Introduction to Chemical and Environmental Engineering – Study Guide
Chemical Engineering Fundamentals
Credit to CBE245 for slides
As a chemical engineer you will encounter many types of processes and will be asked to design, operate or optimize a particular process (CBE Design Course)

What is a process?

**Process**: an operation or series of operations that causes a physical or chemical change, thereby converting raw materials into products

Within any process there are **process streams**: input and output of a process unit; governed by **conservation of mass and energy**: What goes in must come out!

- *input may also be called feed stream*
- *output may also be called the product stream*

Process flowsheet: Input-Output Diagram

Process variables: variables to characterize the streams entering and leaving a process unit. What are some important process variables? **temperature, pressure, composition**...
Let’s take a look at a few examples of processes:

Consider ice-cream making at your favorite place (Thomas Sweets, Bent Spoon, etc…)

**Process flowsheet:**

```
Cream
Sugar
Flavoring
X_i (composition)
Temperature
```

**Process unit:** Ice cream maker

**Process streams:**
- **input** – cream, sugar, flavoring
- **output** – ice cream

This is a **batch** process; it is characterized by chemical and physical changes without materials moving in or out, except at the beginning and at the end of a cycle.

The ingredients are fed into the batch reactor at the beginning of the cycle; ice-cream is removed at the end of the cycle.
Ammonia synthesis example:

[Recall that this is one of the top ten chemical engineering achievements; 35B lbs produced in 1995 (sixth largest chemical production)]

Chemical reaction: \( \text{N}_2(g) + 3\text{H}_2(g) \rightarrow 2\text{NH}_3(g) \)

If the previous example was a batch process, what type of process is the above? It is a **continuous process** and is characterized by chemical and physical changes with material moving in and out.

Process variables in this example includes:

- **Temperature** of the inlet and outlet streams
- **Pressure** of the inlet and outlet streams
- **Compositions** of the inlet and outlet streams
- **Total amount of material** in the inlet and outlet streams
Ammonia Synthesis

Ammonia synthesis process

- 350 tons CH₄/day
- 795 tons H₂O/day
- 825 tons N₂/day
- 1000 tons NH₃/day
- 970 tons CO₂/day

Input-Output Diagram

Block Flow Diagram

Process Flow Diagram
As in the previous example, most process streams consist of a mixture of liquids or gases, or solution of one or more solutes in a liquid solvent.

* When discussing **composition** as a **process variable** we must think in terms of mass, volume, density, moles, etc.

\[
\text{density} \equiv \text{mass per unit volume}; \text{ has dimensions of mass/length}^3 \\
[=] \text{g/cm}^3; \text{ kg/m}^3; \text{ lb}_m/\text{ft}^3
\]

What can you do with density? Use it to determine volume of a given mass or vice versa...

**Density** – a material property but depends on T, P.

How does density change with T and P?

example: Density (\(\rho\)) of water at 4\(^\circ\)C, 1 atm = 1.00000 g/cm\(^3\) \\
Density of water (liquid) at 0\(^\circ\)C, 1 atm = 0.999868 g/cm\(^3\) \\
Density of water (liquid) at 100\(^\circ\)C, 1 atm = 0.95838 g/cm\(^3\)

Water – an “anomaly”; volume expands as you cool from 4 to 0\(^\circ\)C

* Most pure compounds – density decreases with increasing temperature (volume expansion)

* Density of many pure compounds, solutions, and mixtures can be found in standard references including the back of your text book.
Regarding density, in this class we will make the following assumptions (remember, get comfortable making assumptions!):

- solids and liquids are **incompressible**, so density is constant with pressure
- gases and vapors are compressible, so density changes with pressure

Specific volume \( \equiv \) volume occupied by a unit mass of the substance; 
has dimensions of length\(^3\)/mass  
(reciprocal density)

Specific gravity \( \equiv \) the ratio of the density of a substance to a reference density of a reference substance at specific conditions; dimensionless

\[
SG \equiv \frac{\rho(T,P)}{\rho_{\text{ref}}(T,P)}
\]

For solids and liquids, the most common reference is water at \(4^\circ\text{C}, 1\text{ atm}\):

\[
\rho_{\text{water(l)}}(4^\circ\text{C}, 1\text{ atm}) = 1.000 \text{ g/cm}^3 = 1000. \text{ kg/m}^3 = 62.43 \text{ lb}_m/\text{ft}^3
\]

Typically, specific gravity is expressed as:

\[
SG = 0.6_{20^\circ}^{4^\circ} \quad 20^\circ\text{C} = \text{T of sub.} \quad 4^\circ\text{C} = \text{T of ref.}
\]
What is a mole? I am sure everyone can answer this question?

