Chapter 2 – Structure and Synthesis of the Process Flow Diagram

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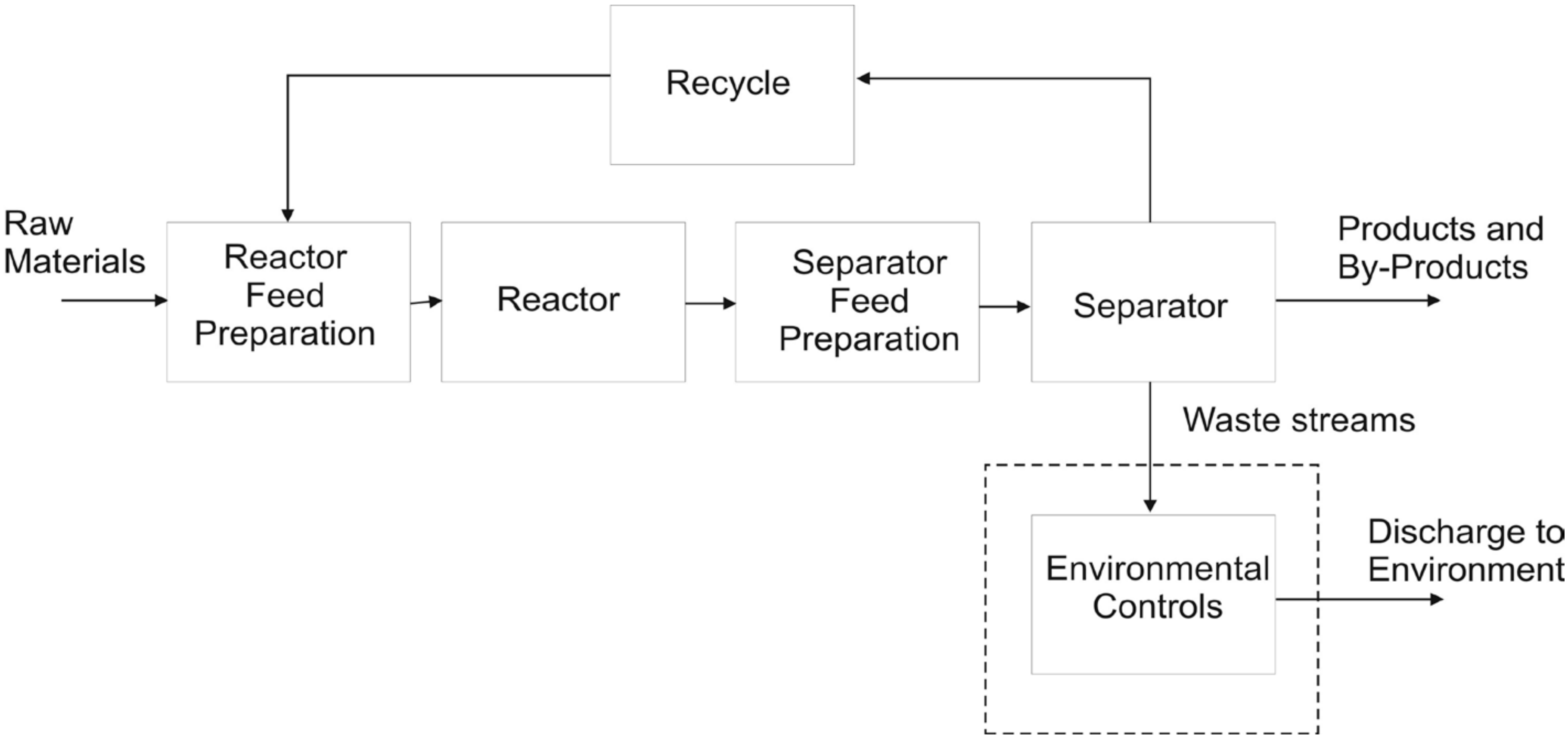
CHE 4101-Plant Design

