

TNT production by Nitration of Toluene

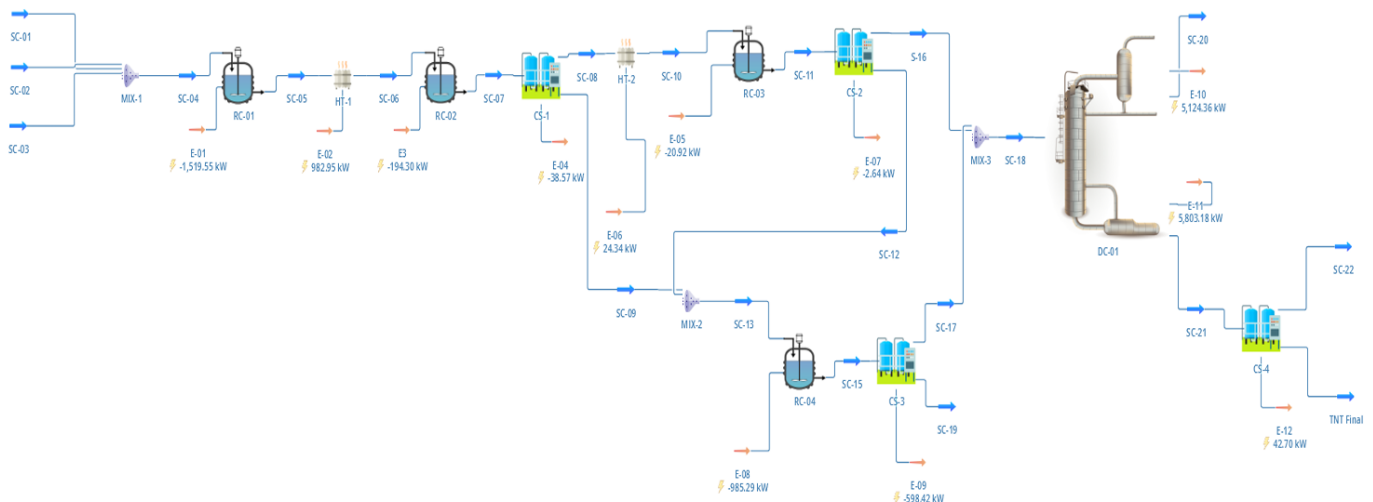
Dhruv Thakare

Visvesvaraya National institute of Technology

Background & Description:

Trinitrotoluene (TNT) is a widely used high-energy material with significant applications in defense, mining, and demolition. Its production involves a multi-stage nitration process, where toluene undergoes sequential nitration using nitric and sulfuric acid mixtures under controlled conditions. Production of TNT from this process is quite difficult due to the formation of various byproducts formed which can be again treated to form the desired product. The concentrations of Sulfuric acid and Nitric acid used are 98% and 90% respectively. The temperatures of reaction are brought till the required limits by using Heaters, mainly for third nitration temperature requirement is 100-115 C. For more concentrated and desired product 3 compound separators are used. Mononitro toluene reacts with nitric acid in the presence of sulfuric acid to give dinitrotoluene, for simplicity it was assumed that only (2,4), (2,6) and (3,4)-DNT are formed. As the reactions get complete, separation needs to take place to separate the desired product from the rest as output stream contains unreacted reactants, side product and spent acid, for this a Distillation Column is used. The difference in boiling points makes it easy to separate DNT and TNT from other unreacted reactants. Though the production of TNT is approximately 15kmol per 100kmol of Toluene (Efficiency of 15%) this can be increased upto a great extent by adding recycling streams which will utilize all the unreacted Toluene, Acids and even MNT, DNT.

Flowsheet:



Results:

Master Property Table											
Object	TNT Final	SC-21	SC-20	SC-18	SC-15	SC-13	SC-11	SC-07	SC-06	SC-04	
Temperature	326.922	326.922	62.1812	72.3072	72.0964	72.0964	110	70	70	34.4576	C
Pressure	1.01325	1.01325	1.01325	3	3	3	3	3	3	3	bar
Mass Flow	545.189	1703.7	10565.5	12269.1	35482.4	35482.4	1067.39	35618.2	35618.2	35618.2	kg/h
Molar Flow	2.40046	8.77569	125.64	134.415	414.4	414.4	7.84939	415	415	415	kmol/h
Volumetric Flow	0.483859	432.094	869.708	12.9709	19.1995	19.0877	1.94323	19.1115	19.047	18.2583	m3/h
Molar Enthalpy (Mixture)	17698.9	72972.8	-30386	-41818.5	-71943.2	-68940.7	-74058.7	-69505.5	-68963.3	-72568.1	kJ/kmol
Molar Entropy (Mixture)	78.026	171.18	-56.4428	-73.0257	-141.517	-139.264	-101.879	-140.747	-140.509	-165.564	kJ/[kmol.K]
Molar Fraction (Vapor)	0	1	0.248552	0	0	0	0.0150063	0	0	0	
Phases	L	V	V+L	L	L	L	V+L	L	L	L	
Energy Flow	22.7399	247.976	-2180.55	-2611.38	-58945.6	-57960.4	-650.193	-58014.1	-57819.8	-57283.2	kW

