

CRYOGENIC ENGINEERING

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Lecture No - 19

Earlier Lecture

- Synthetic membranes, Adsorption, Absorption and distillation are some of the common techniques of Gas Separation.
- Mixing of two different gases is an irreversible process because unmixing or separation requires work input.
- Ideal work requirement per mole of mixture to separate a mixture with **N** constituents is given by

$$\frac{-W_i}{n_m} = \mathfrak{R}T_m \sum_{j=1}^N y_j \ln \left(\frac{1}{y_j} \right)$$

- where y_j is mole fraction of j^{th} component.

Outline of the Lecture

Topic : Gas Separation (contd)

- Ideal Gas Separation System
 - Tutorials
 - Parametric study
 - 3 – Gas mixtures

Mixture Composition

- In general, the composition of any mixture can be specified in three different ways. They are
 - Volume percentage
 - Weight percentage
 - Mole Fraction
- In most of the Gas separation problems, the correlations are based on mole fractions.
- Hence, all percentages have to be ultimately expressed in the mole fractions.

Tutorial – 1

- Consider a mixture of **Gas A** and **Gas B** with a composition of 60% and 40% respectively by weight. Determine the mole fraction of **Gas A** and **Gas B**, if the temperature and the pressure of the mixture are 300 K and 1.013 bar respectively. Given that the molecular weight of **Gas A** and **Gas B** are 28g/mol and 32g/mol respectively.
- Calculate the mole fractions if the above percentages are given on volume basis.

Tutorial – 1

Given

Working Pressure : 1 atm

Temperature : 300 K

Mixture Composition

I | 60% A + 40% B by w/w.

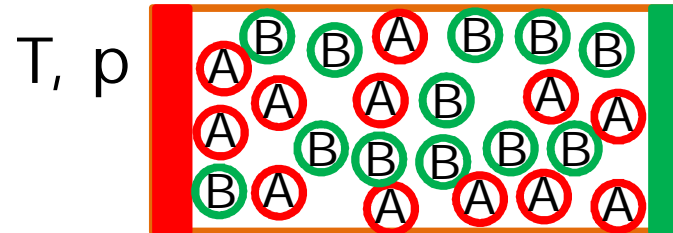
II | 60% A + 40% B by v/v.

For above mixtures, Calculate

1 | y_A and y_B

Tutorial – 1

- 60% A + 40% B w/w.



- Let the mass of the mixture be x gm. Then the mass of the **Gas A** in the mixture is $0.6x$ gm.

- The number of moles of **Gas A** are

$$n_a = \frac{0.6x}{28}$$

- The number of moles of **Gas B** are

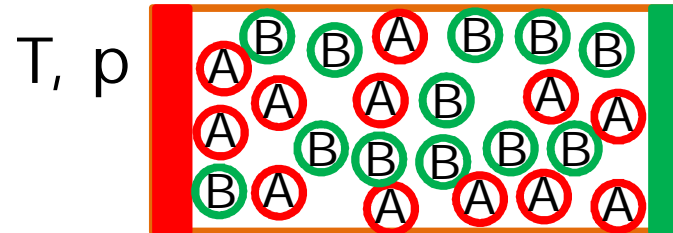
$$n_b = \frac{0.4x}{32}$$

- Total moles in the mixture are

$$n_{tot} = \frac{0.6x}{28} + \frac{0.4x}{32}$$

Tutorial – 1

- 60% A + 40% B w/w.



Gas A

$$y_a = \frac{n_a}{n_{tot}} = \frac{\frac{0.6x}{28}}{\frac{0.6x}{28} + \frac{0.4x}{32}}$$

$$y_a = 0.631$$

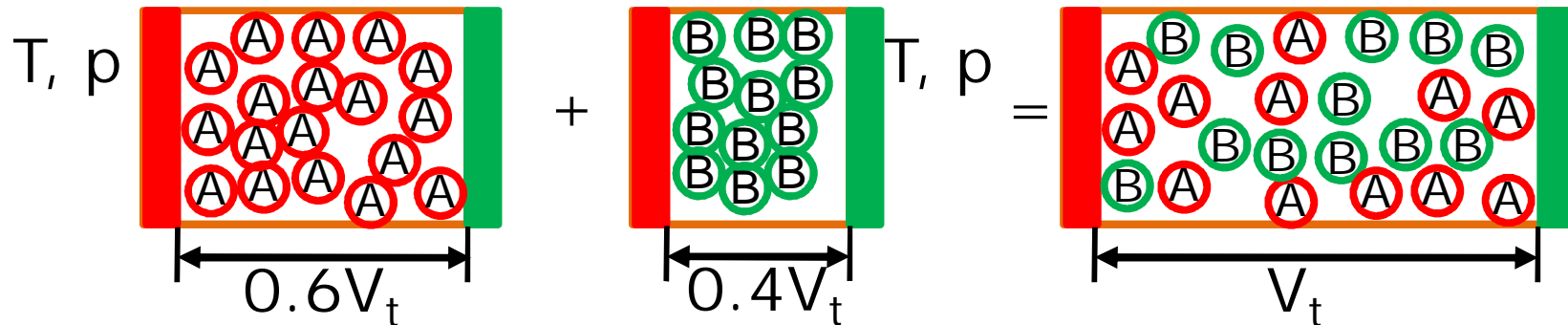
Gas B

$$y_b = \frac{n_b}{n_{tot}} = \frac{\frac{0.4x}{32}}{\frac{0.6x}{28} + \frac{0.4x}{32}}$$

$$y_b = 0.369$$

Tutorial – 1

- 60% A + 40% B v/v.



