CM4310 homework #4

a)
Ideas: In order to calculate the risk indices, we should know the emission rates, concentrations and toxicity parameters.

The emissions for the absorber oil flow rates of 0 and 100 kgmole/hr are given below. n-C14 is the absorber oil.

<table>
<thead>
<tr>
<th>Absorber Oil Flow Rate (kgmol/hr)</th>
<th>Toluene Emission Rate (kg/hr)</th>
<th>Ethyl Acetate</th>
<th>CO2</th>
<th>CO</th>
<th>TOC</th>
<th>NOx</th>
<th>SOx</th>
<th>n-C14</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>193.55</td>
<td>193.55</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>100</td>
<td>0.02</td>
<td>128.07</td>
<td>360</td>
<td>0.129</td>
<td>0.007</td>
<td>0.52</td>
<td>3.39</td>
<td>4.23</td>
</tr>
</tbody>
</table>

The concentrations of each chemical in water and air compartments are calculated by Mackay Level III model using the spreadsheet Dr. Shonnard provided. The data for calculating fate and transport are listed in the table of the assignment.

The concentrations for each chemical in the air and water compartments are listed in the following table.

<table>
<thead>
<tr>
<th>Concentration (g/m³)</th>
<th>Toluene</th>
<th>Ethyl Acetate</th>
<th>CO₂</th>
<th>CO</th>
<th>TOC</th>
<th>NOₓ</th>
<th>SOₓ</th>
<th>n-C14</th>
<th>PCP</th>
</tr>
</thead>
<tbody>
<tr>
<td>In air</td>
<td>1.97x10⁻⁶</td>
<td>4.36x10⁻⁷</td>
<td>9.99x10⁻⁵</td>
<td>9.99x10⁻⁵</td>
<td>1.97x10⁻⁶</td>
<td>2.78x10⁻⁸</td>
<td>5.81x10⁻⁸</td>
<td>1.62x10⁻⁵</td>
<td>7.69x10⁻⁷</td>
</tr>
<tr>
<td>In water</td>
<td>4.00x10⁻⁶</td>
<td>5.00x10⁻⁸</td>
<td>1.05x10⁻⁴</td>
<td>6.52x10⁻⁸</td>
<td>1.50x10⁻⁶</td>
<td>6.33x10⁻⁶</td>
<td>1.90x10⁻⁶</td>
<td>4.10x10⁻⁹</td>
<td>7.83x10⁻³</td>
</tr>
</tbody>
</table>

The environmental indices are calculated as follows:

**Global warming index**: \( I_{GW} = \sum_i (GWP_i \times m_i) \)

The global warming potential for each emitted chemical is given in the table in the assignment.

<table>
<thead>
<tr>
<th>Chemical</th>
<th>GWP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>3.35</td>
</tr>
<tr>
<td>Ethyl acetate</td>
<td>2.0</td>
</tr>
<tr>
<td>Tetradecane</td>
<td>3.1</td>
</tr>
<tr>
<td>Hexane</td>
<td>3.1</td>
</tr>
<tr>
<td>CO₂</td>
<td>1</td>
</tr>
<tr>
<td>CO</td>
<td>2</td>
</tr>
<tr>
<td>NOₓ</td>
<td>40</td>
</tr>
</tbody>
</table>

Absorber oil flow rate: 0 kgmole/hr

\( I_{GW} = (3.35)(193.5 \text{ kg/hr}) + (2)(193.5 \text{ kg/hr}) = 1,035 \text{ kg/hr} \)

Absorber oil flow rate: 100 kgmole/hr
\( I_{GW} = (3.35)(0.02 \text{ kg/hr}) + (2)(128.07 \text{ kg/hr}) + (3.1)(4.23 \text{ kg/hr}) + (3.1)(0.007 \text{ kg/hr}) + (1)(360 \text{ kg/hr}) + (2)(0.129 \text{ kg/hr}) + (40)(0.52 \text{ kg/hr}) = 650 \text{ kg/hr} \)

**Smog Formation Index:** \( I_{SF} = \sum_i (SFP_i \times m_i) \)

The smog formation potential for each chemical is given in the table in the assignment.

