Nature of Invention: Chemical molecule and synthesis route

Applicant: SynergyX

Inventors: Alankrit Gupta

Chemical Formula: $(C_{10}H_8O_4)_n$

Chemical Name: Polyethylene terephthalate(PET)

Chemical synthesis routes:

a. **PRIMARY MODE OF SYNTHESIS:**

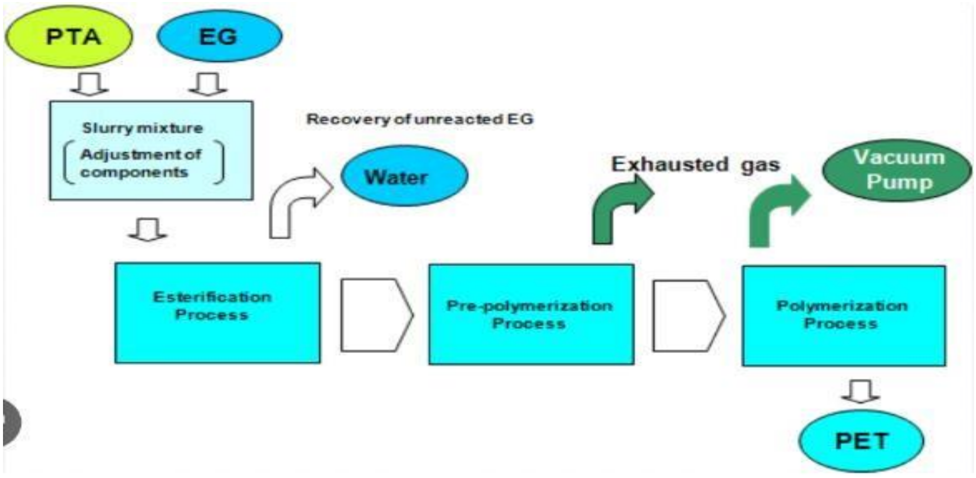
RAW MATERIALS REQUIRED:

1. Pure terephthalic acid (PTA)
2. Ethylene glycol (EG)
3. Antimony Triacetate (Catalyst)

UTILITIES REQUIRED:

1. Paste vessel
2. Esterification Reactor
3. Distillation Column
4. DRR(Disc ring reactor)
5. Pre-Polycondensation Reactor
6. Condenser
7. Emulsion Storage Vessel
8. Coolers
9. Filters

PROCESS ANALYSIS:



1. <u>PASTE PREPARATION:</u>

CONDITIONS: T=328K & P=1 atm

SITE: Paste vessel(Mixer)

CHEMICAL REACTION: Physical heterogeneous mixing(No chemical change)

REACTION YIELD: Mixing to full extent.

DETAILED DESCRIPTION:

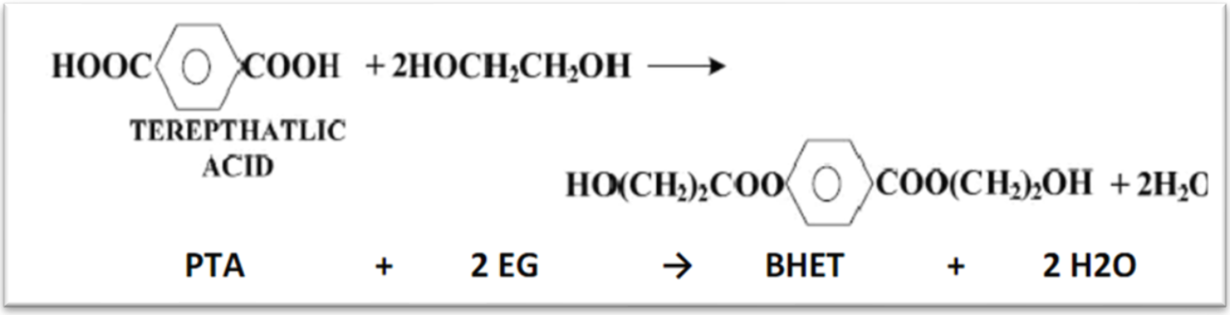
- Raw materials, PTA and MEG, are mixed in a paste tank under controlled conditions at approximately 55°C.
- The mixing ratio is 1.12:1 MEG:PTA to produce 1 PET molecule, with Antimony Triacetate catalyst added to control the ratio and initiate polymerization.
- PTA is continuously added to the paste tank while MEG with catalyst solution is introduced through spray nozzles.
- A control system adjusts the mole ratio of EG solution based on the quantity of PTA added, ensuring the desired ratio of raw materials.
- The paste, after agitation, is transferred into an Esterification reactor for further processing.

