DESIGN PROJECT REVIEW II

MEE 321

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Process description:

Polyol, MDI and 1, 4-Butanediol are the main reactants for the formation of TPU.

Polyol Reactor: Adipic acid and 1, 4-Butanediol are made to react to produce polyester Polyol. Water liberated from the reaction is condensed and treated as effluent. Along with the water some amount of organic material also gets produced which needs to be analysed for the presence of monomers and oligomers.

Polyol Blend Tank: Prepared polyol is melted to liquid state and is fed to the blend tank with additives in a very negligible amount as per application.

The flowrate of raw materials is calibrated to avoid polymer build up. The calibrated reactants cannot be reused again as it gets exposed to air and gets a colour due to oxygen presence.

MDI and BDO Charging: MDI and BDO supplied to the tanks are charged after melting. The flowrate is maintained to maintain the polymer consistency and final quality of the product.

FettAlkohol Tank: Fettalkohol C-8 98% is a chain terminating agent which controls the side reaction of a product which is not desired to be formed.

Extruder: Co-rotating twin reactive screw extruder is used. Mixer product and BDO are sent to the extruder and are fed one by one, with few minutes gap and the material is collected in waste drums till all raw material are mixed and uniform polymer is formed before sending the polymer to pelletisation process. The technique used for making the pellets from the resin is called *Under water pelletisation*. Resin from the extruder passes through a DIE and then pulled out in the required cross sectional area and is cut by the blades of the pelletiser , then cooled by chilled water. A lot of waste is also removed due to pelletiser upset as a result of improper polymer build up.

Dryers: A centrifugal dryer is used. Here the pellets and water gets separated. This water is recycled. The final moisture content present in the pellets after dehumidification (hot air dryer) is 0.05%.

Sieving: The desired shape of pellets is between 3-5mm. Hence the bigger sizes are left on the upper sieves and the required size of pellets are obtained.
Packing: The final product is packed and dispatched to various industries.

The process shows a maximum conversion rate of 96%.

Production of TPU : 350 Kg/hr = 8400 Kg/day = 8.4 tons/day

Composition of the TPU pellets (excluding water content)

POLYOL	48.06%
BDO	10.14%
MDI	41.04%
Additives	0.76%

The additives used are :

Finawax	0.36%
Edenol	0.25%
Irgonax	0.10%
Carbodiimid	0.05%

stream	Temp	specific heat, Cp	ΔH_f
	(K)	(KJ/kg)	(KJ/mol)
water	298	4.18	-242
adipic acid	298	2.43694	-994.3
BDO	298	2.219263205	-503.25
polyol	363	1.89	-1250
MDI	338	1.8	-360
TPU	333	1.65946	-1393

Temp. of reactor (K)	493
Temp. of Extruder (K)	523
Temp. in hot air dyer(K)	368
Temp of water effluent(K)	318
Temp of mixer(K)	373
specific heat of mixer outlet(KJ/kg)	1.78
enthalpy of mixer outlet stream	-1483
Temp of chilled water wash (K)	385.5
temp in centrifugal dryer(K)	298

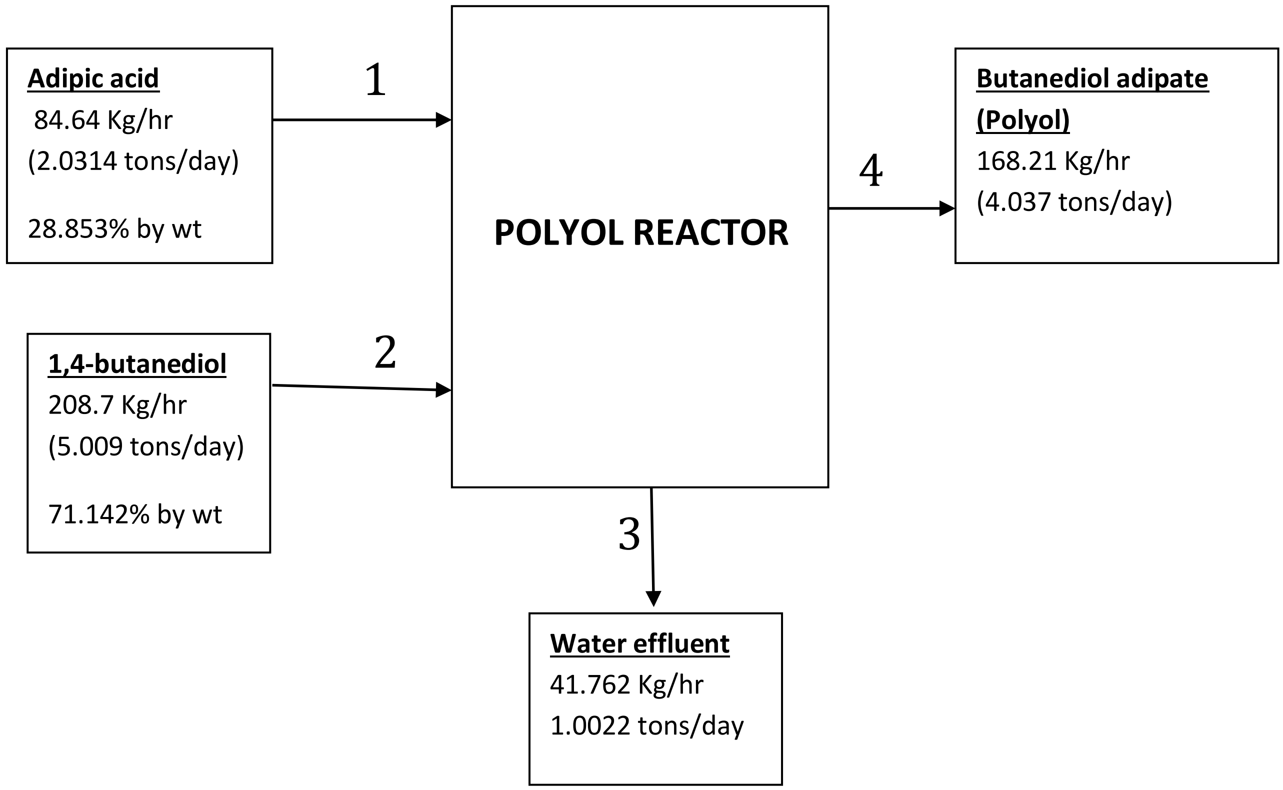
MASS BALANCE

Mass Balance of reactor:

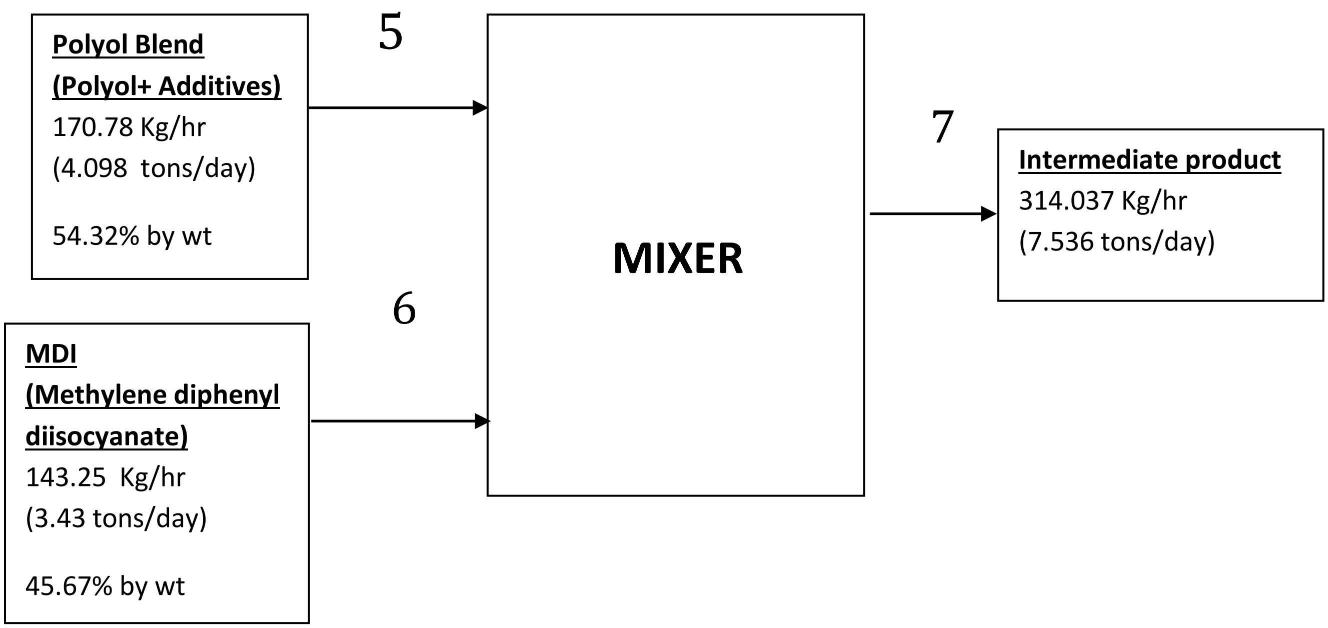
$$R(COOH)_2 + 2R(OH)_2 \rightarrow HO - [R - COO - R - C00 - R] - OH + 2H_20$$

Adipic acid *1,4-butanediol* *butanediol adipate (polyester polyol)* *water*

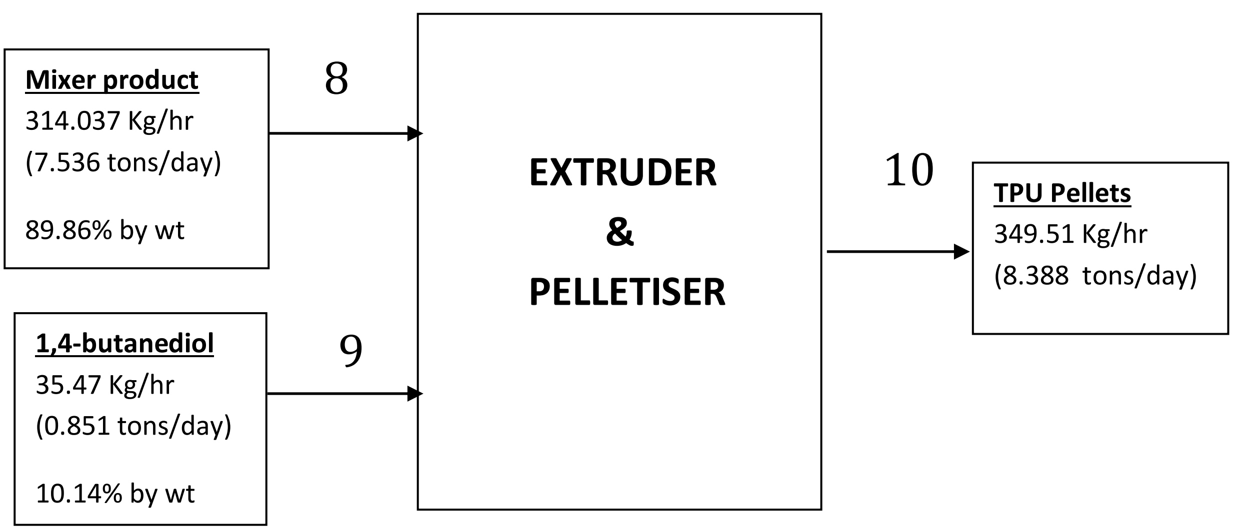
Where $R = C_4H_8$

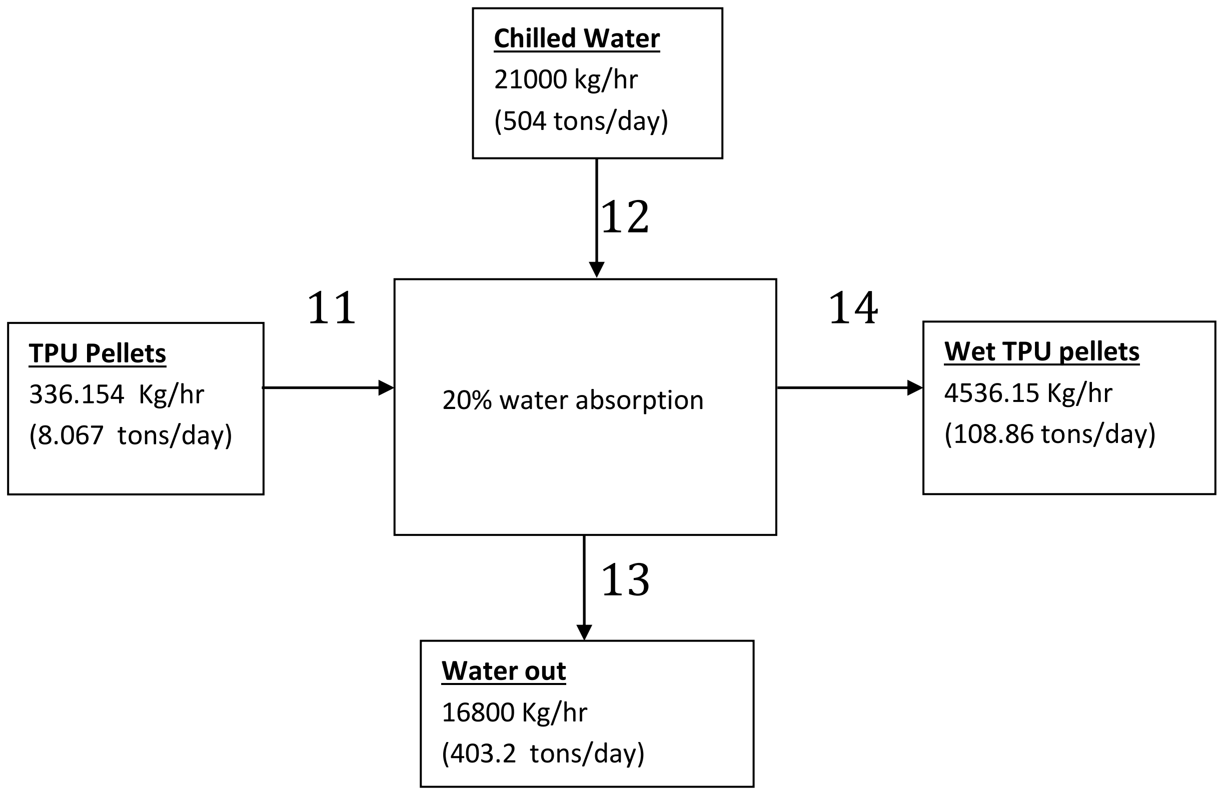

Adipic acid
84.64 Kg/hr
(2.0314 tons/day)
28.853% by wt
1
1,4-butanediol
208.7 Kg/hr
(5.009 tons/day)
71.142% by wt
2
POLYOL REACTOR
3
Water effluent
41.762 Kg/hr
1.0022 tons/day
4
Butanediol adipate
(Polyol)
168.21 Kg/hr
(4.037 tons/day)

Mass Balance of Mixer:

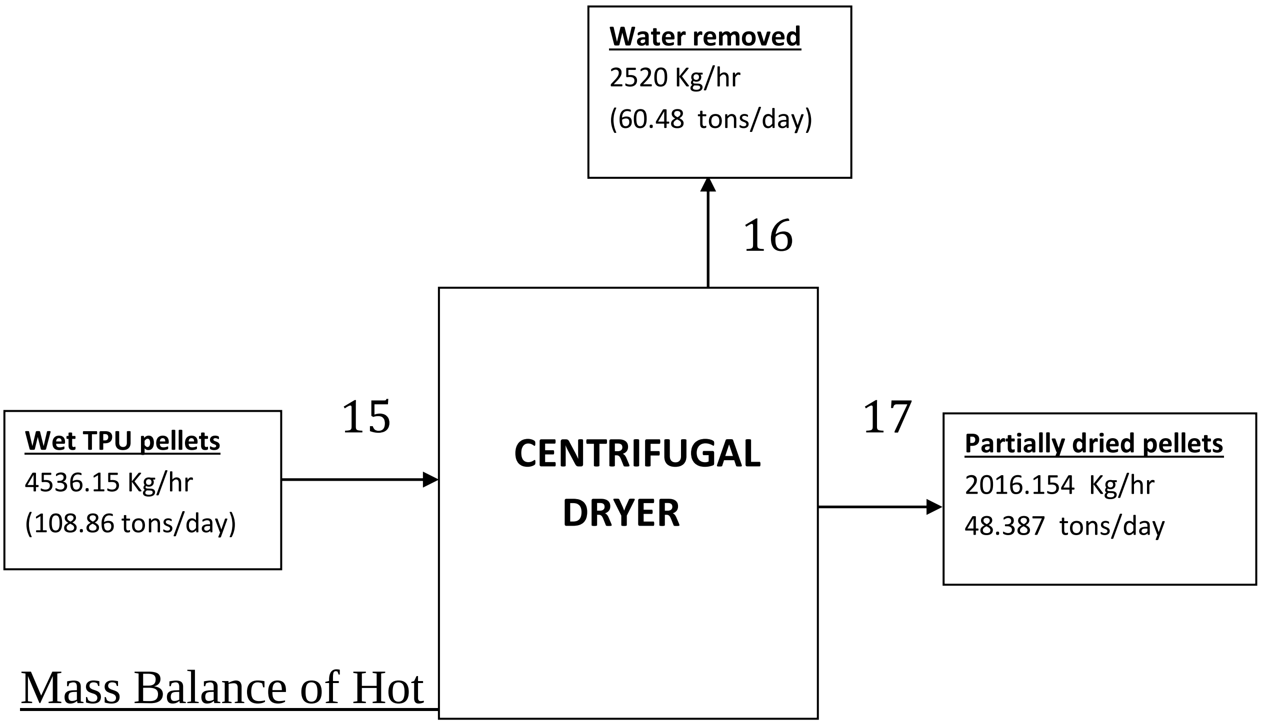


Mass Balance of Extruder and Pelletiser:

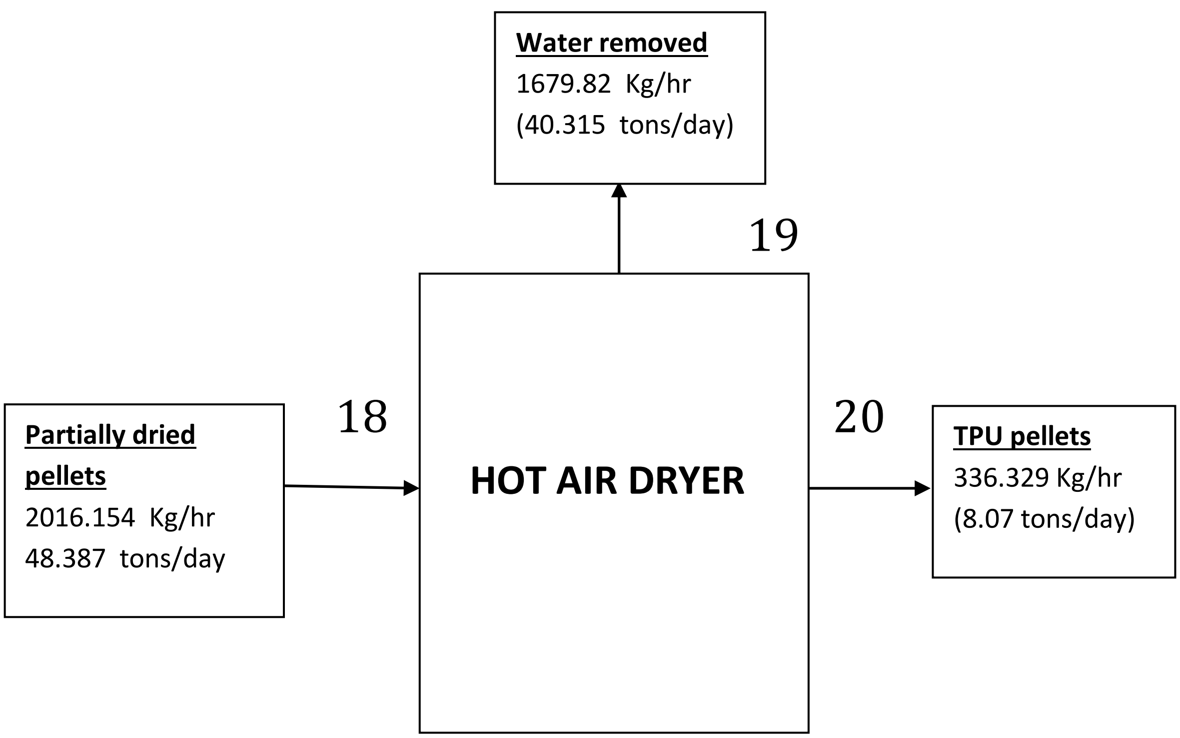



Chilled Water
21000 kg/hr
(504 tons/day)
12
11
TPU Pellets
336.154 Kg/hr
(8.067 tons/day)
20% water absorption
14
Wet TPU pellets
4536.15 Kg/hr
(108.86 tons/day)
13
Water out
16800 Kg/hr
(403.2 tons/day)

Mass Balance of Centrifugal dryer:



Mass Balance of Hot



Assuming no losses : input= output=**350Kg/hr** = 8.4 tons/day

The conversion is **96%** i.e. 4% loss of material = 14Kg/hr = 0.336 tons/day.

Therefore including all the losses ; production =**336.329 Kg/hr** (96.094 % of 350)

These losses accounts for:

1) **Charging and Metering loss :**

   Charging Polyol and MDI from drums gives us loss of 0.15% each. , there is 1 to 2 kg of Polyol left out in the drums, as it cannot be pumped out fully. The flow rate of raw material is very critical as it decides the polymer build up and the final property of the product. So always in any grade, before starting the process, Polyol flow is calibrated and material used for the calibration are not reused as it is exposed to air, and subsequent color build up due to oxygen content, This Polyol is disposed as waste and it works out to be 0.10%.

2) **Extruder start up loss:**

   Systematic feeding sequence is adopted to overcome any material choke in the extruder. So raw material are fed one by one , with few minutes gap and the material is collected in waste drums till all raw material are mixed and formed the uniform polymer before the polymer to pelletisation process. This takes minimum of half an hour to 45 minutes. Material collected during this time is not useful for the regular production. This material is declared as waste and amounts to be 9.0%. This is main area, where maximum waste is generated.

3) **Pelletiser upset loss:**

   TPU process is very difficult one and stabilization requires few hours.

During the startup process or due to slight variation in the flow steams or delay in push up of material in the extruder, improper polymer build up occurs and leads to pelletiser upset. While overcoming the pelletiser upset by way of removing the cutter and cleaning it, polymer passes through the extruder are collected in drums and treated as waste since it cannot be sold to any customer. This is an average, accounts to be 1.6%

The total loss of 336 kgs of material per hour (8.064 tons/day):

LOSSES	%age	Kg/hr	Tons/day
Polyol loss	2.25%	7.728	0.1854
MDI loss	2.25%	7.728	0.1854
Extruder loss	81%	272.16	6.532
Pelletiser loss	14.4%	48.384	1.1612
TOTAL	**100%**	**336**	**8.064**

Calculations:

Since the mass flow rate is 350 kg/hr for TPU pellets. It has 0.05% of moisture and 99.95% of solids and the percentage composition of BDO is 10.14% of the solids. Therefore, the mass flow rate of **stream 9** = 10.14% x 99.95% x 350

= 0.1014 x 0.9995 x 350

= **35.47 Kg/hr = 0.851 tons/day**.

The percentage composition of polyol is 48.06% of solids. Therefore, the mass flow rate of **stream 4** = 48.04% x 99.95% x 350 = 0.4806 x 0.9995 x 350

= **168.125 kg/hr = 4.035 tons/day.**

Now according to the reaction:

$$\boldsymbol{R(COOH)_2 + 2R(OH)_2 \rightarrow HO - \lfloor R - COO - R - C00 - R \rfloor - OH + 2H_20}$$

Adipic acid *1,4-butanediol* *butanediol adipate (polyester polyol)* *water*

Where $\boldsymbol{R} = \boldsymbol{C_4H_8}$

1 mole Adipic acid—2 moles BDO—1 mole polyol—2 moles water

Therefore, mass flow rate of Adipic acid i.e **stream 1** = (168.125/290) x (1x146)
= **84.642 kg/hr =2.031 tons/day.**

Mass flow rate of BDO i.e **stream 2** = [(168.125/290) x 2] x (2 x 90)
= **208.7 kg/hr = 5.009 tons/day.**

Similarly, mass flow rate of water effluent i.e **stream 3** =(168.125/290)x2 x (2x18)
= **41.74 kg/hr = 1.0017 tons/day.**

The percentage composition of MDI is 41.04% of solids. Therefore, the mass flow rate of **stream 6** = 41.04% x 99.95% x350 = 0.4104 x 0.9995 x 350 =143.568 kg/hr.

we know that there is a loss of 2.25% of 4% of 350 i.e 0.315 kg/hr. Therefore (143.568 - 0.315) = **143.25 kg/hr = 3.43 tons/day.**

Stream 5 is a blend of polyol and additives. The percentage composition of additives is 0.76% of solids.
Therefore mass flow rate of **stream 5** = (0.76% x 99.95% x 350) + 168.125
= (0.0076 x 0.9995 x 350) + 168.125
= **170.78 kg/hr = 4.098 tons/day.**

Therefore, now mass flow rate of **stream 7=stream 8** = 170.78 + 143.25
= **314.037 kg/hr = 7.536 tons/day.**

The mass flow rate of **stream 10** = 314.037+35.47= **349.51kg/hr =8.388 tons/day.**

Since the extruder startup loss and pelletiser upset loss contribute to a total loss of 10.1% of 4% of 350 = 11.34 +2.016 =13.356 kg/hr.

Therefore, mass flow rate of **stream 11** = 349.51 – 13.356
= **336.154kg/hr = 8.067 tons/day.**
Now with 21000 kg/hr of chilled water for wash of pellets from extruder and 20% absorption of water by the pellets.
Therefore mass flow rate of **stream 12** = **21000 kg/hr = 504 tons/day**
and that of **stream 13** = 80% of 210 00kg/hr = **16800 kg/hr = 403.2 tons/day.**
Mass flow rate of **stream 14 = stream 15** = 336.154 + (20% of 21000kg/hr)
= 336.154 + 4200
= **4536.154 kg/hr = 108.86 tons/day.**

Since the centrifugal dryer is efficient in removing 60% of the moisture content , therefore mass flow rate of **stream 16** = 60% of 4200

= **2520 kg/hr = 60.4 tons/day.**

After removing 60% moisture, the mass flow rate of **stream 17 = stream 18** = (4536.154 - 2520) = **2016.154 kg/hr = 48.387 tons/day.**

The hot air dryer removes moisture upto 0.05% of 350 i.e. the moisture content in stream 20 is 0.05% x 350 = 0.175 and moisture content in stream 18 = (4200 -2520) =1680.
This implies mass flow rate of **stream 19** = (1680 - 0.175) = **1679.82 kg/hr**

= 40.315tons/day.

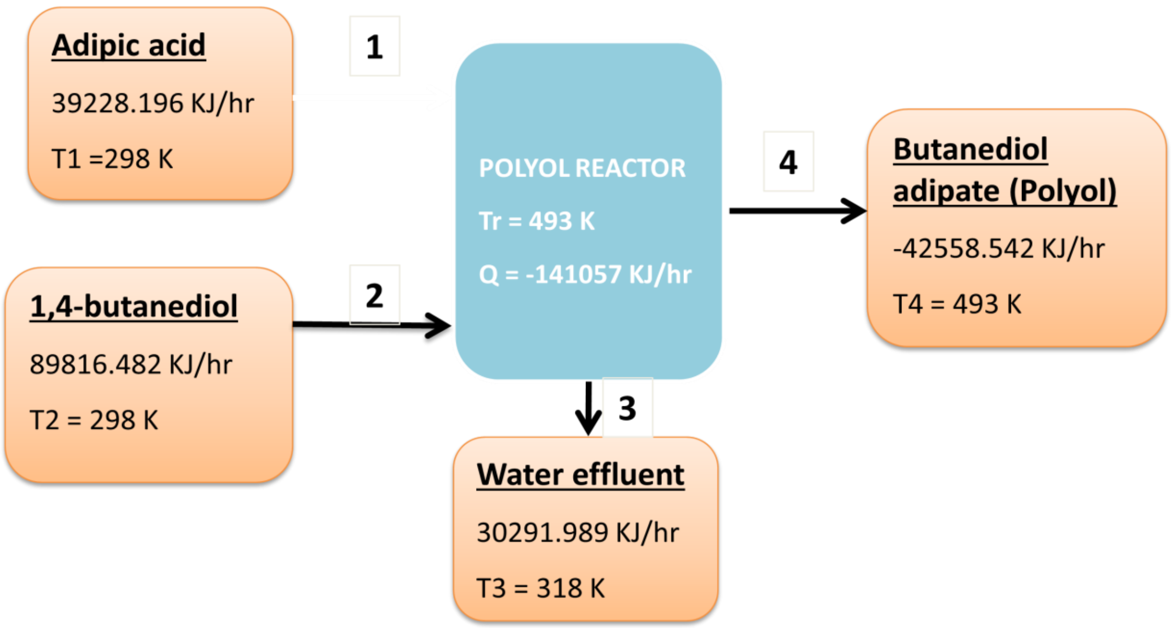
Mass flow rate of **stream 20** = (2016.154 – 1679.82) = **336.329 kg/hr**

= 8.07 tons/day.

Therefore % conversion = 336.329 / 350 x 100 = 96.09%

ENERGY BALANCE

Energy Balance on Reactor:



For Adipic Acid

$\Delta H_1 = \Delta H^0 + m_1 Cp_1(T_r - T_1)$ = (-994.3) + (84.685)(2.4369)(493-298) = 39228.19656 KJ/hr

For 1,4 Butandiol

$\Delta H_2 = \Delta H^0 + m_2 Cp_2(T_r - T_2)$ = -503.25+ (208.812)(2.219) (493- 298) = 89816.482 KJ/hr

For Water

$\Delta H_3 = \Delta H^0 + m_3 Cp_3(T_3 - T_r)$ = (-242) + (41.74)(4.18) (493- 318) = 30291.98912 KJ/hr

For Polyol

$\Delta H_4 = \Delta H^0 + m_4 Cp_4(T_4 - T_r)$ = (-1250) + (168.12)(1.89) (363- 493) = - 42558.542 KJ/hr

Heat Loss In Reactor

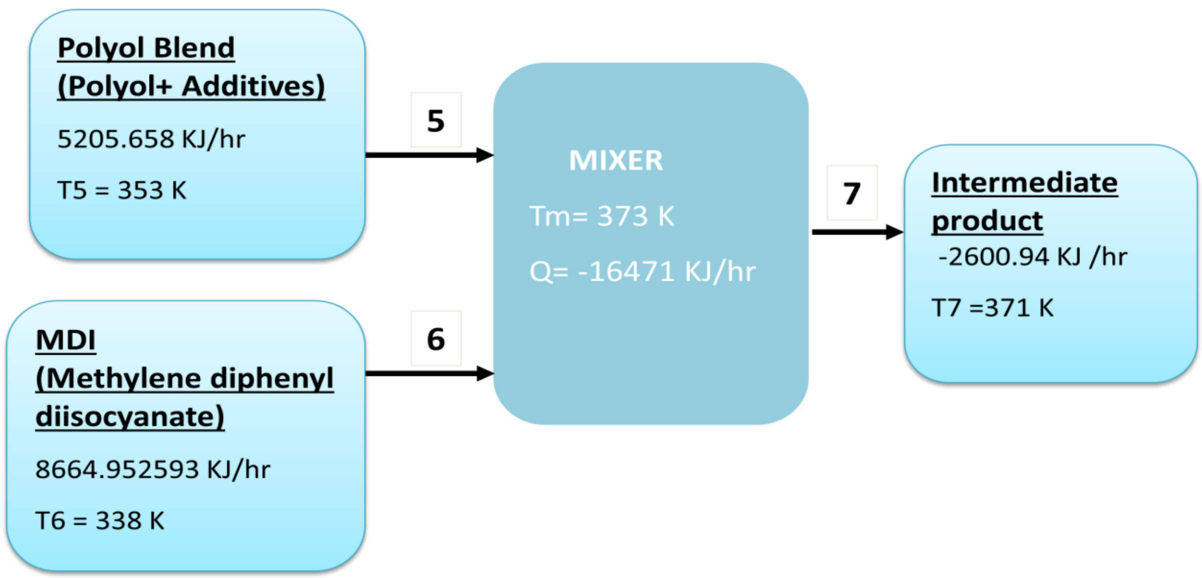
$\Delta H_1 + \Delta H_2 + Q1 = \Delta H_4 + \Delta H_3$
Q_1 = - 141311.23 KJ/hr

Energy Balance On Blending Tank

A blending action is observed. The polyol released from the polyol reactor is mixed with additives like Iragnox and Carbodiimid with the help of an agitator which results in a 10% loss in energy.

$Q_2 = Q_1 - 0.1*Q_1 = -126951$ KJ/hr

Energy Balance On Mixer



For Polyol

$\Delta H_5 = \Delta H^0 + m_5 Cp_5(T_m - T_5)$ = (-1250) + (170.78)(1.89) (373- 353) = **5205.658 KJ/hr**

For Methylene Diamine Isocyanate

$\Delta H_6 = \Delta H^0 + m_6 Cp_6(T_m - T_6)$ = (-360) + (143.25)(1.8) (373-338) = **8664.952593 KJ/hr**

For Stream 7

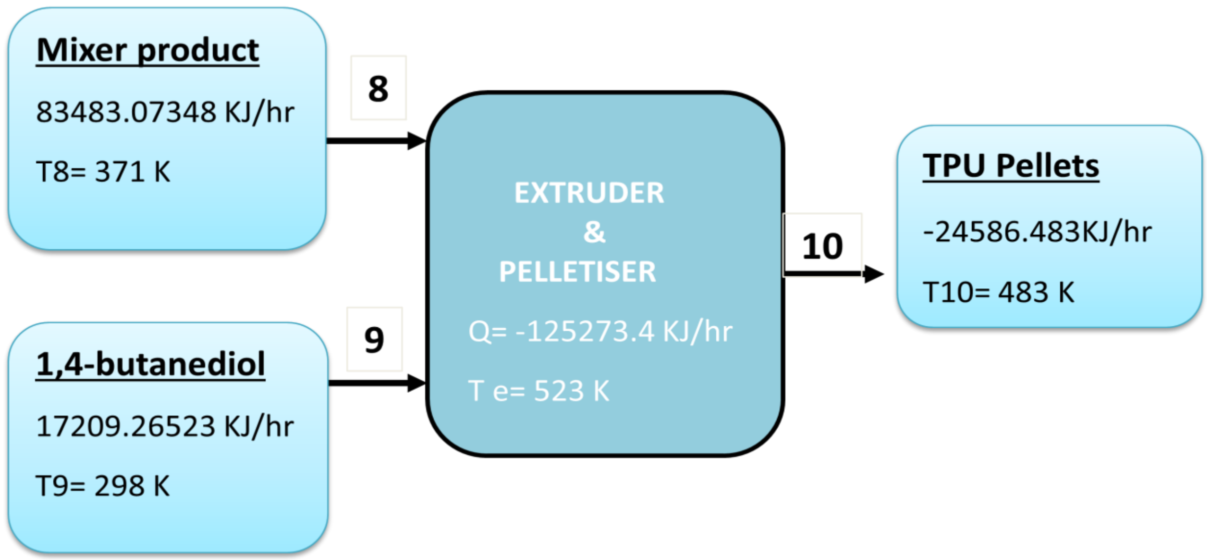
$\Delta H_7 = \Delta H^0 + m_7 Cp_7(T_7 - T_m)$ = (-1483) + (314.03)(1.78) (371-373) = **-2600.9746 KJ/hr**

Heat Loss In Mixer

$\Delta H_5 + \Delta H_6 + Q3 = \Delta H_7$

Q_3 = **-16471.585 KJ/hr**

Energy Balance On Extruder



For Stream 8

$\Delta H_8 = \Delta H^0 + m_8 Cp_8(T_e - T_8)$ = (-1483) + (314.03)(1.78) (523-371) **= 83483.07348 KJ/hr**

For 1,4 Butandiol

$\Delta H_9 = \Delta H^0 + m_9 Cp_9(T_e - T_9)$ = (-503.25) + (35.47)(2.219) (523- 298) = **17209.26523 KJ/hr**

For Stream 10

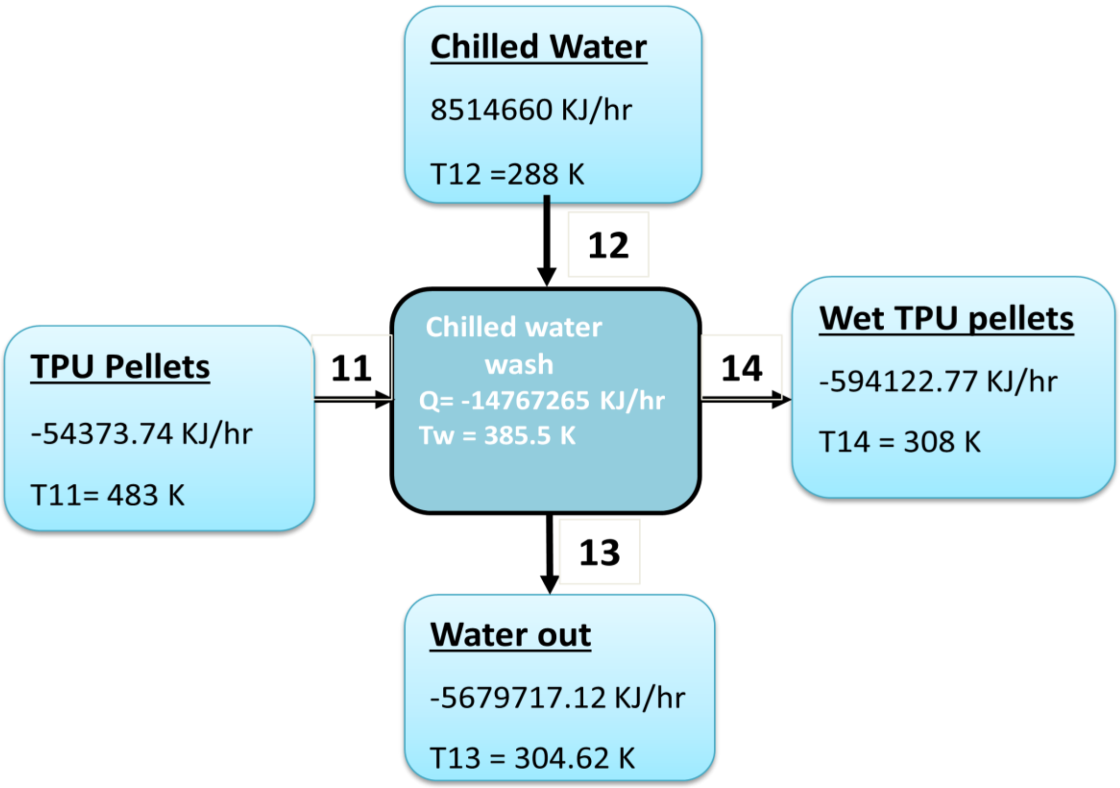
$\Delta H_{10} = \Delta H^0 + m_{10} Cp_{10}(T_{10} - T_e)$ = (-1393) + (349.51)(1.659) (483- 523) = **-24592.9 KJ/hr**

Heat Loss In Extruder

$\Delta H_8 + \Delta H_9 + Q4 = \Delta H_{10}$

Q_4 = **-125285.26 KJ/hr**

Energy Balance of Water Wash



For Extruder Pellet

$\Delta H_{11} = m_{11}\, Cp_{11}(T_w - T_{11})$ = (336.154)(1.659) (385.5- 473) = **-54388.84049 KJ/hr**

For Inlet Chilled Water

$\Delta H_{12} = m_{12}\, Cp_{12}(T_w - T_{12})$ = (21000)(4.18) (385.5- 288) = **8558550 KJ/hr**

For Outlet Water

$\Delta H_{13} = m_{13}\, Cp_{13}(T_{13} - T_w)$ = (16800)(4.18) (304.62-385.5) = **-5679717.12 KJ/hr**

For Wet TPU Pellets

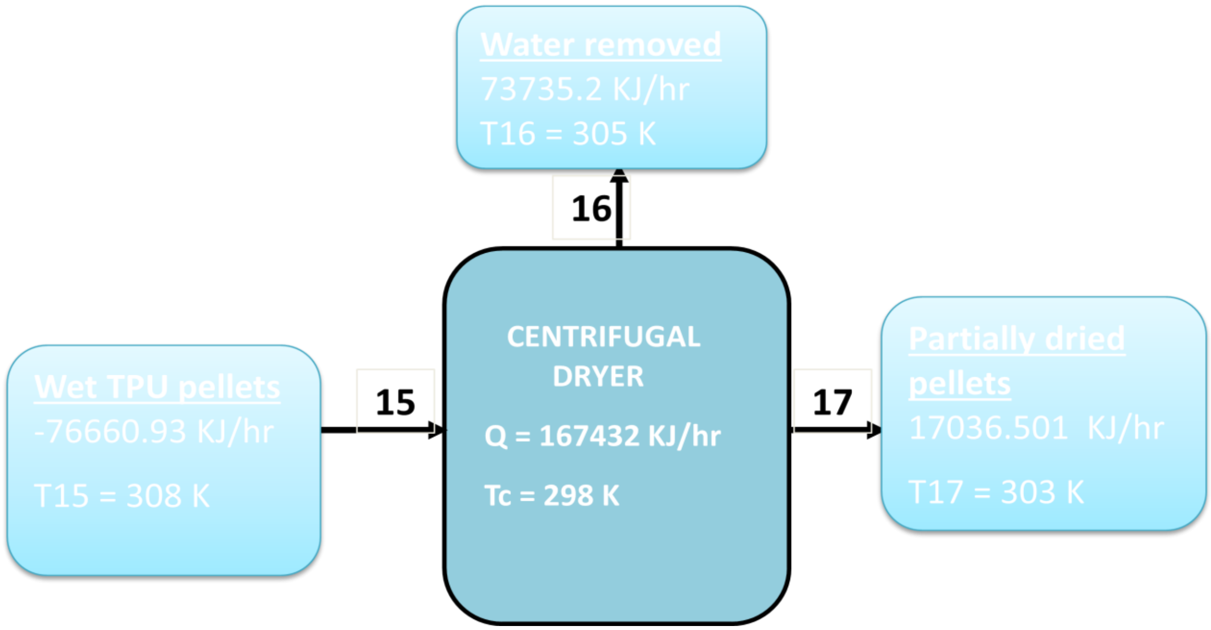
$\Delta H_{14} = m_{14}\, Cp_{14}(T_{14} - T_w)$ = (4536.154)(1.69) (308- 385.5) = **-583386.3853 KJ/hr**

Heat Loss In Water Wash

$\Delta H_{11} + \Delta H_{12} + Q5 = \Delta H_{13} + \Delta H_{14}$

Q_5 = **-14767265**

Energy Balance On Centrifugal Dryer



For Wet TPU Pellets

$\Delta H_{15} = m_{15}\, Cp_{15}(T_c - T_{15})$ = (4536.15)(1.69) (298- 308) = **-75275.66261 KJ/hr**

For Outlet Water

$\Delta H_{16} = m_{16} Cp_{16}(T_{16} - T_c)$ = (2520)(4.18) (305- 298) = **73735.2 KJ/hr**

For Dry TPU

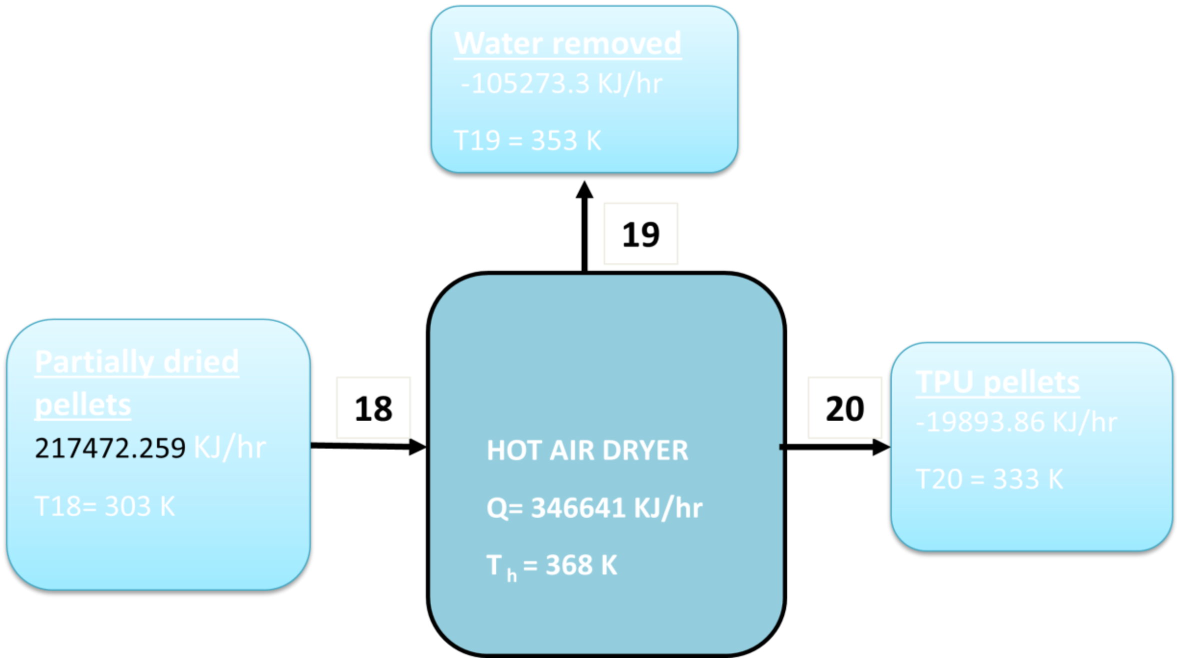
$\Delta H_{17} = m_{17} Cp_{17}(T_{17} - T_c)$ = (2016.154)(1.69) (303- 298) = **16728.6 KJ/hr**

Heat Loss In Centrifugal Dryer

$\Delta H_{15} + Q6 = \Delta H_{16} + \Delta H_{17}$

Q_6 = 165739.498 KJ/hr

Energy Balance On Hot Air Dryer



For Dry TPU Pellets

$\Delta H_{18} = m_{18}Cp_{18}(T_h - T_{18})$ = (2016.15)(1.69) (368- 303) = **217472.259KJ/hr**

For Hot Water Exit

$\Delta H_{19} = m_{19}Cp_{19}(T_{19} - T_h)$ = (1679)(4.18) (353- 368) = **-105325.022KJ/hr**

For Dried TPU

$\Delta H_{20} = m_{20}Cp_{20}(T_{20} - T_h)$ = (336.329)(1.69) (333- 368) = **-19534.36843KJ/hr**

Heat Loss In Hot Air Dryer

$\Delta H_{18} + Q7 = \Delta H_{19} + \Delta H_{20}$

Q_{20} = **-342331.65 KJ/hr**