# Production of cyclohexanol and cyclohexanone through oxidation of cyclohexane

Unit system used – $^0$C, bar, kg/hr, kmol/hr

## Introduction

Cyclohexane is an important commercial component for the preparation of cyclohexanol and cyclohexanone, which are intermediates in the production of adipic acid and caprolactam respectively. These intermediates are important in the manufacture of nylon-6 and nylon-66. Which have become important reference materials in the industries production of polymers and the demand expands over the last few years. In addition, cyclohexanol and cyclohexanone are also used as a solvent for lacquers and varnishes as well as stabilisers and homogenisers for soaps and synthetic detergent emulsions. The other use of cyclohexanone are in the synthesis of insecticides, herbicides and pharmaceutical.

Reaction involved: $1.5C_6H_{12} + 2O_2 = C_6H_{12}O + C_6H_{10}O + H_2O$

Reactor Used: Continuous stir tank reactor

Reactor conditions: Outlet Temperature = 179.027 $^0$C, Pressure Drop = 0atm

## Process Description

Cyclohexane(25$^o$C,1 bar,500 kmol/hr) is first pressurized by a pump to 9 bar , and then it is sent to heat exchanger to reach the temperature of cyclohexane to 160$^o$C. Now pressurized and heated cyclohexane stream which is ready for reaction is mixed with oxygen(30kmol/hr) in mixer unit before it enters to the CSTR. In the the kinetic data of the reaction are given to carry out the liquid phase reaction. After reaction there is a separation unit for separating the major portion of unreacted cyclohexane from products. So there are two rigorous distillation columns are provided. According to relative volatility of cyclohexane, Cyclohexanol and cyclohexanone; cyclohexane first separated from the product mixer in first column as distillate. Around 460 kmol/hr

cyclohexane is obtained from the top as 0.95 mole fraction in distillate mixer. This cyclohexane is first separated from water and other minor component by component separator unit and all 460 kmol/hr cyclohexane is recycled. The bottom of first column goes to the second column where cyclohexanone(0.8477 mole fraction) is separated from the top of second distillation column, while we get Cyclohexanol(0.9085 mole fraction) as bottom of second column.

## Results

| **Master Property Table** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Object** | **oxygen** | **Mixed product** | **Mixed reactant** | **d1** | **d2** | **Cyclohexane in** | **b1** | **b2** | |
| Temperature | 25 | 179.027 | 157.204 | 36.1057 | 139.885 | 25 | 148.178 | 158.388 | C |
| Pressure | 1 | 9 | 9 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | 1.01325 | bar |
| Molar flow | 30 | 520.268 | 530 | 479.466 | 20.7982 | 500 | 40.8 | 20 | kmol/h |
| Vapour phase molar flow | 30 | 223.816 | 105.065 | 0 | 0 | 0 | 0 | 0 | kmol/h |
| Vapour phase molar fraction | 1 | 0.430194 | 0.198236 | 0 | 0 | 0 | 0 | 0 | |
| Liquid phase molar flow | 0 | 296.452 | 424.935 | 479.466 | 20.7982 | 500 | 40.8 | 20 | kmol/h |
| Liquid phase molar fraction | 0 | 0.569806 | 0.801764 | 1 | 1 | 1 | 1 | 1 | |

## Conclusion

The selected flowsheet is simulated in DWSIM software by using their Unit operations and thermodynamics and result is match with literature in which, it was simulated by the commercial simulator; which prove the usefulness of open-source simulator DWSIM.

## References


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(2) E. Bolton , Ind. Eng. Chem (1942).
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(4) Soave G. "Equilibrium constants from a modified Redlich-Kwong equation of state" C.E.S., 27, 6,1197-1203 (1972)