Chapter 4
Processes and Process Variables

Name: ______________
Date: ______________

The goal of Chapter 4 is to introduce students to conservation equations applied to material flows in chemical and manufacturing systems. 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.

4.2-1 The General Balance Equation
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Example 4.2-1 The General Balance Equation

(a) On average during the early part of 2009, the United States imported 12,446 thousand barrels of oil per day. There were also 5,191 thousand barrels of oil per day removed from oil wells. The nation exported 1,826 thousand barrels of oil per day and consumed 18,019 thousand barrels of oil per day. Write a balance on the oil in the nation.

Strategy

To solve this problem, we will use the general material balance equation, given by:

Input + Generation – Output – Consumption = Accumulation

Solution

In terms of thousand barrels of oil per day, we have:

12,446 + ______ – ______ – 18,019 = –______

Thus, there was a net reduction in oil reserves during this time of year.

(b) Prior to the Christmas season, a hydrogen fueling station has a reserve of 500 kg hydrogen. Assume that the station receives hydrogen shipments of 2,740 kg/day. If the current demand is to supply 700 cars/day at a rate of 4 kg per car, in how many days will the reserve be depleted?

Strategy

To solve this problem, we will use the general material balance equation, given by:

Input + Generation – Output – Consumption = Accumulation

Solution

We will model the hydrogen fueling as consumption. We note that there is no generation (hydrogen production) or output (hydrogen shipments) from the station.

In terms of kg per day, we can calculate the hydrogen consumption as:

$$\frac{700\,\text{cars}}{\text{day}}\,\frac{\_\_\_\_\,\text{kg}}{\text{car}} = \_\_\_\_\_\,\frac{\text{kg}}{\text{day}}$$

Now, using the general mass balance equation we have:

_____ + _____ – _____ – 2800 = ______

The net reduction in hydrogen reserves is ____ kg/day. Dividing this into the reserve gives:

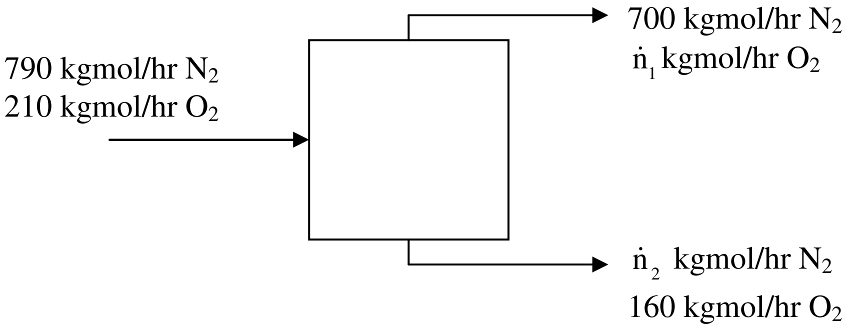
$$\frac{500\,\text{kg}}{\quad}\;\frac{\text{day}}{\underline{\qquad}\ \text{kg}} = \underline{\qquad}\ \text{days}$$

It might be appropriate to have additional hydrogen shipments during this season in order to avoid total depletion of the reserves.

Example 4.2-2 Material Balances on a Continuous Distillation Process

Hydrogen can be produced using a process called coal gasification. It is desired to supply nearly pure oxygen to this process. Oxygen is separated from nitrogen out of the air (79 mol% nitrogen and 21 mol% oxygen) via a process known as cryogenic distillation.

(a) A cryogenic distillation unit has a feed of 1000 kgmol/hr air. The top stream has 700 kgmol/hr nitrogen and the bottom stream has 160 kgmol/hr oxygen. The process is illustrated in the block diagram below. Write balances on the oxygen and nitrogen to determine the unknown component molar flow rates.



Strategy

First, we need to determine the individual molar flow rates into the unit. Then, we can use the overall balance equation at steady state (no accumulation) to determine the unknown quantities. We note that in this system there is also no generation or consumption.

Solution

The molar feed of nitrogen is given by 1000 kgmol/hr (____) = 790 kgmol/hr, and the molar feed of oxygen is given by 1000 kgmol/hr (____) = ____ kgmol/hr.

Using the overall balance on nitrogen gives: In = Out, such that:

$$\_\_\_\_ \text{ kgmol/hr} = 700 \text{ kgmol/hr} + \dot{n}_2 \text{ kgmol/hr}$$

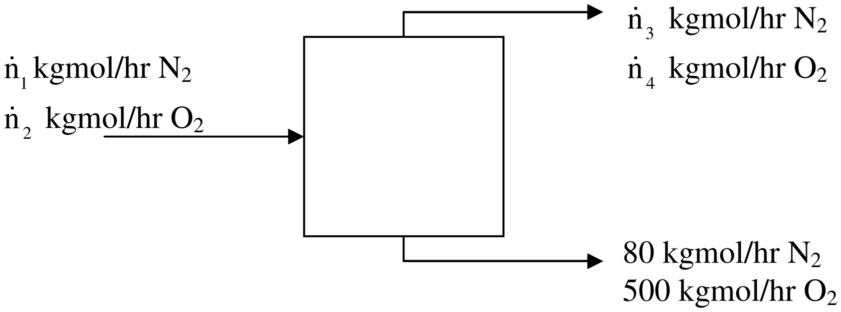
Which can be solved to give $\boxed{\dot{n}_2 = \_\_\_ \text{ kgmol/hr}}$.

Using the overall balance on oxygen gives: In = Out, such that:

$$\_\_\_ \text{ kgmol/hr} = \dot{n}_1 \text{ kgmol/hr} + \_\_\_ \text{ kgmol/hr}$$

Which can be solved to give $\boxed{\dot{n}_1 = \_\_\_ \text{ kgmol/hr}}$.

(b) A coal gasifier requires 500 kgmol/hr oxygen from a cryogenic distillation unit. The distillation unit has 95% of the total oxygen feed in the bottoms product. Determine the air supply rate in kgmol/hr. Also determine the oxygen molar flow rate at the top of the unit. If the nitrogen molar flow rate at the bottom of the unit is 80 kgmol/hr, determine the nitrogen molar flow rate at the top of the unit. A schematic of the unit is seen below.



Solution

We note that 95% of the total oxygen supply comes out of the unit in the bottoms. This can be represented by the equation:

$$500\frac{\text{kgmol}\,O_2}{\text{hr}} = \_\_\_\,\dot{n}_2$$

Which can be solved to give $\dot{n}_2 = \_\_\_\_$ kgmol/hr.

Using the overall balance on oxygen gives: In = Out, such that:

$$\_\_\_\text{ kgmol/hr} = \dot{n}_4\text{ kgmol/hr} + \_\_\_\_\text{ kgmol/hr}$$

Which can be solved to give $\dot{n}_4 = \_\_\_$ kgmol/hr.

We note that the feed contains an oxygen mole fraction of 0.21. Thus,

$$\frac{\dot{n}_2}{\dot{n}_1 + \dot{n}_2} = 0.21$$

This equation can be rearranged to solve for $\dot{n}_1$ as:

$$\dot{n}_1 = \frac{\_\_\_\_\,\dot{n}_2}{0.21}$$

$$\dot{n}_1 = \_\_\_\_\frac{\text{kgmol}\,N_2}{\text{hr}}$$

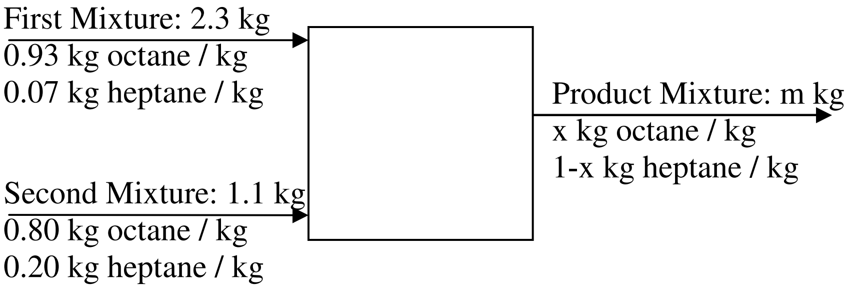
Using the overall balance on nitrogen gives: In = Out, such that:

$$\dot{n}_1\ \text{kgmol/hr} = \_\_\_\ \text{kgmol/hr} + \_\_\_\ \text{kgmol/hr}$$

Which can be solved to give $\boxed{\_\_\_ = 1898\ \text{kgmol/hr}}$

Example 4.2-3 Balances on a Batch Mixing Process

(a) Two octane-heptane mixtures are contained in separate tanks. The first mixture contains 93 wt% octane and the second mixture contains 80 wt% octane. In order to have a fuel that can be used in a vehicle, 2.3 kg of the first mixture is mixed with 1.1 kg of the second mixture. What is the mass and composition of the product? A schematic of the process is shown below.



Strategy

The total mass of the product mixture is m = 2.3 + 1.1 = 3.4 kg. The overall balance equation In = Out will be used for octane to determine the amount in the product mixture. After this is known the value of x can be determined.

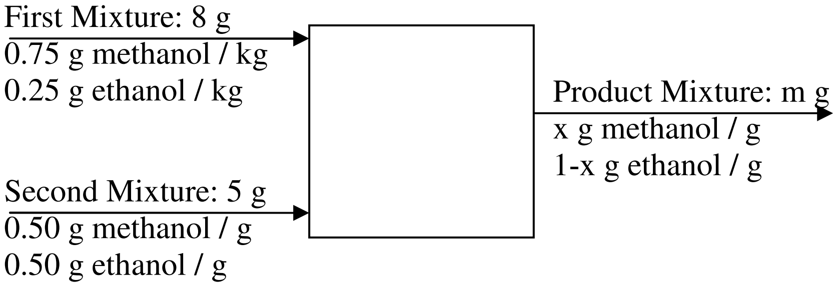
Solution

The amount of octane in the first mixture is 2.3 kg (0.93) = ____ kg. Also, the amount of octane in the second mixture is ____ kg (0.80) = ____ kg.

Thus the total octane is ____ kg which corresponds to a weight fraction of _____.

Note that one can also sum the heptane masses and obtain about ____ kg.

(b) Let us suppose that a new fuel cell can run with methanol or ethanol. Two methanol-ethanol mixtures are contained in separate flasks. The first mixture contains 75 wt% methanol and the second mixture contains 50 wt% methanol. If 8 g of the first mixture is mixed with 5 g of the second mixture, what is the mass and composition of the product? A schematic of the process is shown below.



Strategy

The total mass of the product mixture is m = 8 + 5 = 13 g. The overall balance equation In = Out will be used for methanol to determine the amount in the product mixture. After this is known the value of x can be determined.

Solution

The amount of methanol in the first mixture is __ g (____) = 6 g. Also, the amount of methanol in the second mixture is __ g (0.50) = ____ g.

Thus the total methanol is 8.5 g which corresponds to a weight fraction of ____.

Note that one can also sum the ethanol masses and obtain ____.

Example 4.2-4 Integral Balance on a Semibatch Process

(a) A hydrogen tank on board a car contains 4.1 kg of hydrogen. The car consumes 30 g H_2 / min for 25 minutes of city driving and 17 g H_2 / min for 65 minutes of highway driving per day. After how many days does the driver need to refuel?

Strategy

First, we will determine the total hydrogen consumption per day. This information can be used to determine the number of days the hydrogen tank can hold.

Solution

During city driving the car uses 25 min (30 g / min) = ____ g H_2.

Also, during highway driving the car uses 65 min (___ g / min) = _____ g H_2.

Thus, the total hydrogen consumed on the trip is _____ g.

The tank mass divided by the daily usage will give the number of days before refilling according to:

$$\frac{4.1\,\text{kg}}{}\,\frac{1000\,\text{g}}{\text{kg}}\,\frac{\text{day}}{\_\_\_\_\_\,\text{g}} = \_\_\_\ \text{days}$$

Thus, the car needs to be refilled every 2 days.

(b) A hydrogen tank on board a car is partially full and contains 1.2 kg of hydrogen. The car will consume 15 g H_2 / min at 54 miles per hour of highway driving. The next hydrogen refueling station is at an exit which is 30 miles away. The next station is 90 miles away. Can the driver wait for the 90 miles before refueling?

Strategy

We will use unit conversions to calculate a fuel consumption rate in units of kg H_2 per mile. We can then determine the total distance that we can travel at that rate.

Solution

Using unit conversions we have:

$$\frac{\_\_\_\,\text{g}}{\text{min}}\,\frac{\text{hr}}{\_\_\_\,\text{miles}}\,\frac{60\,\text{min}}{\text{hr}}\,\frac{\text{kg}}{1000\,\text{g}} = \_\_\_\_\_\_\,\frac{\text{kg}}{\text{mile}}$$

Multiplying by the distance to the hydrogen station gives a hydrogen requirement of:

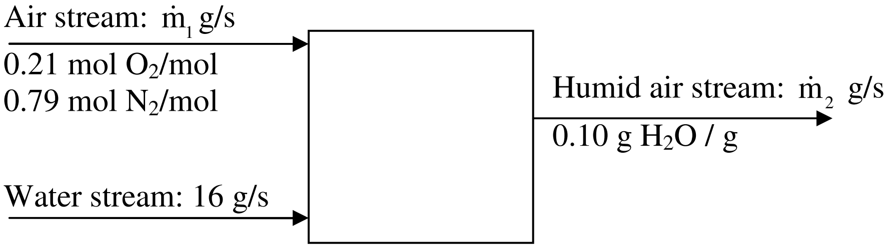
$$\frac{\_\_\_\_\_\_\ \text{kg}}{\text{mile}}\ \frac{\_\_\_\ \text{miles}}{} = \_\_\_\_\ \text{kg}$$

Thus, the car needs to be refilled at the next stop located ___ miles away.

Example 4.3-1 Flowchart of an Air Humidification Process

Fuel cell membranes need to be humidified in order to conduct protons, and therefore lead to electrical current flow. This is often done by adding water in with the incoming air flow.

(a) Suppose you have a water flow of 16 g/s being added to an air stream. The humid air stream is to contain 10 wt% water. Determine the air and effluent flows in g/s and the component mole fractions in the humid air stream. Consider the schematic below.



Strategy

We can use mass balances and molecular weights to solve this problem. However, to convert from mass to moles we will need to select a molar basis.

Solution

Performing a water mass balance gives In = Out, such that we have:

$$0 + 16 = \dot{m}_2\ (\_\_\_\_)\ \text{such that}\ \boxed{\dot{m}_2 = \_\_\_\_\ \text{g/s}}.$$

Performing an overall mass balance gives:

$$\dot{m}_1 + 16 = \dot{m}_2$$

Thus,

$$\dot{m}_1 = \_\_\_\_ - \_\_\_$$

$$\boxed{\dot{m}_1 = \_\_\_\_\ \text{g/s}}.$$

To convert the air stream to moles we need to select a basis. Let us suppose that there are 100 mol/s of air. Using the mole fractions gives: 100 (0.21) = 21 mol/s O_2 and 100 (0.79) = 79 mol/s N_2. Using molecular weights of the gases, we have:

$$\frac{21\,\text{mol}\,O_2}{\text{s}}\ \frac{32\,\text{g}\,O_2}{\text{mol}\,O_2} = \_\_\_\_\ \frac{\text{g}\,O_2}{\text{s}}$$

and:

$$\frac{\_\_\_\ \text{mol N}_2}{\text{s}}\,\frac{28\,\text{g N}_2}{\text{mol N}_2}=\_\_\_\_\,\frac{\text{g N}_2}{\text{s}}$$

such that the total air flow rate is 2884 g/s. Since the actual air flow rate is 144 g/s we can determine the number of moles from the proportion:

$$\_\_\_\_\,\frac{\text{g air}}{\text{s}}\,\frac{\_\_\_\_\ \text{mol air}}{\_\_\_\_\_\ \text{g air/s}}=5.0\,\frac{\text{mol air}}{\text{s}}$$

and we can use the mole fractions to calculate component molar feed flow rates of 5.0 (___) = 1.1 mol/s O_2 and 5.0 (____) = ____ mol/s. The water molar flow rate is given by

$$\frac{\_\_\_\ \text{g H}_2\text{O}}{\text{s}}\,\frac{\text{mol H}_2\text{O}}{\_\_\_\ \text{g H}_2\text{O}}=\_\_\_\_\,\frac{\text{mol H}_2\text{O}}{\text{s}}$$

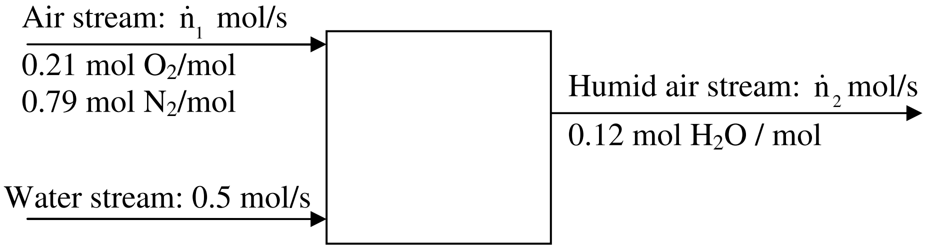
If we add up all of the molar flow rates in the humid air stream, we have ____ mol/s. Thus, we can calculate the mole fractions as:

$$\frac{\_\_\_\ \text{mol H}_2\text{O}}{\text{s}}\,\frac{\text{s}}{\_\_\_\_\ \text{mol total}}=\boxed{0.15\text{ mole fraction water}},$$

$$\frac{\_\_\_\_\ \text{mol O}_2}{\text{s}}\,\frac{\text{s}}{\_\_\_\_\ \text{mol total}}=\boxed{\_\_\_\_\ \text{ mole fraction oxygen}},\text{ and}$$

$$\frac{\_\_\_\_\ \text{mol N}_2\text{O}}{\text{s}}\,\frac{\text{s}}{\_\_\_\_\ \text{mol total}}=\boxed{\_\_\_\_\_\ \text{ mole fraction nitrogen}}.$$

(b) Suppose you have a water flow of 0.5 mol/s being added to an air stream. The humid air stream is to contain 12 mol% water. Determine the air and effluent flows in mol/s and g/s.



