

Nitration Of Benzene process simulation using DWSIM

Nitrobenzene (some time called the oil of Mira-bane) $C_6H_5NO_2$ is pale yellow liquid with an odour that resembles bitter almonds, Depending upon the compounds purity. Its colour various from pale yellow to yellowish brown liquid boiling at 483 K (101 KPa) and freezing at 287.7 K as bright yellow crystals. It is quite toxic to human system.

A continuous process for the production of nitrobenzene has been developed by M / S.Biazzini of Switzerland. The advantages of this process are the lower concentration of mixed acid is used and higher reaction, rates though the sequence of operations is the same as in batch process. Continuous nitrator with capacity of 150 lit. Can produce as a 7500 capacity batch nitrator, but at the same time of quantity a reactants in nitrator is considerably small, unlike the batch process. Mixed acid and benzene are fed to nitrator in such that all nitric acid is utilized for nitration of benzene. The reactants are kept mixed under high speed agitation (600 rpm) and cooling. Due to the controlled feed rate and rapid agitation, the reaction time is 15 to 20 minutes only at reaction mixture is drawn off side of nitrator. The mixture is sent to decanter, where the, product is separated from spent acid for further processing.

Benzene used is of commercial quality. Mixed acid contain of 56 – 60 wt % H_2SO_4 , 20 – 26 wt% nitric acid and 15 – 18% water. Sulphuric acid used is of 94% - 98% concentration and nitric acid commercial grade of 55% - 60% concentration. Benzene is charged to the nitrator. Mixed acid is slowly added on surface of benzene from dosing tank with stirring. The ratio of mixed acid to benzene is kept around 2.5 : 1.0. The temperature mass is maintain initially at 25 – 30°C. So by high speed agitator and proper cooling coils reaction temperature can maintained upto 50 – 55°C. By obvious agitation, the interfacial area, of the reaction mixture is maintained as high as possible, thereby enhancing the mass transfer of reactants and cooling coils, which control the temperature of highly exothermic reaction.

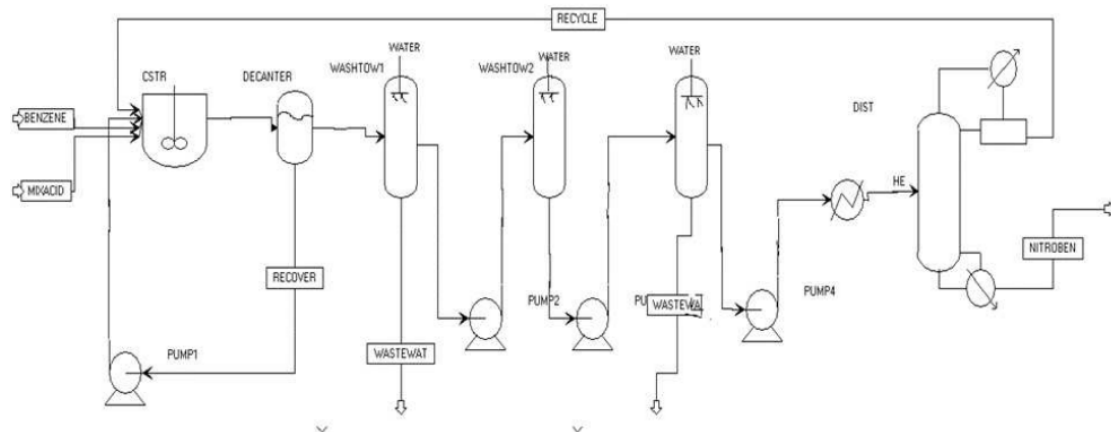
A slight excess of benzene usually is fed into the nitrator to ensure that the nitric acid in mixed acid is formation of denitrobenzene. Reaction time is only 15 – 20 minutes because of rapid and efficient agitation. Nitrobenzene and spent acid are removed from the side reactor and send to decanter unit. Organic and aqueous layers are formed, where two layers are separate in 10 to 20 minutes.

The aqueous phase or spent acid is drawn from the bottom and is concentrated in a sulphuric acid is drawn from the bottom and is concentrated in a sulphuric acid reconcentration step or is recycled to the nitrator, where it is mixed nitric acid and sulphuric acid immediately prior to being fed into nitrator.

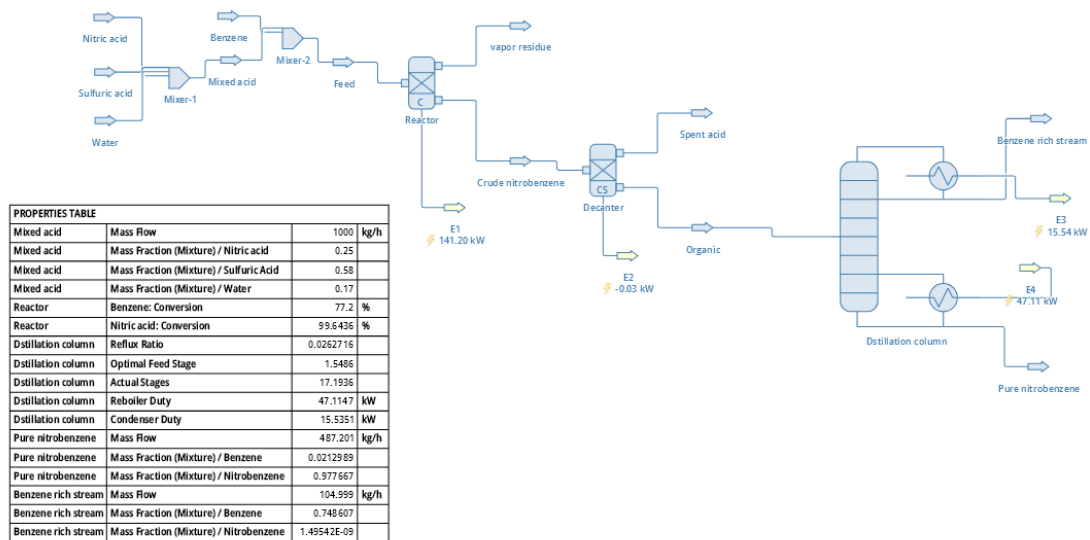
The crude Nitrobenzene can used directly for production of aniline if required, otherwise the crude nitrobenzene flows through a series of washer – separators, where residual acid is removed by washing with a dilute sodium carbonate solution followed by final washing with water. The product is then distilled to remove benzene and the nitrobenzene can be refined by vacuum distillation. Theoretical yields are 96 – 99 %.

The nitration process is unavoidably associated with the disposal of waste water from washing step. This water principally contains Nitrobenzene, some sodium carbonate and inorganic salts from the neutralized spent acid which was present in the product. Generally, the waste water is extracted with benzene to remove the nitrobenzene and the benzene that is dissolved in the water is stripped from water prior to the final waste treatment.

Process diagram



Process simulation Diagram



Conclusion:

1. Achieved 77.2% conversion of benzene in simulation.
2. Achieved 97.7%(by mass) purity of nitrobenzene in Distillation column's bottom stream .