- Let the moles of **Gas A** be n_a . Using the Ideal Gas Law,

$$n_a = \frac{p(0.6V_t)}{\mathcal{R}T}$$

- Similarly, the moles of **Gas B** is

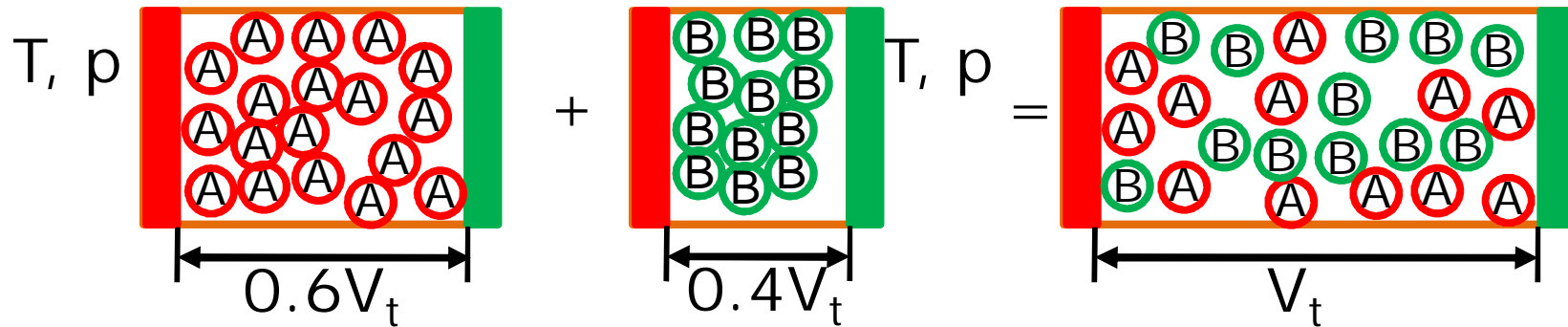
$$n_b = \frac{p(0.4V_t)}{\mathcal{R}T}$$

- The total moles is

$$n_{tot} = \frac{p(0.6V_t)}{\mathcal{R}T} + \frac{p(0.4V_t)}{\mathcal{R}T}$$

Tutorial – 1

- 60% A + 40% B v/v.



$$\frac{n_a}{n_{tot}} = \frac{\boxed{\text{Gas A}} \cancel{0.6} \frac{\cancel{p(V_t)}}{\cancel{\mathcal{R}T}}}{\cancel{0.6} \frac{\cancel{p(V_t)}}{\cancel{\mathcal{R}T}} + \cancel{0.4} \frac{\cancel{p(V_t)}}{\cancel{\mathcal{R}T}}}$$

$$y_a = 0.6$$

$$\frac{n_b}{n_{tot}} = \frac{\boxed{\text{Gas B}} \cancel{0.4} \frac{\cancel{p(V_t)}}{\cancel{\mathcal{R}T}}}{\cancel{0.6} \frac{\cancel{p(V_t)}}{\cancel{\mathcal{R}T}} + \cancel{0.4} \frac{\cancel{p(V_t)}}{\cancel{\mathcal{R}T}}}$$

$$y_b = 0.4$$

Volume fraction = mole fraction

Ideal Separation System

- The Ideal work of separation per mole of mixture (**Gas A** and **Gas B**) is given by

$$\frac{-W_{i,m}}{n_m} = \mathcal{R}T_m \left(y_a \ln \left(\frac{1}{y_a} \right) + y_b \ln \left(\frac{1}{y_b} \right) \right)$$

- On the similar lines, if the mixture is composed of three different gases, say **Gas A**, **Gas B** and **Gas C**, the Ideal work of separation per mole of mixture is given by

$$\frac{-W_{i,m}}{n_m} = \mathcal{R}T_m \left(y_a \ln \left(\frac{1}{y_a} \right) + y_b \ln \left(\frac{1}{y_b} \right) + y_c \ln \left(\frac{1}{y_c} \right) \right)$$

- Where y_a , y_b and y_c are the mole fractions of **Gas A**, **Gas B** and **Gas C** respectively.

Tutorial – 2

- Determine the $W_{i,m}/n_m$, $W_{i,m}/n_{N_2}$, $W_{i,m}/n_{O_2}$ for the separation of mixture of gases consisting of 80% N_2 and 20% O_2 by mole fraction. The mixture is at 300 K and a pressure of 1.013 bar (1 atm). The mol. wt. of N_2 and O_2 are 28 and 32 g/mol respectively.
- For the above problem, also calculate the ideal work requirement for the unit mass of N_2 and O_2 respectively.