Strategy

We can use mass balances and molecular weights to solve this problem.

Solution

Performing a water mole balance gives In = Out, such that we have:

$$0 + 0.5 = \dot{n}_2\ (\underline{\qquad})\ \text{such that}\ \boxed{\dot{n}_2 = \underline{\qquad}\ \text{mol/s}}\,.$$

Performing an overall mass balance gives:

$$\dot{n}_1 + 0.5 = \dot{n}_2$$

Thus,

$$\dot{n}_1 = \underline{\qquad} - 0.5$$

$$\boxed{\dot{n}_1 = \underline{\qquad}\ \text{mol/s}}\,.$$

We can now convert the air stream to grams. Using the mole fractions and molecular weights of the gases, we have:

$$\frac{\underline{\qquad}\,\text{mol air}}{\text{s}}\,\frac{0.21\,\text{mol O}_2}{\text{mol air}}\,\frac{32\,\text{g O}_2}{\text{mol O}_2} = \boxed{\underline{\qquad}\,\frac{\text{g O}_2}{\text{s}}}$$

and:

$$\frac{\underline{\qquad}\,\text{mol air}}{\text{s}}\,\frac{\underline{\qquad}\,\text{mol N}_2}{\text{mol air}}\,\frac{28\,\text{g N}_2}{\text{mol N}_2} = \boxed{\underline{\qquad}\,\frac{\text{g N}_2}{\text{s}}}$$

Thus, the total air mass flow rate is _____ g/s.

For the water stream entering the system we have a mass flow rate of:

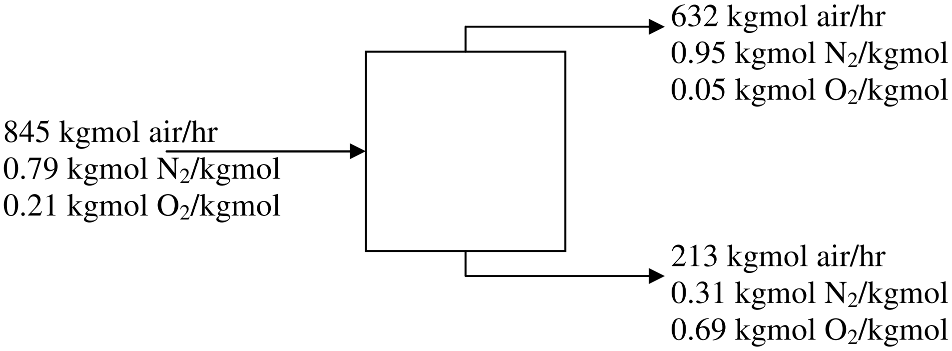
$$\frac{\underline{\qquad}\,\text{mol H}_2\text{O}}{\text{s}}\,\frac{18\,\text{g H}_2\text{O}}{\text{mol H}_2\text{O}} = \boxed{\underline{\quad}\,\frac{\text{g H}_2\text{O}}{\text{s}}}$$

Thus, the total humid air mass flow rate is ____ g/s.

Example 4.3-2 Scale-Up of a Separation Process Flowchart

Hydrogen can be produced using a process called coal gasification. It is desired to supply nearly pure oxygen to this process. Oxygen is separated from nitrogen out of the air (79 mol% nitrogen and 21 mol% oxygen) via a process known as cryogenic distillation.

(a) A cryogenic distillation unit has a feed of 845 kgmol/hr air. The top stream has an overall flow rate of 632 kgmol/hr with a nitrogen mole fraction of 0.95. The bottom stream has an overall flow rate of 213 kgmol/hr with a nitrogen mole fraction of 0.31. The process is illustrated in the block diagram below. Scale up the system for a feed flow rate of 14200 kgmol air/hr.



Strategy

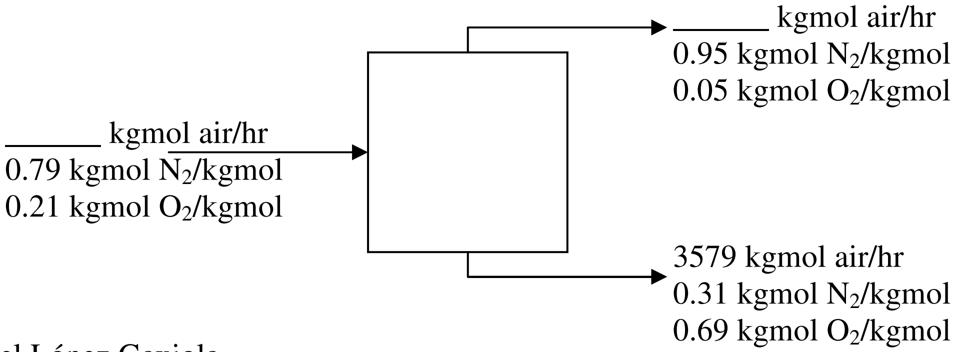
We can use proportions to determine the new molar flow rates in the system. The mole fractions are all unchanged.

Solution

Using the proportion of the current design to the new requirement gives the distillate molar flow rate:

$$632\,\frac{\text{kgmol}}{\text{hr}}\;\frac{\_\_\_\_\_\_\;\text{kgmol air/hr}}{845\;\text{kgmol air/hr}}=\boxed{\_\_\_\_\_\_\;\frac{\text{kgmol}}{\text{hr}}}$$

and the overall balance gives the bottoms molar flow rate as ______ – ______ = 3579 kgmol/hr. The new flow sheet is shown below.



(b) A scale-up of the same cryogenic distillation unit of part (a) requires a bottoms oxygen molar flow rate of 10000 kgmol/hr. Scale up the system accordingly.

Strategy

We can use proportions to determine the new molar flow rates in the system. The mole fractions are all unchanged.

Solution

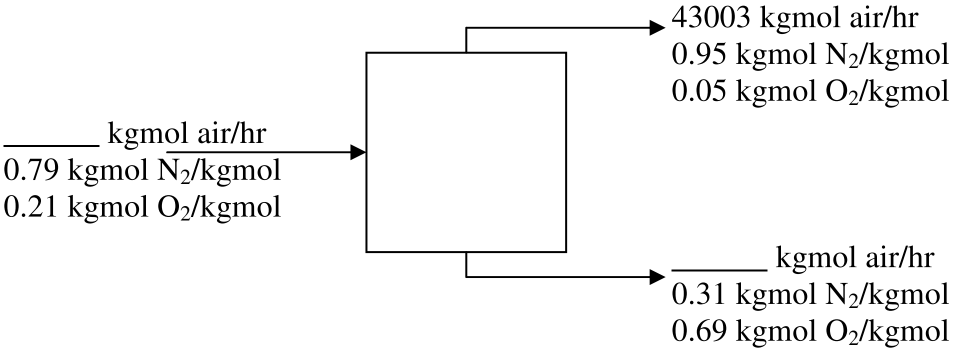
We begin with the mole fraction of oxygen in the bottoms to determine the overall bottoms molar flow rate. We have:

$$10000\frac{\text{kgmol}\,O_2}{\text{hr}}\frac{1\,\text{kgmol bottoms/hr}}{\underline{\hspace{1cm}}\ \text{kgmol}\,O_2/\text{hr}}=\underline{\hspace{1.5cm}}\,\frac{\text{kgmol}}{\text{hr}}$$

Using the proportion of the current design to the new requirement gives the distillate molar flow rate:

$$\underline{\hspace{1cm}}\,\frac{\text{kgmol}}{\text{hr}}\frac{\underline{\hspace{1cm}}\ \text{kgmol air/hr}}{\underline{\hspace{1cm}}\ \text{kgmol air/hr}}=43003\frac{\text{kgmol}}{\text{hr}}$$

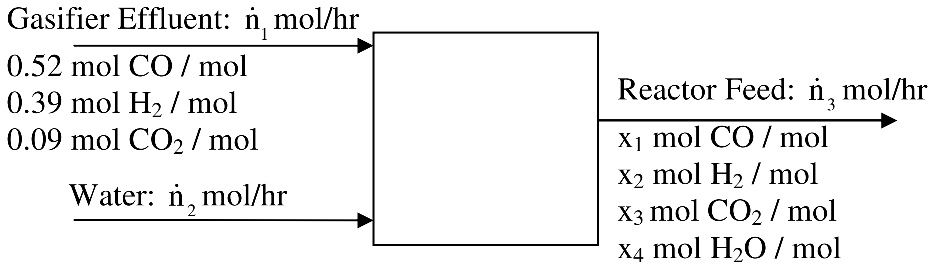
and the overall balance gives the feed molar flow rate as ______ kgmol/hr. The new flow sheet is shown below.



Example 4.3-3 Balances on a Mixing Unit

The effluent from a coal gasifier contains 52 mol% carbon monoxide, 39 mol% hydrogen, and 9 mol% carbon dioxide. The stream is mixed with water before it enters a water-gas shift reactor where the additional hydrogen is formed.

(a) You require a molar water feed that is 10% larger than the carbon monoxide flow rate. Determine the mole fractions in the reactor feed.



Strategy

First, we need to pick a basis for this problem. Let us choose $\dot{n}_1$ = 100 mol/hr. We will then calculate values for $\dot{n}_2$, $\dot{n}_3$, and the mole fractions in the reactor feed.

Solution

The molar flow rate of carbon dioxide in the feed is given as 100 (____) = ___ mol/hr. Thus, we must supply a water molar flow rate of $\dot{n}_2$ = ___ (___) = 57 mol/hr. An overall mass balance gives the reactor molar flow rate of $\dot{n}_3$ = ____ mol/hr. We can now calculate all of the mole fractions:

For carbon monoxide,

$$x_1 = \frac{\dot{n}_1(\;\_\_\_\_\;)}{\_\_\_} = 0.33$$

for hydrogen,

$$x_2 = \frac{\dot{n}_1(\;\_\_\_\_\;)}{\_\_\_} = \_\_\_\_$$

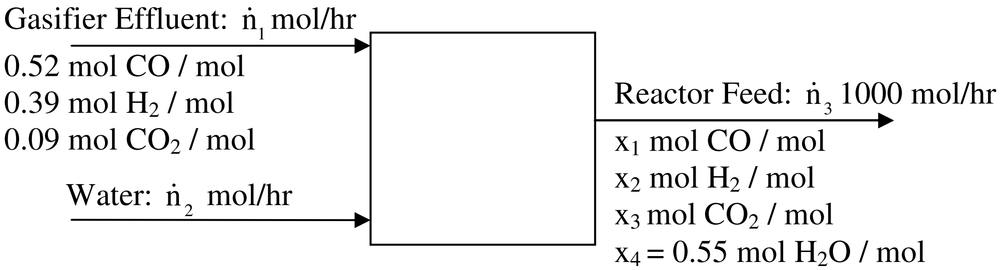
for carbon dioxide,

$$x_3 = \frac{\dot{n}_1(\;\_\_\_\_\;)}{\_\_\_} = \_\_\_\_$$

and for water,

$$x_4 = \frac{\_\_\_}{\_\_\_} = 0.36.$$

(b) Consider the same process outlined in part a) above. However, you require a water mole fraction of 0.55 in the reactor feed. Determine the mole fractions in the reactor feed for a basis of m_3 = 1000 mol/hr.



Strategy

We can use the water mole balance formula to determine $\dot{n}_2$, then use the overall mole balance formula to determine $\dot{n}_1$. We will then calculate the mole fractions in the reactor feed.

Solution

We start with the mole fraction formula for water, $x_4 = \frac{\dot{n}_2}{\_\_\_} = 0.55$, such that $\dot{n}_2$ = ____ mol/hr. Thus, $\dot{n}_1$ = ____ mol/hr. We can now calculate all the mole fractions in the reactor feed:

For carbon monoxide, $x_1 = \frac{\dot{n}_1(0.52)}{\_\_\_} = \_\_\_\_$

for hydrogen, $x_2 = \frac{\dot{n}_1(\ \_\_\_\ )}{\_\_\_} = \_\_\_\_$

for carbon dioxide, $x_3 = \frac{\dot{n}_1(\ \_\_\_\ )}{\_\_} = \_\_\_\_$

Note that the mole fractions sum to unity.

Example 4.3-4 Degree of Freedom Analysis

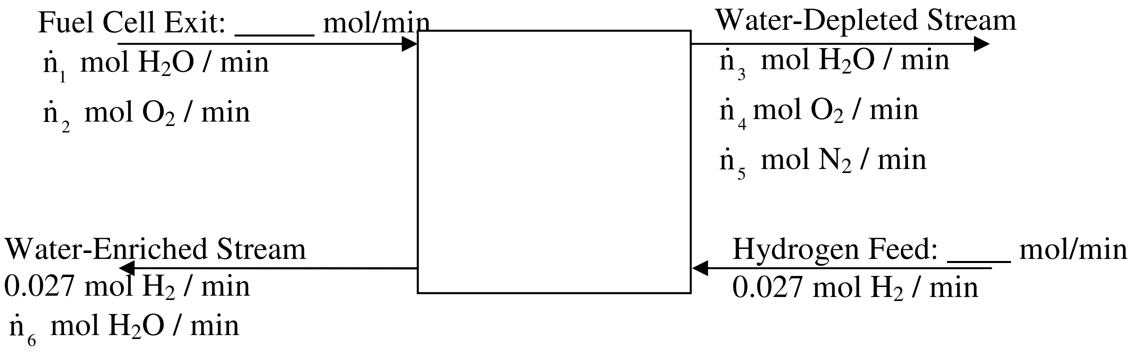
(a) The gas exiting a fuel cell is at a molar flow rate of 0.090 mol/min and contains water vapor, oxygen, and nitrogen. A mass exchange membrane has been proposed to remove water from this stream and add it to the hydrogen feed stream (0.027 mol/min). Half of the water in the exit gas is transferred. Perform a degree of freedom analysis on this system.

Strategy

We will determine the number of degrees of freedom for this system and see if we have enough information to solve the problem.

Solution

All of the information from the problem statement has been supplied in the figure below.



We have four chemicals (H_2O, O_2, N_2, and H_2) and have six unknown quantities on the flow sheet. Thus, we need three additional relationships which we do not have, so we cannot solve this problem.

However, we can see that from an oxygen balance we have $\dot{n}_2 = \dot{n}_4$, from a nitrogen balance we have $\dot{n}_5 = \_\_\_\_ - \_\_\_ - \dot{n}_2$, and from a water balance we have $\dot{n}_3 = \dot{n}_6 = \frac{\_\_\_}{2}$.

(b) Consider the system described in part a with the following additional information: the water in the fuel cell exit makes up 8 mol% of the total and on a water-free basis the oxygen mole fraction is 0.19. Solve for the unknown values if possible.

Strategy

We will re-evaluate the number of degrees of freedom for this system and see if we have enough information to solve the problem.

Solution

The new problem statement provides two additional relationships from which we can solve the system.

The water molar flow rate entering in the fuel cell exit stream is given by:

$$\dot{n}_1 = \_\_\_\_\_ \frac{\text{mol}}{\text{min}} \frac{\_\_\_\ \text{mol } H_2O}{1\,\text{mol}} = 0.007 \frac{\text{mol } H_2O}{\text{min}}$$

From which we can determine $\dot{n}_3$ and $\dot{n}_6$ = ______ mol/min.

