Technical Team

Nature of Invention: Process Flow Diagram and Mass Balance.

Applicant: SynergyX

Inventors: Sanskaar Srivastava, Aditya Gupta, Priyanshu Kamde, Diya Saraf, Sakshi Dargu.

Chemical Formula: TiO_2

Chemical Name: Titanium Dioxide

Process Title: Production of Titanium Dioxide from Titanium Isopropoxide

Raw materials and chemicals Required: Citric acid, Distilled water, TTiP, Ethylene Glycol

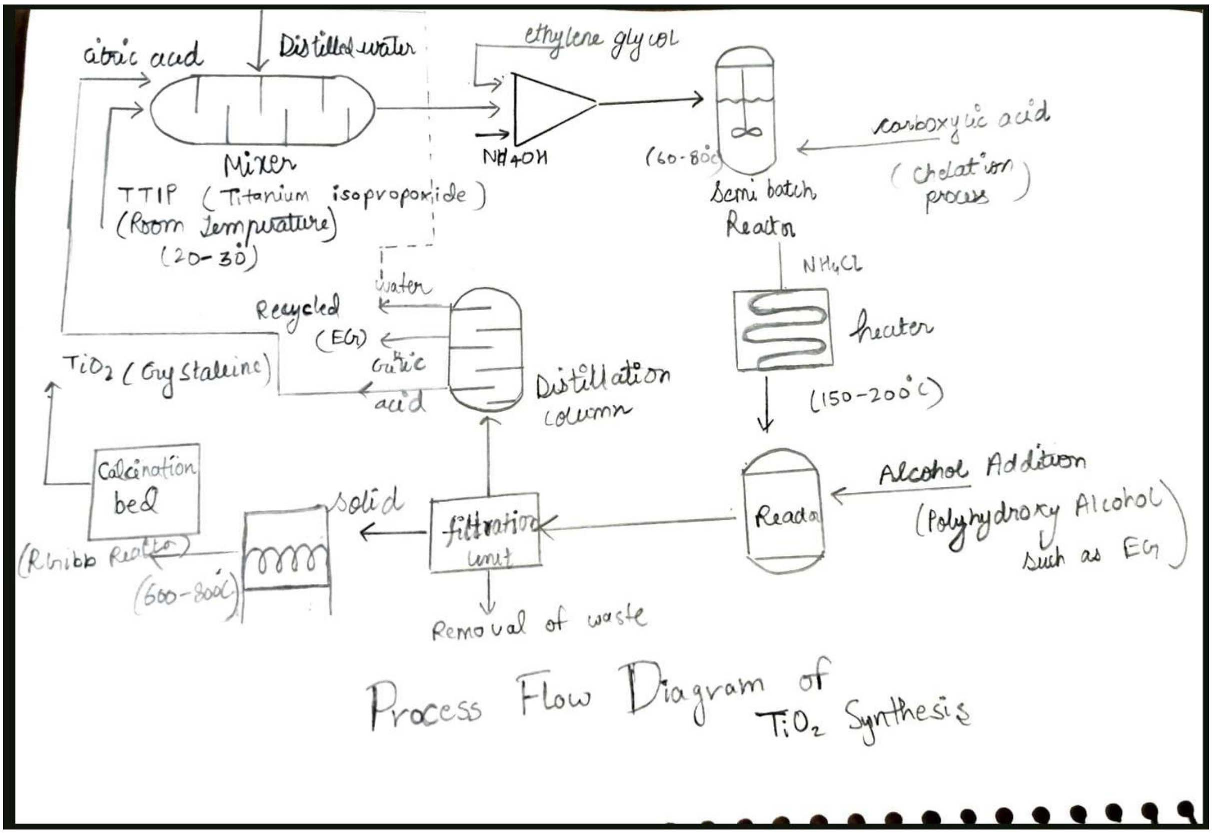
Reason why Pechini method is used instead of Sol gel on industrial scale:

The Pechini method is preferred over the sol-gel method for industrial-scale TiO_2 nanoparticle production due to its scalability, cost-effectiveness, and precise control over processing parameters. Its straightforward mixing of precursor solutions allows for easy scale-up without altering processing conditions significantly, ensuring consistent product quality. Additionally, the method's reliance on citric acid as a chelating agent reduces costs compared to sol-gel processes. Moreover, the Pechini method offers better reproducibility and batch-to-batch consistency while providing versatility to tailor nanoparticle properties for various applications, making it a favorable choice for industrial TiO2 production.

Ultimately pechini is just a modified sol gel process for industrial scale with better compatibility.

Process Description:

Block Diagram:



Material Balance:

→ Mass Balance :-

① Preparation of Polymeric Precursor :-

$$Ti(OCH(CH_3)_2)_4 + 3C_6H_8O_7 \longrightarrow Ti[(C_6H_7O_7)_2(OH)_2]_n + 4C_3H_7OH$$

Assuming the TTIP feed basis to be x Kmol/hr.