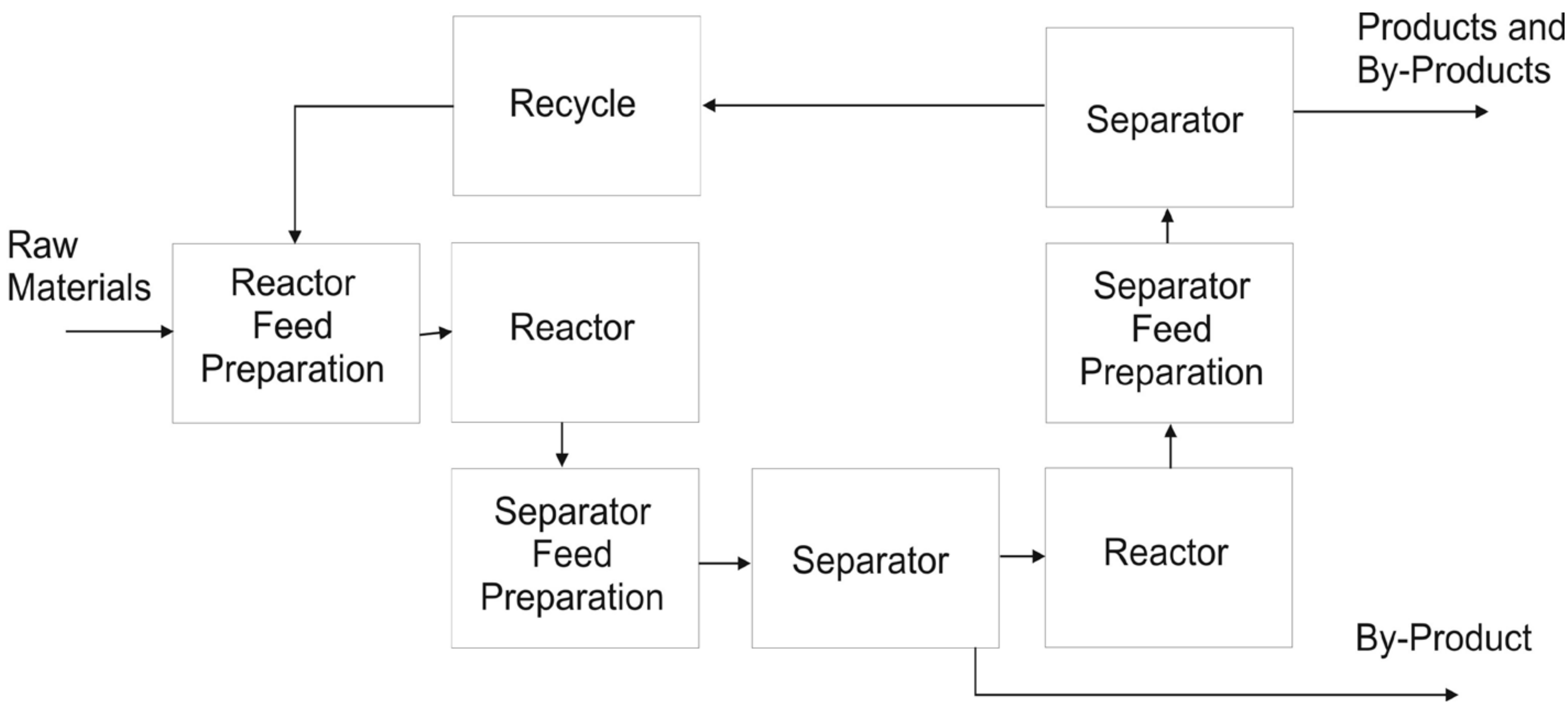
Outline

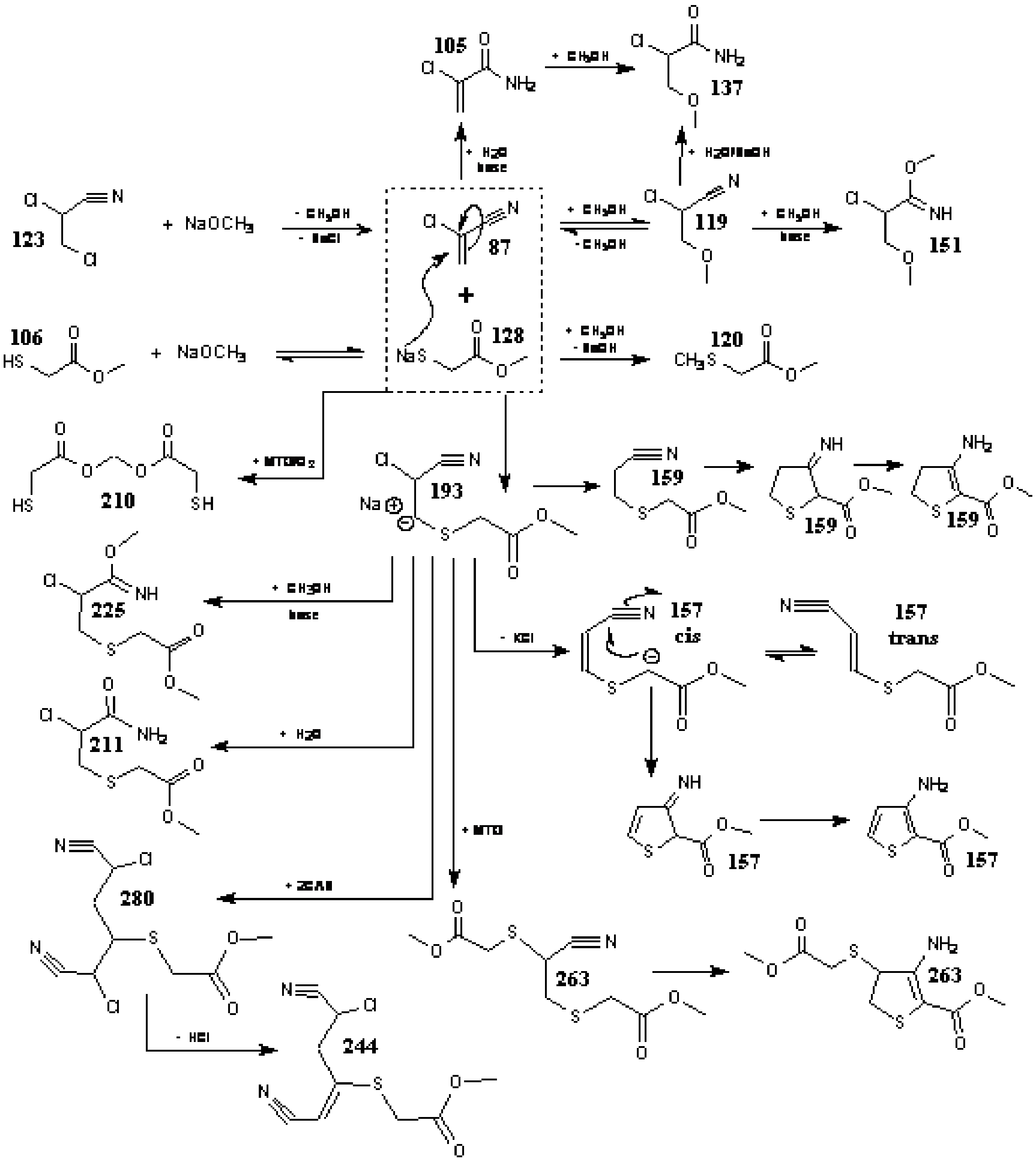
- Generic Structure of Processes
- Process Design Hierarchy
  - Batch vs. Continuous Processes
  - Input – Output Structure
  - Recycle Structure
  - General separation structure of process
  - Heat-exchanger network/process energy recovery