The amount of oxygen and nitrogen molar flow rate entering in the fuel cell exit stream is given by 0.090 – ____ = _____ mol/min. Since the oxygen mole fraction is known on a water free basis, we have:

$$\dot{n}_2 = \dot{n}_4 = \_\_\_\_ \frac{\text{mol}}{\text{min}} \frac{0.19\,\text{mol } O_2}{1\,\text{mol}} = \_\_\_\_\_ \frac{\text{mol } O_2}{\text{min}}$$

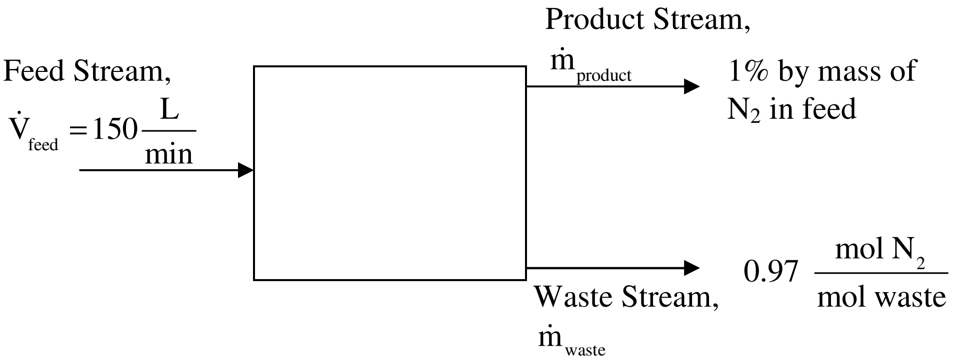
and we can then determine the nitrogen molar flow rate as:

$$\dot{n}_5 = \_\_\_\_\_ - \dot{n}_1 - \_\_\_\_ = \_\_\_\_\_ \frac{\text{mol } N_2}{\text{min}}$$

Example 4.3-5 Material Balances on a Distillation Column

Hydrogen can be produced using a process called coal gasification. It is desired to supply nearly pure oxygen to this process. Oxygen is separated from nitrogen out of the air (79 mol % nitrogen and 21 mol % oxygen) via a process known as cryogenic distillation.

(a) The overhead product stream is leaving the top of the distillation column with 1 % by mass of the nitrogen entering the column and the bottom product stream is leaving with 97 mol % of nitrogen. Liquid air is being fed at a rate of 150 L/min and has a density of 870 kg/m^3. Calculate the molar flow rate of the waste stream.



Strategy

This problem can be solved using mass balances and molecular weight. To determine the mass fractions, a mass basis will be selected for this problem.

Solution

The air flow rate entering the column has to be in a mass basis. This can be done using the density of air given in the problem statement.

$$\dot{m}_1 = 150\,\frac{\text{L}}{\text{min}}\left(\underline{\hspace{1cm}}\,\frac{\text{kg}}{\text{m}^3}\right)\left(\frac{1\ \text{m}^3}{1000\ \text{L}}\right)\left(\frac{\underline{\hspace{0.6cm}}\ \text{min}}{1\ \text{h}}\right) = 7830\,\frac{\text{kg}}{\text{h}}$$

The molar fractions in the feed stream has to be converted to mass fractions. To do this, the molecular weight of the feed and waste stream has to be determined by using the molar fractions and the molecular weight of the gases in the feed and waste stream, respectively:

$$M_{feed} = \underline{\hspace{1cm}}\,\frac{\text{mol O}_2}{\text{mol feed}}\left(\frac{32\text{g O}_2}{\text{mol O}_2}\right) + \underline{\hspace{1cm}}\,\frac{\text{mol N}_2}{\text{mol feed}}\left(\frac{28\text{g N}_2}{\text{mol N}_2}\right) = \underline{\hspace{1cm}}\,\frac{\text{g}}{\text{mol}}$$

$$M_{waste} = \underline{\hspace{1cm}}\,\frac{\text{mol O}_2}{\text{mol feed}}\left(\frac{32\text{g O}_2}{\text{mol O}_2}\right) + \underline{\hspace{1cm}}\,\frac{\text{mol N}_2}{\text{mol feed}}\left(\frac{\underline{\hspace{0.6cm}}\text{g N}_2}{\text{mol N}_2}\right) = \underline{\hspace{1cm}}\,\frac{\text{g}}{\text{mol}}$$

Converting mol fractions to mass fractions in both the feed and waste streams:

$$x_{O_2,\text{feed}} = \underline{\qquad}\ \frac{\text{mol } O_2}{\text{mol feed}}\left(\frac{1 \text{ mol feed}}{\underline{\qquad}\ \text{g}}\right)\left(\frac{32 \text{ g } O_2}{1 \text{ mol } O_2}\right) = \underline{\qquad}\ \frac{\text{g } O_2}{\text{g}}$$

$$x_{N_2,\text{feed}} = \underline{\qquad}\ \frac{\text{mol } N_2}{\text{mol feed}}\left(\frac{1 \text{ mol feed}}{\underline{\qquad}\ \text{g}}\right)\left(\frac{28 \text{ g } N_2}{1 \text{ mol } N_2}\right) = \underline{\qquad}\ \frac{\text{g } N_2}{\text{g}}$$

$$x_{O_2,\text{waste}} = \underline{\qquad}\ \frac{\text{mol } O_2}{\text{mol waste}}\left(\frac{1 \text{ mol waste}}{\underline{\qquad}\ \text{g}}\right)\left(\frac{32 \text{ g } O_2}{1 \text{ mol } O_2}\right) = \underline{\qquad}\ \frac{\text{g } O_2}{\text{g}}$$

$$x_{N_2,\text{waste}} = \underline{\qquad}\ \frac{\text{mol } N_2}{\text{mol waste}}\left(\frac{1 \text{ mol waste}}{\underline{\qquad}\ \text{g}}\right)\left(\frac{28 \text{ g } N_2}{1 \text{ mol } N_2}\right) = \underline{\qquad}\ \frac{\text{g } N_2}{\text{g}}$$

Performing a nitrogen balance gives:

$$\text{In} = \text{Out}$$

$$x_{N_2,\text{feed}}\dot{m}_{\text{feed}} = x_{N_2,\text{product}}\dot{m}_{\text{product}} + x_{N_2,\text{waste}}\dot{m}_{\text{waste}}$$

The problem is not showing the value of $x_{N2,\text{product}}$, but we can calculate this, since the amount of nitrogen exiting in the product stream is 1 % by mass of the amount of nitrogen in the feed stream. This information can be written as

$$x_{N_2,\text{feed}}\dot{m}_{\text{feed}} = 0.01 x_{N_2,\text{feed}}\dot{m}_{\text{feed}} + x_{N_2,\text{waste}}\dot{m}_{\text{waste}}$$

$$\underline{\qquad}\ \frac{\text{kg } N_2}{\text{kg}}\left(\underline{\qquad}\ \frac{\text{kg}}{\text{h}}\right) = 0.01\left(\underline{\qquad}\ \frac{\text{kg } N_2}{\text{kg}}\right)\left(\underline{\qquad}\ \frac{\text{kg}}{\text{h}}\right) + \left(\underline{\qquad}\ \frac{\text{kg } N_2}{\text{kg}}\right)\dot{m}_{\text{waste}}$$

Thus:

$$\dot{m}_{\text{waste}} = \frac{\underline{\qquad}\ \frac{\text{kg } N_2}{\text{kg}}\left(7830\ \frac{\text{kg}}{\text{h}}\right) - 0.01\left(0.767\ \frac{\text{kg } N_2}{\text{kg}}\right)\left(\underline{\qquad}\ \frac{\text{kg}}{\text{h}}\right)}{\left(\underline{\qquad}\ \frac{\text{kg } N_2}{\text{kg}}\right)}$$

$$\boxed{m_{\text{waste}} = \underline{\qquad}\ \frac{\text{kg waste}}{\text{hr}}}$$

(b) Determine the mass fractions in the product stream.

If an overall mass balance is done for the distillation column, the product stream can be determined:

$$\text{In} = \text{Out}$$
$$\dot{m}_{\text{feed}} = \dot{m}_{\text{product}} + \dot{m}_{\text{waste}}$$
$$\dot{m}_{\text{product}} = \underline{\qquad} - \underline{\qquad}$$
$$\dot{m}_{\text{product}} = \underline{\qquad}\ \frac{\text{kg}}{\text{h}} - \underline{\qquad}\ \frac{\text{kg}}{\text{h}}$$
$$\boxed{\dot{m}_{\text{product}} = \underline{\qquad}\ \frac{\text{kg}}{\text{h}}}$$

The mass fraction of oxygen in the product stream can be calculated by performing an oxygen mass balance:

$$x_{O_2,\text{product}}\dot{m}_{\text{product}} = x_{O_2,\text{feed}}\dot{m}_{\text{feed}} - x_{O_2,\text{waste}}\dot{m}_{\text{waste}}$$

Solving for $x_{O_2,\text{product}}$:

$$x_{O_2,\text{product}} = \frac{\underline{\qquad\quad} - x_{O_2,\text{waste}}\dot{m}_{\text{waste}}}{\underline{\qquad\quad}}$$

$$x_{O_2,\text{product}} = \frac{\underline{\qquad}\ \frac{\text{kg } O_2}{\text{kg}}\ \underline{\qquad}\ \frac{\text{kg}}{\text{h}} - \underline{\qquad}\ \frac{\text{kg } O_2}{\text{kg}}\ \underline{\qquad}\ \frac{\text{kg}}{\text{h}}}{\underline{\qquad}\ \frac{\text{kg}}{\text{h}}}$$

$$\boxed{x_{O_2,\text{product}} = \underline{\qquad}\ \frac{\text{kg } O_2}{\text{kg}}}$$

Since there is only nitrogen and oxygen in the product stream, the sum of the mass fractions for oxygen and nitrogen must be equal to unity. Thus:

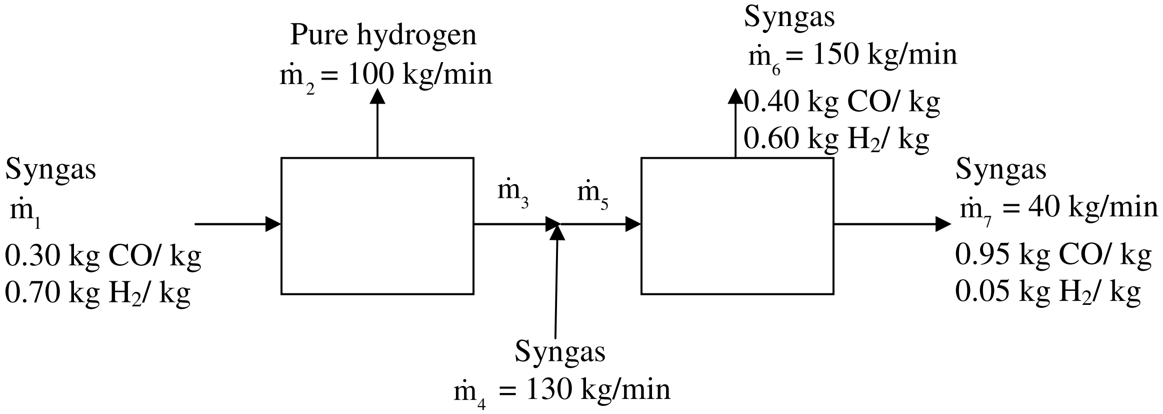
$$x_{N_2,\text{product}} = \underline{\quad} - \underline{\qquad} = \underline{\quad} - \underline{\qquad}$$

$$\boxed{x_{N_2,\text{product}} = 0.036\ \frac{\text{kg } N_2}{\text{kg}}}$$

Example 4.4-1 Two-Unit Process

Hydrogen can be produced by the processes of coal gasification and methane steam reforming. Both processes generate syngas as a byproduct, which contains CO and H_2. The syngas obtained by coal gasification process will be fed to a water gas shift reactor to produce pure hydrogen for use in Proton Exchange Membrane Fuel Cells (PEMFC).

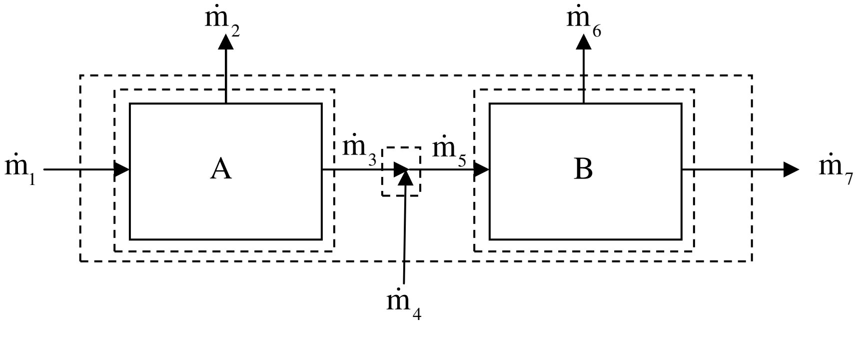
The unreacted syngas combines with a stream of syngas exiting a steam methane reforming reactor and enters a purification unit. The product stream from the purification process will be stored for use in Solid Oxide Fuel Cells (SOFC). A diagram of this process is shown below:



(a) Determine the unknown flow rates m_1, m_3 and m_5.

Strategy

The unknown flow rates can be determined by performing overall mass balances on the different boundaries of this process, as shown in next figure.



Solution

Overall Mass Balance

In = Out

$$\dot{m}_1 + \dot{m}_4 = \dot{m}_2 + \dot{m}_6 + \dot{m}_7$$

$$\dot{m}_1 + \underline{\qquad}\ \frac{\text{kg}}{\text{min}} = \underline{\qquad}\ \frac{\text{kg}}{\text{min}} + \underline{\qquad}\ \frac{\text{kg}}{\text{min}} + 40\ \frac{\text{kg}}{\text{min}}$$

$$\dot{m}_1 = \underline{\qquad}\ \frac{\text{kg}}{\text{min}} + \underline{\qquad}\ \frac{\text{kg}}{\text{min}} + \underline{\qquad}\ \frac{\text{kg}}{\text{min}} - \underline{\qquad}\ \frac{\text{kg}}{\text{min}}$$

$$\boxed{\dot{m}_1 = \underline{\qquad}\ \frac{\text{kg}}{\text{min}}}$$

Overall Mass Balance on Unit B:

$$\text{In} = \text{Out}$$

$$\dot{m}_5 = \underline{\qquad\qquad}$$

$$\dot{m}_5 = \underline{\qquad}\ \frac{\text{kg}}{\text{min}} + \underline{\qquad}\ \frac{\text{kg}}{\text{min}}$$

$$\boxed{\dot{m}_5 = \underline{\qquad}\ \frac{\text{kg}}{\text{min}}}$$

Overall Mass Balance on Unit A:

$$\text{In} = \text{Out}$$

$$\dot{m}_1 = \underline{\qquad} + \underline{\qquad}$$

$$\dot{m}_3 = \underline{\qquad\qquad}$$

$$\dot{m}_3 = \underline{\qquad}\ \frac{\text{kg}}{\text{min}} - \underline{\qquad}\ \frac{\text{kg}}{\text{min}}$$

$$\boxed{\dot{m}_3 = \underline{\qquad}\ \frac{\text{kg}}{\text{min}}}$$

(b) Determine the unknown mass compositions x_1, x_3 and x_5.

Strategy

To calculate the compositions of the unknown streams on the middle point of the process, component mass balances will have to be performed for either CO or H_2.

