OUTLINE OF CHAPTER 2

Conservation of any (extensive) property

\[ \frac{\theta(t + \Delta t) - \theta(t)}{\Delta t} = \left( \text{Rate at which } \theta \text{ enters the system} \right) \]
\[ - \left( \text{Rate at which } \theta \text{ leaves the system} \right) \]
\[ + \left( \text{Rate at which } \theta \text{ is generated} \right) \]

\( \theta = \text{Mass, Moles or Energy(not specific)} \)

For mass:

\[ \frac{dM}{dt} = \sum_{k=1}^{\kappa} M_k \]
For moles: can be anything (chemical reactions), but if no generation takes place (no chemical reactions)

\[
\frac{dN}{dt} = \sum_{k=1}^{K} \dot{N}_k
\]

**Integral form**

\[
\int_{t_1}^{t_2} \frac{dM}{dt} \, dt = \sum_{k=1}^{K} \int_{t_1}^{t_2} \dot{M}_k \, dt
\]

**Left side**

\[
\int_{t_1}^{t_2} \frac{dM}{dt} \, dt = \int_{M(t_1)}^{M(t_2)} dM = M(t_2) - M(t_1) = \text{(Change in total mass of system between } t_1 \text{ and } t_2)
\]

**Right side**

\[
\int_{t_1}^{t_2} \dot{M}_k \, dt = \text{(Mass that entered the system at the } k\text{th entry port between } t_1 \text{ and } t_2) = \Delta M_k
\]

Then

\[
M(t_2) - M(t_1) = \sum_{k=1}^{K} \Delta M_k
\]

If flowrates are constant (steady flows)

\[
\int_{t_1}^{t_2} \dot{M}_k \, dt = \dot{M}_k \int_{t_1}^{t_2} dt = \dot{M}_k \Delta t
\]
and therefore

\[ M(t_2) - M(t_1) = \sum_{k=1}^{K} \dot{M}_k \Delta t \quad \text{(steady flows)} \]

**Steady state:**

\[ \frac{dM}{dt} = 0 \quad \text{and} \quad \dot{M}_k = \text{constant} \]

Then

\[ \sum_{k=1}^{K} \dot{M}_k = 0 \quad \text{(the classical, what goes in, goes out).} \]

**Summary**

<table>
<thead>
<tr>
<th>Table 2.2-1 The Mass Conservation Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Rate-of-change form of the mass balance</strong></td>
</tr>
<tr>
<td>General equation</td>
</tr>
<tr>
<td>( \frac{dM}{dt} = \sum_{k=1}^{K} \dot{M}_k )</td>
</tr>
<tr>
<td>Special case:</td>
</tr>
<tr>
<td>Closed system</td>
</tr>
<tr>
<td>( \frac{dM}{dt} = 0 )</td>
</tr>
<tr>
<td>( M = \text{constant} )</td>
</tr>
<tr>
<td><strong>Difference form of the mass balance</strong></td>
</tr>
<tr>
<td>General equation</td>
</tr>
<tr>
<td>( M_2 - M_1 = \sum_{k=1}^{K} \Delta M_k )</td>
</tr>
<tr>
<td>Special cases:</td>
</tr>
<tr>
<td>Closed system</td>
</tr>
<tr>
<td>( M_2 = M_1 )</td>
</tr>
<tr>
<td>Steady flow</td>
</tr>
<tr>
<td>( M_2 - M_1 = \sum_{k=1}^{K} \dot{M}_k \Delta t )</td>
</tr>
</tbody>
</table>

*Here we have used the abbreviated notation \( M_i = M(t_i) \) and \( N_i = N(t_i) \).
**Multicomponent Systems with chemical reactions:**

We need to use moles, so now, the equation

\[
\frac{dN}{dt} = \sum_{k=1}^{K} \dot{N}_k
\]

Has to be written for each specie!! And generation needs to be added.