Generic Structure of Process Flow Diagrams



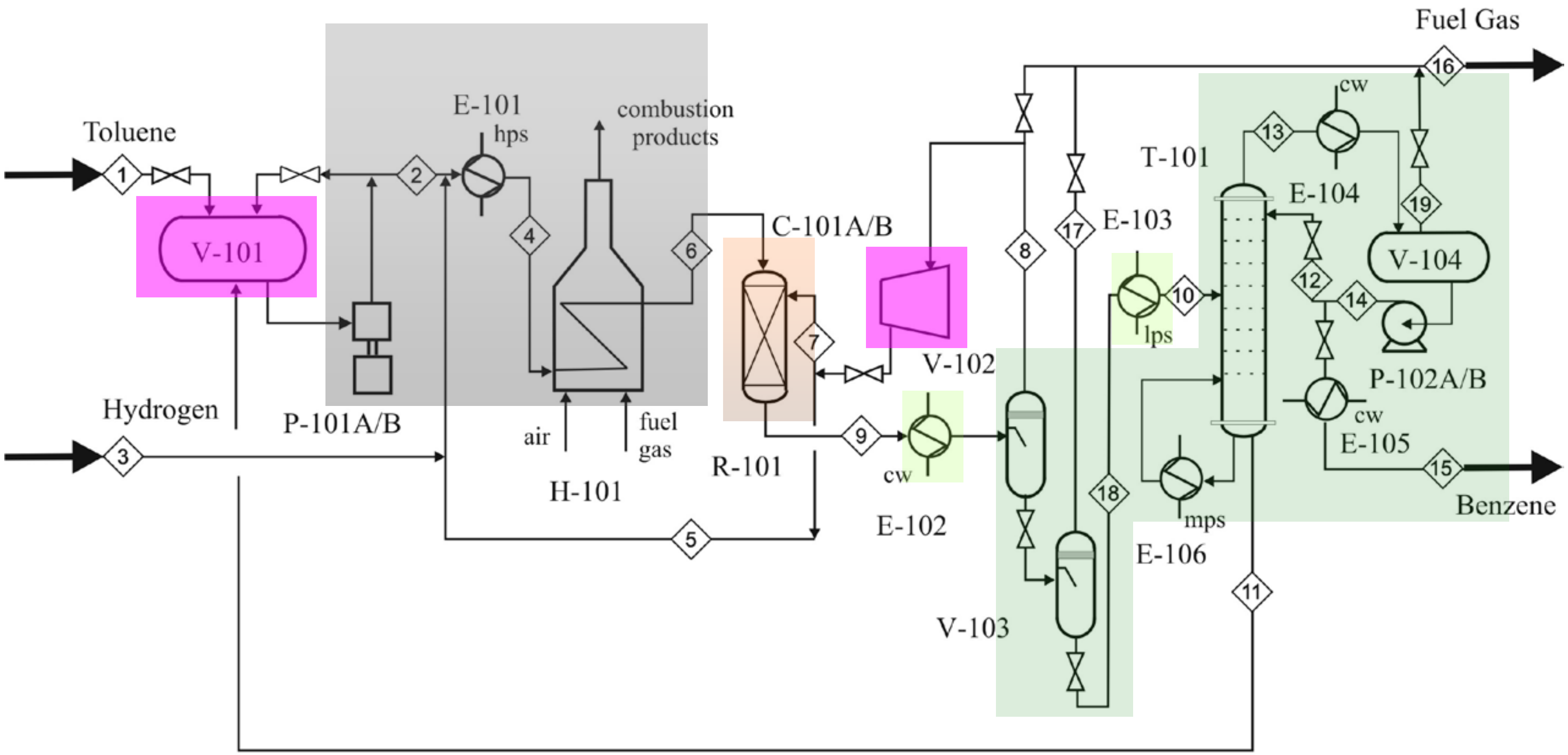
Generic Structure of Process Flow Diagrams





must know complete stoichiometry, including all by-products

Generic Structure of Process Flow Diagrams



Input/Output Stream

$$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$$

Figure 2.2 Input Output Streams on Toluene Hydrodealkylation PFD

Environmental Control

- End of Pipe vs. Green Approach
  - Most significant changes obtained by changing process chemistry within reactor – eliminate/minimize unwanted by-products
- End of Pipe vs. Common Units
  - Fired Heaters - excess oxygen
  - low sulfur fuel - NO_X control
  - Wastewater (biological, sedimentation/filtration)

Approach of Douglas[1]

