STEADY STATE SIMULATION OF PRODUCTION OF ACRYLONITRILE BY PROPYLENE AMMOXIDATION

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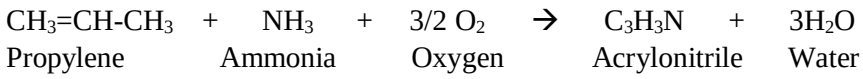
INTRODUCTION:

Acrylonitrile is a chemical compound with the formula C_3H_3N. This is colourless liquid often appears yellow due to impurities in terms of its molecular structure, it consists of a vinyl group to a nitrile. It is an important monomer for the manufacture of polyacrylonitrile(PAN). It is used as comonomer in the production of acrylonitrile butadiene styrene(ABS) and styrene acrylonitrile(SAN). Acrylic fiber is used for clothing, carpeting. It is used in the production of plastics, surface coatings, nitrile elastomers, barrier resins, adhesives. It is also used as intermediate for synthesis of various antioxidants, pharmaceuticals, dyes, surface active agents, flour milling, food processing. United States is one of the major producers and largest exporter of acrylonitrile. India accounts to produce ABS, majority of the demand for acrylonitrile are fulfilled by domestic production. Some of the major operating markets are Bhansali engineering polymers, INEOS Styrolution, LG chemical, Lotte chemical cooperation, Formosa plastic group.

BACKGROUND AND DESCRIPTION:

- The simulation was conducted for the production of acrylonitrile by propylene ammoxidation with the aid of the software ‘’DWSIM”.
- Acrylonitrile is commercially produced by a reaction of propylene and ammonia in the presence of a catalyst.
- Main reaction:

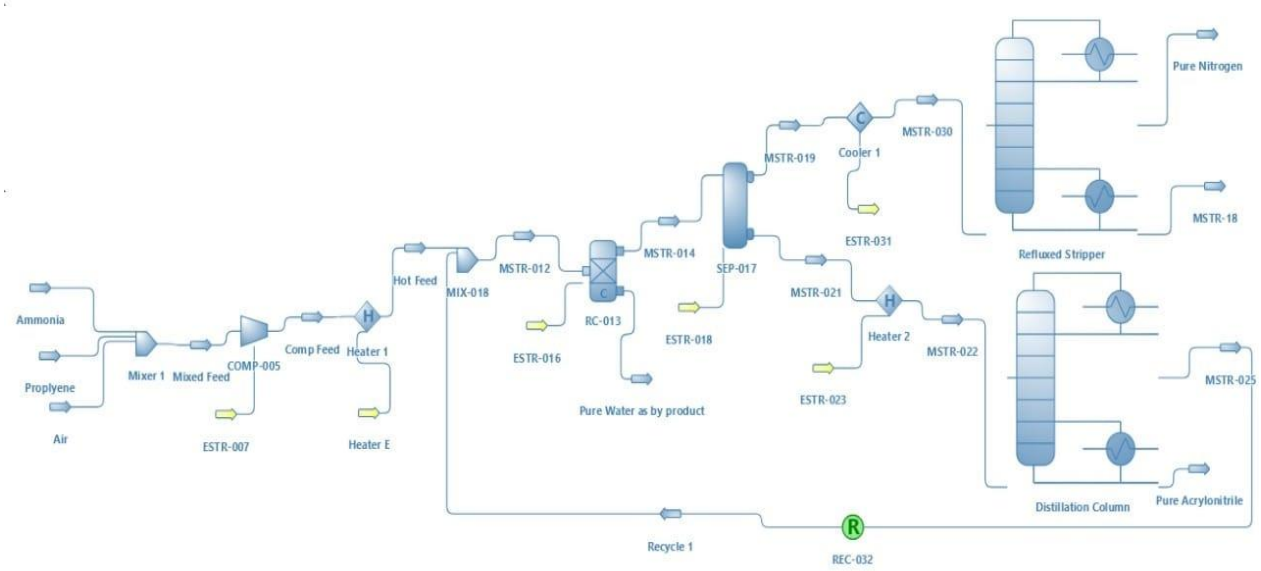


- Oxygen is introduced bellow the bottom grid with the mixed propylene and ammonia. The catalysts play an important role in preserving the safety as scavenger for oxygen radicals.
- The catalysts used in this process are mostly mixed metal oxides such as bismuth-molybdenum oxide, uranium-antimony oxide, tellurium-molybdenum oxide etc.
- Some of the wastes that are generated from the process are ammonium sulphate and the aqueous wastes containing cyanides, sulphates etc.

- Propylene, Ammonia and Air are sent into the ‘Reactor’ in the ratio of 1:1.2:5 at the temperature 298.15 K and pressure 101.325 kPa.
- The reactant feed is mixed. This mixed feed is sent into the ‘Adiabatic compressor’ at 297.951 K and 101325 Pa, where there is rise in pressure. The pressure rise is 121.590 kPa, hence the outlet pressure is 222.915 kPa.
- The compressed feed is sent to ‘Material team heater’ at 379.938 K and 222.915 kPa. the temperature change is -29.9384 K, therefore the outlet temperature being 350 k.
- This hot feed at 350 K and 192.518 kPa is sent into the ‘Mixer’. This mixed feed enters into the ‘Conversion reactor’. The pure water is separated as by product.
- Now this mixture is sent into the ‘Vapour-Liquid separator’, where it is separated into vapour and liquid phases.

- The separated vapour phase mixture enters 'Cooler' where there is pressure drop of 253.31.3 kPa and outlet temperature 173.15 K. This enters refluxed stripper and pure nitrogen is obtained.
- The separated liquid phase mixture enters 'Heater' where there is pressure drop of 40.530 kPa and outlet temperature 400 K, and enters distillation column where pure acrylonitrile is obtained.

FLOW DIAGRAM:



MASTER PROPERTY TABLE:

Master Property Table						
Object	Pure Water as by product	Pure Nitrogen	Propylene	Ammonia	Air	
Temperature	310	80.8439	298.15	298.15	298.15	K
Pressure	192518	150000	101325	101325	101325	Pa
Molar Flow	94306	59617.5	23764.4	70461.7	172831	mol/s
Molar Fraction (Mixture) / Acrylonitrile	1.80182E-06	1.41261E-20	0	0	0	
Molar Fraction (Mixture) / Propylene	2.69472E-09	0	1	0	0	
Molar Fraction (Mixture) / Ammonia	0.00315943	1.49802E-24	0	1	0	
Molar Fraction (Mixture) / Nitrogen	1.37124E-07	1	0	0	0.77	
Molar Fraction (Mixture) / Water	0.996839	0	0	0	0	
Molar Fraction (Mixture) / Oxygen	1.02611E-07	1.04365E-20	0	0	0.23	

REFERENCE:

Aman agarwal, Ankesh kumar singh, Pratik chaplop, Rahul gupta, Raju Mishra, Sachin goel., "Acrylonitrile by Propylene Ammoxidation" thesis Dr. R.G.Pala, 2013, page 1-44.

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