PRODUCTION OF DNT FROM TOLUENE

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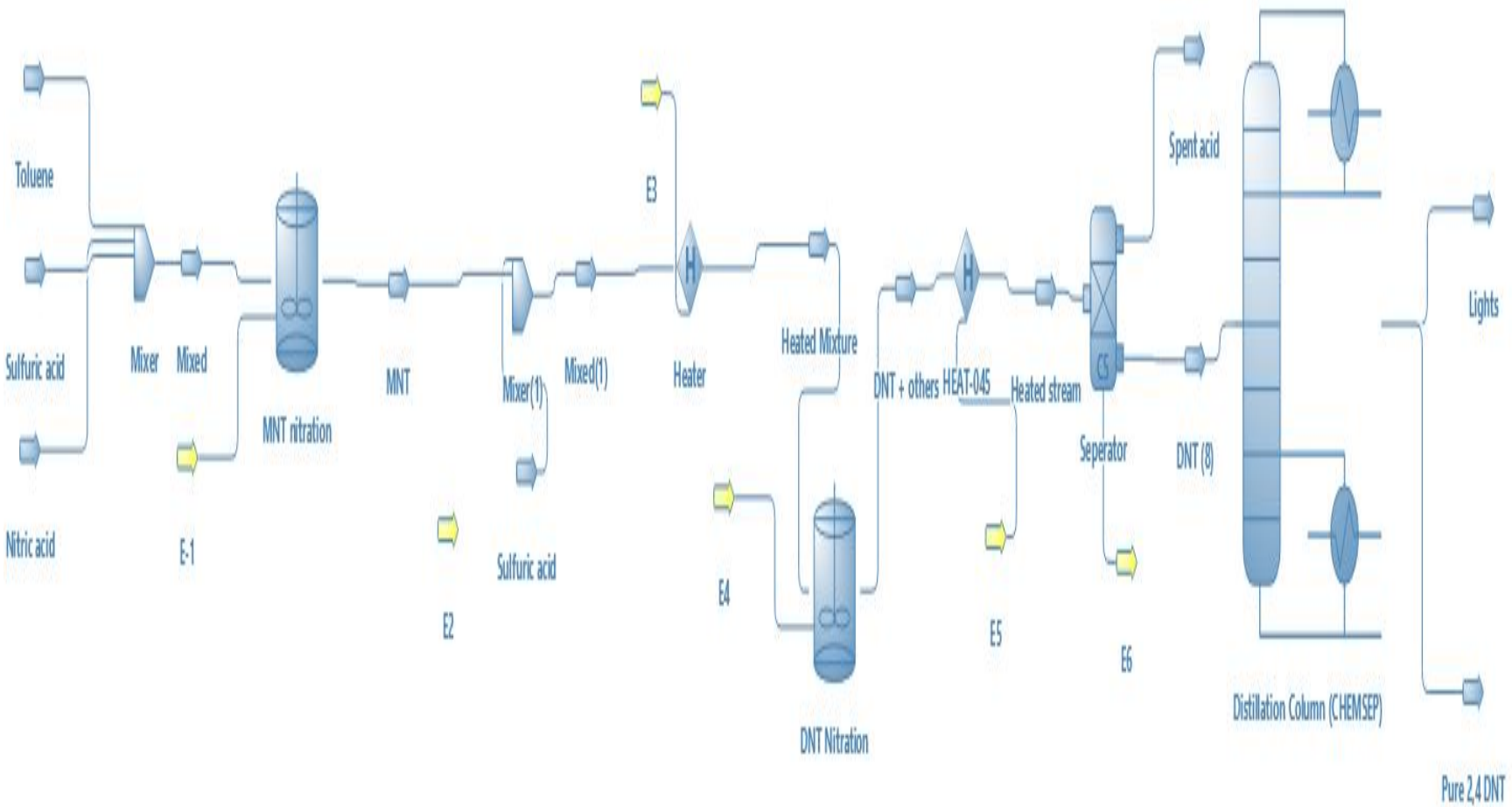
Process Description:

For this process, UNIFAC is selected as property package. Toluene & Nitric acid are reactants. Sulfuric acid is used as catalyst in this process. After mixing of reactants, the mixed stream is supplied to a kinetic reactor wherein reaction between Toluene and Nitric acid occurs. The reaction is assumed to be first order wrt both Toluene and Nitric acid to produce o,p and m-nitrotoluene in the proportional of 58:39.5:2.5 respectively; giving 99.5% conversion of Toluene. The reaction occurs at 310K and at atmospheric pressure. The outlet stream from the reactor is again mixed with Sulfuric acid so as to ensure high rates of reaction in the further process. This mixed stream is passed through the heater so as to ensure favourable reaction conditions upstream to the reactor by heating it to 343K (reaction temperature). In the reactor, Mononitro toluene reacts with nitric acid in the presence of sulfuric acid to give dinitrotoluene, for simplicity it was assumed that only 2,4 and 2,6-DNT are formed in the proportion of 77: 23 respectively. For the later reactor, there are two reactions taking place. One is the production of 2,4-DNT from o-nitrotoluene and other is the production of 2,6-DNT from p-nitrotoluene. Order of reactions here too is first order wrt each reactant. In these reactions, 60% conversion of o-nitrotoluene and 47.5% conversion of p-nitrotoluene were recorded. Then the desired product is 2,4 DNT.