- 5-step process to conceptual process design
  - batch vs. continuous
  - input-output structure
  - identify and define recycle structure of process
  - identify and design
    - general structure of separation system
    - heat-exchanger network
      or process energy recovery system

1 – Douglas, J.M., Conceptual Design of Chemical Processes, McGraw-Hill, NY, 1988

Batch vs. Continuous

- Variables to Consider:
  - Size
    - Batch < 500 ton/yr ~ 1.5 ton/day (< 2 m^3 of liquid or solid per day)
    - Continuous > 5,000 ton/yr
  - Flexibility
    - Batch can handle many different feeds and products – more flexible
    - Continuous is better for smaller product slate and fewer feeds

Batch vs. Continuous (cont.)

- Other considerations:
  - Continuous allows the process to benefit from the "Economy of Scale," but the price is less flexibility
  - Batch scale-up consists of multiple parallel units
  - Accountability and quality control – FDA requires batch accountability
  - batch is more accident prone (safety)
  - Equipment scheduling is very important issue
  - Seasonal issues: e.g., antifreeze, food products

Input – Output Structure
(Process Concept Diagram)

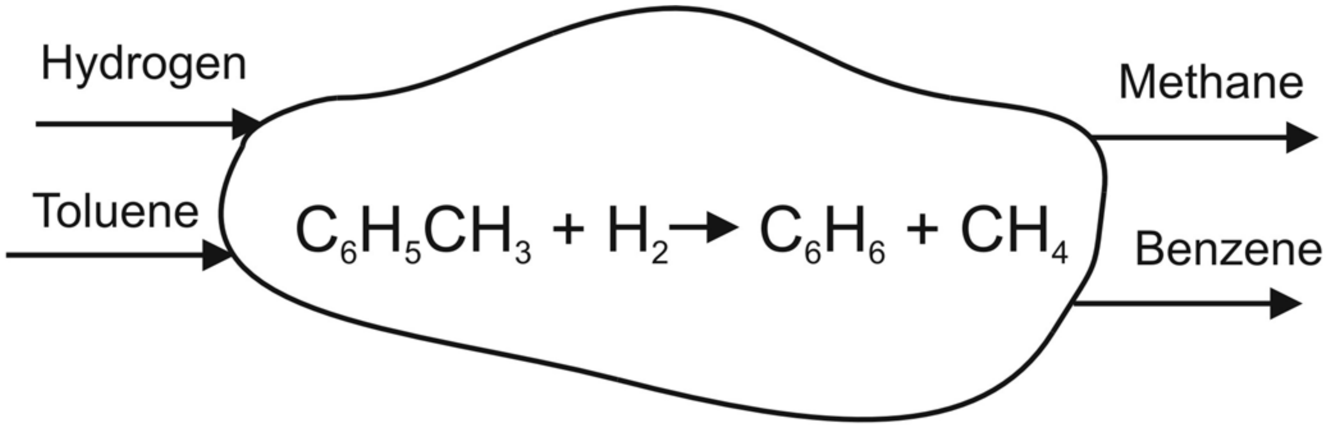


Figure 2.1: Input-Output Structure of Process Concept Diagram for the Toluene Hydrodealkylation Process

