Chapter 2
The Structure and Synthesis of Process Flow Diagrams

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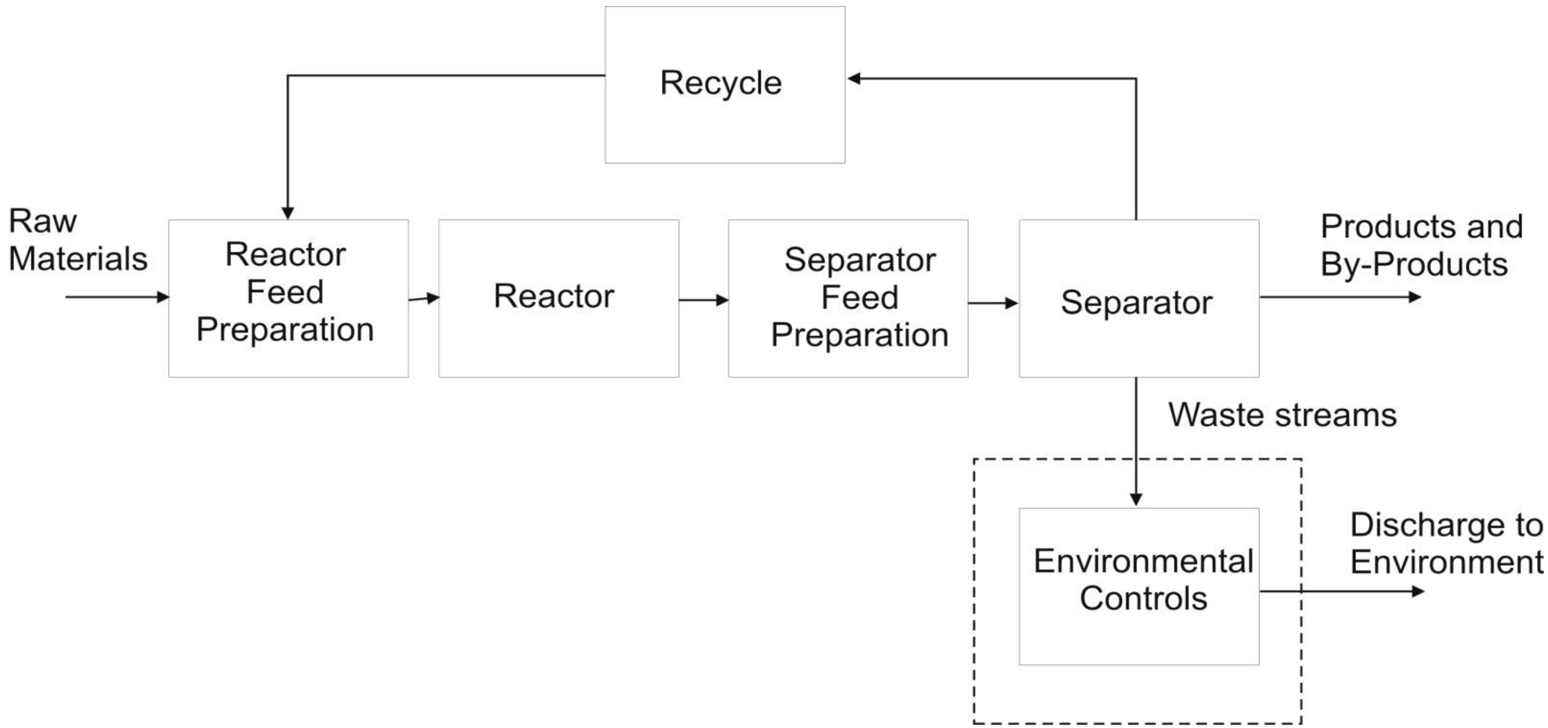