- Toluene: \( SFP_i = 0.87 \)
- Ethyl acetate: \( SFP_i = 0.32 \)
- Tetradecane: \( SFP_i = 0.1 \)

Absorber oil flow rate: 0 kgmole/hr

\[ I_{SF} = (0.87)(193.5 \text{ kg/hr}) + (0.32)(193.5 \text{ kg/hr}) = 230 \text{ kg/hr} \]

Absorber oil flow rate: 100 kgmole/hr

\[ I_{SF} = (0.87)(0.02 \text{ kg/hr}) + (0.32)(128.07 \text{ kg/hr}) + (0.1)(4.23 \text{ kg/hr}) = 41.4 \text{ kg/hr} \]

**Acid Rain Index:** \( I_{AR} = \sum_i (ARP_i \times m_i) \)

The acid rain potential for each chemical is given in the table in the assignment.

- NO\(_X\): \( ARP_i = 0.7 \)
- SO\(_X\): \( ARP_i = 1 \)

Absorber oil flow rate: 0 kgmole/hr

\[ I_{SF} = (0.7)(0 \text{ kg/hr}) + (1)(0 \text{ kg/hr}) = 0 \text{ kg/hr} \]

Absorber oil flow rate: 100 kgmole/hr

\[ I_{SF} = (0.7)(0.52 \text{ kg/hr}) + (1)(3.39 \text{ kg/hr}) = 3.754 \text{ kg/hr} \]

**Ozone Depletion Index:** There are no ozone depleting chemicals emitted for this case.

**Non-Carcinogenic Ingestion Toxicity Index:** \( I_{ING} = \sum_i (INGTP_i \times m_i) \)

The ingestion toxicity potential is given by eqn. 11.3-14

\[ INGTP_i = \frac{(C_{i,w})}{(RfD_{i})} = \frac{(LD_{50,i})}{(LD_{so,i})} \]

Toluene: \( INGTP_i = [(4.0x10^{-7} \text{ g/m}^3)/(0.2 \text{ mg/kg/day})] / [(4.0x10^{-7} \text{ g/m}^3)/(0.2 \text{ mg/kg/day})] = 1.0 \)

Ethyl acetate: \( INGTP_i = [(5.0x10^{-6} \text{ g/m}^3)/(0.9 \text{ mg/kg/day})] / [(4.0x10^{-7} \text{ g/m}^3)/(0.2 \text{ mg/kg/day})] = 2.8 \)

TOC: \( INGTP_i = [(1.50x10^{-9} \text{ g/m}^3)/(28700 \text{ mg/kg})] / [(4.0x10^{-7} \text{ g/m}^3)/(5000 \text{ mg/kg})] = 6.5x10^{-4} \)

Absorber oil flow rate: 0 kgmole/hr

\[ I_{ING} = (1.0)(193.5 \text{ kg/hr}) + (2.8)(193.5 \text{ kg/hr}) = 735 \text{ kg/hr} \]
Absorber oil flow rate: 100 kgmole/hr
\[ I_{\text{ING}} = (1.0)(0.02 \text{ kg/hr}) + (2.8)(128.07 \text{ kg/hr}) + (6.5 \times 10^{-4})(0.007 \text{ kg/hr}) = 358.6 \text{ kg/hr} \]

**Non-Carcinogenic Inhalation Toxicity Index**: \[ I_{\text{INH}} = \sum_i (\text{INHTP}_i \times m_i) \]

The ingestion toxicity potential is given by eqn. 11.3-14
\[ \text{INHTP}_i = \frac{C_{i,a}}{RfC_{i}} \]

\[ \text{INGTP}_i = \frac{(C_{i,a}) / (LC_{50,i})}{(C_{\text{Toluene},a}) / (LC_{50,\text{Toluene}})} \]

depending upon the availability of data.