Input-Output on PFD

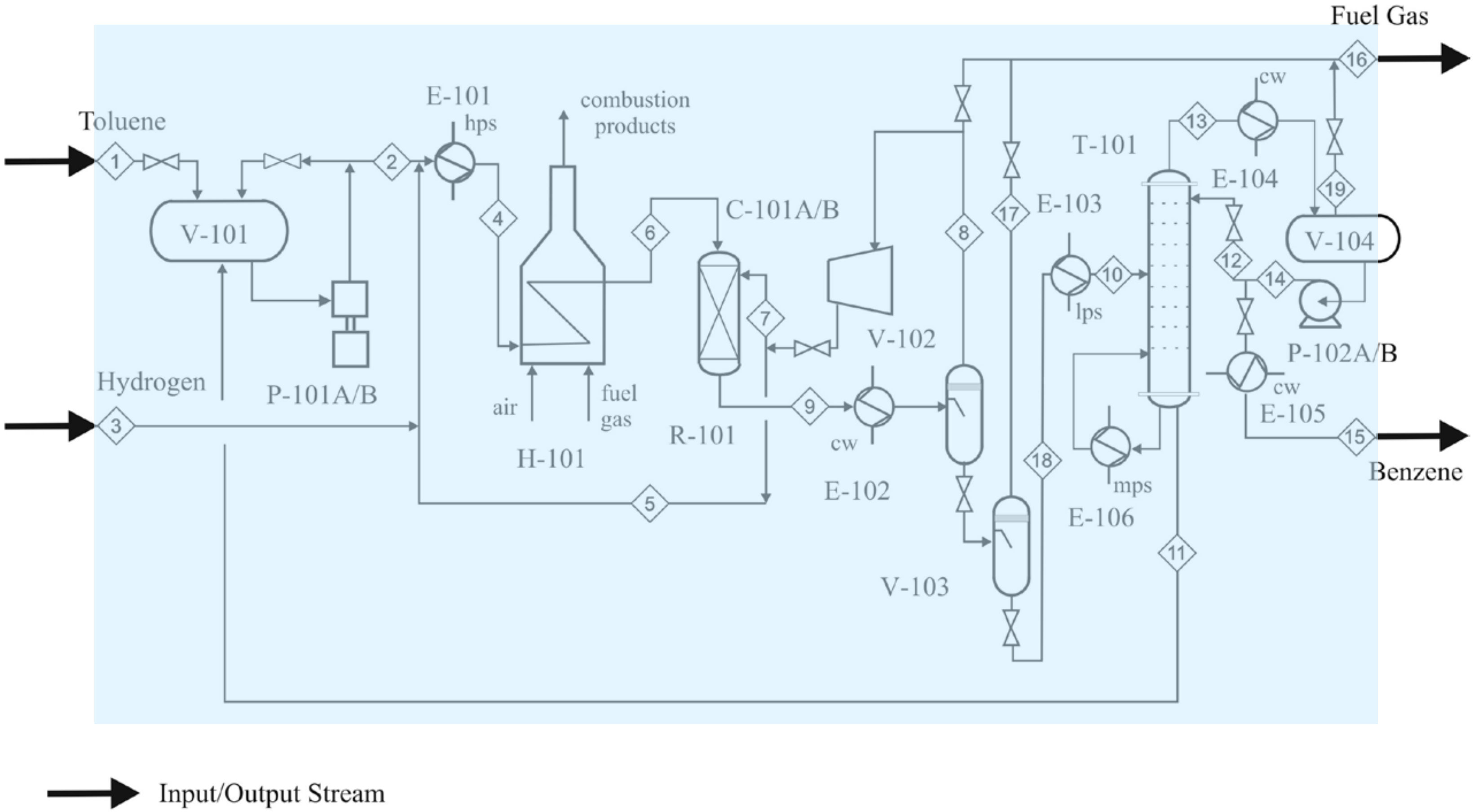


Figure 2.2 Input Output Streams on Toluene Hydrodealkylation PFD

Input-Output – Utility Streams

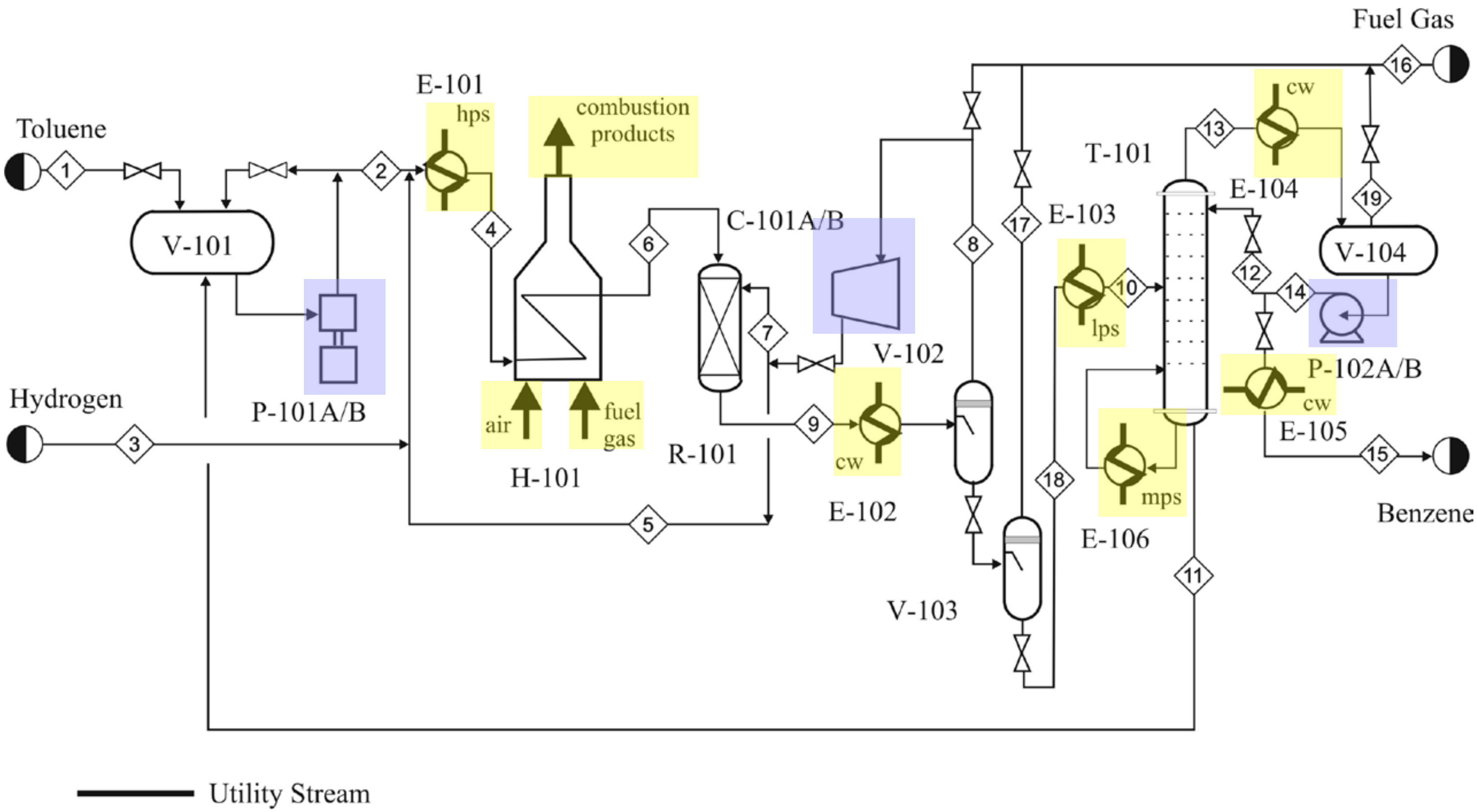


Figure 2.3: Identification of Utility Streams on the Toluene HDA PFD

Other Input – Output Issues

- Purify Feed ?
- Feed purity and trace components
  - Small quantities and “inerts” – do not separate
  - Example
    - H_2 in feed contains CH_4
    - CH_4 does not react
    - so – do not remove

Other Input – Output Issues (cont)

- If separation of impurities is difficult… Do not separate
  - azeotrope – (water and ethanol)
  - gases (requires high P and low T)

How would you remove CH_4 from H_2?