Tutorial – 2

Given

Working Pressure : 1 atm

Temperature : 300 K

Mixture : 80% N₂ + 20% O₂ by mole fraction

For above mixture, Calculate

$W_{i,m}/n_m$	Work of separation of mixture/mole of mixture
$W_{i,m}/n_{O_2}$	Work of separation of mixture/mole of Oxygen
$W_{i,m}/n_{N_2}$	Work of separation of mixture/mole of Nitrogen
$W_{i,m}/m_{O_2}$	Work of separation of mixture/mass of Oxygen
$W_{i,m}/m_{N_2}$	Work of separation of mixture/mass of Nitrogen

Tutorial – 2

- Ideal Work/mole of mixture

$$\frac{-W_{i,m}}{n_m} = \mathcal{R}T_m \left(y_a \ln \left(\frac{1}{y_a} \right) + y_b \ln \left(\frac{1}{y_b} \right) \right)$$

Data

$$\mathcal{R} = 8.314 \text{ J/mol} - \text{K}$$

$$T_m = 300 \text{ K}$$

$$y_a = 0.8 \text{ (mole fraction of N}_2\text{)}$$

$$y_b = 0.2 \text{ (mole fraction of O}_2\text{)}$$

$$\frac{-W_{i,m}}{n_m} = (8.314)(300) \left(0.8 \ln \left(\frac{1}{0.8} \right) + 0.2 \ln \left(\frac{1}{0.2} \right) \right) = 1248.1 \text{ J / mol}$$

Tutorial – 2

- Ideal Work/mole of N₂

$$\frac{-W_{i,m}}{n_{N_2}} = \left(\frac{-W_{i,m}}{n_m} \right) \left(\frac{n_m}{n_{N_2}} \right) \left(\frac{n_m}{n_{N_2}} \right) = \frac{1}{y_{N_2}}$$

$$\frac{-W_{i,m}}{n_{N_2}} = \left(\frac{-W_{i,m}}{n_m} \right) \left(\frac{1}{y_{N_2}} \right)$$

$$\frac{-W_{i,m}}{n_m} = 1248.1 \quad y_{N_2} = 0.8$$

$$\frac{-W_{i,m}}{n_{N_2}} = \frac{1248.1}{0.8} = 1560.1 \text{ J / mol - N}_2$$

Tutorial – 2

- Ideal Work/mole of O₂

$$\frac{-W_{i,m}}{n_{O_2}} = \left(\frac{-W_{i,m}}{n_m} \right) \left(\frac{1}{y_{O_2}} \right)$$

$$\frac{-W_{i,m}}{n_m} = 1248.1$$

$$y_{O_2} = 0.2$$

$$\frac{-W_{i,m}}{n_{O_2}} = \frac{1248.1}{0.2} = 6240.5 \text{ J / mol - O}_2$$

Tutorial – 2

- Ideal Work/mass of N₂

$$\left(\frac{-W_{i,m}}{m_{N_2}} \right) = \left(\frac{-W_{i,m}}{n_{N_2}} \right) \left(\frac{n_{N_2}}{m_{N_2}} \right) \quad \frac{n_{N_2}}{m_{N_2}} = \left(\frac{1}{molw_{N_2}} \right)$$

$$\frac{-W_{i,m}}{m_{N_2}} = \left(\frac{-W_{i,m}}{n_{N_2}} \right) \left(\frac{1}{molw_{N_2}} \right)$$

$$\frac{-W_{i,m}}{n_{N_2}} = 1560.1 \quad molw_{N_2} = 28$$

$$\frac{-W_{i,m}}{m_{N_2}} = \frac{1560.1}{28} = 55.71 \text{ J / gm} - N_2$$

Tutorial – 2

- Ideal Work/mass of O₂

$$\frac{-W_{i,m}}{m_{O_2}} = \left(\frac{-W_{i,m}}{n_{O_2}} \right) \left(\frac{1}{molw_{O_2}} \right)$$

$$\frac{-W_{i,m}}{n_{O_2}} = 6240.5$$

$$molw_{O_2} = 32$$

$$\frac{-W_{i,m}}{m_{O_2}} = \frac{6240.5}{32} = 195.01 \text{ J / gm-O}_2$$

Tutorial – 2

- Tabulating the results, we have

Work	300 K, 1 atm	
$W_{i,m}/n_m$	1248.1	
$W_{i,m}/n_{N_2}$	1560.1	$W_{i,m}/m_{N_2}$ 55.71
$W_{i,m}/n_{O_2}$	6240.5	$W_{i,m}/m_{O_2}$ 195.01

- $W_{i,m}/n_m$ is always less than the $W_{i,m}/n_{N_2}$ or $W_{i,m}/n_{O_2}$ because $n_m = n_{N_2} + n_{O_2}$.

