Lecture 5.

Ideal Gas Calculations
What is an ideal gas?

An ideal gas is an imaginary gas that obeys exactly the following relationship:

\[ PV = nRT \]

where

\( P \) = absolute pressure of the gas
\( V \) = total volume occupied by the gas
\( n \) = number of moles of the gas
\( R \) = ideal gas constants in appropriate units
\( T \) = absolute temperature of the gas
The Ideal Gas Constant, $R$

$$R = 1.987 \text{ cal/(gmol)(K)}$$
$$= 1.987 \text{ Btu/(lbmol)(^0R)}$$
$$= 10.73 \text{ (psia)(ft}^3\text{)/(lbmol)(^0R)}$$
$$= 8.314 \text{ (kPa)(m}^3\text{)/(kmol)(K)}$$
$$= 8.314 \text{ J/(gmol)(K)}$$
$$= 82.06 \text{ (atm)(cm}^3\text{)/(gmol)(K)}$$
$$= 0.08206 \text{ (atm)(L)/(gmol)(K)}$$
$$= 21.9 \text{ (in. Hg)(ft}^3\text{)/(lbmol)(^0R)}$$
$$= 0.7302 \text{ (atm)(ft}^3\text{)/(lbmol)(^0R)}$$
**Standard Conditions for the Ideal Gas**

Several arbitrarily specified standard states of temperature and pressure have been selected by custom.

<table>
<thead>
<tr>
<th>System</th>
<th>$T_S$</th>
<th>$P_S$</th>
<th>$V_S$</th>
<th>$n_S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SI</td>
<td>273.15 K</td>
<td>101.325 kPa</td>
<td>22.415 m$^3$</td>
<td>1 kmol</td>
</tr>
<tr>
<td>Am. Eng.</td>
<td>492$^0$R</td>
<td>1 atm</td>
<td>359.05 ft$^3$</td>
<td>1 lbmol</td>
</tr>
<tr>
<td>Natural Gas Industry</td>
<td>333.15 K</td>
<td>14.696 psia</td>
<td>379.4 ft$^3$</td>
<td>1 lbmol</td>
</tr>
</tbody>
</table>
**Example 5-1. Ideal Gas Calculation**

Butane (C$_4$H$_{10}$) at 360$^\circ$C and 3.00 atm absolute flows into a reactor at a rate of 1100 kg/h. Calculate the volumetric flow rate of this stream.

**Method A.** Computation using a known value of R.

The ideal gas equation in terms of flowrate:

\[
\frac{PV}{t} = \frac{nRT}{t} \quad \text{or} \quad P \left( \frac{V}{t} \right) = \left( \frac{n}{t} \right) RT
\]

\[\rightarrow \rightarrow \]

\[PV = nRT\]
Example 5-1. Ideal Gas Calculation

Solving for volumetric flowrate:

$$\dot{V} = \frac{n \, RT}{P}$$

Obtaining the molar flowrate from mass flowrate:

$$\dot{n} = \frac{m}{MW} = \frac{1100 \, \text{kg/h}}{58 \, \text{kg/kmol}} = 19.0 \, \text{kmol/h}$$

Using absolute temperatures and pressure:

$$T = 633 \, \text{K} \text{ and } P = 3 \, \text{atm}$$
Example 5-1. Ideal Gas Calculation

Using the following value of \( R \):

\[
R = 0.08206 \text{ L- atm} / \text{gmol-K} \left( \frac{1000 \text{ gmol}}{1 \text{ kmol}} \right) = 82.06 \text{ L- atm} / \text{kmol-K}
\]

The volumetric flowrate is

\[
\vec{V} = \frac{nRT}{P} = \frac{(19.0 \text{ kmol/h})(82.06 \text{ L-atm/kmol-K})(633 \text{ K})}{3 \text{ atm}}
\]

\[
\vec{V} = 328,978.5 \frac{\text{L}}{\text{h}} \left( \frac{1 \text{ m}^3}{1000 \text{ L}} \right) = 329 \frac{\text{m}^3}{\text{h}}
\]
Example 5-1. Ideal Gas Calculation

Method B. By comparison to standard conditions

\[
\frac{PV}{P_s V_s} = \frac{nT}{n_s T_s}
\]

Using a basis of 1 hr, then \( n = 19 \) kmol

The following standard conditions will be used.