Solution

H_2 Mass Balance on Unit B:

$$\text{In} = \text{Out}$$

$$x_{H_2,5}\dot{m}_5 = \underline{\qquad\qquad\qquad}$$

$$x_{H_2,5} = \frac{\underline{\qquad\quad} + \underline{\qquad\quad}}{\underline{\qquad}}$$

$$x_{H_2,5}=\frac{0.60\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\qquad}\,\frac{\text{kg}}{\text{min}}+\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\quad}\,\frac{\text{kg}}{\text{min}}}{\underline{\qquad}\,\frac{\text{kg}}{\text{min}}}$$

$$\boxed{x_{H_2,5}=\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}}$$

H_2 Mass Balance on Overall Process:

In = Out

$$x_{H_2,1}\dot{m}_1+x_{H_2,4}\dot{m}_4=x_{H_2,2}\dot{m}_2+x_{H_2,6}\dot{m}_6+x_{H_2,7}\dot{m}_7$$

$$x_{H_2,4}=\frac{\underline{\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad}}{\dot{m}_4}$$

$$x_{H_2,4}=\frac{1.00\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\qquad}\,\frac{\text{kg}}{\text{min}}+\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}\,150\,\frac{\text{kg}}{\text{min}}+\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\quad}\,\frac{\text{kg}}{\text{min}}-\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\quad}\,\frac{\text{kg}}{\text{min}}}{\underline{\qquad}\,\frac{\text{kg}}{\text{min}}}$$

$$\boxed{x_{H_2,4}=\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}}$$

H_2 Mass Balance on Unit A:

In = Out

$$x_{H_2,1}\dot{m}_1=\underline{\qquad\qquad\qquad\qquad}$$

$$\underline{\qquad}=\frac{x_{H_2,1}\dot{m}_1-\underline{\qquad\qquad}}{\dot{m}_3}$$

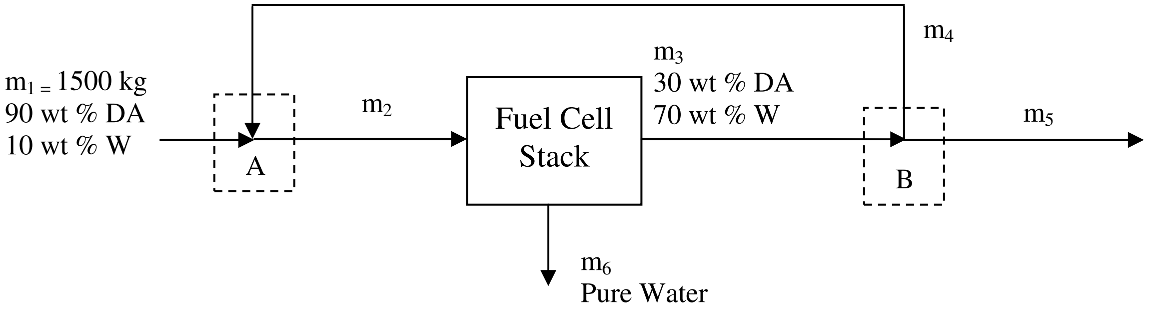
$$\underline{\qquad}=\frac{\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\qquad}\,\frac{\text{kg}}{\text{min}}-\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}\,\underline{\qquad}\,\frac{\text{kg}}{\text{min}}}{60\,\frac{\text{kg}}{\text{min}}}$$

$$\boxed{\underline{\qquad}=\underline{\qquad}\,\frac{\text{kg H}_2}{\text{kg}}}$$

Example 4.5-1 Material and Energy Balances on an Air Conditioner

In a Proton Exchange Membrane Fuel Cell, the polymer membrane separating the anode and the cathode must be kept at a certain degree of humidity. This way, the membrane will allow the flow of hydrogen protons to the cathode side, to form water as a product of the process inside the fuel cell.

A fuel cell stack is fed with 1500 kg of moist air. The exhaust gas exiting the stack contains air and water. 60 % of this humid air will be returned to the feed air stream, and the rest will leave through the exhaust gas stream. A diagram of this process is shown in the figure below:



DA=dry air (21 mol % O_2, 79 mol % N_2), W = water

(a) Determine the amount of humid air in all of the unknown streams for this process.

Strategy

We can perform element mass balances on each of the units of this process, for either dry air or water.

Solution

Overall water balance:

$$\text{In} = \text{Out}$$
$$x_1 m_1 = x_5 m_5$$
$$m_5 = \_\_\_\_\_$$

The diagram for the process described in the problem statement is not showing the composition for the exhaust gases. However, since there is no additional water entering or exiting the splitting point B, the composition of the streams m_3, m_4 and m_5 will be the same. Thus,

$$x_3 = x_4 = x_5 = \_\_\_\_\_$$

$$m_5 = \frac{0.10(\underline{\hspace{2em}}\ \text{kg})}{\underline{\hspace{2em}}}$$

$$\boxed{m_5 = 214.3\ \text{kg}}$$

It is known that 60 % of the amount of humid air exiting the fuel cell will be recycled and the rest will exit through the exhaust gases stream. This information can be written as:

$$m_4 = \underline{\hspace{2em}}\, m_3$$

and,

$$m_3 = m_4 + m_5$$

such that:

$$m_5 = \underline{\hspace{3em}}$$

$$m_5 = (\underline{\hspace{1.5em}} - \underline{\hspace{1.5em}})\, m_3$$

$$m_5 = \underline{\hspace{2em}}\, m_3$$

With these equations we can solve for m_3 and m_4.

$$m_3 = \frac{m_5}{\underline{\hspace{1.5em}}}$$

$$m_3 = \frac{\underline{\hspace{2em}}\ \text{kg}}{\underline{\hspace{1.5em}}}$$

$$\boxed{m_3 = \underline{\hspace{2em}}\ \text{kg}}$$

This value for m_3 can be substituted in the equation solved for m_4:

$$m_4 = \underline{\hspace{2em}}\, m_3$$

$$m_4 = \underline{\hspace{1.5em}}(535.7\ \text{kg})$$

$$\boxed{m_4 = \underline{\hspace{2em}}\ \text{kg}}$$

To solve for m_2, we need to do an overall mass balance in the mixing point A:

Overall mass balance in the mixing point A

$$\text{In} = \text{Out}$$

$$m_1 + m_4 = m_2$$

$$m_2 = \underline{\hspace{2em}}\ \text{kg} + \underline{\hspace{2em}}\ \text{kg}$$

$$\boxed{m_2 = \underline{\hspace{2.5em}}\ \text{kg}}$$

Finally, to determine the amount of condensed water leaving the fuel cell stack, an overall mass balance can be done on the fuel cell stack.

Overall mass balance in the Fuel Cell Stack

$$\begin{aligned}
&\text{In} = \text{Out} \\
&m_2 = \underline{\hspace{2.5cm}} \\
&\underline{\hspace{0.8cm}} = m_2 - m_3 \\
&\underline{\hspace{0.8cm}} = 1821.4\text{ kg} - \underline{\hspace{1.4cm}}\text{ kg} \\
&\boxed{\underline{\hspace{0.8cm}} = 1285.7\text{ kg}}
\end{aligned}$$

(b) Determine the amount of water entering the fuel cell

Strategy

This problem can be solved by doing a water mass balance in point where the recycle and fresh air stream mix.

Solution

Water mass balance in the mixing point A

$$\begin{aligned}
&\text{In} = \text{Out} \\
&x_1 m_1 + x_4 m_4 = x_2 m_2 \\
&x_2 = \frac{\underline{\hspace{2.8cm}}}{\underline{\hspace{0.6cm}}} \\
&x_2 = \frac{0.1(\underline{\hspace{1.4cm}}\text{ kg}) + \underline{\hspace{0.8cm}}(\underline{\hspace{1.4cm}}\text{ kg})}{\underline{\hspace{1.6cm}}\text{ kg}} \\
&\boxed{x_2 = \underline{\hspace{1cm}}}
\end{aligned}$$

Example 4.6-1 Reaction Stoichiometry

Hydrogen can be obtained from methane by the steam methane reforming reaction:

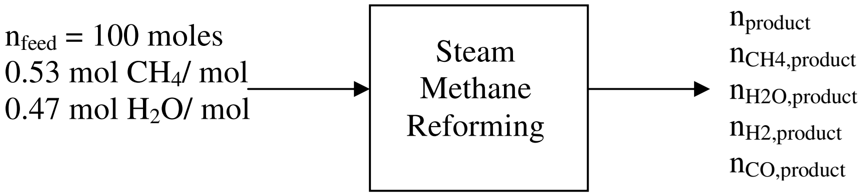
$$CH_4 + H_2O \rightleftarrows CO + 3H_2$$

A gas mixture containing 53 mole % methane and 47 mole % water is fed into a reactor.

(a) Determine which component in the gas mixture is the limiting reactant. Select a basis of 100 moles of gas in the feed stream.

Strategy

We can start to analyze this problem by making a diagram of the reactor. For this we will have to consider that both reactants are exiting the reactor, because we do not know which gas is the limiting reactant.



Solution

First, we can determine the number of moles of each reactant entering the reactor:

$$n_{CH_4,feed} = 0.53\ \frac{\text{mol } CH_4}{\text{mol}}(100\text{ mol}) = \_\_\_\text{ mol}$$

$$n_{H_2O,feed} = \_\_\_\ \frac{\text{mol } CH_4}{\text{mol}}(\_\_\_\text{ mol}) = \_\_\_\text{ mol}$$

If we look at the reaction occurring in this process, it can be seen that 1 mol of methane is reacting with 1 mol of water, i.e. the ratio of the moles of methane to the moles of water is equal to one. If this ratio is calculated using the number of moles being fed into the reactor, the limiting reactant can be determined:

$$\frac{n_{H_2O,feed}}{n_{CH_4,feed}} = \frac{\_\_\_\text{ mol } CH_4}{\_\_\_\text{ mol } H_2O} = 0.89$$

Since the ratio is less than one, water is the limiting reactant.

(b) Determine the percentage by which the other reactant is in excess.

Strategy

To determine the percentage of methane in excess, the stoichiometric amount of methane corresponding to the limiting reactant in the feed must be determined.

Solution

$$n_{CH_4,stoich} = 47 \text{ mol } H_2O\left(\frac{\_\_\_ \text{ mol } CH_4}{\_\_\_ \text{ mol } H_2O}\right) = \_\_\_ \text{ mol } CH_4$$

Knowing the stoichiometric amount, the percentage of methane in excess can be calculated by dividing the amount of methane in excess, by the stoichiometric amount:

$$(\% \text{ excess})_{CH_4} = \frac{n_{CH_4,feed} - n_{CH_4,stoich}}{n_{CH_4,stoich}} \text{ x } 100$$

$$(\% \text{ excess})_{CH_4} = \frac{\_\_\_ \text{ mol } CH_4 - \_\_\_ \text{ mol } CH_4}{\_\_\_ \text{ mol } CH_4} \text{ x } 100$$

$$\boxed{(\% \text{ excess})_{CH_4} = \_\_\_\_\_ \ \%}$$

(c) Determine the amount of each gas exiting the reactor, if the conversion of the limiting reactant is 25 %.

Strategy

The amount of each gas exiting in the product stream, will depend on the amount of the limiting reactant consumed in the reaction. Because of this, we need to start to solve this problem by determining the water consumed, also called the extent of reaction.

Solution

If the fractional conversion of the water is 25 %, then:

$$n_{H_2O,product} = (1 - 0.25)\_\_\_\_\_$$

$$n_{H_2O,product} = (0.75)\_\_\_\_\_\_$$

$$n_{H_2O,product} = (0.75)(\ \_\_\_\_\_\_\_\_\_\ )$$

$$\boxed{n_{H_2O,product} = \_\_\_\_ \text{ mol } H_2O}$$

The extent of reaction will be given by the difference between the water fed into the reactor and the amount of water exiting in the product stream:

$$\xi = \_\_\_\_\_\_\_\_ - \_\_\_\_\_\_\_\_$$

$$\xi = \_\_\_ \text{ mol } H_2O - \_\_\_\_ \text{ mol } H_2O$$

$$\xi = \_\_\_\_ \text{ mol } H_2O$$

The amount of each gas exiting the reactor is given by the equation:

$$n_{i,product} = n_{i,feed} + \nu_i \xi$$

where ν_i is the coefficient of the species i in the reaction and it has a negative value for reactants.

Applying this equation to all the gases in the reaction:

$$n_{CH_4,product} = n_{CH_4,feed} - \_\_\_$$
$$n_{H_2O,product} = \_\_\_\_\_\_\_ - \_\_$$
$$n_{CO,product} = \_\_\_\_\_\_\_ + \_\_$$
$$n_{H_2,product} = n_{H_2,feed} + \_\_\_\_$$

Substituting the values of each gas in the feed, and the value found for the extent of reaction:

$$n_{CH_4,product} = 53 \text{ mol} - \_\_\_\_ \text{ mol}$$
$$\boxed{n_{CH_4,product} = \_\_\_\_ \text{ mol}}$$

$$n_{CO,product} = \_\_\_\_ \text{ mol} + \_\_\_\_ \text{ mol}$$
$$\boxed{n_{CO,product} = 11.7 \text{ mol}}$$

$$n_{H_2,product} = \_\_\_\_ \text{ mol} + (3 \times \_\_\_\_ \text{ mol})$$
$$\boxed{n_{H_2,product} = \_\_\_\_ \text{ mol}}$$

Example 4.6-2 Calculation of an Equilibrium Composition

Hydrogen can be obtained from natural gas through a process that involves two steps: steam methane reforming and water gas shift reactions. In the water gas shift reaction, carbon monoxide obtained from the steam methane reforming process reacts with steam to produce hydrogen by the following reaction:

Water-Gas Shift Reaction: $CO + H_2O \rightleftarrows CO_2 + H_2$

The water-gas shift reaction reaches equilibrium at a temperature of 1300 K, with a value for the equilibrium constant *K*, of 0.55 and given by:

$$K(T)=\frac{y_{CO_2}y_{H_2}}{y_{CO}y_{H_2O}}$$

Suppose a reactor is being fed with a stream containing 3 moles of CO and 4 moles of H_2O.

(a) Calculate the composition in the reactor, assuming that the reaction mixture reaches equilibrium at 1300 K.

Strategy

The number of moles of the products of the water-gas shift reaction will depend on the extent of reaction at equilibrium. Since the value of the equilibrium constant *K*, is known, we can express the mole fractions as functions of the extent of reaction at equilibrium.

Solution

First we need to express the number of moles of each gas at equilibrium, using the equation:

$$n_{i,product} = n_{i,feed} + \nu_i \xi_e$$

where ξ_e is the extent of reaction and equilibrium, and ν_i is the coefficient of the species *i* in the reaction. The variable ν_i has a negative value for reactants.

$$n_{CO,product} = n_{CO,feed} - \xi_e = \_\_ \text{ moles} - \xi_e$$
$$n_{H_2O,product} = n_{H_2O,feed} - \xi_e = \_\_ \text{ moles} - \xi_e$$
$$n_{CO_2,product} = \xi_e$$
$$n_{H_2,product} = \xi_e$$

The terms accounting for the moles of hydrogen and carbon dioxide in the feed stream are not considered since they are not entering the reactor.

It is known that the molar fraction is given by:

$$y_i = \frac{\_\_\_\_}{n_{total}}$$

The total number of moles can be determined as a function of the extent of reaction, by adding the equations for the number of moles of each species in the product stream.

$$n_{total} = n_{CO,product} + n_{H_2O,product} + n_{CO_2,product} + n_{H_2,product}$$

$$n_{total} = \_\_\_\_\_\_ - \_\_ + \_\_\_\_\_\_ - \_\_ + \_\_ + \_\_$$

$$n_{total} = \_\_\_\_\_\_ + \_\_\_\_\_\_$$

$$n_{total} = \_\_ \text{ moles} + \_\_ \text{ moles}$$

$$n_{total} = \_\_\_\_\_\_\_$$

Now that we know the number of moles of each gas and the total number of moles at equilibrium, the molar fractions can be expressed as:

$$y_{CO} = \frac{n_{CO}}{n_{total}} = \frac{\_\_\_\_\_\_}{\_\_\_\_\_}$$

$$y_{H_2O} = \frac{n_{H_2O}}{n_{total}} = \frac{\_\_\_\_\_\_\_}{\_\_\_\_\_}$$

$$y_{CO_2} = \frac{n_{CO_2}}{n_{total}} = \frac{\_\_\_}{\_\_\_\_}$$

$$y_{H_2} = \frac{n_{H_2}}{n_{total}} = \frac{\_\_\_}{\_\_\_\_\_\_\_}$$

Now we can substitute the expressions for the molar fractions in the equation for the equilibrium constant, to yield:

$$K(T)=\frac{y_{CO_2}y_{H_2}}{y_{CO}y_{H_2O}}=\frac{\left(\frac{\_\_\_}{\_\_\ \text{mol}}\right)\left(\frac{\_\_\_}{\_\_\ \text{mol}}\right)}{\left(\frac{\_\_\_\_-\_\_}{\_\_\ \text{mol}}\right)\left(\frac{\_\_\_\_-\_\_}{\_\_\ \text{mol}}\right)}$$

$$K(T)=\frac{\_\_\_^{2}}{(\_\_\ \text{mol}-\_\_)(\_\_\ \text{mol}-\_\_)}=0.55$$

This equation can be solved for the extent of reaction to find:

$$\xi_e = \_\_\_\_\ \text{mol}$$

Substituting this value in the equations for the mol fractions:

$$y_{CO}=\frac{\_\_\ \text{mol}-\_\_\_\ \text{mol}}{\_\_\ \text{mol}}$$

$$\boxed{y_{CO}=\_\_\_\_}$$

$$y_{H_2O}=\frac{\_\_\ \text{mol}-\_\_\_\ \text{mol}}{\_\_\ \text{mol}}$$

$$\boxed{y_{H_2O}=\_\_\_\_}$$

$$y_{CO_2}=\frac{\_\_\_\_\ \text{mol}}{\_\_\ \text{mol}}$$

$$\boxed{y_{CO_2}=\_\_\_\_}$$

$$y_{H_2}=\frac{\_\_\_\_\ \text{mol}}{\_\_\ \text{mol}}$$

$$\boxed{y_{H_2}=\_\_\_\_}$$

(b) Determine which of the two gases in the feed stream is the limiting reactant

Strategy

To solve this problem, we need to find the ratio of the moles of each gas fed into the reactor and compare it to the ratio shown in the reaction.