Parametric Study

- As mentioned earlier, the ideal work of separation for a mixture of **Gas A** and **Gas B** is given by

$$\frac{-W_{i,m}}{n_m} = \mathcal{R}T_m \left(y_a \ln \left(\frac{1}{y_a} \right) + y_b \ln \left(\frac{1}{y_b} \right) \right)$$

- Since, y_a and y_b are the mole fractions of **Gas A** and **Gas B** respectively, the following condition is true at all times.

$$y_a + y_b = 1 \longrightarrow y_b = 1 - y_a$$

- Substituting, we have

$$\frac{-W_{i,m}}{n_m} = \mathcal{R}T_m \left(y_a \ln \left(\frac{1}{y_a} \right) + (1 - y_a) \ln \left(\frac{1}{1 - y_a} \right) \right)$$

Parametric Study

$$\frac{-W_{i,m}}{n_m} = RT_m \left(y_a \ln \left(\frac{1}{y_a} \right) + (1 - y_a) \ln \left(\frac{1}{1 - y_a} \right) \right)$$

- It is clear that the ideal work of separation for a mixture is dependent on the mole fractions (y_a and y_b) of **Gas A** and **Gas B** respectively.
- Also, the work requirement decreases with the decrease in the temperature.
- The effect of y_a and the separation temperature on the ideal work requirement is studied in a greater detail through the next tutorial.

Tutorial – 3

- Consider mixtures of **Gas A** and **Gas B** with the following compositions in mole fractions.

Mixture Composition

I	30% A + 70% B
II	50% A + 50% B
III	60% A + 40% B
IV	80% A + 20% B

- Determine the $W_{i,m}/n_m$, $W_{i,m}/n_A$, $W_{i,m}/n_B$ for the separation of this mixture given that the mixture is at 300 K and 200 K. The mixture pressure is 1.013 bar (1 atm).

Tutorial – 3

Given

Working Pressure : 1 atm

Temperature : 300 K and 200 K

Mixture Composition

I	30% A + 70% B
II	50% A + 50% B
III	60% A + 40% B
IV	80% A + 20% B

For above mixtures, Calculate

$W_{i,m}/n_m$	Work of separation of mixture/mole of mixture
$W_{i,m}/n_A$	Work of separation of mixture/mole of Gas A
$W_{i,m}/n_B$	Work of separation of mixture/mole of Gas B

Methodology

- The two separation temperatures under study are 300 K and 200 K.
- In this tutorial, the $W_{i,m}/n_m$, $W_{i,m}/n_A$, $W_{i,m}/n_B$ are calculated only for 300 K and mixture III.
- All other calculations pertaining to 200 K and other mixtures are left as an exercise to the students.
- The data is plotted graphically in the further slides.

Tutorial – 3

- Ideal Work/mole of mixture – III

$$\frac{-W_{i,m}}{n_m} = \mathcal{R}T_m \left(y_A \ln \left(\frac{1}{y_A} \right) + y_B \ln \left(\frac{1}{y_B} \right) \right)$$

Data

$$\mathcal{R} = 8.314 \text{ J/mol} \cdot \text{K}$$

$$T_m = 300 \text{ K}$$

$$y_A = 0.6 \text{ (mole fraction of A)}$$

$$y_B = 0.4 \text{ (mole fraction of B)}$$

$$\frac{-W_{i,m}}{n_m} = (8.314)(300) \left(0.6 \ln \left(\frac{1}{0.6} \right) + 0.4 \ln \left(\frac{1}{0.4} \right) \right) = 1678.6 \text{ J/mol}$$

Tutorial – 3

- Ideal Work/mole of A

$$\frac{-W_{i,m}}{n_A} = \left(\frac{-W_{i,m}}{n_m} \right) \left(\frac{1}{y_A} \right)$$

$$\frac{-W_{i,m}}{n_m} = 1678.6 \quad y_A = 0.6$$

$$\frac{-W_{i,m}}{n_A} = \frac{1678.6}{0.6} = 2797.6 \text{ J / mol - A}$$

Tutorial – 3

- Ideal Work/mole of B

$$\frac{-W_{i,m}}{n_B} = \left(\frac{-W_{i,m}}{n_m} \right) \left(\frac{1}{y_B} \right)$$

$$\frac{-W_{i,m}}{n_m} = 1678.6 \quad y_B = 0.4$$

$$\frac{-W_{i,m}}{n_B} = \frac{1678.6}{0.4} = 4196.5 \text{ J / mol - B}$$

Tutorial – 3

- Extending the calculations for all other mixtures at 300 K temperature, we have the following table.

300 K	$W_{i,m}/n_m$	$W_{i,m}/n_A$	$W_{i,m}/n_B$
0.3A + 0.7B	1523	5078	2176
0.5A + 0.5B	1728	3457	3457
0.6A + 0.4B	1678	2797	4196
0.8A + 0.2B	1248	1560	6240

- For any given mixture, applying the same analogy, the $W_{i,m}/n_m$ is always less as compared to either $W_{i,m}/n_A$ or $W_{i,m}/n_B$.