2. <u>ESTERIFICATION:</u>

CONDITIONS: T=529K & P=0.14bar

SITE: Batch Reactor

CHEMICAL REACTION:



REACTION YIELD: 90%

DETAILED DESCRIPTION:

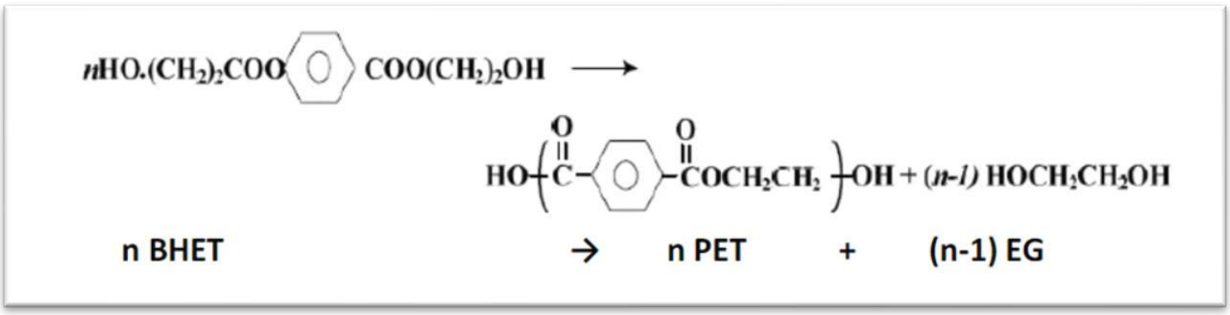
- In Reactor PTA reacts with MEG under high temperature and pressure to produce monomers of DGT (Diethylene-Glycol-Terephthalate), accompanied by the release of water and initiation of polycondensation reactions.
- Vapors containing spent ethylene glycol (SEG) and water are removed from the top of the reactor. These vapors are then directed into a distillation column where ethylene glycol (EG) is separated from water.
- The separated EG is further utilized as EGR (ethylene glycol recycle), while the water from the distillation column is directed towards condensers where it undergoes temperature changes and is employed as reflux in the distillation process.

3. <u>PRE-POLYCONDENSATION:</u>

CONDITIONS: T=545K & P=19-20mbar

SITE: Batch Reactor

CHEMICAL REACTION:



REACTION YIELD:92%

DETAILED DESCRIPTION:

- In the pre-polycondensation reactor, monomers and oligomers from the Esterification stage undergo condensation polymerization, resulting in the elimination of MEG. Antimony Triacetate catalyst is activated in this reactor, initiating chain growth.
- Step growth-polymerization occurs as product monomers, containing carboxyl and hydroxyl functional groups, react to grow molecular chains. This reaction facilitates the growth of molecules through the interaction of these functional groups.
- Ethylene glycol (EG) vapors produced during the process are captured by a scraper condenser to efficiently condense the vapors. The condensed liquid is transferred to an emulsion storage vessel, where EG is pumped to coolers before being recycled for use in EG showers.

4. <u>DRR (Disc Ring Reactor):</u>

CONDITIONS: T= 548K & P= 1.5-1.2mbar
SITE: DRR Reactor
CHEMICAL REACTION: Polymerisation of PET chains
REACTION YIELD: 96%

DETAILED DESCRIPTION:

- The DRR (Double Ribbon Reactor) features a cage of rings attached to the inner side of the reactor shaft, continuously cutting through the thick, semi-solid material at high temperature and low pressure to achieve the desired intrinsic viscosity, up to 0.620.
- Material within the DRR is exposed to very high temperature and low pressure, sliding through the surfaces of the rings attached to the slowly revolving shaft. EG and water vapors exit from the top of the reactor, passing through a horizontal scraper condenser.
- Product from the DRR is pumped by self-lubricated gear-type pre-polymer pumps into a viscometer and then to candle filters with stainless steel candles for filtration. After filtration, the product is directed to the drying section.

5. <u>EG RECOVERY SECTION:</u>

CONDITIONS: P= 260mbar.
SITE: Distillation column, Scraper Condenser
CHEMICAL REACTION: Separation of EG from water and recycling
PURITY: 98-99%

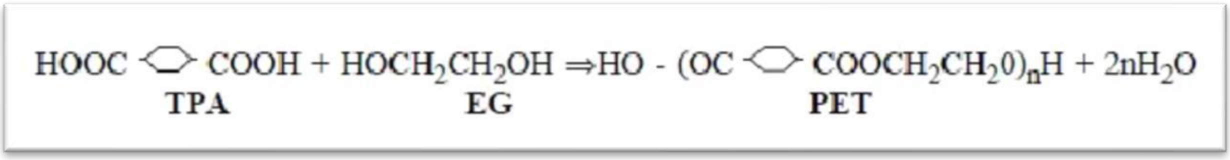
DETAILED DESCRIPTION:

- EG recovery from both reactors and scraper condensers is achieved through a distillation column, where EG is separated for reuse, while water is condensed for reflux, and any remaining components are evaporated.