Solution

To solve this problem, we need to find the ratio of the moles of each gas fed into the reactor and compare it to the ratio of the number of moles of both species in the reaction.

$$\frac{n_{H_2O,feed}}{n_{CO,feed}} = \frac{\_\_\text{ mol } H_2O}{\_\_\text{ mol CO}} = \_\_\_\_$$

Since this value is greater than 1 (ratio of number of moles of water to the number of moles of carbon monoxide from the reaction), the limiting reactant is carbon monoxide.

(c) Determine the fractional conversion of the limiting reactant.

Strategy

Since the extent of reaction is known after solving part (a) of this problem, the amount of carbon monoxide in the product stream can be calculated.

Solution

It is known that the fractional conversion is given by:

$$f_{CO} = \frac{\xi_e}{n_{CO,feed}}$$

$$f_{CO} = \frac{\_\_\_\_\text{ mol}}{\_\_\text{ mol}}$$

$$\boxed{f_{CO} = \_\_\_\_}$$

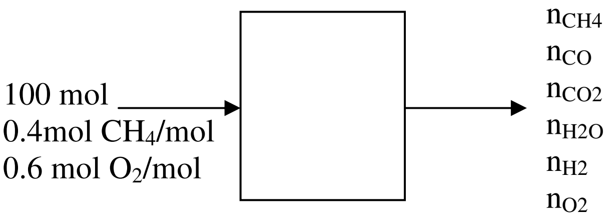
Example 4.6-3 Yield and Selectivity in Partial Oxidation of Natural Gas

Hydrogen can be produced by an incomplete combustion of natural gas in a steam methane reforming process. The two reactions taking place are the following:

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

$$CH_4 + \frac{1}{2}O_2 \longrightarrow CO + 2H_2$$

The feed to this reactor contains 60 mol % oxygen and the rest is methane.



(a) If the fractional conversion of methane is 0.57 and the fractional yield of hydrogen is 0.49, determine the molar composition of the product gas.

Strategy

The number of moles of each gas exiting the reactor, can be written in terms of the extents of reaction ξ_1, ξ_2. A basis of 100 moles in the feed will be selected.

Solution

The number of moles of each gas exiting in the product stream, will be given as:

$$n_{CH_4} = 40 - \xi_1 - \xi_2$$

$$n_{CO} = \underline{\hspace{1.5em}}$$

$$n_{CO_2} = \underline{\hspace{1.5em}}$$

$$n_{H_2O} = \underline{\hspace{2em}}$$

$$n_{H_2} = \underline{\hspace{2em}}$$

$$n_{O_2} = \underline{\hspace{6em}}$$

The amount of methane leaving the reactor can be determined using the fractional conversion given in the problem statement.

$$n_{CH_4} = \underline{\hspace{4em}}\frac{\text{moles of } CH_4 \text{ unreacted}}{\text{moles of } CH_4 \text{ fed}}\left(\underline{\hspace{2em}} \text{ moles of } CH_4 \text{ fed}\right)$$

$$n_{CH_4} = \underline{\hspace{2em}} \text{ moles of } CH_4 = 40 - \xi_1 - \xi_2$$

We also have information about the hydrogen yield, which is defined as:

$$\text{Yield}_{H_2} = \frac{\text{moles of } H_2 \text{ produced}}{\text{maximum possible } H_2 \text{ produced}}$$

If there was a fractional conversion of methane of 1.00 for this process, the maximum possible amount of hydrogen that could be produced would be:

$$\text{Maximum possible } H_2 \text{ produced} = \left(\underline{\hspace{1.5em}} \text{ moles of } CH_4 \text{ fed}\right)\left(\frac{2 \text{ moles of } H_2 \text{ produced}}{1 \text{ mol of } CH_4 \text{ fed}}\right)$$

$$\text{Maximum possible } H_2 \text{ produced} = \underline{\hspace{1.5em}} \text{ moles of } H_2$$

Substituting this value into the definition of hydrogen yield:

$$\text{Yield}_{H_2} = \frac{2\xi_1}{80 \text{ moles}} = \underline{\hspace{2em}}$$

Solving for the extent of reaction ξ_1:

$$\xi_1 = \frac{\underline{\hspace{2em}}(80 \text{ moles})}{2}$$

$$\xi_1 = \underline{\hspace{2em}} \text{ moles}$$

This value can be substituted into the equation for the number of moles of methane exiting the reactor, in terms of the extents of reactions ξ_1 and ξ_2:

$$40 - \xi_1 - \xi_2 = \underline{\hspace{2em}} \text{ moles of } CH_4$$

Solving for the extent of reaction ξ_2:

$$\xi_2 = 40 - \xi_1 - \underline{\hspace{2em}}$$

$$\xi_2 = 40 - \underline{\hspace{2em}} - \underline{\hspace{2em}}$$

$$\xi_2 = \underline{\hspace{1.5em}} \text{ moles}$$

Now that both values for the extents of reaction are known, the number of moles of each gas can be calculated:

n_{CH_4} = ____ moles
n_{CO} = ____ moles
n_{CO_2} = ____ moles
n_{H_2} = ____ moles
n_{H_2O} = ____ moles
n_{O_2} = ____ moles

The total number of moles can be determined by adding the number of moles of each gas, to yield:

n_T = ____ moles

Thus, the composition of the product stream will be:

x_{CH_4} = ____
x_{CO} = ____
x_{CO_2} = ____
x_{H_2} = ____
x_{H_2O} = ____
x_{O_2} = ____

(b) Calculate the selectivity of hydrogen to water production.

Strategy

This problem can be solved using the amounts of each gas calculated in part (a)

Solution

Since the problem is asking for the selectivity of hydrogen to methane:

$$\text{Selectivity} = \frac{\text{moles of hydrogen in the product}}{\text{moles of water in the product}}$$

$$\text{Selectivity} = \frac{\underline{\hspace{2em}}\ \text{moles } H_2}{\underline{\hspace{2em}}\ \text{moles } H_2O}$$

$$\boxed{\text{Selectivity} = \underline{\hspace{2em}}\ \frac{\text{moles } H_2}{\text{moles } H_2O}}$$

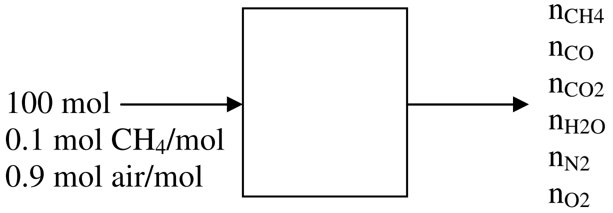
Example 4.7-1 Incomplete Combustion of Methane

Consider the reaction occurring inside the firebox in a steam-methane reforming process for hydrogen production:

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

$$CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O$$

The feed stream entering the firebox has a composition of 10 mol % methane and 90 mol % air. If the conversion of methane is 95 %, determine the molar composition of the product stream. It is known that the ratio of the number of moles of CO_2 to the number of moles of CO in the product is 10.



Strategy

The composition of the product stream can be determined using either molecular species balances, atomic species balances or using the extents of reaction. For this problem we will use atomic species balances. A 100 mol of feed basis will be selected.

Solution

We will start by calculating the number of moles of methane that did not react. It is known that 95 % of the methane entering the process is consumed:

$$n_{CH_4} = \_\_\_\_(10 \text{ mol CH}_4 \text{ fed}) = \_\_\_ \text{ mol CH}_4$$

For nitrogen, the same amount entering the process will be exiting in the product stream, since it is a nonreactive specie in this reaction. The composition of air will be considered to be 21 mol % oxygen and 79 mol % nitrogen.

$$n_{N_2} = \_\_\_\_\left(\frac{\text{mol N}_2}{\text{mol air}}\right)(90 \text{ mol air fed}) = \_\_\_\_ \text{ mol N}_2$$

Now we will proceed to perform atomic species balances on carbon, oxygen and hydrogen. We will do this by taking into account all the molecular species where this elements are present:

C balance

Input = Output

$$10\text{ mol CH}_4\left(\frac{1\text{ mol C}}{1\text{ mol CH}_4}\right)=n_{CH_4}\text{ mol CH}_4\left(\frac{1\text{ mol C}}{1\text{ mol CH}_4}\right)+n_{CO}\text{ mol CO}\left(\frac{1\text{ mol C}}{1\text{ mol CO}}\right)$$
$$+n_{CO_2}\text{ mol CO}_2\left(\frac{1\text{ mol C}}{1\text{ mol CO}_2}\right)$$

Substituting for n_{CH4} and since the ratio of the number of moles of carbon dioxide to the number of moles of carbon monoxide is 10, we have:

$$10\text{ mol CH}_4\left(\frac{1\text{ mol C}}{1\text{ mol CH}_4}\right)=\_\_\_\_\text{ mol CH}_4\left(\frac{1\text{ mol C}}{1\text{ mol CH}_4}\right)+n_{CO}\text{ mol CO}\left(\frac{1\text{ mol C}}{1\text{ mol CO}}\right)$$
$$+10n_{CO}\text{ mol CO}_2\left(\frac{1\text{ mol C}}{1\text{ mol CO}_2}\right)$$

Solving for n_{CO}:

$$n_{CO}=\frac{10\text{ mol CH}_4\left(\frac{1\text{ mol C}}{1\text{ mol CH}_4}\right)-\_\_\_\text{ mol CH}_4\left(\frac{1\text{ mol C}}{1\text{ mol CH}_4}\right)}{\_\_\_\left(\frac{1\text{ mol C}}{1\text{ mol CO}}\right)}$$

$$n_{CO}=\_\_\_\text{ mol CO}$$

With the number of moles of carbon monoxide, we can solve for the number of moles of carbon dioxide:

$$\frac{n_{CO_2}}{n_{CO}}=\_\_\_\left(\frac{\text{mol CO}_2}{\text{mol CO}}\right)$$

$$n_{CO_2}=\_\_\_n_{CO}\text{ mol CO}\left(\frac{\text{mol CO}_2}{\text{mol CO}}\right)$$

$$n_{CO_2}=\_\_\_(\_\_\_\_\text{ mol CO})\left(\frac{\text{mol CO}_2}{\text{mol CO}}\right)$$

$$n_{CO_2} = \_\_\_ \text{ mol } CO_2$$

We will continue to do balances on hydrogen:

H balance

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

$$10 \text{ mol } CH_4 \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } CH_4} \right) = n_{CH_4} \text{ mol } CH_4 \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } CH_4} \right) + n_{H_2O} \text{ mol } H_2O \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } H_2O} \right)$$

Substituting for n_{CH4} and since the problem states that the number of moles of hydrogen produced for each mol of water produced is 7, we have:

$$10 \text{ mol } CH_4 \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } CH_4} \right) = \_\_\_ \text{ mol } CH_4 \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } CH_4} \right) + n_{H_2O} \text{ mol } H_2O \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } H_2O} \right)$$

Solving for n_{H2O}:

$$n_{H_2O} = \frac{\_\_\_ \text{ mol } CH_4 \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } CH_4} \right) - \_\_\_ \text{ mol } CH_4 \left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } CH_4} \right)}{\left(\frac{\_\_ \text{ mol H}}{1 \text{ mol } H_2O} \right)}$$

$$n_{H_2O} = \_\_\_\_ \text{ mol } H_2O$$

Now we need to determine the excess oxygen that is fed into the reactor, which will be exiting in the product stream.

O balance

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

First we need to determine the amount of oxygen entering in the feed stream. This can be done by multiplying the number of moles of air entering the process by the composition of air:

$$n_{O_2 \cdot in} = \_\_\_\_ \left(\frac{\text{mol } O_2}{\text{mol air}} \right) (\_\_\_ \text{ mol air fed}) = \_\_\_\_ \text{ mol } O_2$$

Performing the oxygen balance we have:

$$\_\_\_\_ \text{ mol } O_2\left(\frac{2 \text{ mol O}}{1 \text{ mol } O_2}\right) = n_{O_2} \text{ mol } O_2\left(\frac{2 \text{ mol O}}{1 \text{ mol } O_2}\right) + n_{CO} \text{ mol CO}\left(\frac{1 \text{ mol O}}{1 \text{ mol CO}}\right)$$
$$+ n_{CO_2} \text{ mol } CO_2\left(\frac{2 \text{ mol O}}{1 \text{ mol } CO_2}\right) + n_{H_2O} \text{ mol } H_2O\left(\frac{1 \text{ mol O}}{1 \text{ mol } H_2O}\right)$$

Substituting the known values of n_{CO}, n_{CO2} and n_{H2O} we have:

$$\_\_\_\_ \text{ mol } O_2\left(\frac{2 \text{ mol O}}{1 \text{ mol } O_2}\right) = n_{O_2} \text{ mol } O_2\left(\frac{2 \text{ mol O}}{1 \text{ mol } O_2}\right) + \_\_\_\_ \text{ mol CO}\left(\frac{1 \text{ mol O}}{1 \text{ mol CO}}\right)$$
$$+ \_\_\_ \text{ mol } CO_2\left(\frac{2 \text{ mol O}}{1 \text{ mol } CO_2}\right) + \_\_\_\_ \text{ mol } H_2O\left(\frac{1 \text{ mol O}}{1 \text{ mol } H_2O}\right)$$

Solving for n_{O2}:

$$n_{O_2} = \frac{\_\_\_\_ \text{ mol O} - \_\_\_\_ \text{ mol O} - \_\_\_\_ \text{ mol O} - \_\_\_\_ \text{ mol O}}{\left(\frac{2 \text{ mol O}}{1 \text{ mol } O_2}\right)}$$

$$n_{O_2} = \_\_\_ \text{ mol } O_2$$

Now the composition of the product stream can be calculated. The total number of moles exiting the process is given by:

$$n_T = n_{O_2} + n_{N_2} + n_{H_2O} + n_{CO} + n_{CO_2} + n_{CH_4}$$
$$n_T = \_\_\_ + \_\_\_\_ + \_\_\_\_ + \_\_\_ + \_\_\_ + \_\_\_$$
$$n_T = \_\_\_\_ \text{ moles}$$

Hence, the composition will be obtained by dividing the amount of moles of each individual species by the total number of moles:

$$\boxed{x_{O_2} = \_\_\_\_\_} \qquad \boxed{x_{CO} = \_\_\_\_\_}$$
$$\boxed{x_{N_2} = \_\_\_\_\_} \qquad \boxed{x_{CO_2} = \_\_\_\_\_}$$
$$\boxed{x_{H_2O} = \_\_\_\_\_} \qquad \boxed{x_{CH_4} = \_\_\_\_\_}$$

Example 4.7-2 Product Separation and Recycle in a Steam-Methane Reforming Process

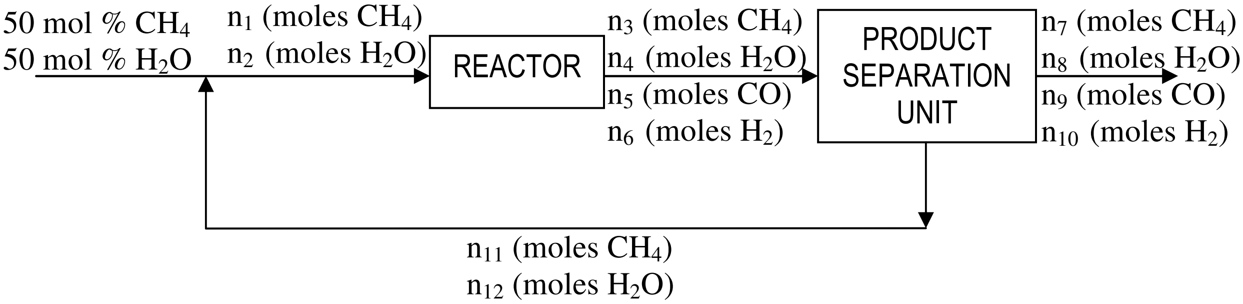
A common process used to obtain hydrogen from natural gas for use in polymer electrolyte membrane fuel cells is the steam methane reforming reaction. The products of this reaction will enter a separation unit.

The natural gas that did not react is returned to the reactor to produce more hydrogen. The rest of the products will enter another reactor where the water-gas shift reaction will take place.

The reaction occurring in the steam-methane reforming process is shown below:

$$CH_4 + H_2O \longrightarrow CO + 3H_2$$

The following diagram represents the steam-methane reforming process for this problem:



This process was designed to achieve a 95 % overall conversion of methane. It is also known that 92 % of the methane that does not react is returned to the reactor and that 40 % of the unreacted water will be fed to the water-gas shift reaction unit.

Calculate the molar fractions of each component in the overall product of the steam-methane reforming process, the ratio of the recycled moles to the moles of feed, and the methane conversion in the reactor.