\[
\frac{dN_i}{dt} = \sum_{k=1}^{K} (\dot{N}_i)_k + \left(\frac{dN_i}{dt}\right)_{rxn}
\]

or

\[
N_i(t_2) - N_i(t_1) = \sum_{k=1}^{K} \int_{t_1}^{t_2} (N_i)_k \, dt + (\Delta N_i)_{rxn} = \sum_{k=1}^{K} \Delta N_k + (\Delta N_i)_{rxn}
\]

and if the flow rate of a stream is steady (i.e. \((\dot{N}_i)_k\) is constant), then

\[
(\Delta N_i)_k = (\dot{N}_i)_k \Delta t
\]

**Example:** Reactor where the following reaction takes place:

\[
\text{C}_2\text{H}_4 + \text{Cl}_2 \rightarrow \text{C}_2\text{H}_4\text{Cl}_2
\]

The balance equations are
but from stoichiometry:

\[
\left( \frac{dN_{C_2H_4Cl_2}}{dt} \right)_{\text{rxn}} = -\left( \frac{dN_{C_2H_4}}{dt} \right)_{\text{rxn}} = -\left( \frac{dN_{Cl_2}}{dt} \right)_{\text{rxn}}
\]

Then we can use only one of them by simply replacing.

**NOTATION ON CHEMICAL REACTIONS**

Any reaction

\[
\alpha A + \beta B + \cdots \rightleftharpoons \rho R + \cdots
\]

Is written as follows:

\[
\rho R + \cdots - \alpha A - \beta B - \cdots = 0
\]

or

\[
\sum_{i} \nu_i I = 0
\]

where \( \nu_i \) are the stoichiometric coefficients.
Example:

\[ \text{H}_2\text{O} = \text{H}_2 + \frac{1}{2}\text{O}_2 \]

is written

\[ \text{H}_2 + \frac{1}{2}\text{O}_2 - \text{H}_2\text{O} = 0, \]

so that \( \nu_{\text{H}_2\text{O}} = -1, \nu_{\text{H}_2} = +1, \text{and } \nu_{\text{O}_2} = +\frac{1}{2}. \)

\( \nu_i \) are the stoichiometric coefficients.

**MOLAR EXTENT OF REACTION**

We write:

\[ N_i = N_{i,0} + \nu_i X \]

where \( X \) is the extent of reaction (molar!!!), which can also be viewed as

\[ X = \frac{N_i - N_{i,0}}{\nu_i} \]

which is not restricted to lie between 0 and 1 (i.e. it is not fractional conversion)
Then
\[
\left( \frac{dN_i}{dt} \right)_{\text{rxn}} = \nu_i \dot{X}
\]

and therefore
\[
\frac{dN_i}{dt} = \sum_{k=1}^{K} (\dot{N}_i)_k + \left( \frac{dN_i}{dt} \right)_{\text{rxn}}
\]

and
\[
N_i(t_2) - N_i(t_1) = \sum_{k=1}^{K} \int_{t_1}^{t_2} (\dot{N}_i)_k \, dt + (\Delta N_i)_{\text{rxn}} = \sum_{k=1}^{K} \Delta N_k + (\Delta N_i)_{\text{rxn}}
\]

Thus in the previous example

\[
C_2H_4: \quad \left( \frac{dN_{C_2H_4}}{dt} \right) = (\dot{N}_{C_2H_4})_1 + (\dot{N}_{C_2H_4})_3 - \frac{dX}{dt}
\]

\[
Cl_2: \quad \left( \frac{dN_{Cl_2}}{dt} \right) = (\dot{N}_{Cl_2})_2 + (\dot{N}_{Cl_2})_3 - \frac{dX}{dt}
\]

\[
C_2H_4Cl_2: \quad \left( \frac{dN_{C_2H_4Cl_2}}{dt} \right) = (\dot{N}_{C_2H_4Cl_2})_3 + \frac{dX}{dt}
\]