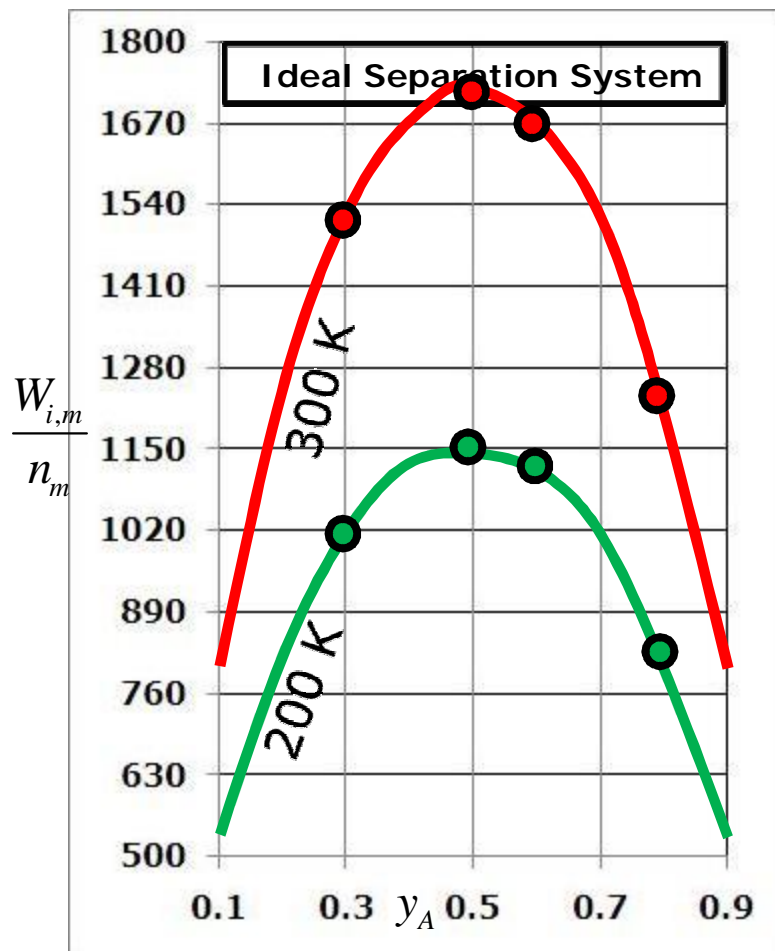
Tutorial – 3

- Similarly, the calculations for all other mixtures at 200 K temperature, the results are as tabulated below.

200 K	$W_{i,m}/n_m$	$W_{i,m}/n_A$	$W_{i,m}/n_B$
0.3A + 0.7B	1015	3385	1451
0.5A + 0.5B	1152	2305	2305
0.6A + 0.4B	1119	1865	2797
0.8A + 0.2B	832	1040	4160

Tutorial – 3

- $W_{i,m}/n_m$ v/s. y_A



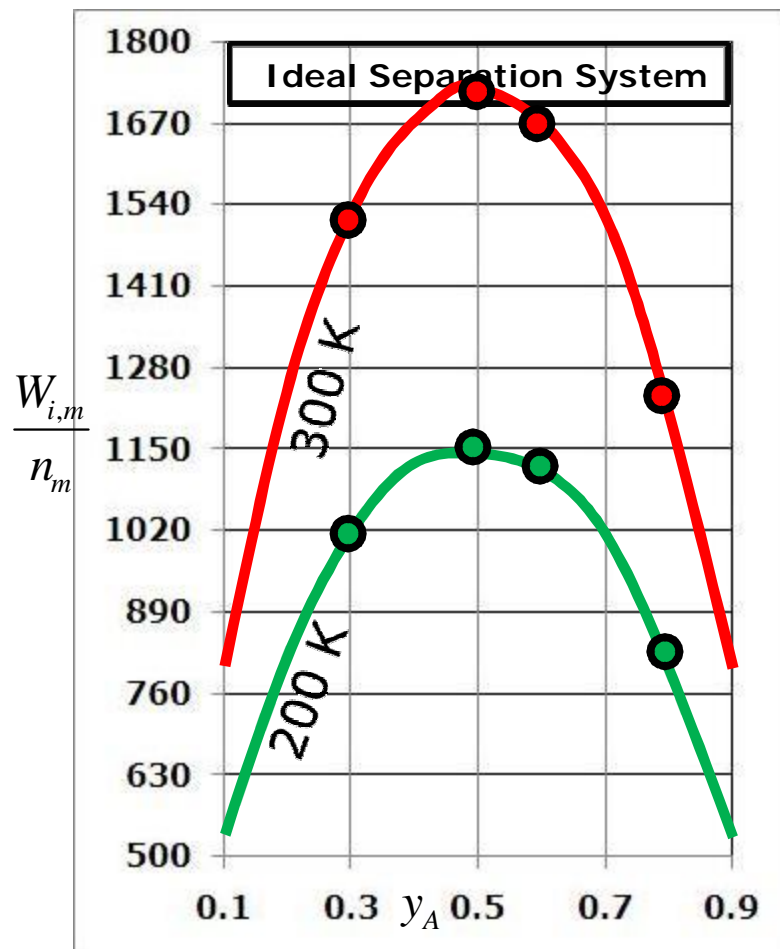
- The Plot for $W_{i,m}/n_m$ versus y_A for 300 K and 200 K are as shown.

