Production of Terepthalic Acid from oxidation of p-Xylene

Dwsim Version-6.0 update-4

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Background:

Terephthalic acid is an aromatic carboxylic acid core to polyester fibers production. A large majority of the production of terephthalic acid is via aerobic catalytic oxidation of p-xylene with air in acetic acid medium in a process commonly known as the Amoco process. Terephthalic acid history is closely related to polyester history. Terepthalic acid is primarily utilized as a raw material to make polyester PET, a polymer used to make a variety of household items such as clothing and plastic bottles.

Process Description:

$$CH_3(C_6H_4)CH_3 + 3O_2 \text{ <--> } COOH(C_6H_4)COOH + 2HOH$$

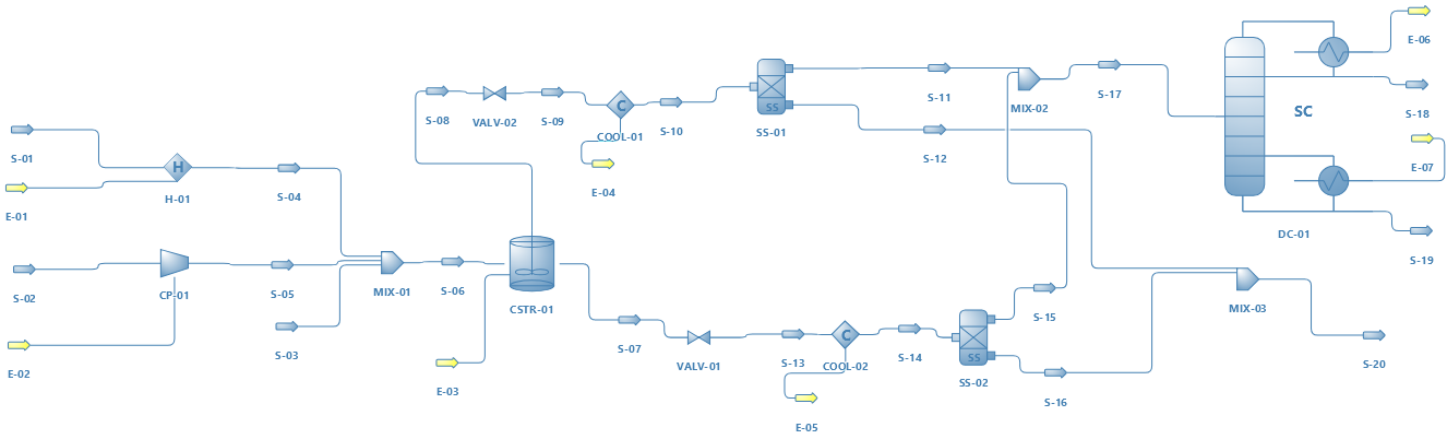
p-Xylene + Oxygen <--> Terepthalic Acid + Water

P-xylene (S-01), Oxygen (S-02) are used as feed which are prepared before mixing via treatment of p-xylene through heater and oxygen to be compressed. Thus in a mixer (MIX-01) treated p-xylene (S-04), compressed oxygen (S-05) and mixture of Acetic acid as solvent and trace of terepthalic acid via. (S-03) is fed. After gaining optimum temperature (474.63K) and pressure(4.34 bar), mixed feed (S-06)is introduced into a CSTR reactor (CSTR-01).

Reaction takes place at 731K and 4.34 bar pressure gives two product streams; out of which stream (S-07) contains large amount product Terepthalic acid while stream (S-08) posses in minor fraction. Both product stream are cooled and with the help of Solid separator, crystals of TPA (S-20) is obtained while remaining by-product like water, unreacted p-xylene and solvent Acetic acid is recovered with the help of distillation column.

Distillation column (DC-01) is operated at atmospheric pressure and 393.07K temperature, feed stream (S-17) containing p-xylene and acetic acid is separated as boiling point of Acetic Acid is 391.15K. We get Acetic Acid as top product (S-18) and P-xylene (S-19) as bottom product.

Flowsheet:



Results:

Result-1								
Object	**S-08**	**S-07**	**S-05**	**S-04**	**S-03**	**S-02**	**S-01**	
Temperature	731.801	731.836	573.561	448.15	448.15	298.15	298.15	**K**
Pressure	4.34658	4.34658	11.0133	1.01325	1.01325	1.01325	1.01325	**bar**
Mass Flow	10346.2	44148.2	15999.4	10616.5	27878.5	15999.4	10616.5	**kg/h**
Molar Flow	91.2917	268.199	500	100	400	500	100	**kmol/h**
Vapor Phase Mass Flow	10346.2	282.271	15999.4	10616.5	21487.1	15999.4	0	**kg/h**
Vapor Phase Molar Flow	91.2917	4.15431	500	100	357.791	500	0	**kmol/h**
Liquid Phase (1) Mass Flow	0	43866	0	0	6391.49	0	10616.5	**kg/h**
Liquid Phase (1) Molar Flow	0	264.045	0	0	42.2085	0	100	**kmol/h**
Molar Fraction (Mixture) / Terephthalic acid	0.480111	0.984905	0	0	0.0909174	0	0	

Result-2					
Object	**S-20**	**S-19**	**S-18**	**S-06**	
Temperature	725.35	411.305	124.309	474.63	**K**
Pressure	1.01325	1.01325	1.01325	4.34658	**bar**
Mass Flow	51164.4	516.277	2813.75	54494.4	**kg/h**
Molar Flow	307.977	4.88183	46.6326	1000	**kmol/h**
Vapor Phase Mass Flow	0	0.51012	9.21875E-06	48066.4	**kg/h**
Vapor Phase Molar Flow	0	0.00484895	2.88097E-07	957.595	**kmol/h**
Liquid Phase (Mixture) Mass Flow	51164.4	515.784	2813.74	6428.02	**kg/h**
Liquid Phase (Mixture) Molar Flow	307.977	4.87698	46.6326	42.4046	**kmol/h**
Molar Fraction (Mixture) / Terephthalic acid	1	0.000909666	1.84632E-236	0.0363669	
Mass Fraction (Mixture) / Terephthalic acid	1	0.001429	5.08349E-236	0.110868	
Molar Flow (Mixture) / Terephthalic acid	307.977	0.00444084	8.60988E-235	36.3669	**kmol/h**

References:

Cao, Na; Chang, Eric; and Kaufman, Maria, "New Terephthalic Acid Process" (2011). Senior Design Reports (CBE). 2.
http://repository.upenn.edu/cbe_sdr/24