c} = \frac{\text{_____ bar} \left( \frac{1 \text{ atm}}{1.01325 \text{ bar}} \right)}{\text{_____ atm}}$$

$$P'_r = \text{_____}$$

Since the partial oxidation of coal process described in this problem is taking place at high pressures, the generalized compressibility chart for high pressures (Figure 5.4-4 in Felder & Rousseau) can be used to determine the compressibility factor for the syngas, at the reduced temperature and pressure just calculated. At  $T'_r = \text{_____}$  and  $P'_r = \text{_____}$ :

$$z_m \approx 1.0$$

Recalling the definition of the compressibility factor  $z$ :

$$z_m = \frac{P\hat{V}}{RT}$$

Solving for the molar volume  $\hat{V}$  from this equation yields:

$$\hat{V} = \frac{z_m RT}{P}$$

Substituting the known values into this equation gives:

$$\hat{V} = \frac{1.0 \left( 0.08206 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \right) ( \text{_____ K} )}{\text{_____ bar} \left( \frac{1 \text{ atm}}{\text{_____ bar}} \right)}$$

$$\hat{V} = \text{_____} \frac{\text{L}}{\text{mol}}$$