300K	y_A	$W_{i,m}/n_m$
I	0.3	1523
II	0.5	1728
III	0.6	1678
IV	0.8	1248

200K	y_A	$W_{i,m}/n_m$
I	0.3	1015
II	0.5	1152
III	0.6	1119
IV	0.8	832

Tutorial – 3

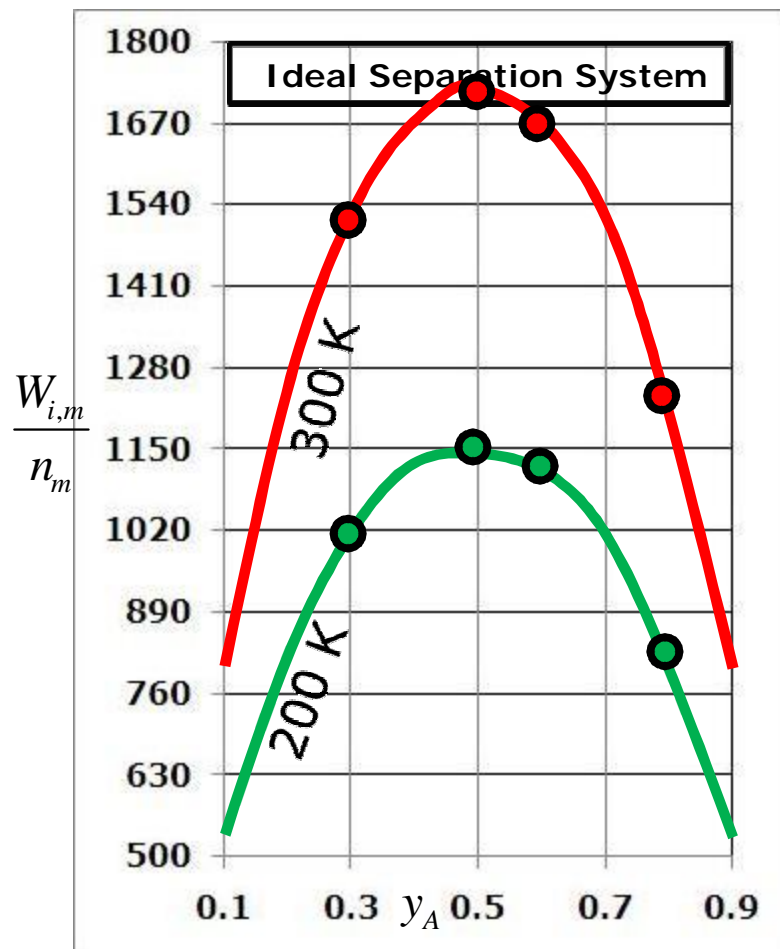
- $W_{i,m}/n_m$ v/s. y_A



- It is clear that the $W_{i,m}/n_m$ decreases with the decrease in the separation temperature.
- Also for a given mixture and temperature, the $W_{i,m}/n_m$ crosses a maxima.
- This maxima occurs when the mole fractions of **Gas A** and **Gas B** are equal.

Tutorial – 3

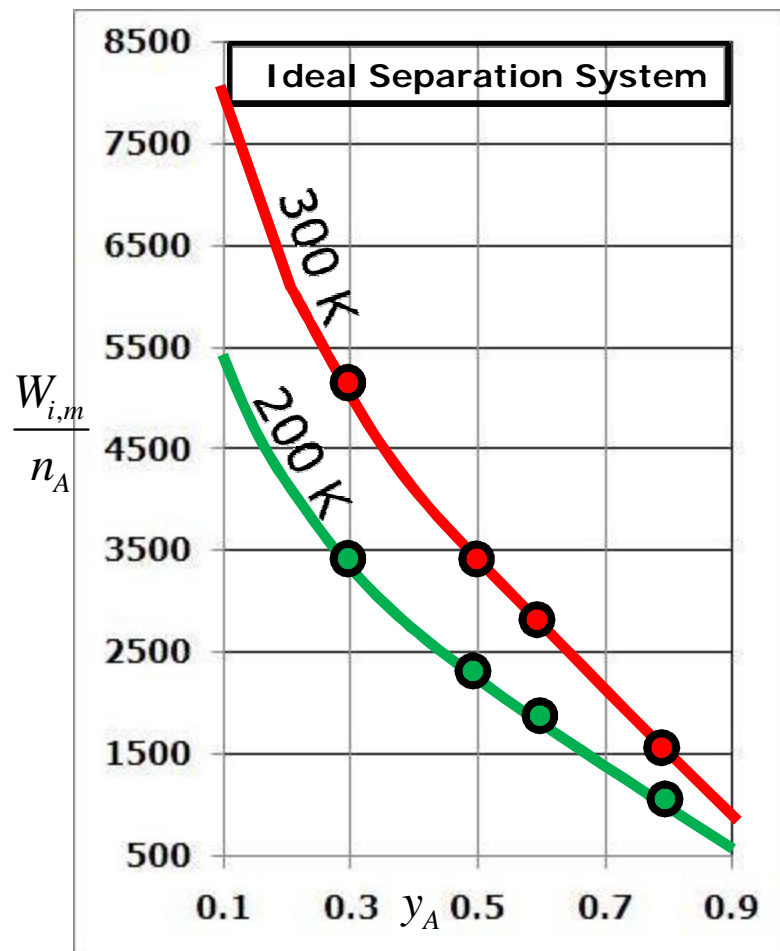
- $W_{i,m}/n_m$ v/s. y_A



- In case of a three gas mixture say **Gas A, B** and **C**, the horizontal position of maxima occurs when
 - $y_A = y_B = y_C = 0.33$
- This position of the maxima is independent of the separation temperature.