Toluene: \[ \text{INHTP}_i = \frac{[(1.97 \times 10^{-7} \text{ g/m}^3)/(4,000 \text{ ppm})]}{[(1.97 \times 10^{-7} \text{ g/m}^3)/(4,000 \text{ ppm})]} = 1.0 \]

Ethyl acetate: \[ \text{INHTP}_i = \frac{[(4.36 \times 10^{-7} \text{ g/m}^3)/(3200 \text{ ppm})]}{[(1.97 \times 10^{-7} \text{ g/m}^3)/(4,000 \text{ ppm})]} = 2.8 \]

TOC: \[ \text{INHTP}_i = \frac{[(1.97 \times 10^{-7} \text{ g/m}^3)/(0.2 \text{ mg/m}^3)]}{[(1.97 \times 10^{-7} \text{ g/m}^3)/(0.4 \text{ mg/m}^3)]} = 2.0 \]

CO: \[ \text{INHTP}_i = \frac{[(9.99 \times 10^{-7} \text{ g/m}^3)/(1807 \text{ ppm})]}{[(1.97 \times 10^{-7} \text{ g/m}^3)/(4,000 \text{ ppm})]} = 11.23 \]

SOX: \[ \text{INHTP}_i = \frac{[(5.81 \times 10^{-8} \text{ g/m}^3)/(2520 \text{ ppm})]}{[(1.97 \times 10^{-7} \text{ g/m}^3)/(4,000 \text{ ppm})]} = 0.47 \]

NOX: \[ \text{INHTP}_i = \frac{[(2.78 \times 10^{-14} \text{ g/m}^3)/(88 \text{ ppm})]}{[(1.97 \times 10^{-7} \text{ g/m}^3)/(4,000 \text{ ppm})]} = 6.4 \times 10^{-6} \]

Absorber oil flow rate: 0 kgmole/hr
\[ I_{\text{INH}} = (1.0)(193.5 \text{ kg/hr}) + (2.8)(193.5 \text{ kg/hr}) = 735 \text{ kg/hr} \]

Absorber oil flow rate: 100 kgmole/hr
\[ I_{\text{INH}} = (1.0)(0.02 \text{ kg/hr}) + (2.8)(128.07 \text{ kg/hr}) + (6.5 \times 10^{-4})(0.007 \text{ kg/hr}) + (11.23)(0.129 \text{ kg/hr}) + (0.47)(3.39 \text{ kg/hr}) + (6.4 \times 10^{-6})(0.52 \text{ kg/hr}) = 361.7 \text{ kg/hr} \]

b) **Fish Toxicity Index**: \[ I_{\text{FT}} = \sum_i (I_{\text{FT}}^* \times m_i) \]

The fish toxicity potential is given by the following equation,
\[ I_{\text{FT}}^* = \frac{C_{i,w}/FLC_{50,j}}{C_{\text{PCP,w}}/FLC_{50,\text{PCP}}} \]

Toluene: \[ I_{\text{FT}}^* = \frac{[(4.00 \times 10^{-7} \text{ g/m}^3)/(31.7 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 3.88 \times 10^{-5} \]

Ethyl acetate: \[ I_{\text{FT}}^* = \frac{[(5.00 \times 10^{-6} \text{ g/m}^3)/(13 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 1.18 \times 10^{-3} \]

Tetradecane: \[ I_{\text{FT}}^* = \frac{[(4.10 \times 10^{-9} \text{ g/m}^3)/(0.0018 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 7.01 \times 10^{-3} \]

TOC: \[ I_{\text{FT}}^* = \frac{[(1.50 \times 10^{-9} \text{ g/m}^3)/(9 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 5.13 \times 10^{-7} \]

CO2: \[ I_{\text{FT}}^* = \frac{[(1.05 \times 10^{-7} \text{ g/m}^3)/(123.162 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 2.63 \times 10^{-6} \]

CO: \[ I_{\text{FT}}^* = \frac{[(6.52 \times 10^{-12} \text{ g/m}^3)/(10.39 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 1.93 \times 10^{-9} \]

