Simulation and study of production process of Nitrobenzene

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Background

Nitrobenzene is an organic liquid having colorless to pale yellowish oily color. It is having odour like bitter almond tree or polish. Another name of nitrobenzene is “Oil of Mirbane”. Depending upon the purity, its color varies from pale-yellow to yellowish to caramel.

Nitrobenzene is prepared by direct nitration of benzene with mixed acid. Mixed acid is that the mixture of nitric acid, sulfuric acid and water. Several methods are available for technical nitration of benzene. Like isothermal nitration, adiabatic nitration, by using nitrogen dioxide gas etc.

In continuous isothermal process, the heat of nitration is removed by providing cooling to the nitrator. Benzene and also the nitrating acid (56-65 wt % H_2SO_4, 20-26 wt % HNO_3, and 15-18 wt % H_2O) are feed into the nitrator, the reaction mixture is stirred with high speed agitation and internal cooling coils and external heat exchangers. The temperature is maintained at 50 to 60 °C. There are three sorts of reactor mechanism. After the Nitration, Crude nitrobenzene separated from spent acid in gravity separator, then washings and distillation. (1) (2) (3)

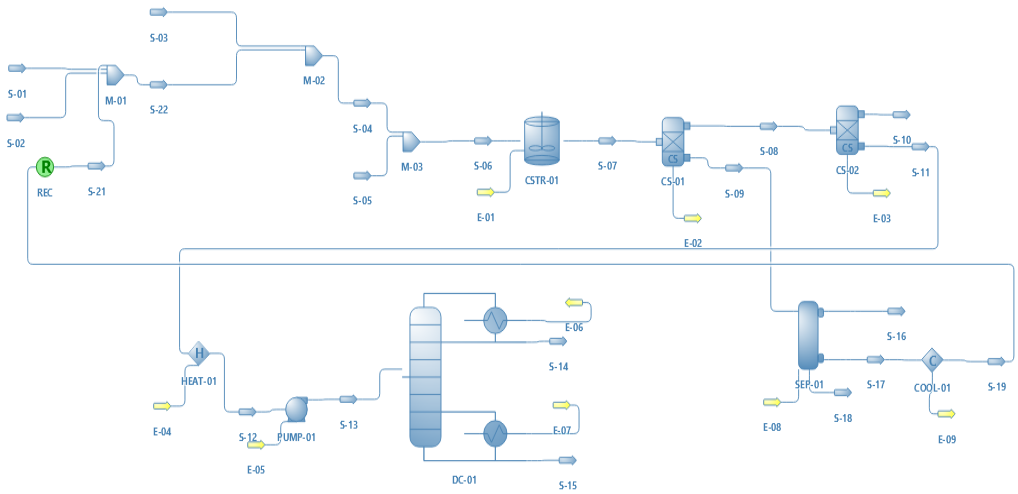

Figure 1: Flowsheet for production of Nitrobenzene from Benzene and Nitric acid

Process Description

Sulphuric acid (S-01) and Water (S-02) feeds along with Recycle water and sulphuric acid stream (S-021) in to (M-01) and now this mixture stream (S-022) and Nitric acid (S-03) feeds into mixture (M-02). Now this mixture stream (S-04) and Benzene (S-05) introduced in the Continuous stirred tank reactor (CSTR-01). Here reaction takes place between the Benzene and Nitric acid in the presence of Sulphuric acid and reaction is exothermic, so need to maintain temperature 50 to 60 °C and pressure 1 bar. The product mixture (S-07) leaving the reactor is

introduced in the gravity separation unit (CS-01), in which Crude Nitrobenzene (S-08) separated from the Spent acid (S-09). Now the Crude Nitrobenzene (S-08) feed in the washer in which sulphuric acid and water removed with Sodium carbonate and Calcium sulphate respectively. Now Crude mixture (S-11) are feed in to the pre-heater, in which mixture is pre-heated up to 192.2 °C. Using centrifugal pump (PUMP-01) feed in to the Distillation column (DC-01), in which Nitrobenzene is separated.

Spent acid (S-09) is in introduced in Gas- Liquid separation unit (SEP-01), in which excess water (S-16) are remove from the sulphuric acid and water stream (S-17). Now using cooler (COOL-01) Temperature reduce up to 25 °C and use as recycling (S-21).

Results

It was observed that at a temperature and pressure of 55 °C and 1 bar, the product stream from reactor contained nitrobenzene in large quantity of around 9722 kg/hr is produced. Even though large amount of nitrobenzene was produced, it was a diluted stream with mass fraction of about 0.37 (37 %). Its purity was improved using gravity separation and distillation column. After sensitivity analysis of Benzene flowrate (S-05) and benzene conversion in reactor we get maximum conversion 96.9386 % at flowrate of 6342.09 kg/hr.

Nitric acid is limiting reactant and its presence in reaction mixture creates byproducts. Thus, we increase Conversion of Nitric acid is 100 %.

Sulfuric acid is recovered and reconcentrate and recycled to inlet mixture. By performing sensitivity analysis of evaporator, we get desired composition of stream at 116.3 ° C. The % Recovery of sulfuric acid in reconcentrate is 98.99 %.

The crude nitrobenzene is distilled to get purer product. The obtained nitrobenzene in bottom product is of 99.97 % purity. The desired quantity of nitrobenzene production is 9722.22 kg/hr but the actual achieved production is 9023.15 kg/hr. Hence % Recovery of nitrobenzene is 92.81 %.

Conclusion and recommendation

Process simulation for the production of nitrobenzene by isothermal nitration of benzene was done using DWSIM. Gravity separation, Washing and distillation is performed to obtain considerable purity of the final nitrobenzene product. Three sensitivity analysis were performed. we find that how actually parameters mention above may affect each stream. For example, we first added calculated amount of extra water to decanter, but from that action we know that how much extent it affects each stream, so we are finally able to find the optimum amount of water required for operation and using sensitivity analysis we increase 4% conversion of Benzene.

While working with DWSIM, the team felt that the Sensitivity analysis parameters could be improved i.e. a greater number of dependent and independent variable combinations could be added in the software, because, even after trying to perform different types of analysis on the process, the desired results were not obtained from the software. It was possible only after manually changing the specifications of the unit. Also, the software could include other objects like decanter, crystallizer, extractor, dryer etc. to improve the simulation and flowsheet design.

Reference:

[1] Krik and Other, “Encyclopedia of Chemical Technology”, Vol.15, 3rd Ed., page (918-931),

[2] Munnig, J., et al. (2013). Process for the continuous preparation of nitrobenzene,

[3] Ullmann’s Encyclopedia of Industrial Chemistry, 2005 Wiley-VCH Verlag GmbH & Co. KGaA.