OVERALL:

OVERALL YIELD:96%

OVERALL REACTION:



b. ALTERNATE PRODUCTION PROCESS:EASTMAN INTEGREX PROCESS

NOTE: Most of the alternate pathways have little change in either raw material or process control, which mainly depends on availability and feasibility of process at the particular time and place

RAW MATERIALS REQUIRED:

1. Pure terephthalic acid (PTA)
2. Ethylene glycol (EG)
3. Antimony Triacetate (Catalyst)

UTILITIES REQUIRED:

1. Paste Tank
2. Pipe reactor
3. Vacuum Distillation Column

4. Heat Exchanger
5. Vent lines and pipes

PROCESSANALYSIS:

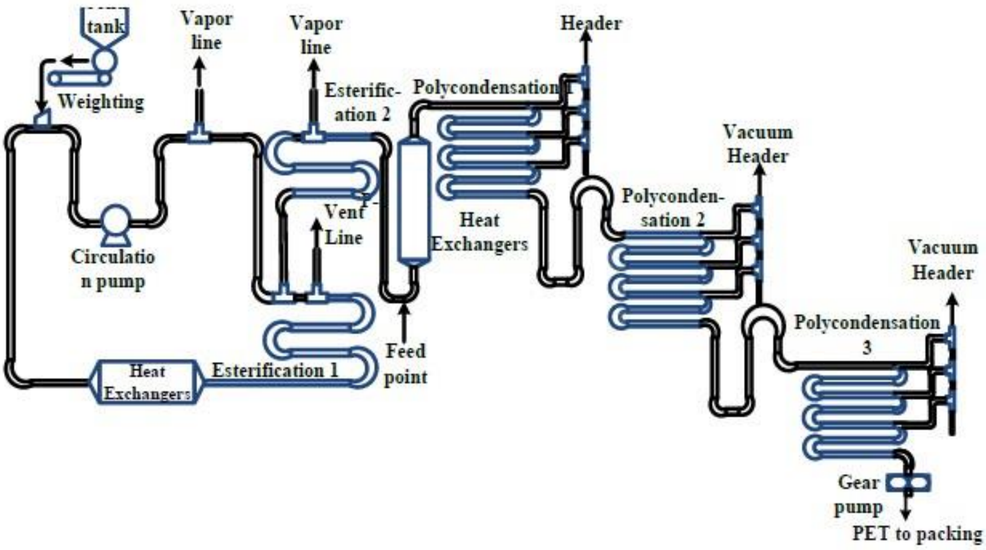


Figure 16: Combined Esterification Polycondensation Pipe Reactor Developed by Eastman-IntegRex

1. This application introduces a novel pipe reactor design for esterification or polycondensation processes.
2. The pipe reactor's flexible orientation and layout enable plant design for limited space condition, eliminating the need for level or pressure control.
3. Traditional equipment such as pumps, agitators, screws, and seal systems are eliminated or minimized in the pipe reactor design, reducing operational complexity and equipment costs.
4. Welding the pipe reactors without gaskets reduces emissions and air leakage, improving product quality and environmental performance.
5. This innovative technology produces PET of lower intrinsic viscosity (IV) polyester or PET resin in the melt phase, up to an IV of 0.75.
6. Eastman's pipe reactor design addresses mass transfer issues by applying vacuum, facilitating easy removal of by-products.

7. In Eastman's process, feed materials such as TPA and EG are introduced into a circulation loop, where esterification occurs at elevated temperatures.
8. Vent gases from esterification are separated in a distillation column, with water removed from EG.
9. BHET produced from esterification is polymerized in the pipe reactor, divided into sections to gradually increase IV, with vent vapors condensed and recycled.
10. The produced PET is then cut to crystals and stored in silos for further use.
11. Cost of applying vacuum and converting reactant into low viscous fluid is high and due to less opportunity and purity of recycling process, the yield is reduced.
12. Overall Yield is down to around 88%.
13. Other sub-reaction yield are highly variable and generally around same as before.

References:

1. https://www.scribd.com/document/433599901/Production-of-PolyethyleneTerephthalate-PET-Resin-From-PTA-and-EG
2. https://www3.epa.gov/ttnchie1/ap42/ch06/final/c06s06-2.pdf
3. https://austinpublishinggroup.com/chemical-engineering/fulltext/ace-v8id1083.php#:~:text=In%20order%20to%20produce%20PET,and%20Dimethyl%20Terephthalate%20(DMT).

List the contributions of author :Alankrit Gupta

- Designed and implemented a chemical synthesis route for the production of Polyethylene Terephthalate (PET), including raw material selection and process design.
- Contributed to the development and optimization of various stages in the synthesis process, such as paste preparation, esterification, pre-polycondensation, DRR operation, and EG recovery.
- Collaborated on the design and implementation of a novel pipe reactor technology for esterification and polycondensation processes, resulting in significant cost savings and operational simplifications.

- Conducted experiments and optimized reaction conditions to enhance reaction efficiency and overall yield, contributing to a comprehensive understanding of the reaction mechanisms involved.
- Played a role in evaluating alternative production processes, such as the Eastman IntegRex process, and provided insights into their feasibility and potential yield improvements, contributing to the overall efficiency and effectiveness of the synthesis process.

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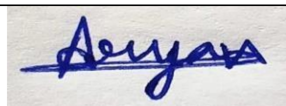
Aryan Nigam	220227	
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