Tutorial – 3

- $W_{i,m}/n_A$ v/s. y_A



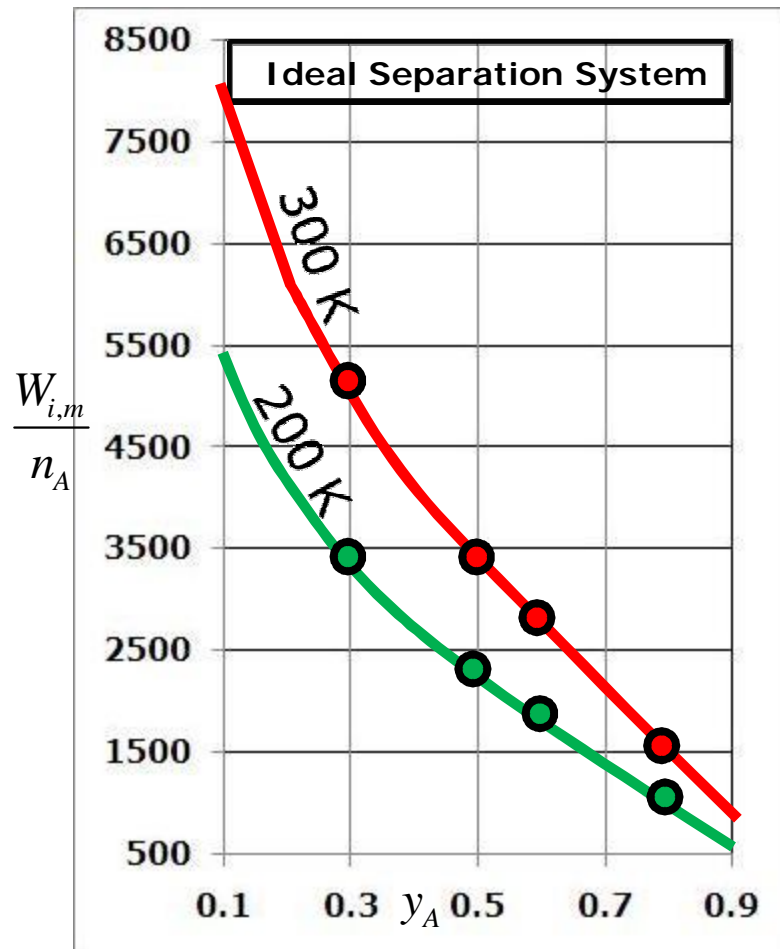
- The Plot for $W_{i,m}/n_A$ versus y_A for 300 K and 200 K are as shown.

300K	y_A	$W_{i,m}/n_A$
I	0.3	5078
II	0.5	3457
III	0.6	2797
IV	0.8	1560

200K	y_A	$W_{i,m}/n_A$
I	0.3	3385
II	0.5	2305
III	0.6	1865
IV	0.8	1040

Tutorial – 3

- $W_{i,m}/n_A$ v/s. y_A



- It is clear that the $W_{i,m}/n_A$ decreases with the decrease in the separation temperature.
- Also for a given mixture and temperature, there is a steep decrease in the $W_{i,m}/n_A$ with the increase in the concentration of a particular ingredient (here **Gas A**).

Gas Separation

- For a mixture with two ingredients, the separation results into two separate components.
- But, for a mixture with three ingredients, say **Gas A**, **Gas B** and **Gas C**, the following cases of separation are possible.
 - All three gases are separated from each other.
 - Only one gas is separated leaving the other two mixed.
- The following tutorial is taken up to have a better understanding of these concepts.

Tutorial – 4

- Consider Air as a mixture of 78% N₂, 21% O₂ and 1% Argon by mole fractions. Determine the work requirement per unit mole of Argon, when all the three gases are separated and only when Argon is separated. The mixture is at 300 K and at a pressure of 1.013 bar (1 atm).
- For the above problem, calculate the above parameters for the case of Oxygen. Comment on the results.

Tutorial – 4

Given

Working Pressure : 1 atm

Temperature : 300 K

Mixture : 78% N₂ + 21% O₂ + 1% (mol. fr.)

Calculate

$W_{i,m}/n_m$	$W_{i,m}/n_{Ar}$
$W_{i,Ar}/n_m$	$W_{i,m}/n_{O_2}$
$W_{i,O_2}/n_m$	$W_{i,Ar}/n_{Ar}$
	$W_{i,O_2}/n_{O_2}$

Tutorial – 4

- $W_{i,m}/n_m$

$$\frac{-W_{i,m}}{n_m} = \mathfrak{R}T_m \left(y_{Ar} \ln \left(\frac{1}{y_{Ar}} \right) + y_{O_2} \ln \left(\frac{1}{y_{O_2}} \right) + y_{N_2} \ln \left(\frac{1}{y_{N_2}} \right) \right)$$

