# Production of Toluene by Dehydrogenation of Normal Heptane

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**Background & Description:**

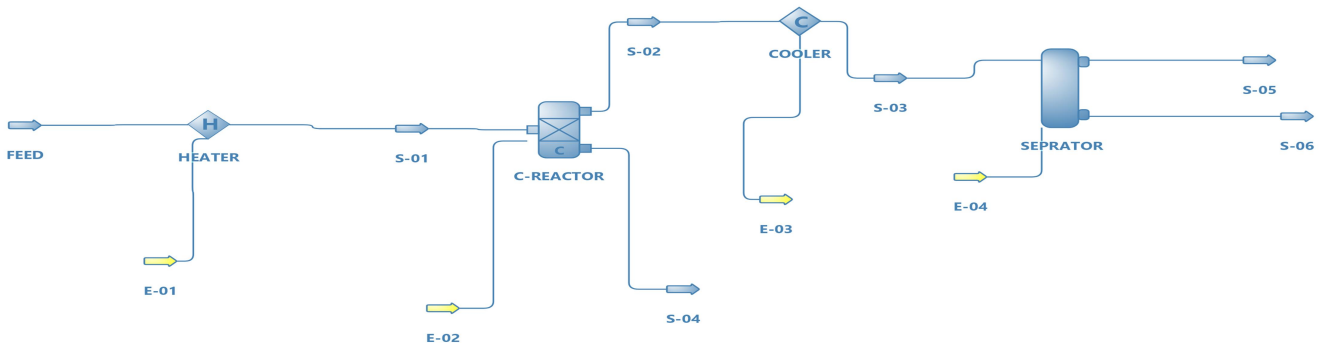
Toluene is produced from n-heptane by dehydrogenation over a $Cr_2O_3$ catalyst, The reaction for the same is given below:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_3 \longrightarrow C_6H_5CH_3 + 4H_2$$

In this process Toluene is formed along with Hydrogen as shown in the reaction.

The process flowsheet shows the conversion of n-heptane to toluene using a catalytic reactor working on the reaction shown above. The toluene production process is started by heating n-heptane from 65 to 800°F in a heater. It is fed to a catalytic reactor, which operates isothermally and converts 15 mol percent of the n- heptane to toluene. Its effluent is cooled to 65°F and fed to a separator (flash). Assuming that all of the units operated at atmospheric pressure, The species flow rate and other properties are determined in every stream.

**Flowsheet :**



## Results:

| Master Property Table | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Object** | **S-06** | **S-05** | **S-04** | **S-03** | **S-02** | **S-01** | **FEED** | |
| **Temperature** | 18.3333 | 18.3333 | 426.667 | 18.3333 | 426.667 | 426.667 | 18.3333 | **C** |
| **Pressure** | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | **bar** |
| **Mass Flow** | 3459.13 | 140.875 | 0 | 3600 | 3600 | 3600 | 3600 | **kg/h** |
| **Molar Flow** | 34.9817 | 22.5022 | 0 | 57.4839 | 57.4839 | 35.9274 | 35.9274 | **kmol/h** |
| **Volumetric Flow** | 4.87186 | 538.07 | 0 | 542.942 | 3294.47 | 2051.58 | 5.24272 | **m3/h** |
| **Mixture Molar Enthalpy** | -37374.2 | -232.34 | 0 | -22834.9 | 63516.6 | 99373.3 | -37435.2 | **kJ/kmol** |
| **Mixture Molar Entropy** | -95.4591 | 0.396744 | 0 | -57.9361 | 227.384 | 201.948 | -102.485 | **kJ/[kmol.K]** |
| **Vapor Phase Molar Fraction** | 0 | 1 | 0.352309 | 0.391453 | 1 | 1 | 0 | |
| **Phases** | Liquid Only | Vapor Only | Mixed | Mixed | Vapor Only | Vapor Only | Liquid Only | |
| **Energy Flow** | -363.17 | -1.45227 | 0 | -364.622 | 1014.22 | 991.73 | -373.598 | **kW** |

| Master Property Table | | | |
|---|---|---|---|
| **Object** | **S-06** | **S-05** | |
| **Molar Fraction (Mixture) / Toluene** | 0.150629 | 0.00532612 | |
| **Mass Fraction (Mixture) / Toluene** | 0.140354 | 0.0783869 | |
| **Molar Flow (Mixture) / Toluene** | 5.26927 | 0.119849 | **kmol/h** |
| **Mass Flow (Mixture) / Toluene** | 485.502 | 11.0427 | **kg/h** |

| PROPERTIES TABLE | | | |
|---|---|---|---|
| **C-REACTOR** | **Toluene Formation: Extent** | 15 | % |
| **C-REACTOR** | **N-heptane: Conversion** | 15 | % |

## Conclusion:

Toluene is formed with a conversion rate of 15%.

## Reference:


1. HYSYS:An Introduction to Chemical Engineering Simulation by Mohd.Kamaruddin Abd Hamid chapter-13 page no-146