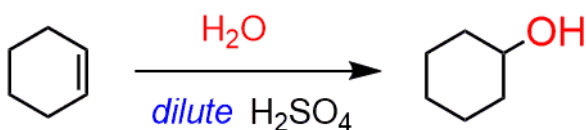


Reactive Distillation Process for the Production of Cyclohexanol via direct Hydration of Cyclohexene

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Introduction and Background :

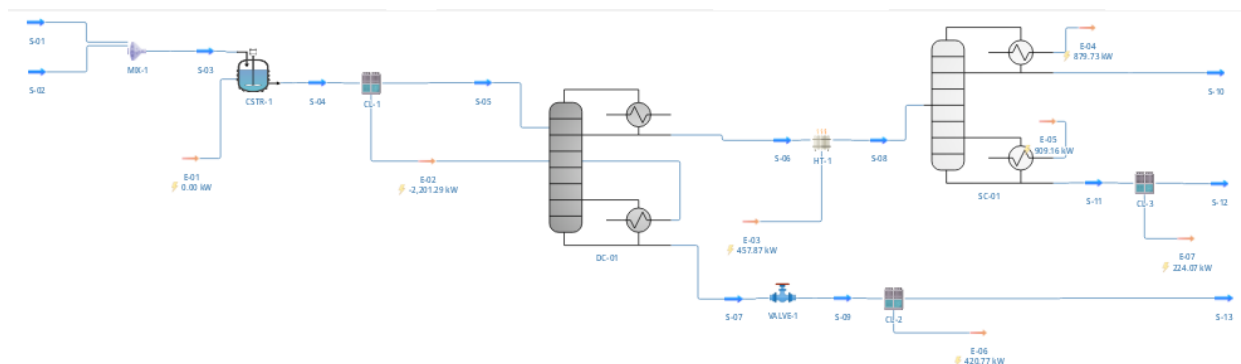
Cyclohexanol is an important precursor essential for the synthesis of Nylon-6 polymer which is used very widely. The amount of cyclohexanol produced annually exceeds 1 million tons. The traditional process is to hydrogenate benzene to produce cyclohexane, and then cyclohexane can be oxidized by air to form a mixture containing cyclohexanol and cyclohexanone.^{1,2} However, the drawbacks of this process are the low selectivity of cyclohexanol, the explosion risk, high energy requirement, and numerous side product formations. To counter these issues, cyclohexanol can be produced directly by hydrating cyclohexene in the required amounts via the AMberlyst catalyzed reaction given below.



Description of the Flowsheet :

In the given flowsheet, the two streams of water and cyclohexene are first mixed and added to the CSTR for the rapid production of Cyclohexanol under the given kinetic conditions. Thereafter, the product stream from CSTR enters the reactive distillation column for separation of cyclohexanol from cyclohexene and water. An additional shortcut column is added for the distillate stream of the distillation output in order to obtain higher purity of Cyclohexene. The Cyclohexanol from the raffinate stream of the distillation column is cooled and stored. One CSTR, three coolers, one mixer, one distillation column, one shortcut column and one valve has been used to accomplish the flowsheet simulation. The mass, energy and reaction balance perfectly to yield Cyclohexanol as the product.

Flowsheet and Master Property Table :



| Master Property Table | | | | | | | | | | | | | |
|--------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|---------|----------|
| Object | S-13 | S-12 | S-11 | S-10 | S-09 | S-08 | S-07 | S-06 | S-05 | S-04 | S-03 | S-02 | S-01 |
| Temperature | 41.0193 | 39.2647 | 159.265 | 83.1211 | 161.019 | 100 | 184.709 | -22.0105 | 107.541 | 181.917 | 128.645 | 126 | 134.1 |
| Pressure | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 2.01325 | 1.01325 | 3.014 | 3.014 | 3.014 | 3.014 | 3.025 |
| Mass Flow | 3605.72 | 2381.43 | 2381.43 | 3308.22 | 3605.72 | 9689.38 | 3605.72 | 5689.38 | 9295.28 | 9295.28 | 9295.28 | 8214.36 | 1080.92 |
| Molar Flow | 36 | 23.8229 | 23.8229 | 40.1875 | 36 | 64.007 | 36 | 64.007 | 100.007 | 100.007 | 100.007 | 160 | 60 |
| Volumetric Flow | 3.85224 | 2.54422 | 2.90599 | 4.4006 | 228.984 | 207.332 | 4.54339 | 6.34089 | 11.5042 | 975.253 | 1764.4 | 1101.04 | 671.579 |
| Molar Enthalpy (Mixture) | -57937.4 | -58063.7 | -24202.6 | -24110.8 | -15860.3 | -25801.3 | -15860.3 | -51553.4 | -32061.6 | 14735.2 | 9210.14 | 12514.2 | 3703.41 |
| Molar Entropy (Mixture) | -184.239 | -185.16 | -46.4926 | -65.5467 | -27.3917 | -61.1131 | -28.404 | -198.21 | -83.9912 | 39.5608 | 28.9168 | 26.8118 | 1.48544 |
| Molar Fraction (Vapor) | 0 | 0 | 0 | 0 | 0.175718 | 0.10246 | 0 | 0 | 0 | 0.774382 | 0.994931 | 1 | 1 |
| Phases | L | L | L | L | V+L | V+L | L | L | L | V+L | V+L | V | V |
| Energy Flow | -3441.37 | -2259.25 | -2035.17 | -351.508 | -3020.6 | -2416.1 | -3020.6 | -2873.96 | -5710.8 | -4410.8 | -3746.45 | 222.061 | -3968.51 |
| | | | | | | | | | | | | | kW |

Reference :

Reactive-Distillation Process for Direct Hydration of Cyclohexene to Produce Cyclohexanol Bor-Chang Chen, Bor-Yih Yu, Yuan-Lin Lin, Hsiao-Ping Huang, and I-Lung Chien Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan.