Nature of Invention: Process design

Applicant: CHEMINOVA

Inventors: Rohan Batra and Anubhav Vashishtha

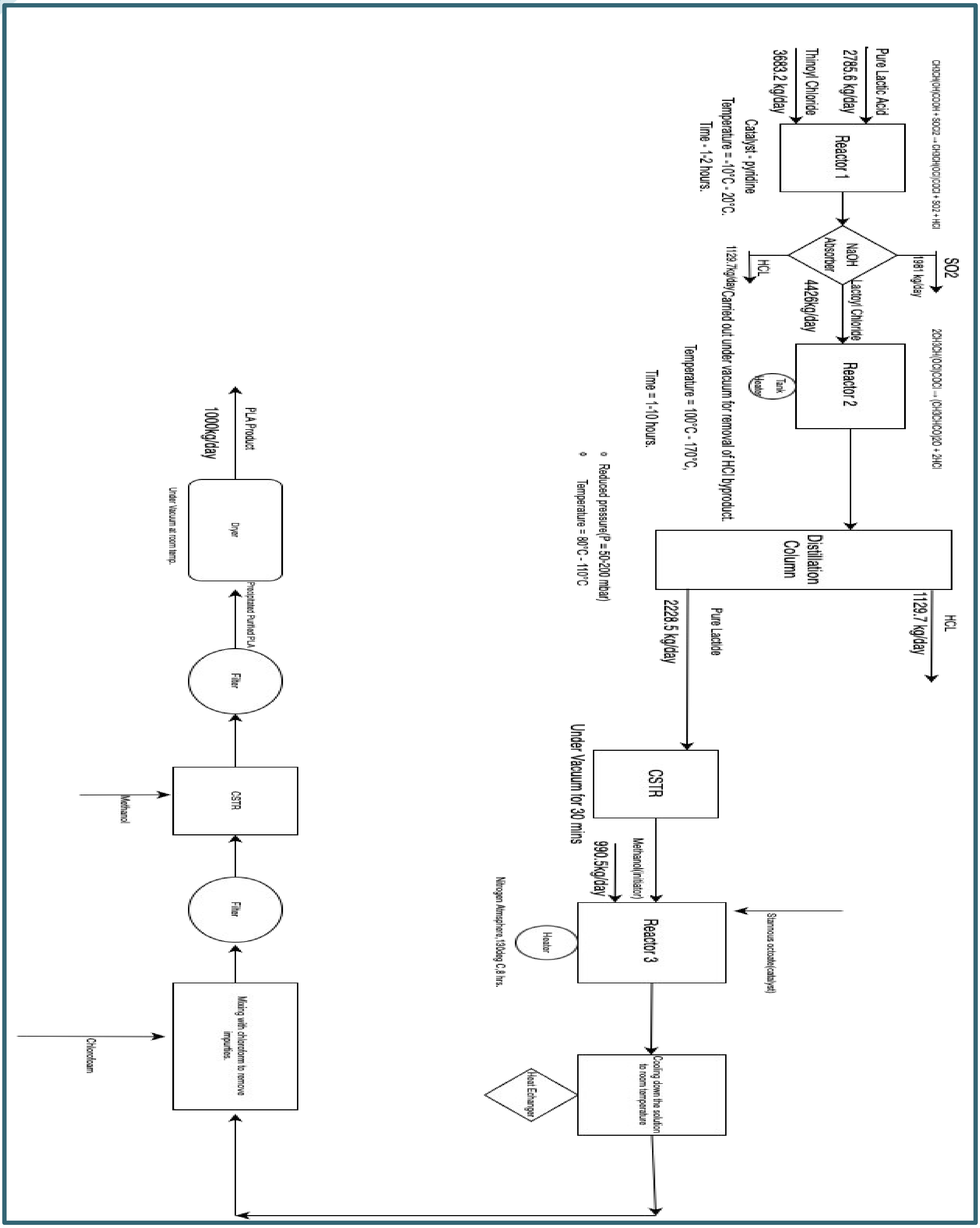
Chemical Formula:-(C3H4O2)n

Chemical Name:-Poly Lactic Acid(PLA)

Process Title: PLA preparation using **US5247059A**

Process Description:

a. Give the block diagram for the feasible process (as determined in market analysis report). List all unit operations and process conditions.


Pure Lactic Acid
2785.6 kg/day
Thinoyl Chloride
3683.2 kg/day
Reactor 1
Catalyst - pyridine
Temperature = -10°C - 20°C.
Time - 1-2 hours.
SO2
1981 kg/day
NaOH
Absorber
HCL
1129.7kg/day
Lactoyl Chloride
4426kg/day
Reactor 2
Tank
Heater
Carried out under vacuum for removal of HCl byproduct.
Temperature = 100°C - 170°C,
Time = 1-10 hours.
Reduced pressure(P = 50-200 mbar)
Temperature = 80°C - 110°C
Distillation
Column
HCL
1129.7 kg/day
Pure Lactide
2228.5 kg/day
CSTR
Under Vacuum for 30 mins
Methanol(initiator)
990.5kg/day
Reactor 3
Heater
Stannous octoate(catalyst)
Cooling down the solution to room temperature
Heat Exchanger
PLA Product
1000kg/day
Dryer
Under Vacuum at room temp.
Precipitated Purified PLA
Filter
CSTR
Methanol
Filter
Mixing with chloroform to remove impurities.
Chloroform

b. Give the material balance for a scaled-up process plant with capacity of 1000 kg/day. (If needed, simplify the calculations by stating assumptions)

CHE261 PLA Plant Mass Balance

We are assuming 100% efficiency of purification processes like filtration, precipitation etc hence in order to get output of 1000kg/day of pure PLA, we will need 1000kg/day of PLA from Reactor 3.

MASS BALANCE ON REACTOR 1

Reaction:

Amount of lactoyl chloride to be produced = 4426 kg/day

Amount of lactic acid required = $\frac{4426}{143} \times 90$ kg/day

$\boxed{\text{Amount of lactic acid required} = 2785.6 \text{ kg/day}}$

Amount of thionyl chloride required = $\frac{4426}{143} \times 119$ kg/day

$\boxed{\text{Amount of thionyl chloride required} = 3683.2 \text{ kg/day}}$

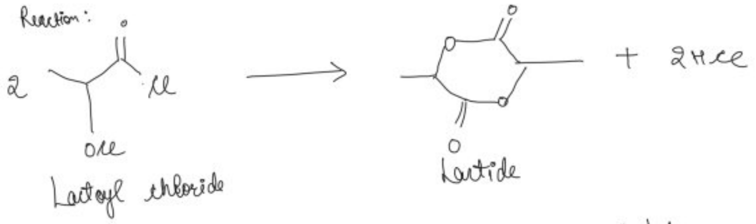
Amount of SO_2 generated = $\frac{4426}{143} \times 64$

$\boxed{\text{Amount of } SO_2 \text{ generated} = 1981 \text{ kg/day}}$

Amount of HCl generated = $\frac{4426}{143} \times 36.5$

$\boxed{\text{Amount of HCl generated} = 1129.7 \text{ kg/day}}$

MASS BALANCE ON REACTOR 2



Amount of lactide to be produced = 2228.5 kg/day

Amount of lactoyl chloride = $2 \times \frac{2228.5}{144} \times 143$ kg/day

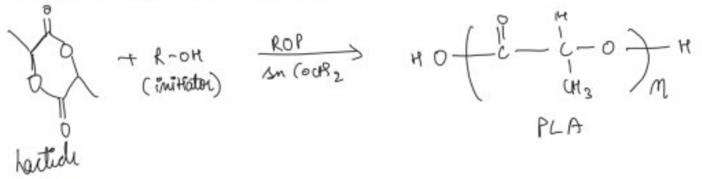
$\boxed{\text{Amount of lactoyl chloride required} = 4426 \text{ kg/day}}$

Amount of HCl produced = $2 \times \frac{2228.5}{144} \times 36.5$ kg/day

$\boxed{\text{Amount of HCl produced} = 1129.7 \text{ kg/day}}$

MASS BALANCE ON REACTOR 3

The reaction taking place in Reactor is



Yield of the reaction =89%
So the industrially produced valuable PLA has degree of polymerisation(n) between 100-200. The initial concentrations of Methanol and Lactide are chosen with this in objective.For our process, we will take n=150.

Number of lactide molecules = DP - 1 = 150 - 1 = 149
Number of methanol molecules = 2 x (DP - 1) = 2 x (150 - 1) = 298

149 molecules of lactide + 298 molecules of Methanol $\xrightarrow{\text{catalyst}}$ 1 polymer chain of PLA

$149 \times 144\,g + 298 \times 32\,g \longrightarrow (72 \times 150 + 18)\,g$

The required amount of PLA is 1000 kg/h and since the yield of the reaction is 89%, corresponding amount of lactide and methanol required are:

Amount of lactide required = $\frac{149 \times 144}{(72 \times 150 + 18)} \times \frac{1000}{0.89}$ kg/day

$\boxed{\text{Amount of lactide required} = 2228.5 \text{ kg/day}}$

Amount of Methanol required = $\frac{298 \times 32}{(72 \times 150 + 18)} \times \frac{1000}{0.89}$ kg/day

c. List the capacity of reactors needed and evaluate the cost. Use Glass lined Carbon steel (GS lined CS) as the material of construction (MOC). Use the pressure according to reaction conditions. You will use only 70% of the total volume. If you design a 1000 L reactor, you can only fill 700 L reaction mixture.

Capital cost (only for the reactor):

example:

Equipment	Design Capacity (L)	No. of units	Cost/unit ($ for year 2014)	Total Cost ($ for year 2014)
Reactor 1 (Jacketed reactor, agitated, Glass lined Carbon steel, atm. pressure)	5000	1	54,400	54,400
Scrubber (Wet centrifugal,carbon steel,atm. pressure)	---	1	11700	11,700
Reactor 2 (Jacketed reactor, agitated, Glass lined Carbon steel, pressure=1-2atm)	10000	1	78,500	78,500
Tank Heater [Pressure=150 psi, Carbon steel]	Area = 150sqft	1	10100	10100
Distillation Column	20,000	1	37,500	37,500
CSTR (Jacketed reactor, agitated, Glass lined Carbon steel, vacuum)	500	1	16,000	16,000

Reactor 3 (Jacketed reactor, agitated, Glass lined Carbon steel, vacuum)	20000	1	113,400	113,400
Heat exchanger [vacuum, Carbon steel]	Area = 150sqft	1	10,200	10,200
CSTR (Jacketed reactor, agitated, Glass lined Carbon steel, **vacuum**)	1000	1	23200	23200
Filter [disc]	Area =200sqft	1	147500	147500
CSTR (Jacketed reactor, agitated, Glass lined Carbon steel, **vacuum**)	5000	1	54,400	54,400
Filter [gravity]	Area =200sqft	1	115,000	115,000
Dryer [drum double vacuum]	Area =200sqft	1	254,800	254,800

References: Provide reference for a research paper or an actual patent.

1. http://www.matche.com/equipcost/Reactor.html
2. https://patents.google.com/patent/US5247059A/en

List the contributions of each author:

- Rohan Batra:- Made the entire block diagram and did the material balance.
- Anubhav Vashishtha:- found the patent and did the economic analysis of the entire reactor arrangement.

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