A certain amount of material corresponding to a specific number of molecules, atoms, electrons, or any specified type of particles?

The word mole is derived from the Latin word *moles* meaning *heap* or *pile*. So basically a mole is a large heap of particles.

Official definition: the amount of a substance that contains as many entities as there are atoms in 12 gm of carbon. Number of entities = \(6.023 \cdot 10^{23}\) atoms

g-mole (mol) — amount of substance whose mass is expressed in grams; is equivalent to the molecular weight of the substance (in grams)

Example: CO has a molecular weight of 28 gm/mol — 1 mol of CO contains 28 gm of CO and 1 mol of CO contains \(6.023 \cdot 10^{23}\) molecules

<table>
<thead>
<tr>
<th>CGS</th>
<th>SI</th>
<th>American</th>
</tr>
</thead>
<tbody>
<tr>
<td>g</td>
<td>(k_g)</td>
<td>(lb_m)</td>
</tr>
<tr>
<td>mol</td>
<td>kmol</td>
<td>lb-mole</td>
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<tr>
<td>g/mol</td>
<td>(k_g/kmol)</td>
<td>(lb_m/lb-mole)</td>
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Lets look at an example:

How many of each of the following are contained within 100 gm of CO$_2$? $M_w = 44.01$ g/mol (44.01 lb$_m$/lb-mol, 44.01 kg/kmol)

a) mol of CO$_2$?

\[ 100.0 \text{ gm} \times \frac{1 \text{ mol CO}_2}{44.01 \text{ gm CO}_2} = 2.273 \text{ mol CO}_2 \]

b) lb-moles of CO$_2$?

\[ 100.0 \text{ gm} \times \frac{1 \text{ lb}_m}{453.6 \text{ gm}} \times \frac{1 \text{ lb mol}}{44.01 \text{ lb}_m} = 5.011 \times 10^{-3} \text{ lb mol CO}_2 \]

c) mol of O?

\[ 100.0 \text{ gm} \times \frac{1 \text{ mol CO}_2}{44.01 \text{ gm}} \times \frac{2 \text{ mol O}}{1 \text{ mol CO}_2} = 4.546 \text{ mol O} \]

d) molecules of CO$_2$?

\[ 2.273 \text{ mol CO}_2 \times \frac{6.02 \times 10^{23} \text{ molecules}}{1 \text{ mol}} = 1.37 \times 10^{24} \text{ molecules} \]
Defining Composition:

A mass fraction is the mass of particular compound in a mixture divided by the total mass

\[ x_A = \frac{\text{mass of } A}{\text{total mass}} = \frac{kg \; A}{kg \; \text{total}} = \frac{g \; A}{g \; \text{total}} = \frac{lbm \; A}{lbm \; \text{total}} \]

mole fraction:

\[ y_A = \frac{\text{moles of } A}{\text{total moles}} = \frac{kg \; \text{mol } A}{kg \; \text{mol total}} = \frac{gmol \; A}{gmol \; \text{total}} = \frac{lbm \; \text{mol } A}{lbm \; \text{mol total}} \]

volume fraction:

\[ v_A = \frac{\text{volume of } A}{\text{total volume}} = \frac{m^3 \; A}{m^3 \; \text{total}} = \frac{cm^3 \; A}{cm^3 \; \text{total}} = \frac{ft^3 \; A}{ft^3 \; \text{total}} \]

* Fractions are unitless!

Generalizations:

• solids and liquids generally go by mass or mole fractions
• gases and vapors generally go by mole or volume fractions
Chemical engineers are not only interested in content (composition) but are also interested in quantity as most processes involve the movement of material from one point to another.

Where is material moved? Between process units or between production facilities, etc..