Other Input – Output Issues (cont)

- If impurities foul or poison catalyst, **separate!**
  - Sulfur – Group VIII Metals (Pt, Pd, Ru, Rh)
  - CO in platinum PEM fuel cells

Note: S and CO may be present in very small amounts (ppm)

Other Input – Output Issues (cont)

- If impurity reacts to form difficult-to-separate material or hazardous product then separate
- Phosgene Example
  - $CH_4 + H_2O \rightarrow CO + 3H_2$
  - $CO + Cl_2 \rightarrow COCl_2$
  - Any $H_2 \rightarrow HCl$

Other Input – Output Issues (cont)

- Impurity in large quantities then purify – why?
  - A notable exception is air

Add Materials to Feed

- To stabilize products

- To enable separation/minimize side reactions
  - Anti-oxidants and scavengers
  - Solvents and catalysts

Inert Feeds

- Control exothermic reactions
  - Steam controls oxidation reactions (and may eliminate or modify explosion limits)
  - Reduces coke formation on catalyst
- Control equilibrium
  - Adding inerts shifts equilibrium to the right

    e.g., styrene reaction

$$C_6H_5CH_2CH_3 \leftrightarrow C_6H_5CHCH_2 + H_2$$

Profit Margin

- If $ Products - $ Raw Material < 0,
- then do not bother to pursue this process, start looking for an alternate route

hydrodealkylation vs. disproportionation

$$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$$

$$2C_6H_5CH_3 \rightarrow C_6H_6 + C_6H_4(CH_3)_2$$

Toluene used more efficiently

Selection of Reaction Path by Economic Potential

- There are typically a variety of reaction paths available to a given product. Paths that use the cheapest raw materials (commodities) and produce fewest by-products are preferred.

Selection of Reaction Path by Economic Potential

- Early in design process, decisions can be made based on the economic potential (EP) of the process, where EP is the difference in value between the products and the reactants.

Selection of Reaction Path by Economic Potential (cont'd)

1. $C_2H_2 \ + \ HCl \rightarrow C_2H_3Cl$

2. $C_2H_4 \ + \ Cl_2 \rightarrow C_2H_4Cl_2$
   $C_2H_4Cl_2 \ + \ \Delta \rightarrow C_2H_3Cl \ + \ HCl$

3. $C_2H_4 \ + \ \tfrac{1}{2}O_2 \ + \ 2HCl \rightarrow C_2H_4Cl_2 \ + H_2O$
   $C_2H_4Cl_2 \ + \ \Delta \rightarrow C_2H_3Cl \ + \ HCl$

Selection of Reaction Path by Economic Potential (cont'd)

- Cost & MW data for mat'ls in Paths 1-3:

Material	MW	value
Acetylene	26	$0.94/kg
Chlorine	71	$0.21/kg
Ethylene	28	$0.53/kg
HCl	36	$0.35/kg
Vinyl chloride	62	$0.42/kg

Selection of Reaction Path by Economic Potential (cont'd)

- Path 1 $C_2H_2 + HCl \rightarrow C_2H_3Cl$

- Economic Potential for Path 1
  = (62 x 0.42) – (26 x 0.94 + 36 x 0.35)
  = -$11.0/kmol VCM

Selection of Reaction Path by Economic Potential (cont'd)

- Path 2 $C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$

  $C_2H_4Cl_2 + \Delta \rightarrow C_2H_3Cl + HCl$

- Economic Potential for Path 2

  = [(62)(0.42)+(36)(0.35)]–[(28)(0.53)+(71)(0.21)]

  = $8.89/kmol VCM

- Assuming HCl by product cannot be sold,

  =[(62)(0.42)]–[(28)(0.53)+(71)(0.21)]

  = -$3.71/kmol VCM

Selection of Reaction Path by Economic Potential (cont'd)

- Path 3

  $C_2H_4 + \frac{1}{2}O_2 + 2HCl \rightarrow C_2H_4Cl_2 + H_2O$

  $C_2H_4Cl_2 + \Delta \rightarrow C_2H_3Cl + HCl$

- Economic Potential for Path 3

  = (62 x 0.42) – (28 x 0.53 + 36 x 0.35)

  = -$1.40/kmol VCM

Selection of Reaction Path by Economic Potential (cont'd)

- Path 1 = -$11.0/kmol VCM

- Path 2 = $8.89/kmol VCM
  - HCl unsaleable = -$3.71/kmol VCM

- Path 3 = -$1.40/kmol VCM

Recycle

- Since raw materials make up from 25 to 75% of total operating costs, should recover as much raw material as possible
- Exception is when raw materials are very cheap

For example, Air Separation