Strategy

We will perform overall material balances on the atomic species to determine the composition of the product gas that will enter the water-gas shift reaction unit.

Since there is no reaction involved in the separation unit and in the mixing point of the fresh feed with the recycle stream, we can do molecular balances to determine the inner streams in this process.

A basis of 100 moles of fresh feed will be selected for simplicity.

Solution

We can first determine the amount of methane leaving in the product stream, by using the information about the overall methane conversion.

$$n_7 = \underline{\qquad}(50 \text{ moles of } CH_4 \text{ fed})$$

$$n_7 = \underline{\qquad} \text{ moles of } CH_4$$

Now we proceed to do the overall balances on the atomic species.

Overall C balance

$$\underline{\quad}\ \text{mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol } CH_4}\right) = n_7 \text{ mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol } CH_4}\right) + \underline{\quad}\ \text{mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol CO}}\right)$$

$$\underline{\quad}\ \text{mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol } CH_4}\right) = \underline{\qquad}\ \text{mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol } CH_4}\right) + n_9 \text{ mol CO}\left(\frac{1 \text{ mol C}}{\text{mol CO}}\right)$$

Solving for n_9:

$$n_9 = \frac{\underline{\quad}\ \text{mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol } CH_4}\right) - \underline{\quad}\ \text{mol } CH_4\left(\frac{1 \text{ mol C}}{\text{mol } CH_4}\right)}{\left(\frac{1 \text{ mol C}}{\text{mol CO}}\right)}$$

$$n_9 = \underline{\qquad}\ \text{mol CO}$$

Overall O balance

$$\underline{\quad}\ \text{mol } H_2O\left(\frac{1 \text{ mol O}}{\text{mol } H_2O}\right) = n_8 \text{ mol } H_2O\left(\frac{1 \text{ mol O}}{\text{mol } H_2O}\right) + \underline{\quad}\ \text{mol CO}\left(\frac{1 \text{ mol O}}{\text{mol CO}}\right)$$

Substituting for n_9 and solving for n_8:

$$n_8 = \frac{\underline{\quad}\ \text{mol } H_2O\left(\frac{1 \text{ mol O}}{\text{mol } H_2O}\right) - \underline{\qquad}\ \text{mol CO}\left(\frac{1 \text{ mol O}}{\text{mol CO}}\right)}{\left(\frac{1 \text{ mol C}}{\text{mol } H_2O}\right)}$$

$$n_8 = \underline{\quad}\ \text{mol } H_2O$$

Overall H balance

$$\_\_\_\ \text{mol CH}_4\left(\frac{\_\_\ \text{mol H}}{\text{mol CH}_4}\right)+\_\_\_\ \text{mol H}_2\text{O}\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2\text{O}}\right)=n_7\ \text{mol CH}_4\left(\frac{\_\_\ \text{mol H}}{\text{mol CH}_4}\right)+\_\_\ \text{mol H}_2\text{O}\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2\text{O}}\right)$$

$$+\_\_\ \text{mol H}_2\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2}\right)$$

Substituting the known values for n_7,n_8 and solving for n_{10}:

$$n_{10}=\frac{\_\_\ \text{mol CH}_4\left(\frac{\_\_\ \text{mol H}}{\text{mol CH}_4}\right)+\_\_\ \text{mol H}_2\text{O}\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2\text{O}}\right)}{\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2}\right)}$$

$$\frac{-\_\_\_\_\ \text{mol CH}_4\left(\frac{\_\_\ \text{mol H}}{\text{mol CH}_4}\right)-\_\_\_\_\ \text{mol H}_2\text{O}\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2\text{O}}\right)}{\left(\frac{\_\_\ \text{mol H}}{\text{mol H}_2}\right)}$$

$$n_{10}=\_\_\_\_\_\ \text{mol H}_2$$

The total number of moles in the product stream is given by:

$$n_T=n_7+\_\_+\_\_+n_{10}$$

$$n_T=\_\_\_\_\ \text{moles}$$

Now we can determine the composition of the overall product of this process:

$$x_7=\frac{n_7}{n_T}\qquad x_7=\frac{\_\_\_\ \text{moles CH}_4}{\_\_\_\ \text{moles}}\qquad \boxed{x_7=0.013}$$

$$x_8=\frac{n_8}{n_T}\qquad x_8=\frac{\_\_\_\ \text{moles H}_2\text{O}}{\_\_\_\ \text{moles}}\qquad \boxed{x_8=\_\_\_\_\_}$$

$$x_9=\frac{n_9}{n_T}\qquad x_9=\frac{\_\_\_\ \text{moles CO}}{\_\_\_\ \text{moles}}\qquad \boxed{x_9=\_\_\_\_\_}$$

$$x_{10}=\frac{n_{10}}{n_T}\qquad x_{10}=\frac{\_\_\_\ \text{moles H}_2}{\_\_\_\ \text{moles}}\qquad \boxed{x_{10}=\_\_\_\_\_}$$

The recycle ratio we need to calculate to solve this problem is defined as:

$$r = \frac{n_{11} + n_{12}}{\text{moles of feed}}$$

However, the number of moles n_{11} and n_{12} are unknown, but can be determined by doing molecular balances on the separation unit.

CH_4 balance on the Separation Unit

$$n_3 = n_7 + n_{11}$$

For this steam-methane reforming process, 92 % of the unreacted methane leaving the reactor will be returned to the reactor to further produce hydrogen:

$$n_{11} = 0.92\ \_\_\_$$

$$n_7 = \_\_\_\_\_\ n_3$$

Since we calculated the value for n_7, this last equation can be used to solve for n_3.

$$n_3 = \frac{n_7}{\_\_\_\_} = \frac{\_\_\_\ \text{moles of } CH_4}{\_\_\_\_} = \_\_\_\_\_\ \text{moles of } CH_4$$

In a similar way, we can calculate the number of moles of methane in the recycle stream.

$$n_{11} = 0.92\,\_\_ = 0.92(\ \_\_\_\_\_\ \text{moles}) = \_\_\_\_\_\ \text{moles of } CH_4$$

The amount of moles of water in the recycle stream, can be calculated also by molecular balances in the separation unit.

H_2O balance on the Separation Unit

$$n_4 = n_8 + n_{12}$$

It is known that 40 % of the moles that did not react will be entering the water-gas shift reaction. This means that 40 % of the unreacted moles of water will be exiting in the product stream for this process. This can be written as:

$$n_8 = 0.4\ n_4$$

$$\_\_\_ = 0.6\ n_4$$

From the equation for n_8 in terms of n_4, we can solve for the amount of water exiting the reactor, n_4.

$$n_4 = \frac{n_8}{0.4} = \frac{\_\_\_\_ \text{ moles of } H_2O}{0.4} = \_\_\_\_ \text{ moles of } H_2O$$

In a similar way, we can calculate the number of moles of methane in the recycle stream.

$$\_\_\_\_ = 0.6\ n_4 = 0.6\ (\ \_\_\_\_ \text{ moles}) = \_\_\_\_ \text{ moles of } H_2O$$

Now the recycle ratio can be calculated.

$$r = \frac{\_\_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles}}{\_\_\_\_ \text{ moles}}$$

$$\boxed{r = \_\_\_\_ \frac{\text{mol recycle}}{\text{mol fresh feed}}}$$

With the data we have of the methane entering the reactor and the number of moles of methane that did not react, the conversion in the reactor can be determined with the following equation:

$$f = \frac{\_\_\_\_\_}{n_1} \times 100\ \%$$

The number of moles of methane entering the reactor can be determined by performing a methane balance in the mixing point of the fresh feed and the recycle stream.

CH_4 balance on the Mixing Point

$$\_\_\_ \text{ moles of } CH_4 + n_{11} = n_1$$

After substituting the value for n_{11} into the balance equation, the value of n_1 can be calculated.

$$n_1 = \_\_\_ \text{ moles of } CH_4 + \_\_\_\_\_ \text{ moles of } CH_4$$

$$n_1 = \_\_\_\_\_ \text{ moles of } CH_4$$

Substituting the values for n_1 and n_3 into the definition of the fractional conversion in the reactor, we have:

$$f = \frac{\_\_\_\_\_ - \_\_\_\_\_}{\_\_\_\_\_} \times 100\ \%$$

$$\boxed{f = \_\_\_\_\_\ \%}$$

Example 4.7-3 Recycle and Purge in the Synthesis of Methanol for use in Direct-Methanol Fuel Cells

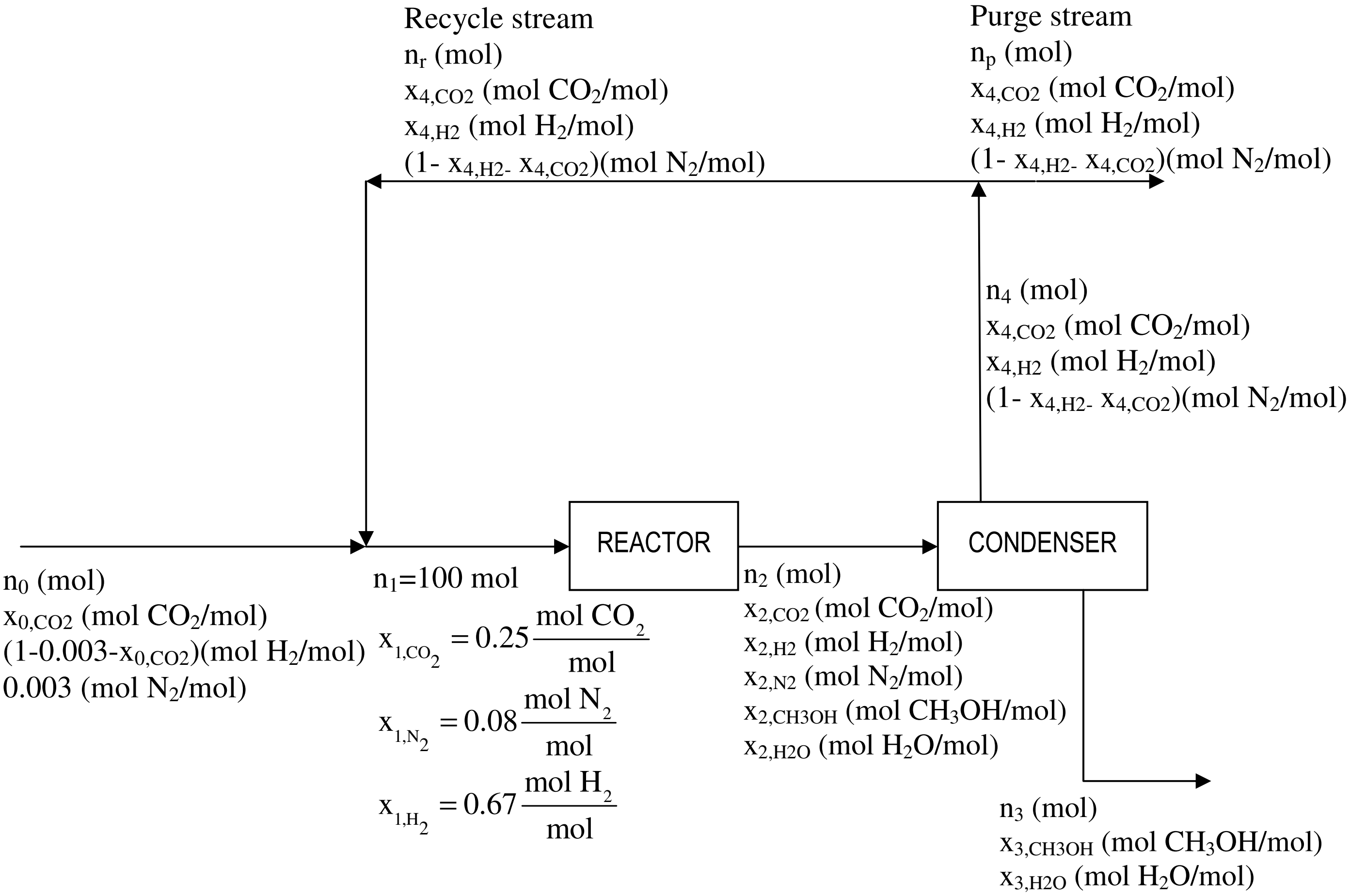
Direct-methanol fuel cells or DMFCs are a subcategory of fuel cells in which methanol is used as the fuel. This type of fuel cells are used especially in portable equipment and have the advantages of providing higher energy density than batteries and faster recharging.

Methanol used in DMFCs is produced in the reaction of carbon dioxide and hydrogen:

$$CO_2 + 3H_2 \longrightarrow CH_3OH + H_2O$$

The fresh feed to the process contains hydrogen, carbon dioxide and 0.3 mol % of nitrogen. The stream exiting the reactor enters a condenser that removes the methanol and water, and returns the unreacted gases to the feed to the reactor. To avoid accumulation of inert gases in the system, a purge stream is withdrawn from the recycle.

The reactor will be fed with a gas containing 25 mol % of CO_2, 67 mol % of H_2 and 8 mol % of N_2. Calculate the number of moles and the composition of the fresh feed, feed to condenser, recycle and purge streams for a conversion of hydrogen of 70 %. A diagram of this process is shown below:



Strategy

For this problem, it is convenient to select a basis of 100 moles for the stream entering the reactor. This can be done when the composition of the stream is known.

Since there is only one reaction occurring in this process, molecular balances can be performed on the different units of this process.

Solution

We will start by performing molecular balances on the reactor. The problem states that the single-pass conversion of hydrogen in the reactor is 70 %, which can be written as:

Reactor Analysis

$$n_{2,H_2} = \underline{\qquad} \frac{\text{mol } H_2 \text{ unreacted}}{\text{mol } H_2 \text{ fed}} \times (\underline{\quad} \text{ mol } H_2 \text{ fed})$$

$$n_{2,H_2} = \underline{\quad} \text{ mol } H_2$$

With this information we can now determine the amount of hydrogen that reacted.

H balance

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

$$\text{Consumption} = \underline{\quad} \text{ moles of } H_2 - 20.1 \text{ moles of } H_2$$

$$\text{Consumption} = \underline{\quad} \text{ moles of } H_2$$

Based on the stoichiometry of the reaction, the amount of hydrogen consumed in the reactor can be used to determine the amount of carbon dioxide consumed and the amount of methanol and water produced in the reactor.

CO_2 balance

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

$$n_{2,CO_2} = \underline{\quad} \text{ moles of } CO_2 - \underline{\quad} \text{ moles of } H_2 \text{ consumed} \left(\frac{1 \text{ mol } CO_2 \text{ consumed}}{\underline{\quad} \text{ moles of } H_2 \text{ consumed}} \right)$$

$$n_{2,CO_2} = \underline{\quad} \text{ moles of } CO_2$$

CH_3OH balance

$$\text{Output} = \text{Generation}$$

$$n_{2,CH_3OH} = \_\_\_\_ \text{ moles of } H_2 \text{ consumed} \left(\frac{1 \text{ mol } CH_3OH \text{ produced}}{\_\_ \text{ moles of } H_2 \text{ consumed}} \right)$$

$$n_{2,CH_3OH} = \_\_\_\_ \text{ moles of } CH_3OH$$

H_2O balance

$$\text{Output} = \text{Generation}$$

$$n_{2,H_2O} = \_\_\_\_ \text{ moles of } H_2 \text{ consumed} \left(\frac{1 \text{ mol } H_2O \text{ produced}}{\_\_ \text{ moles of } H_2 \text{ consumed}} \right)$$

$$n_{2,H_2O} = \_\_\_\_ \text{ moles of } H_2O$$

N_2 balance

Since nitrogen is a gas that is not participating in the reaction, the number of moles of nitrogen fed to the reactor will be the same as the number of moles exiting the reactor:

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

$$n_{2,N_2} = \_\_\_ \text{ moles of } N_2$$

Now that the numbers of moles of all the species exiting the reactor are known, the composition of this stream can be determined. For this, the total number of moles will be given as:

$$n_2 = \_\_\_\_ + n_{2,H_2} + \_\_\_\_ + n_{2,CH_3OH} + \_\_\_\_$$

$$n_2 = \_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles}$$

$$n_2 = \_\_\_\_\_ \text{ moles}$$

The molar fraction results for this stream are shown below:

$$x_{2,i} = \frac{n_{2,i}}{n_2}$$

$$x_{2,CO_2} = \_\_\_\_\_$$

$$x_{2,H_2} = \_\_\_\_\_$$

$$x_{2,N_2} = \_\_\_\_\_$$

$$x_{2,CH_3OH} = \_\_\_\_\_$$

$$x_{2,H_2O} = \_\_\_\_\_$$

The numbers of moles of each gas exiting the reactor are now known. Using these values we can calculate the amount and composition of the gas that will be split into the recycle and purge streams.