According to stoichiometric Analysis :-

Moles flow rate of $C_6H_8O_7$ needed :- $3x$ Kmol/hr

→ Molar flow rate $Ti[(C_6H_7O_7)_2(OH)_2]_n$:- x Kmol/hr

② Polymerization Process :- (Acetic Acid formulation)

$$Ti(OH)_4 + 2CH_3COOH \longrightarrow \underset{\text{M-L Complex}}{Ti[(CH_3COO)_2(H_2O)]_n} + 4H_2O$$

→ Stoichiometric Analysis :-

Ti

Moles of CH_3COOH needed :- $2x$ Kmol/hr

Also $Ti(OH)_4 + 3EG \longrightarrow Ti(EG)_3 + 3H_2O$

∴ EG needed :- $3x$ Kmol/hr

The reaction for the formed M-L Complex to TiO_2 involves a stoichiometric coefficient of 1.

∴ TiO_2 (Amorphous) formed $\longrightarrow$ x Kmol/hr

(3) Calcination

TiO_2 (Amorphous) $\longrightarrow$ TiO_2 (Crystalline)

∴ TiO_2 (Crystalline) formed $\longrightarrow$ x Kmol/hr.

(4) Distillation Column for recycle :

Assuming a 90% yield there may be an ample amount of Citric Acid and EG left which may be used to enhance productivity.

∴ Distilled EG :- $0.3x$ Kmol/hr.

Distilled $C_6H_8O_7$:-

∴ Total EG feed :- $3.3x$ Kmol/hr.

Total Citric Acid feed :- $0.3x$ Kmol/hr + $3x$ Kmol/hr

$\Rightarrow$ $3.3x$ Kmol/hr.

Energy Balance:

In semi-batch reactor from $25^\circ C$ to $70^\circ C$.

Specific heat capacity of $Ti(OH)_4$ is $0.84\ J/g^\circ C$

$\dot{Q} = S\,\Delta T$ (calculating in per mole)

$= 0.84\,(70-25)$

$= 37.8\ KJ/kg(hr)$

In heater befor alcohol addition ($70^\circ C$ to $200^\circ C$)

Specific heat of TiO_2 is $0.7\ J/g^\circ C$

$\dot{Q} = S\,\Delta T$

$= 0.7\,(200-70)$

$= 91\ KJ/kg(hr)$

In Calcination bed heating is from $200^\circ C$ to $800^\circ C$

$\dot{Q} = S\,\Delta T$

$= 0.7\,(800-200)$

$= 420\ KJ/kg(hr)$

List the contributions of each author:

Process Flow Design:-Aditya Gupta,Sanskaar Srivastava, Priyanshu Kamde

Material Balance: Priyanshu Kamde, Sanskaar Srivastava, Aditya Gupta

Energy Balance: Sakshi Dargu, Diya Saraf

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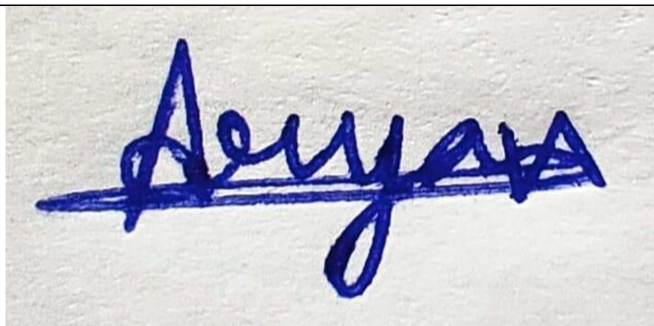
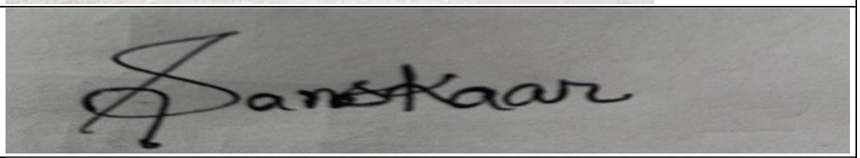
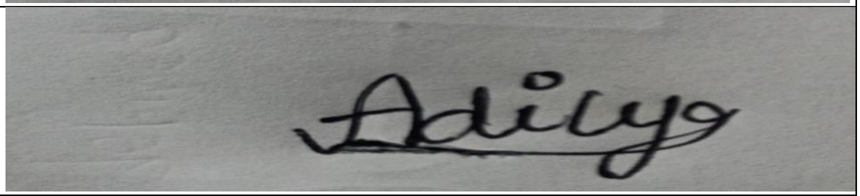
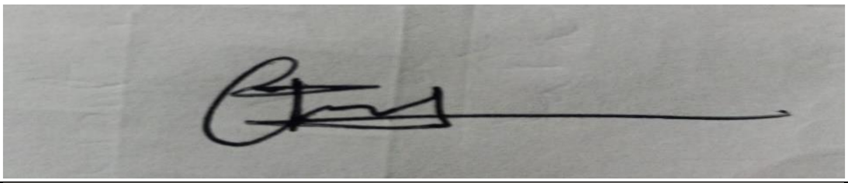
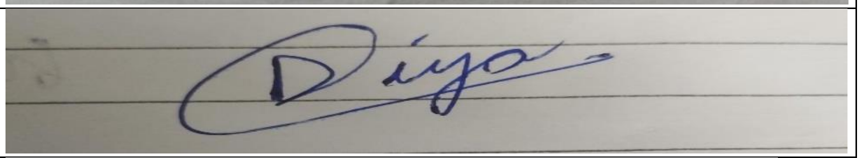
Aryan Nigam	220227	
Sanskaar Srivastava	220967	
Aditya Gupta	220066	
Priyanshu Kamde	220494	
Diya Saraf	220383	
Sakshi dargu	220323