INTRODUCTION TO CHEMICAL PROCESS SIMULATORS

DWSIM Chemical Process Simulator

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October 2016
Introduction to Chemical Process Simulators

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Ethylene Glycol Production

http://pubs.acs.org/doi/abs/10.1021/ie901037w
Ethylene Glycol Production

\[ \begin{align*}
W + \text{EtO} & \rightarrow \text{MEG} \quad k1 \\
\text{MEG} + \text{EtO} & \rightarrow \text{DEG} \quad k2 \\
\text{DEG} + \text{EtO} & \rightarrow \text{TEG} \quad k3 \\
\text{TEG} + \text{EtO} & \rightarrow \text{TTEG} \quad k4
\end{align*} \]

Kinetics in COCO

\[ k1 = \exp(13.62-8220/T)/60/1000*\text{C(\text{Water})}\times\text{C("Ethylene oxide")}) \]

\[ k2 = \exp(15.57-8700/T)/60/1000*\text{C("Monoethylene glycol")}\times\text{C("Ethylene oxide")}) \]

\[ k3 = \exp(16.06-8900/T)/60/1000*\text{C("Diethylene glycol")}\times\text{C("Ethylene oxide")}) \]

\[ k4 = \exp(16.3-9000/T)/60/1000*\text{C("Triethylene glycol")}\times\text{C("Ethylene oxide")}) \]
Pressure Swing Distillation of Acetone-Methanol


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Ammonia Synthesis

Ammonia is produced by reacting nitrogen from the air with hydrogen. Hydrogen is usually obtained from steam reformation of methane, and nitrogen is obtained from deoxygenated air. The chemical reaction is shown below:

\[ N_2 + 3H_2 \rightleftharpoons 2NH_3 \]

Our goal is to produce a simulation for the production of ammonia using DWSIM. A diagram and the data needed to simulate this process is given below.

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>0.7371</td>
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<tr>
<td>Ammonia</td>
<td>0</td>
</tr>
<tr>
<td>CO</td>
<td>0.0024</td>
</tr>
<tr>
<td>Argon</td>
<td>0.0027</td>
</tr>
<tr>
<td>Methane</td>
<td>0.0103</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.2474</td>
</tr>
</tbody>
</table>
Ammonia Synthesis
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DWSIM Chemical Process Simulator

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