We are interested in the rate at which materials are being transported through the process line.

\[
\text{mass flow rate} = \dot{m} \quad \frac{\text{mass}}{\text{time}}
\]

\[
\text{volumetric flow rate} = \dot{V} \quad \frac{\text{volume}}{\text{time}}
\]

Suppose a fluid (gas or liquid) flows in a cylindrical pipe shown below, and the shaded area represents a section perpendicular to flow. If the mass flow rate is known, then every sec \( m \) kilograms pass through the area. If the volumetric flow rate is known, then every second \( V \) cubic meters of fluid pass through the area. Are the two \( m \) and \( V \) independent?

\[
\text{Density} = \frac{m}{V} \quad \frac{\dot{m}}{\dot{V}}
\]

Mass flow rate must be known for many calculations, yet in practice volumetric flow rate is measured.
Example: Conversion between mass fraction and mole fraction

An industrial-strength drain cleaner contains 5.00 kg of water and 5.00 kg of NaOH. What are the mass fractions and mole fractions of each component in the drain container?

You are giving the masses, so it is easy to calculate the mass fractions. The masses have to be converted in moles, so that mole fractions can be determined.

Conversion of masses to moles.....

\[
\begin{align*}
5.00\text{kg}H_2O \times \frac{1\text{kgmol}H_2O}{18.0\text{kg}H_2O} &= 0.278\text{kgmol}H_2O \\
5.00\text{kg}NaOH \times \frac{1\text{kgmol}NaOH}{40.0\text{kg}NaOH} &= 0.125\text{kgmol}NaOH
\end{align*}
\]

Calculate mass and mole fractions.....

\[
\begin{align*}
m_{H_2O} &= \frac{5\text{kg}}{10\text{kg}} = 0.5 \\
m_{NaOH} &= \frac{5\text{kg}}{10\text{kg}} = 0.5 \\
n_{H_2O} &= \frac{0.278}{0.278 + 0.125} = 0.69 \\
n_{NaOH} &= \frac{0.125}{0.278 + 0.125} = 0.31
\end{align*}
\]
Example: A mixture of gases has the following composition by mass:

- $O_2$: 16%
- CO: 4.0%
- $CO_2$: 17%
- $N_2$: 63%

What is the molar composition?

Set a basis of 100 gm of mixture

Mass fraction of $O_2 = \frac{16}{100} = 0.16 = X_{O_2}$

Mass of $O_2 = m_{O_2} = X_{O_2} \times m_{total} = 0.16 \times 100 = 16 \text{ gm}$

Mol of $O_2 = n_{O_2} = \frac{m_{O_2}}{M_{w_{O_2}}} = \frac{16\text{ gm}}{32\text{gmmol}^{-1}} = 0.5 \text{ mol}$

Perform the same calculations for CO, $CO_2$, and $N_2$

Mol of CO = 0.143
Mol of $CO_2$ = 0.386
Mol of $N_2$ = 2.250

Total moles = $n_{CO} + n_{CO_2} + n_{N_2} + n_{O_2} = 3.279$

Molar composition = $y_i = \frac{n_i}{n_{total}}$

$y_{O_2} = \frac{0.5}{3.279} = 0.150; \ y_{CO} = 0.044; \ y_{CO_2} = 0.120; \ y_{N_2} = 0.690$
Environmental Engineering Fundamentals
Credit to CEE304 for slides/information
Water consumption refers to the permanent withdrawal (no longer available in its original form, i.e. evaporation) of water from its source, while water withdrawal refers to water merely withdrawn or diverted from its source.
Equations

Efficiency: \[ \eta = \frac{\text{Energy}_{\text{out}}}{\text{Energy}_{\text{in}}} \]

Energy: \[ \frac{\text{Power}}{\text{Area}} = \frac{\text{Energy}}{(\text{Time})(\text{Area})} \]

\[ \left( \frac{W}{m^2} \right) = \left( \frac{J}{s\ m^2} \right) \]
Rankine cycle

**T-s diagram for steam turbine**

- **Superheat cycle**: Define turbine start with temp. and pressure.
- **Normal cycle**: Turbine starts with sat vap.
Ideal (Air) Brayton Cycle

1 $\rightarrow$ 2: Isentropic compression
2 $\rightarrow$ 3: Isobaric heat addition
3 $\rightarrow$ 4: Isentropic expansion
4 $\rightarrow$ 1: Isobaric heat rejection
PU "Cogen Plant" uses steam for heating and cooling instead of steam turbine.
OTEC

Ocean Thermal Energy Conversion (OTEC) uses the temperature difference between surface and deep ocean water to generate electricity. Warm surface water vaporizes ammonia, which drives a turbine to generate electricity. Deep ocean water cools the gas, turning it back into a liquid in the condenser. The process is cyclic, with water being pumped from the deep ocean to the surface and back again.
Pressurized Water Nuclear Reactor
Once-Through Cooling Water System