\[
\begin{align*}
P_s &= 1 \text{ atm} \\
V_s &= 22.41 \text{ m}^3 \\
n_s &= 1 \text{ kmol} \\
T_s &= 273 \text{ K}
\end{align*}
\]
**Example 5-1. Ideal Gas Calculation**

Solving for $V$:

$$V = \left( \frac{n}{n_S} \right) \left( \frac{T}{T_S} \right) \left( \frac{P_S}{P} \right) V_S$$

$$V = \left( \frac{19.0 \text{ kmol}}{1 \text{ kmol}} \right) \left( \frac{633 \text{ K}}{273 \text{ K}} \right) \left( \frac{1 \text{ atm}}{3 \text{ atm}} \right) 22.415 \text{ m}^3$$

$$V = 329 \text{ m}^3$$

In terms of volumetric flowrate

$$\vec{V} = 329 \text{ m}^3 \text{ h}^{-1}$$
Example 5-2. Ideal Gas at Two Different Conditions

Ten cubic feet of air at 70°F and 1 atm is heated to 610°F and compressed to 2.5 atm. What volume does the gas occupy in its final state?

Let 1 denote the initial state of the gas and 2 the final state.

\[
\frac{P_1V_1}{P_2V_2} = \frac{n_1T_1}{n_2T_2} = \frac{T_1}{T_2}
\]

Solving for \( V_2 \):

\[
V_2 = V_1 \left( \frac{P_1}{P_2} \right) \left( \frac{T_2}{T_1} \right) = 10.0 \text{ ft}^3 \left( \frac{1.00 \text{ atm}}{2.50 \text{ atm}} \right) \left( \frac{1070 \, {}^0\text{R}}{530 \, {}^0\text{R}} \right) = 8.08 \text{ ft}^3
\]
**Example 5-3. Calculation of Ideal Gas Density**

What is the density of $\text{N}_2$ at $27^0\text{C}$ and $100 \text{ kPa}$ in SI units?

$$\frac{PV}{P_s V_s} = \frac{n T}{n_s T_s}$$

Solving for $(n/V)$ and obtaining the density from this:

$$\rho = \frac{n}{V} \times MW = \left[ \left( \frac{n_s}{V_s} \right) \left( \frac{P}{P_s} \right) \left( \frac{T_s}{T} \right) \right] \times MW$$

$$\rho = \left( \frac{1 \text{ kmol}}{22.41 \text{ m}^3} \right) \left( \frac{100 \text{ Pa}}{101.3 \text{ kPa}} \right) \left( \frac{273 \text{ K}}{300 \text{ K}} \right) \left( \frac{28 \text{ kg}}{\text{ kmol}} \right) = 1.123 \frac{\text{ kg}}{\text{ m}^3}$$
Ideal Gas Mixtures and Partial Pressures

In a mixture of ideal gases, the partial pressure of a gas component is the pressure that would be exerted by a that component if it existed by itself in the same volume as occupied by the mixture and the same temperature of the mixture.

\[ P_i V_{\text{total}} = n_i R T_{\text{total}} \]

where \( P_i \) and \( n_i \) are the partial pressure and number of moles of component \( i \).
Ideal Gas Mixtures and Partial Pressures

For the gas mixture:

\[ P_{\text{total}} V_{\text{total}} = n_{\text{total}} R T_{\text{total}} \]

Dividing the two equations,

\[ \frac{P_i V_T}{P_T V_T} = \frac{n_i R T_T}{n_T R T_T} \quad \text{or} \quad P_i = \frac{n_i}{n_T} P_T = y_i P_T \]

According to Dalton,

\[ P_A + P_B + P_C + \ldots = P_{\text{total}} \]
**Example 5-4. Ideal Gas Mixtures and Partial Pressures**

A flue gas analyzes 14.0% CO₂, 6.0% O₂, and 80.0% N₂. The mixture is at 400°F and 765 mmHg pressure. Calculate the partial pressure of each component.

<table>
<thead>
<tr>
<th>Component</th>
<th>( y )</th>
<th>( P_i ) (mmHg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>0.140</td>
<td>0.140(765) = 107.1</td>
</tr>
<tr>
<td>O₂</td>
<td>0.060</td>
<td>0.060(765) = 45.9</td>
</tr>
<tr>
<td>N₂</td>
<td>0.800</td>
<td>0.800(765) = 612.0</td>
</tr>
<tr>
<td>Total</td>
<td>1.000</td>
<td>765 mmHg</td>
</tr>
</tbody>
</table>