Data

$$\mathfrak{R} = 8.314 \text{ J/mol} - \text{K}$$

$$T_m = 300 \text{ K}$$

Data

$$y_{N_2} = 0.78 \text{ (N}_2\text{)}$$

$$y_{O_2} = 0.21 \text{ (O}_2\text{)}$$

$$y_{Ar} = 0.01 \text{ (Ar)}$$

$$\frac{-W_{i,m}}{n_m} = (8.314)(300) \left(\begin{array}{l} 0.78 \ln \left(\frac{1}{0.78} \right) + 0.21 \ln \left(\frac{1}{0.21} \right) \\ + 0.01 \ln \left(\frac{1}{0.01} \right) \end{array} \right) = 1415.6 \text{ J/mol}$$

Tutorial – 4

- $W_{i,m}/n_{Ar}$

$$\frac{-W_{i,m}}{n_m} = 1415.6$$

$$y_{Ar} = 0.01$$

$$\frac{-W_{i,m}}{n_{Ar}} = \frac{1415.6}{0.01} = 141560 \text{ J / mol - Ar}$$

Tutorial – 4

- $W_{i,m}/n_{O_2}$

$$\frac{-W_{i,m}}{n_m} = 1415.6$$

$$y_{O_2} = 0.21$$

$$\frac{-W_{i,m}}{n_{O_2}} = \frac{1415.6}{0.21} = 6740.9 \text{ J / mol - O}_2$$

Tutorial – 4

- $W_{i,Ar}/n_m$

$$\frac{-W_{i,Ar}}{n_m} = \mathfrak{R}T_m \left(y_{Ar} \ln \left(\frac{1}{y_{Ar}} \right) + y_{O_2+N_2} \ln \left(\frac{1}{y_{O_2+N_2}} \right) \right)$$

Data

$$\mathfrak{R} = 8.314 \text{ J/mol} - \text{K}$$

$$T_m = 300 \text{ K}$$

$$y_{Ar} = 0.01 \text{ (Ar)}$$

$$y_{O_2+N_2} = 0.99 \text{ (N}_2\text{+O}_2\text{)}$$

$$\frac{-W_{i,Ar}}{n_m} = (8.314)(300) \left(0.99 \ln \left(\frac{1}{0.99} \right) + 0.01 \ln \left(\frac{1}{0.01} \right) \right) = 139.6 \text{ J/mol}$$

Tutorial – 4

- $W_{i,Ar}/n_{Ar}$

$$\frac{-W_{i,Ar}}{n_m} = 139.6$$

$$y_{Ar} = 0.01$$

$$\frac{-W_{i,Ar}}{n_{Ar}} = \frac{139.6}{0.01} = 13960 \text{ J / mol - Ar}$$

Tutorial – 4

- $W_{i,O_2}/n_m$

$$\frac{-W_{i,O_2}}{n_m} = \mathcal{R}T_m \left(y_{O_2} \ln \left(\frac{1}{y_{O_2}} \right) + y_{Ar+N_2} \ln \left(\frac{1}{y_{Ar+N_2}} \right) \right)$$

Data

$$\mathcal{R} = 8.314 \text{ J/mol} - \text{K}$$

$$T_m = 300 \text{ K}$$

$$y_{O_2} = 0.21 \text{ (O}_2\text{)}$$

$$y_{N_2+O_2} = 0.78 \text{ (N}_2\text{+Ar)}$$

$$\frac{-W_{i,O_2}}{n_m} = (8.314)(300) \left(0.78 \ln \left(\frac{1}{0.78} \right) + 0.21 \ln \left(\frac{1}{0.21} \right) \right) = 1300.8 \text{ J/mol}$$

Tutorial – 4

- $W_{i,O_2}/n_{O_2}$

$$\frac{-W_{i,O_2}}{n_m} = 1300.8 \quad y_{O_2} = 0.21$$

$$\frac{-W_{i,O_2}}{n_{O_2}} = \frac{1300.8}{0.21} = 6194.3 \text{ J / mol - O}_2$$

Tutorial – 4

- Tabulating the results, we have

Work	300 K	Work	300 K
$W_{i,m}/n_m$	1415.6	$W_{i,m}/n_{Ar}$	141560
$W_{i,Ar}/n_m$	139.6	$W_{i,m}/n_{O_2}$	6740.9
$W_{i,O_2}/n_m$	1300.8	$W_{i,Ar}/n_{Ar}$	13960
		$W_{i,O_2}/n_{O_2}$	6194.3

Summary

- In general, the composition of any mixture can be specified in three different ways. They are Volume percentage, Weight percentage and Mole Fraction.
- Work/mole of mixture is always less than work/mole of its constituents for any mixture.
- $W_{i,m}/n_m$ is maximum when the percentage compositions of all its ingredients are equal.
- With the decrease in the percentage, the work/mole of that component increases.

Assignment

- Consider a mixture of 75% **A**, 22% **B** and 3% **C** by mole fractions. Determine the work requirement per unit mole of **C**, when all the three gases are separated and only when **C** is separated. The mixture is at 300 K and at a pressure of 1.013 bar (1 atm).
- For the above problem, calculate the above parameters for the case of **B**. Comment on the results.

Answers

Work	300 K	Work	300 K
$W_{i,m}/n_m$	1631.3	$W_{i,m}/n_c$	54379
$W_{i,c}/n_m$	336.0	$W_{i,m}/n_B$	2471.7
$W_{i,B}/n_m$	1314.2	$W_{i,c}/n_c$	11202
		$W_{i,B}/n_B$	5973.6

Thank You!