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. Effluent is sent to separator wherein spent acid is separated before it is sent to the distillation column. This is due to the fact that separating spent acid with the use of a distillation column is not favourable as it consumes a lot of energy as the heat of vaporization. Impure DNT stream after removal of spent acid now goes into the distillation column. The input to DC contains isomers of both MNT and DNT, from which 2,4 DNT needs to be separated majorly. Here the almost pure (99%) stream comes out from the bottom and rest goes out as Lights from the top. It is recycled in the actual plant process. It is to be noted that the complete process is conducted at atmospheric pressure.

Flowsheet:


Toluene
Sulfuric acid
Nitric acid
Mixer
Mixed
E-1
MNT nitration
MNT
E2
Mixer(1)
Sulfuric acid
Mixed(1)
E3
Heater
Heated Mixture
E4
DNT Nitration
DNT + others
HEAT-045
Heated stream
E5
Seperator
E6
Spent acid
DNT (8)
Distillation Column (CHEMSEP)
Lights
Pure 2,4 DNT

Flowsheet data:

	MNT	Mixed	Spent acid	Heated stream	DNT + others	Nitric acid	Toluene	Sulfuric acid	Mixed(1)	Sulfuric acid	Heated Mixture	DNT (8)	Lights	Pure 2,4 DNT
Temperature (K)	310.155	310.155	450	450	343	310	310	298.15	308.565	310.5	343	450	511.936	592.22
Mass Flow (kg/s)	8.22223	8.22223	4.83171	10.1667	10.1667	4.16667	3.05556	1.94444	10.1667	1	10.1667	5.33496	3.21523	2.11972
Molar Flow (mol/s)	109.652	109.652	96.6645	129.806	129.806	66.1241	33.1627	20.1541	129.806	10.365	129.806	33.1414	21.5031	11.6383
Mixture Density (kg/m3)	1232.28	1249.97	1.35372	2.56564	4.4933	1487.95	854.084	2376.72	1332.06	2347.67	5.35627	1104.59	976.487	1058.06
Mixture Specific Enthalpy (kJ/kg)	-672.755	-550.012	112.113	21.1224	-251.472	-586.609	-391.782	-898.872	-716.001	-881.004	-287.624	-164.916	-45.4696	65.4491
Mixture Thermal Conductivity (W/[m.K])	0.154888	0.157076	0.023267	0.040456	0.060951	0.287892	0.129717	1.97E-05	0.113499	2.02E-05	0.070283	0.12139	0.104081	0.103002
Vapor Phase Density (kg/m3)	0	0	1.35372	1.61985	1.65388	0	0	0	0	0	1.88434	0	3.3645	0
Vapor Phase Heat Capacity Ratio (Cp/Cv)	NaN	NaN	1.28537	1.1823	1.33028	NaN	NaN	NaN	NaN	NaN	1.30556	NaN	1.04474	NaN

Important stream compositions:

1. Stream leaving 1st reactor:

Compound	Amount
Sulfuric Acid	0.092635769
Air	0
Nitrogen	0
Toluene	0.00019424646
O-nitrotoluene	0.17227805
P-nitrotoluene	0.11938566
M-nitrotoluene	0.010578477
2,4-dinitrotoluene	0
2,6-dinitrotoluene	0
3,4-dinitrotoluene	0
2,5-dinitrotoluene	0
3,5-dinitrotoluene	0
Water	0.30413271
2,4,6-trinitrotoluene	0
Nitric acid	0.30079508

2. Stream leaving 2nd reactor:

Compound	Amount
Sulfuric Acid	0.2304108
Air	0
Nitrogen	0
Toluene	0.00016408712
O-nitrotoluene	0.058190973
P-nitrotoluene	0.052922642
M-nitrotoluene	0.0089360282
2,4-dinitrotoluene	0.095853638
2,6-dinitrotoluene	0.03941181
3,4-dinitrotoluene	0
2,5-dinitrotoluene	0
3,5-dinitrotoluene	0
Water	0.3952828
2,4,6-trinitrotoluene	0
Nitric acid	0.11882722

3. Product stream:

Compound	Amount
Sulfuric Acid	0
Air	0
Nitrogen	0
Toluene	0
O-nitrotoluene	6.1747996E-09
P-nitrotoluene	4.1921672E-07
M-nitrotoluene	1.0623073E-08
2,4-dinitrotoluene	0.99
2,6-dinitrotoluene	0.009999564
3,4-dinitrotoluene	0
2,5-dinitrotoluene	0
3,5-dinitrotoluene	0
Water	0
2,4,6-trinitrotoluene	0
Nitric acid	0