Condenser Analysis

Overall balance

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

$$n_{2,CO_2} + \underline{\quad\quad} + n_{2,N_2} + \underline{\quad\quad} + n_{2,H_2O} = n_{3,CH_3OH} + \underline{\quad\quad} + n_4$$

Since all the amount of methane and water entering the condenser, will be exiting as a product in the liquid phase:

$$n_{2,CH_3OH} = n_{3,CH_3OH}$$

$$n_{2,H_2O} = n_{3,H_2O}$$

After applying this to the overall balance equation for the condenser, we get:

$$n_{2,CO_2} + \underline{\quad\quad} + n_{2,N_2} + \underline{\quad\quad} + n_{2,H_2O} = n_{2,CH_3OH} + \underline{\quad\quad} + n_4$$

Reducing this equation yields:

$$n_{2,CO_2} + n_{2,H_2} + n_{2,N_2} = n_4$$

Substituting the values for $n_{2,CO2}$, $n_{2,H2}$ and $n_{2,N2}$:

$$n_4 = \underline{\quad\quad}\ \text{moles} + \underline{\quad\quad}\ \text{moles} + \underline{\quad\quad}\ \text{moles}$$

$$n_4 = \underline{\quad\quad\ }\ \text{moles}$$

CO_2 balance

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

$$n_{2,CO_2} = n_4 x_{4,CO_2}$$

Solving for $x_{4,CO2}$ and substituting the known values of $n_{2,CO2}$ and n_4:

$$x_{4,CO_2} = \frac{\underline{\quad\quad}}{n_4} = \frac{\underline{\quad\quad}\ \text{moles}}{\underline{\quad\quad\ }\ \text{moles}}$$

$$x_{4,CO_2} = \underline{\quad\quad}$$

H balance

$$\text{Input} = \text{Output}$$
$$n_{2,H_2} = n_4 x_{4,H_2}$$

Solving for $x_{4,H2}$ and substituting the known values of $n_{2,H2}$ and n_4:

$$x_{4,H_2} = \frac{n_{2,H_2}}{n_4} = \frac{\_\_\_\_\ \text{moles}}{\_\_\_\_\_\_\ \text{moles}}$$

$$x_{4,H_2} = \_\_\_\_$$

N_2 balance

$$\text{Input} = \text{Output}$$
$$n_{2,N_2} = n_4 x_{4,N_2}$$

Solving for $x_{4,N2}$ and substituting the known values of $n_{2,N2}$ and n_4:

$$x_{4,N_2} = \frac{n_{2,N_2}}{n_4} = \frac{\_\_\ \text{moles}}{\_\_\_\_\_\_\ \text{moles}}$$
$$x_{4,N_2} = \_\_\_\_\_$$

The composition in the purge and recycle streams will be the same, since it is only a splitting point and there is no reaction occurring.

The only remaining unknown quantities, are the number of moles in the recycle stream, n_r, the number of moles of fresh feed, n_0 and the number of moles in the purge stream, n_p. The unknown variables n_r and n_0, can be determined by doing molecular balances in the mixing point of the recycle stream with the fresh feed.

Mixing Point Analysis

Overall balance

$$\text{Input} = \text{Output}$$
$$n_0 + n_r = \_\_\_\_\ \text{moles}$$

N_2 balance

$$\text{Input} = \text{Output}$$
$$\_\_\_\_\_\ n_0 + \_\_\_\_\_\ n_r = \_\_\ \text{moles}$$

Solving for n_0 and substituting the known values for the compositions $x_{4,N2}$ and $x_{0,N2}$:

$$n_0 = \frac{\_\_\ \text{moles} - \_\_\_\_\_}{\_\_\_\_\_}$$

$$n_0 = \frac{\_\_\ \text{moles} - \_\_\_\_\_}{\_\_\_\_\_}$$

Substituting this equation for n_0, into the overall balance equation:

$$\frac{\_\_\ \text{moles} - \_\_\_\_\ n_r + \_\_\_\_\ n_r}{0.003} = 100\ \text{moles}$$

This equation can be solved for n_r to yield:

$$n_r = \frac{\left(100\ \text{moles} - \frac{\_\_\ \text{moles}}{\_\_\_\_}\right) \times 0.003}{-\_\_\_\_}$$

$$n_r = \_\_\_\_\_\ \text{moles}$$

Substituting this value into the overall balance equation, we can solve for n_0:

$$n_0 + n_r = 100\ \text{moles}$$
$$n_0 = 100\ \text{moles} - \_\_\_\_\_\ \text{moles}$$
$$n_0 = \_\_\_\_\_\ \text{moles}$$

The compositions in the fresh feed stream of hydrogen and carbon dioxide are unknown, but can be calculated by doing a molecular balance of any of this gases in the fresh-feed and recycle streams mixing point.

H balance

$$\text{Input} = \text{Output}$$
$$\_\_\_\_\_\ n_0 + x_{4,H_2} n_r = \_\_\_\ \text{moles}$$

Solving for the unknown composition and substituting the known values for n_0, n_r and $x_{4,H2}$:

$$x_{0,H_2} = \frac{\_\_\_\ \text{moles} - x_{4,H_2} n_r}{n_0} = \frac{\_\_\_\ \text{moles} - \_\_\_(\_\_\_\ \text{moles})}{\_\_\_\ \text{moles}}$$

$$x_{0,H_2} = \_\_\_\_$$

Since there is only hydrogen, nitrogen and carbon dioxide in the fresh feed stream, the following equation can be used to determine the molar fraction of carbon dioxide:

$$x_{0,H_2} + x_{0,CO_2} + x_{0,N_2} = 1$$
$$x_{0,CO_2} = 1 - \_\_\_\_ - \_\_\_\_$$
$$x_{0,CO_2} = 1 - \_\_\_\_ - \_\_\_\_$$
$$x_{0,CO_2} = \_\_\_\_$$

Finally, an overall balance must be done in the recycle-purge splitting point so the number of moles in the purge stream, n_p, can be determined.

Splitting Point Analysis

Overall balance

$$n_4 = n_r + n_p$$

Solving for n_p and substituting the known values for n_r and n_4:

$$n_p = \_\_\_ - \_\_\_ = \_\_\_\_\_\_ \text{ moles} - \_\_\_\_\_\_ \text{ moles}$$
$$n_p = \_\_\_\_ \text{ moles}$$

Summarizing the results:

Fresh feed

$\boxed{n_0 = \_\_\_\_\_ \text{ moles}}$

$\boxed{\_\_\_\_ \text{ mol \% } CO_2}$

$\boxed{\_\_\_ \text{ mol \% } N_2}$

$\boxed{\_\_\_\_ \text{ mol \% } H_2}$

Feed to reactor

$\boxed{\_\_\_\_ \text{ moles}}$

$\boxed{\_\_\_ \text{ mol \% } CO_2}$

$\boxed{\_\_ \text{ mol \% } N_2}$

$\boxed{\_\_\_ \text{ mol \% } H_2}$

Feed to condenser

$\boxed{n_2 = \_\_\_\_\_ \text{ moles}}$

$\boxed{\_\_\_\_ \text{ mol \% } CO_2}$

$\boxed{\_\_\_\_ \text{ mol \% } N_2}$

$\boxed{\_\_\_\_ \text{ mol \% } H_2}$

$\boxed{\_\_\_\_ \text{ mol \% } CH_3OH}$

$\boxed{\_\_\_\_ \text{ mol \% } H_2O}$

Recycle

n_r = ____ moles

____ mol % CO_2

____ mol % N_2

____ mol % H_2

Purge

n_p = ____ moles

____ mol % CO_2

____ mol % N_2

____ mol % H_2

Example 4.8-1 Composition on Wet and Dry Bases

The gases exiting through the stack on a fuel cell vehicle contain 65 mol % H_2O, 0.5 mol % H_2, 7.3 mol % O_2 and the rest is exiting as N_2.

(a) Determine the molar composition of the exhaust gases on a dry basis.

Strategy

With the composition of the exhaust gases given in the problem statement, the composition on a dry basis can be calculated. A basis of 100 moles of wet gas will be selected.

Solution

The number of moles of each component in the exhaust gases will be:

$$
\begin{aligned}
n_{H_2O} &= \_\_\_(100 \text{ moles}) = \_\_\_ \text{ moles } H_2O\\
n_{H_2} &= \_\_\_\_\_(\_\_\_\_ \text{ moles}) = \_\_\_ \text{ moles } H_2\\
n_{O_2} &= \_\_\_\_\_(\_\_\_\_ \text{ moles}) = \_\_\_ \text{ moles } O_2\\
n_{N_2} &= (\_\_\_\_)(\_\_\_\_ \text{ moles}) = \_\_\_\_\_ \text{ moles } N_2
\end{aligned}
$$

For the dry-basis analysis, only the moles of N_2, O_2 and H_2 will be considered. Thus, the total number of moles on a dry-basis will be given by:

$$
\begin{aligned}
n_T &= n_{H_2} + n_{O_2} + n_{N_2}\\
n_T &= \_\_\_\_ \text{ moles } H_2 + \_\_\_\_ \text{ moles } O_2 + \_\_\_\_ \text{ moles } N_2\\
n_T &= \_\_\_ \text{ moles}
\end{aligned}
$$

And the molar fractions of each gas will be:

$$
x_{H_2} = \frac{n_{H_2}}{n_T} \qquad x_{O_2} = \frac{n_{O_2}}{n_T} \qquad x_{N_2} = \frac{n_{N_2}}{n_T}
$$

$$
x_{H_2} = \frac{\_\_\_ \text{ moles } H_2}{\_\_\_ \text{ moles}} \qquad x_{O_2} = \frac{\_\_\_ \text{ moles } O_2}{\_\_\_ \text{ moles}} \qquad x_{N_2} = \frac{\_\_\_\_ \text{ moles } N_2}{\_\_\_ \text{ moles}}
$$

$$
\boxed{x_{H_2} = \_\_\_\_\_} \qquad \boxed{x_{O_2} = \_\_\_\_\_} \qquad \boxed{x_{N_2} = \_\_\_\_\_}
$$

(b) The analysis of the exhaust gases of a fuel cell engine yields that the composition on a dry basis is 59 mol % N_2 and 41 mol % O_2. Determine the composition of this gas on a wet basis if a humidity measurement shows that the mole fraction of H_2O in the stack gases is 0.38.

Strategy

With the mole fraction of water given, the molar fraction of the dry gas can be calculated. This result can be used to determine the molar fraction of water in the dry gas. For simplicity, a basis of 100 moles of dry gas will be selected.

Solution

It is known that the sum of the molar fractions of all the components of the exhaust gases is equal to 1. This can be written as:

$$x_{H_2O} + x_{\text{dry gas}} = 1$$

We can substitute the molar fraction of water, x_{H2O} and solve for the molar fraction, $x_{\text{dry gas}}$:

$$x_{\text{dry gas}} = 1 - \underline{\hspace{1.5em}}$$

$$x_{\text{dry gas}} = \underline{\hspace{1.5em}}\,\frac{\text{moles dry gas}}{\text{moles wet gas}}$$

Now the molar fraction of water in the dry gas can be calculated:

$$\frac{\underline{\hspace{1.5em}}\,\dfrac{\text{moles } H_2O}{\text{moles wet gas}}}{\underline{\hspace{1.5em}}\,\dfrac{\text{moles dry gas}}{\text{moles wet gas}}} = \underline{\hspace{1.5em}}\,\frac{\text{moles } H_2O}{\text{moles dry gas}}$$

This value of the molar fraction of water can be used to determine the number of moles of water, by multiplying the molar fraction by the basis of 100 moles of dry gas we selected:

$$n_{H_2O} = \underline{\hspace{1.5em}}\,\frac{\text{moles } H_2O}{\text{moles dry gas}}(100 \text{ moles dry gas}) = \underline{\hspace{1.5em}} \text{ moles } H_2O$$

Now that the moles of water are known, we need to calculate the number of moles of the other gases and use these results to determine the composition of the exhaust gases on a wet basis.

$$n_{N_2} = \underline{\hspace{1.5em}}\,\frac{\text{moles } N_2}{\text{moles dry gas}}(100 \text{ moles dry gas}) = \underline{\hspace{1.5em}} \text{ moles } N_2$$

$$n_{O_2} = \_\_\_\_ \frac{\text{moles } H_2O}{\text{moles dry gas}}(100 \text{ moles dry gas}) = \_\_\_ \text{ moles } O_2$$

The total number of moles of wet gas is given by:

$$n_T = n_{H_2O} + n_{N_2} + n_{O_2}$$

Substituting the known values:

$$n_T = \_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles} = \_\_\_\_ \text{ moles}$$

And the molar fractions of each gas will be:

$$x_{H_2O} = \frac{n_{H_2O}}{n_T} \qquad x_{N_2} = \frac{n_{N_2}}{n_T} \qquad x_{O_2} = \frac{n_{O_2}}{n_T}$$

$$x_{H_2O} = \frac{\_\_\_ \text{ moles } H_2O}{\_\_\_\_ \text{ moles}} \qquad x_{N_2} = \frac{\_\_\_ \text{ moles } N_2}{\_\_\_\_ \text{ moles}} \qquad x_{O_2} = \frac{\_\_\_ \text{ moles } O_2}{\_\_\_\_ \text{ moles}}$$

$$\boxed{x_{H_2} = \_\_\_\_} \qquad \boxed{x_{N_2} = \_\_\_\_} \qquad \boxed{x_{O_2} = \_\_\_\_}$$

Example 4.8-2 Theoretical and Excess Air in Partial Oxidation of Methane

An alternative process to steam-methane reforming process to produce hydrogen from methane is partial oxidation. This process takes place in a high pressure reactor. The overall exothermic reaction taking place in this process is:

$$CH_4 + \frac{1}{2}O_2 \rightleftarrows CO + 2H_2$$

(a) Determine the percent excess air if the flow rate of methane is 100 mol / h and the air flow rate is 200 mol / h

Strategy

We will start by determining the air flow rate from the stoichiometric equation and the flow rate of methane entering the reactor.

Solution

The theoretical amount of oxygen required by the two reactions to occur, can be determined from the flow rate of methane entering the combustion reactor:

$$(\dot{n}_{O_2})_{\text{theoretical}} = \frac{\underline{\qquad}\ \text{moles } CH_4}{\text{h}}\left(\frac{\underline{\qquad}\ \text{moles } O_2 \text{ required}}{\text{mol } CH_4}\right)$$

$$(\dot{n}_{O_2})_{\text{theoretical}} = \underline{\qquad}\ \frac{\text{moles } O_2}{\text{h}}$$

With the composition of air, the theoretical amount of air that needs to be fed into the reactor is given by:

$$(\dot{n}_{\text{air}})_{\text{theoretical}} = \frac{\underline{\qquad}\ \text{moles } O_2}{\text{h}}\left(\frac{1 \text{ mol air}}{\underline{\qquad}\ \text{mol } O_2}\right)$$

$$(\dot{n}_{\text{air}})_{\text{theoretical}} = \underline{\qquad}\ \frac{\text{moles air}}{\text{h}}$$

The definition of the percent excess air is given by the following equation:

$$\%\ \text{excess air} = \frac{(\dot{n}_{\text{air}})_{\text{fed}} - (\dot{n}_{\text{air}})_{\text{theoretical}}}{(\dot{n}_{\text{air}})_{\text{theoretical}}} \times 100\%$$

Substituting the calculated values of $(\dot{n}_{\text{air}})_{\text{fed}}$ and $(\dot{n}_{\text{air}})_{\text{theoretical}}$:

$$\%\ \text{excess air} = \frac{\underline{\quad\quad}\ \frac{\text{mol}}{\text{h}} - \underline{\quad\quad}\ \frac{\text{mol}}{\text{h}}}{\underline{\quad\quad}\ \frac{\text{mol}}{\text{h}}} \times 100\%$$

It can be seen that the reactor is being fed with a smaller amount than the required oxygen. Hence there will be a deficiency of oxygen for this process, obtained from the following equation:

$$\%\ \text{deficiency air} = \frac{\underline{\quad\quad}\ \frac{\text{mol}}{\text{h}} - \underline{\quad\quad}\ \frac{\text{mol}}{\text{h}}}{\underline{\quad\quad}\ \frac{\text{mol}}{\text{h}}} \times 100\%$$

$$\boxed{\%\ \text{deficiency air} = \underline{\quad\quad}\ \%}$$

This can be also explained by saying that only 84 % of the air required by this process, is being fed into the reactor.

(b) In order to minimize the production of carbon dioxide, methane and coke, and maximize the yield of hydrogen and carbon monoxide, a ratio of methane to air of 0.47 is recommended in the feed stream. What would be the theoretical flow rate of oxygen if the flow rate of methane is 100 mol / h?

Strategy

This problem can be solved in a similar way as part (a) only that for this case, we need to use the methane/air ratio given in the problem statement instead of the stoichiometric equation.