SOX: \[ I_{\text{FT}}^* = \frac{[(1.90 \times 10^{-6} \text{ g/m}^3)/(1.0 \times 10^{5} \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 5.85 \times 10^{-8} \]

NOX: \[ I_{\text{FT}}^* = \frac{[(6.33 \times 10^{-4} \text{ g/m}^3)/(114.3 \text{ mg/L})]}{[(7.83 \times 10^{-5} \text{ g/m}^3)/(0.2409 \text{ mg/L})]} = 1.70 \times 10^{-2} \]

Absorber oil flow rate: 0 kgmole/hr
\[ I_{FT} = (3.88 \times 10^{-5})(193.55 \text{ kg/hr}) + (1.18 \times 10^{-3})(193.55 \text{ kg/hr}) = 0.236 \text{ kg/hr} \]

Absorber oil flow rate: 100 kgmole/hr
\[ I_{FT} = (3.88 \times 10^{-5})(0.02 \text{ kg/hr}) + (1.18 \times 10^{-3})(128.07 \text{ kg/hr}) + (7.01 \times 10^{-7})(0.007 \text{ kg/hr}) + (2.63 \times 10^{-6})(360 \text{ kg/hr}) + (1.93 \times 10^{-5})(0.129 \text{ kg/hr}) + (5.85 \times 10^{-8})(3.39 \text{ kg/hr}) + (1.70 \times 10^{-7})(0.52 \text{ kg/hr}) = 0.191 \text{ kg/hr} \]

**c) Process Composite Index**

Process composite index is calculated by the following equations,
\[
I_N^k = \frac{I_k}{I^k_{PC}}
\]
\[
I_{PC} = \sum_k (I_N^k \times W_k)
\]

<table>
<thead>
<tr>
<th>Weighting Factors</th>
<th>National Index (kg/yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>global warming</td>
<td>5.48E+12</td>
</tr>
<tr>
<td>ozone depletion</td>
<td>1.96E+05</td>
</tr>
<tr>
<td>smog formation</td>
<td>6.80E+09</td>
</tr>
<tr>
<td>acid rain</td>
<td>1.85E+10</td>
</tr>
<tr>
<td>carcinogenic</td>
<td>4.21E+06</td>
</tr>
<tr>
<td>noncarcinogenic</td>
<td>1.41E+11</td>
</tr>
<tr>
<td>ecotoxicity</td>
<td>9.70E+08</td>
</tr>
</tbody>
</table>

Absorber oil flow rate: 0 kgmole/hr
\[ I_{PC} = [(1035 \text{ kg/hr})/(5.48 \times 10^{12} \text{ kg/hr})](2.5) + [(230 \text{ kg/hr})/(6.80 \times 10^9 \text{ kg/hr})](2.5) + [(0 \text{ kg/hr})/(1.85 \times 10^{10} \text{ kg/hr})](10) + [(735 \text{ kg/hr})/(1.55 \times 10^{12} \text{ kg/hr})](5) + [(735 \text{ kg/hr})/(1.41 \times 10^{11} \text{ kg/hr})](5) + [(0.236 \text{ kg/hr})/(9.70 \times 10^8 \text{ kg/hr})](10) = 1.16 \times 10^{-7} \]

Absorber oil flow rate: 100 kgmole/hr
\[ I_{PC} = [(650 \text{ kg/hr})/(5.48 \times 10^{12} \text{ kg/hr})](2.5) + [(41.4 \text{ kg/hr})/(6.80 \times 10^9 \text{ kg/hr})](2.5) + [(3.754 \text{ kg/hr})/(1.85 \times 10^{10} \text{ kg/hr})](10) + [(358.6 \text{ kg/hr})/(1.55 \times 10^{12} \text{ kg/hr})](5) + [(361.7 \text{ kg/hr})/(1.41 \times 10^{11} \text{ kg/hr})](5) + [(0.191 \text{ kg/hr})/(9.70 \times 10^8 \text{ kg/hr})](10) = 3.35 \times 10^{-8} \]