Basics in Process Design

Mass balances for process system analysis/modeling/design
- Block flow diagrams
- Calculate flows from mass and energy balances
- Rough sizing of equipment for
  - storage
  - preprocessing
  - reaction
  - separation,
  - heat exchange
  - transport
- Instrumentation
- Cost estimates
Today

- Basic mass balance
- Process system
- Balance modeling
- Example
- Exercise
- Questions?
Basic mass balance

- Conservation of mass
- Total balance
  - In, out, accumulation
- Partial balances for components
  - In, out, generation or consumption, accumulation

\[
\dot{m}_{\text{in}} = \dot{m}_{\text{out}} + \frac{d m_{\text{accumulated}}}{dt}
\]

\[
\dot{m}_{\text{in}} + \frac{d m_{\text{generated}}}{dt} = \dot{m}_{\text{out}} + \frac{d m_{\text{accumulated}}}{dt}
\]

\[
\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}
\]
Process system

- Basic chemical production process
  - Raw materials
  - Mixing
  - Reaction
  - Separation
  - Product
  - Recirculation
Balance modeling

- **By hand**
  - Draw a block diagram
  - Name the flows and the units/operations
  - List known information
  - Select suitable boundaries
  - Set up balance equations
  - Solve equations or equation systems

- **Computer simulation**
  - Make your own programs in Excel, Matlab, …
  - Use simulation packages like Pro/II, Aspen Plus, …

- **End result – mass balance table**
Possible “problems”

- Not mass flows – volume flows, mol flows, concentrations... → convert to mass flows
- Too many unknowns... → search, ask, measure, estimate, assume
- Too many variables... → organize
- Too many equations... → methods for equation systems, equation-variable grids, iterative solution
Example

Conventional Ammonia Plant

Demineralized water → Feed pretreatment → Primary reformer → Secondary reformer → HT shift → LT shift → CO2 removal → Methanation → Ammonia synthesis → Purge gas separation → CO2 → NH3
Example

Ammonia is synthesized from hydrogen gas (H₂) and nitrogen gas (N₂) in the Haber-Bosch process. The design production rate is 450 ton/day of ammonia.

\[
\text{N}_2 + 3 \text{H}_2 \leftrightarrow 2 \text{NH}_3
\]

The conversion of nitrogen in the reactor (here defined as mol nitrogen gas reacted/mol nitrogen gas in) is assumed to be about 17%. Unreacted hydrogen and nitrogen is separated from the ammonia product and recirculated to the reactor.

a) Draw a block flow diagram that describes this process.

b) Calculate the size and composition of the flows in this process.
Block flow diagram

N₂: H₂ → REACT → SEP → N₂H₂, NH₃

17% conversion of N₂

450 kg/day
Total balance + Stoichiometry

\[
\dot{m}_1 = \dot{m}_3
\]

\[
\frac{\dot{m}_1, N_2 + \dot{m}_1, H_2}{2} = \dot{m}_3, NH_3
\]

\[
\dot{n}_{1, N_2} = \frac{1}{2} \cdot \dot{n}_{3, NH_3}
\]

\[
\dot{n}_{1, H_2} = \frac{3}{2} \cdot \dot{n}_{3, NH_3}
\]

\[
\dot{n}_{3, NH_3} = \frac{\dot{m}_{3, NH_3}}{M_{NH_3}} = \frac{450 \text{ ton/ \(\text{a}\)}}{17.04 \text{ kmol/kg}}
\]

26408 \(\text{kmol/ \(\text{a}\)}\)
\[
\frac{1}{2} \hat{n}_{2, \text{NH}_3} = \frac{n_{1, \text{N}_2} + n_{4, \text{N}_2} - n_{3, \text{N}_2}}{n_{1, \text{N}_2} + n_{4, \text{N}_2}} = 0.17
\]

\[
\frac{1}{2} \hat{n}_{3, \text{NH}_3} = \frac{(450 \text{ torr})}{26400 \text{ W/m}^2} = 0.17
\]
<table>
<thead>
<tr>
<th></th>
<th>N$_2$</th>
<th>H$_2$</th>
<th>NH$_3$</th>
<th>tot</th>
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<td>4</td>
<td>1971.21</td>
<td>426.04</td>
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</tr>
</tbody>
</table>

ton/day
Questions?