Process Descriptions for Simulations Purposes

1. Titanium Dioxide Production via Chloride Route (Synthetic Rutile Feed)

Objective: Simulate the chloride route for TiO_2 production using synthetic rutile (~92% TiO_2) as feedstock.

Feedstock:

- **Synthetic Rutile**
  - Flowrate: 5000 tonnes/year
  - Composition: 92 wt% TiO_2, 3% Fe_2O_3, 2% SiO_2, 3% others
  - Solid granular, particle size: 200–300 µm
- **Chlorine Gas (Cl_2)**
  - Flowrate: Based on stoichiometric requirement + 10% excess
  - Purity: 99.5%
- **Coke (Carbon)**
  - Flowrate: Based on reducing requirement, 20% stoichiometric excess

Process Units:

1. **Fluidized Bed Chlorinator**
   - Reaction: $TiO_2 + 2Cl_2 + C \rightarrow TiCl_4 + CO_2$
   - Temperature: 900–1000 °C
   - Pressure: 1 atm
   - Residence time: ~1.5 h

2. **$TiCl_4$ Condensation Column**
   - Temp: 150–200 °C (to condense $TiCl_4$)
3. **Purification Train**
   - Units: Distillation column or absorber/stripper combo
   - Removes: $FeCl_3$, VCl_4, $SiCl_4$
4. **Oxidation Reactor**
   - $TiCl_4 + O_2 \rightarrow TiO_2 + 2Cl_2$
   - Temp: 1000–1100 °C
   - Pressure: 1.2 atm
5. **Product Recovery (TiO_2 pigment)**
   - Cooling and solid separation, filtering, milling

Product:

- TiO_2 pigment: ~4600 tonnes/year (based on 92% conversion and recovery)
- Chlorine: Recovered and recycled (~95%)

Assumptions:

- Heat integration considered (recover from oxidation step)
- No Cl_2 loss in simulation (ideal separation)

2. Chlor-Alkali Process via Membrane Cell (Industrial Salt Feed)

Objective: Model a chlor-alkali process to produce NaOH and Cl_2 from NaCl (brine) solution.

Feedstock:

- **Brine solution**
  - Flowrate: 100 m^3/h
  - NaCl Concentration: 300 g/L
  - Temperature: 25 °C
- **Deionized water** for cathode compartment

Process Units:

1. **Brine Pre-treatment Unit**
   - Filtration + $Ca(OH)_2$ treatment + Activated carbon
2. **Membrane Electrolyzer**
   - Electrodes: Graphite anode, Nickel cathode
   - Membrane: Nafion
   - Reactions:
     - Anode: $2Cl^- \rightarrow Cl_2(g) + 2e^-$
     - Cathode: $2H_2O + 2e^- \rightarrow H_2(g) + 2OH^-$
     - Net: $2NaCl + 2H_2O \rightarrow Cl_2 + H_2 + 2NaOH$
   - Voltage: 3.2 V per cell
   - Current density: 3 kA/m^2
   - Temp: 80 °C
   - Pressure: 1.5 atm
3. **Product Separation Unit**
   - Gas-liquid separators for Cl_2 and H_2
   - NaOH liquor: 32 wt%

Product Output:

- NaOH: ~8.5 tonnes/h
- Cl_2: ~7.5 tonnes/h
- H_2: ~0.2 tonnes/h

Assumptions:

- 90% cell current efficiency
- Full water availability at cathode side

3. Phosphoric Acid Production from Pyrite and Phosphate Rock

Objective: Simulate the production of H_3PO_4 using pyrite as the source of sulfur for sulfuric acid generation, which reacts with phosphate rock.

Feedstock:

- **Pyrite (FeS_2)**
  - Flowrate: 10 tonnes/h
  - Purity: 95%
- **Phosphate Rock ($Ca_3(PO_4)_2$)**
  - Flowrate: 12 tonnes/h
  - P_2O_5 content: 30 wt%
- **Water**
  - Flowrate: 20 tonnes/h

Process Units:

1. **Roasting Furnace (for SO_2 production)**
   - $FeS_2 + 11/2\ O_2 \rightarrow Fe_2O_3 + 2SO_2$
   - Temp: 800–900 °C
   - Air excess: 20%
2. **Contact Process (H_2SO_4 production)**
   - $SO_2 + O_2 \rightarrow SO_3$ (catalytic converter, V_2O_5)
   - $SO_3 + H_2O \rightarrow H_2SO_4$ (absorber)
   - Conversion: 97%
3. **Reaction with Phosphate Rock**
   - $Ca_3(PO_4)_2 + 3H_2SO_4 \rightarrow 2H_3PO_4 + 3CaSO_4$
   - Temperature: 70 °C
   - Slurry concentration: 25% solids
4. **Filtration Unit**
   - To separate gypsum ($CaSO_4$)
   - Recycle water used

Product Output:

- H_3PO_4: ~5.5 tonnes/h (28% P_2O_5 basis)

- Gypsum: ~8 tonnes/h

Assumptions:

- Heat recovery from roasting used for preheating streams
- Conversion of pyrite to SO_2 is 95%
- Efficient separation assumed in filters