Solution

The ratio of the number of moles of methane to air is given by:

$$r = \frac{\underline{\quad\quad}}{\underline{\quad\quad}} = \underline{\quad\quad}$$

Substituting the flow rate of methane, $\dot{n}_{CH_4}$ and solving for $\dot{n}_{\text{air}}$:

$$\dot{n}_{\text{air}} = \frac{\underline{\quad\quad}\ \frac{\text{moles}}{\text{h}}}{\underline{\quad\quad}}$$

$$\boxed{\dot{n}_{\text{air}} = \underline{\quad\quad}\ \frac{\text{moles}}{\text{h}}}$$

Example 4.8-3 Combustion of Methane in a Steam-Methane Reforming Process

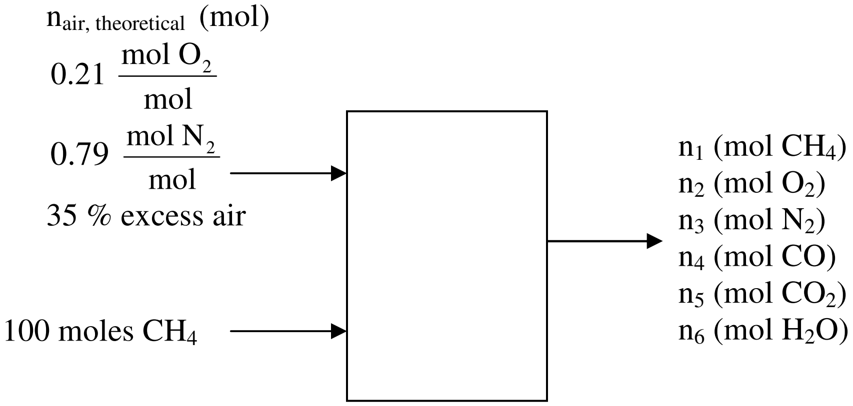
The reactions occurring in a steam-methane reforming process for producing hydrogen are endothermic. Additional methane is being combusted in this process in order to supply the required amount of heat for the steam-methane reforming reaction to occur. The combustion of methane is described by the following stoichiometric equations:

$$CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O$$

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

100 moles of methane are being burned in a combustion reactor with 35 % excess air. It is known that 95 % of the methane fed into the combustion reactor converts into products. 10 % of the methane consumed by this process is converted into CO and the balance reacts to form CO_2.

Determine the amount of air fed into the reactor and the composition of the stack gases. A diagram of this process is shown below:



Strategy

The theoretical amount of air required by this process can be determined from the stoichiometric equations. To calculate the composition of the stack gases, material balances on the different atomic species participating in the reaction can be performed.

Solution

From the stoichiometric equations, the amount of oxygen required can be determined from the ratio of moles consumed by each mol of methane.

$$n_{O_2,\text{theoretical}} = \_\_\_ \text{ moles } CH_4 \left(\frac{\_\_\_ \text{ moles } O_2}{1 \text{ mol } CH_4} \right)$$

$$n_{O_2,\text{theoretical}} = \_\_\_ \text{ moles } O_2$$

Using the composition of air of 21 mol % O_2 and 79 mol % of N_2 and the percent excess of air, the air required by this process can now be determined:

$$n_{\text{air,theoretical}} = \_\_\_\left(\frac{\_\_\_ \text{ moles } O_2}{\_\_\_ \dfrac{\text{moles } O_2}{\text{mol air}}}\right)$$

$$\boxed{n_{\text{air,theoretical}} = \_\_\_\_\_ \text{ moles air}}$$

The amount of methane exiting in the product stream using the information about the fractional conversion and the 100 moles of fuel fed into the reactor:

$$n_1 = \_\_\_\_\_(100 \text{ moles } CH_4)$$
$$n_1 = \_\_\_ \text{ moles } CH_4$$

The number of moles of CO and CO_2 exiting in the stack gases, is determined from the moles of fuel consumed and the selectivities of these species to the consumed methane:

$$n_4 = (100 \text{ moles } CH_4 \text{ fed})\left(\_\_\_\_\_ \frac{\text{moles } CH_4 \text{ consumed}}{\text{mol } CH_4 \text{ fed}}\right)\left(\_\_\_\_\_ \frac{\text{moles CO produced}}{\text{mol } CH_4 \text{ consumed}}\right)$$
$$n_4 = \_\_\_\_ \text{ moles CO}$$

The number of moles of carbon dioxide, n_5 can be calculated in a similar way:

$$n_5 = (100 \text{ moles } CH_4 \text{ fed})\left(\_\_\_\_\_ \frac{\text{moles } CH_4 \text{ consumed}}{\text{mol } CH_4 \text{ fed}}\right)\left(\_\_\_\_\_ \frac{\text{moles } CO_2 \text{ produced}}{\text{mol } CH_4 \text{ consumed}}\right)$$
$$n_5 = \_\_\_\_\_ \text{ moles } CO_2$$

The number of moles of nitrogen in the stack gases will be the same amount entering the reactor, since nitrogen does not participate in the reactions:

$$n_3 = \_\_\_\_\_ \frac{\text{moles } N_2}{\text{mol air}}(\ \_\_\_\_\_ \text{ moles air})$$

$$n_3 = \_\_\_\_\_ \text{ moles } N_2$$

To determine the remaining unknown values, we will proceed to do atomic balances for hydrogen and oxygen.

H balance:

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

$$100\text{ moles CH}_4\left(\underline{\quad}\frac{\text{moles H}}{\text{mol CH}_4}\right)=n_1\text{ moles CH}_4\left(\underline{\quad}\frac{\text{moles H}}{\text{mol CH}_4}\right)+n_6\text{ moles H}_2\text{O}\left(\underline{\quad}\frac{\text{moles H}}{\text{mol H}_2\text{O}}\right)$$

substituting the known value of n_1 and solving for n_6:

$$n_6=\frac{\underline{\quad\quad}\text{ moles CH}_4\left(\underline{\quad}\frac{\text{moles H}}{\text{mol CH}_4}\right)}{\left(\underline{\quad}\frac{\text{moles H}}{\text{mol H}_2\text{O}}\right)}$$

$$n_6=\underline{\quad\quad}\text{ moles H}_2\text{O}$$

O_2 balance:

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

$$\underline{\quad\quad\quad}\text{ moles air}\left(\underline{\quad\quad}\frac{\text{moles O}_2}{\text{moles air}}\right)\left(\underline{\quad}\frac{\text{moles O}}{\text{mol O}_2}\right)=n_2\text{ moles O}_2\left(\underline{\quad}\frac{\text{moles O}}{\text{mol O}_2}\right)+n_4\text{ moles CO}\left(\underline{\quad}\frac{\text{moles O}}{\text{mol CO}}\right)$$

$$+n_5\text{ moles CO}_2\left(2\frac{\text{moles O}}{\text{mol CO}_2}\right)+n_6\text{ moles H}_2\text{O}\left(1\frac{\text{mol O}}{\text{mol H}_2\text{O}}\right)$$

substituting the known values of n_4, n_5 and n_6, and solving for n_2:

$$n_2=\frac{\underline{\quad\quad\quad}\text{ moles O}-\underline{\quad\quad}\text{ moles O}-\underline{\quad\quad\quad}\text{ moles O}-\underline{\quad\quad\quad}\text{ moles O}}{\left(\underline{\quad}\frac{\text{moles O}}{\text{mol O}_2}\right)}$$

$$n_2=\underline{\quad\quad\quad}\text{ moles O}_2$$

Now that the amounts of moles of each molecular specie exiting the reactor are known, the molar fractions can be calculated as shown below:

$$x_i=\frac{n_i}{n_T}$$

where the sub index *i*, represents each of the species present in the stack gases.

In order to use this equation, first we need to determine the total number of moles exiting the reactor, n_T:

$$n_T = n_1 + n_2 + n_3 + n_4 + n_5 + n_6$$

substituting the number of moles of each gas:

$$n_T = \_\_ \text{ moles} + \_\_\_\_\_ \text{ moles} + \_\_\_\_\_ \text{ moles} + \_\_\_ \text{ moles} + \_\_\_\_\_ \text{ moles} + \_\_\_\_ \text{ moles}$$

$$n_T = \_\_\_\_\_ \text{ moles}$$

And the composition of the gas produced by the combustion process is calculated as follows:

$$x_1 = \frac{n_1}{n_T} = \frac{\_\_ \text{ moles } CH_4}{\_\_\_\_\_ \text{ moles}}$$

$$\boxed{x_1 = \_\_\_\_\_ \frac{\text{moles } CH_4}{\text{mol}}}$$

$$x_4 = \frac{n_4}{n_T} = \frac{\_\_\_\_ \text{ moles } CO}{\_\_\_\_\_ \text{ moles}}$$

$$\boxed{x_4 = \_\_\_\_\_ \frac{\text{moles } CO}{\text{mol}}}$$

$$x_2 = \frac{n_2}{n_T} = \frac{\_\_\_\_ \text{ moles } O_2}{\_\_\_\_\_ \text{ moles}}$$

$$\boxed{x_2 = \_\_\_\_\_ \frac{\text{moles } O_2}{\text{mol}}}$$

$$x_5 = \frac{n_5}{n_T} = \frac{\_\_\_\_ \text{ moles } CO_2}{\_\_\_\_\_\_ \text{ moles}}$$

$$\boxed{x_5 = \_\_\_\_\_ \frac{\text{moles } CO_2}{\text{mol}}}$$

$$x_3 = \frac{n_3}{n_T} = \frac{\_\_\_\_\_ \text{ moles } N_2}{\_\_\_\_\_ \text{ moles}}$$

$$\boxed{x_3 = \_\_\_\_\_ \frac{\text{moles } N_2}{\text{mol}}}$$

$$x_6 = \frac{n_6}{n_T} = \frac{\_\_\_\_ \text{ moles } H_2O}{\_\_\_\_\_ \text{ moles}}$$

$$\boxed{x_6 = \_\_\_\_\_ \frac{\text{moles } H_2O}{\text{mol}}}$$

Example 4.8-4 Combustion of a Hydrocarbon Fuel of Unknown Composition

A hydrocarbon gas is burned in the firebox of a steam-methane reforming process. The composition of the stack gases exiting the firebox is 1.6 mol % CO, 9.6 mol % CO_2, 4.9 mol % O_2 and 83.9 mol % N_2 on a dry basis.

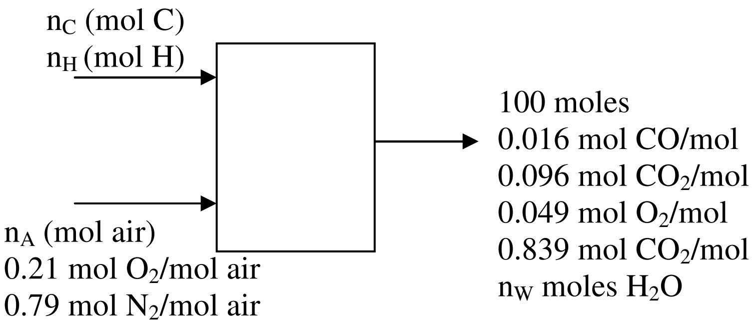
(a) Determine what is the fuel entering the combustion reactor, by calculating the ratio of hydrogen to carbon in the fuel.

Strategy

This problem can be solved using material balances on the atomic species. Since the composition of the fuel is unknown, we need to solve for the number of carbon and hydrogen atoms. A basis of 100 moles of dry stack gases will be selected.

Solution

We will start by making a diagram of this process:



Water will be exiting in the stack gases because the fuel being burned is a hydrocarbon.

The carbon and hydrogen in the fuel will produce carbon monoxide, carbon dioxide and water according to the following reactions:

$$C + O_2 \longrightarrow CO_2$$

$$2C + O_2 \longrightarrow 2CO$$

$$4H + O_2 \longrightarrow 2H_2O$$

Since the nitrogen is not reacting, we can perform material balances and use the molar fraction of nitrogen in the product and in the air streams to determine the amount of air being fed into the reactor.

N balance

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

$$n_A\left(\_\_\_\_\_\ \frac{\text{moles } N_2}{\text{mol air}}\right) = \_\_\_\_\_\ \text{moles}\left(\_\_\_\_\_\ \frac{\text{moles } N_2}{\text{mol}}\right)$$

$$n_A = \_\_\_\_\_\ \text{moles } N_2$$

The number of carbons entering the reactor, can be calculated by doing material balances on atomic carbon.

C balance

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

$$n_C = \_\_\_\_\_\ \text{moles}\left[\left(\_\_\_\_\_\ \frac{\text{moles CO}}{\text{mol}}\right)\left(\frac{1 \text{ mol C}}{\text{mol CO}}\right) + \left(\_\_\_\_\_\ \frac{\text{moles } CO_2}{\text{mol}}\right)\left(\frac{1 \text{ mol C}}{\text{mol } CO_2}\right)\right]$$

$$n_C = \_\_\_\_\_\ \text{moles C}$$

Now that the number of carbons entering the reactor is known, the relationship between the hydrogen feed rate n_H, and the water production rate n_W, can be determined from a hydrogen balance:

H balance

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

$$n_H = \_\_\_\left(\frac{2 \text{ moles } H_2}{\text{mol } H_2O}\right)$$

As it can be seen, the number of moles of water exiting the firebox is still unknown, but we can calculate it from a material balance on oxygen.

O balance

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

$$0.21\ \_\_\_\left(\frac{2 \text{ mol O}}{\text{mol } O_2}\right) = n_W \text{ mol } H_2O\left(\frac{1 \text{ mol O}}{\text{mol } H_2O}\right) + 100 \text{ moles}\left[\left(\_\_\_\_\_\ \frac{\text{moles CO}}{\text{mol}}\right)\left(\frac{1 \text{ mol O}}{\text{mol CO}}\right)\right.$$

$$\left. + \left(\_\_\_\_\_\ \frac{\text{moles } CO_2}{\text{mol}}\right)\left(\frac{2 \text{ mol O}}{\text{mol } CO_2}\right) + \left(\_\_\_\_\_\ \frac{\text{moles } O_2}{\text{mol}}\right)\left(\frac{2 \text{ mol O}}{\text{mol } O_2}\right)\right]$$

Solving for n_W:

$$n_W = \_\_\_\_\_\ \text{moles } H_2O$$

This value for the number of moles of water can be substituted into the hydrogen balance equation to determine the number of hydrogen atoms entering the combustion chamber.

$$n_H = \underline{\qquad} \text{ moles } H_2O\left(\frac{2 \text{ moles H}}{\text{mol } H_2O}\right)$$

$$n_H = \underline{\qquad} \text{ moles H}$$

The hydrogen to carbon ratio will be given by:

$$\frac{n_H}{n_C} = \frac{\underline{\qquad} \text{ moles H}}{\underline{\qquad} \text{ moles C}}$$

$$\boxed{\frac{n_H}{n_C} = \underline{\qquad} \frac{\text{moles H}}{\text{moles C}}}$$

The composition of the fuel will be then described by the general formula: $(CH\_\_)_N$. This general equation can be multiplied by a factor *N*=__ in order to get an even number of hydrogen atoms. This will yield:

$$\boxed{(CH\_\_)\_ = C\_H\_\_}$$

Hence, the fuel being used in this process is butane.

(b) Determine the percent excess air for the complete combustion of the carbon and hydrogen in the fuel.

Strategy

First, the theoretical amount of oxygen must be determined. For this, we will consider only the reaction for the complete combustion of the fuel (no carbon monoxide will be produced).

Solution

The reactions occurring in this problem are:

$$C + O_2 \longrightarrow CO_2$$

$$4H + O_2 \longrightarrow 2H_2O$$

These equations can be used to determine the theoretical oxygen required:

$$n_{O_2,\text{theoretical}} = \underline{\qquad} \text{ moles C}\left(\frac{1 \text{ mol } O_2}{1 \text{ mol C}}\right) + \underline{\qquad} \text{ moles H}\left(\frac{1 \text{ mol } O_2}{\underline{\quad} \text{ mol H}}\right)$$

$$n_{O_2,\text{theoretical}} = \underline{\qquad}\ \text{moles } O_2$$

The actual amount of oxygen being fed into the reactor is given by:

$$n_{O_2,\text{fed}} = \underline{\qquad}\ \text{moles air}\left(\underline{\qquad}\ \frac{\text{mol } O_2}{\text{mol air}}\right)$$

$$n_{O_2,\text{fed}} = \underline{\qquad}\ \text{moles } O_2$$

Now, from the definition of percent excess air:

$$\%\ \text{excess air} = \frac{\underline{\qquad\qquad}}{n_{O_2,\text{theoretical}}} \times 100 = \frac{\underline{\qquad\qquad\qquad}}{\underline{\qquad\qquad\qquad}} \times 100$$

$$\boxed{\%\ \text{excess air} = \underline{\qquad}\ \%}$$