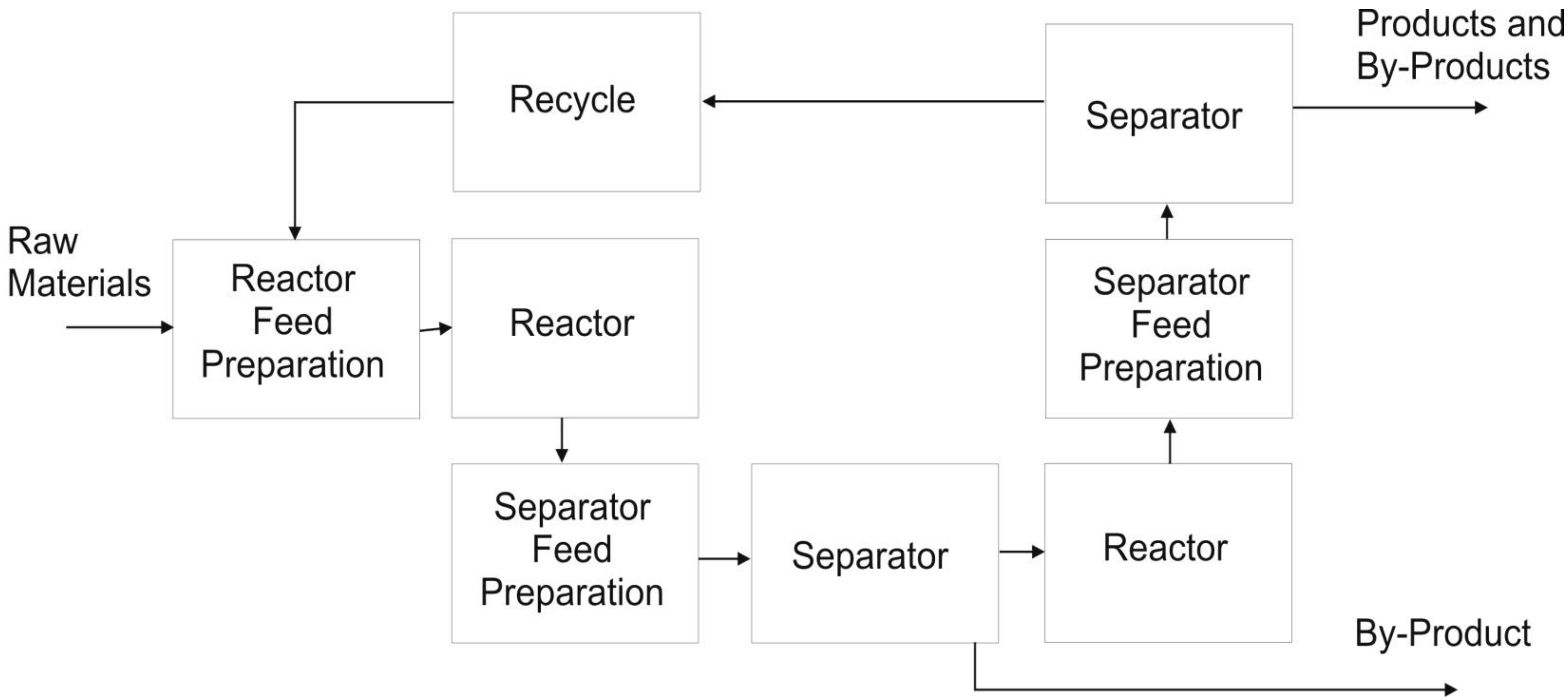
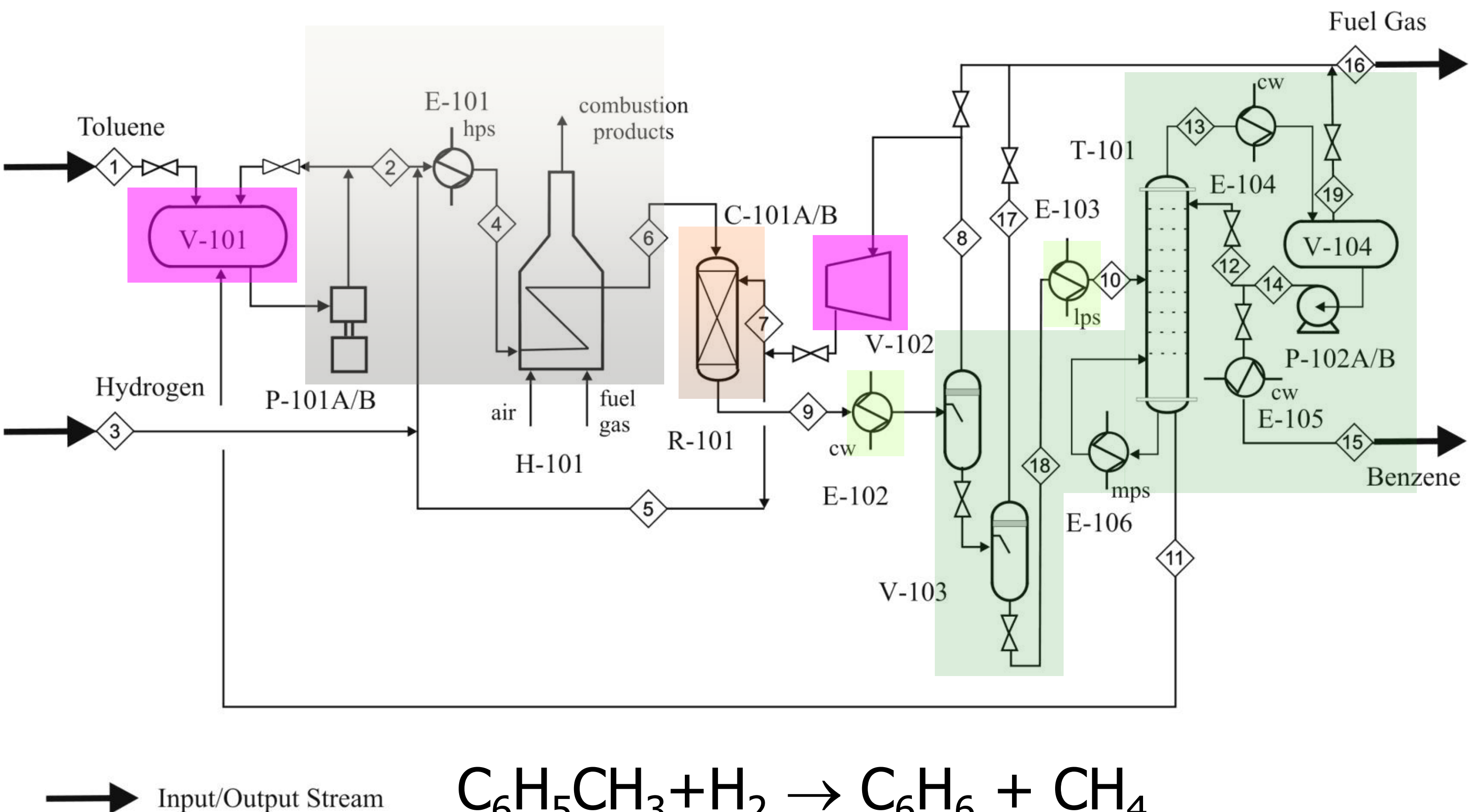
Generic Structure of Process Flow Diagrams



Generic Structure of Process Flow Diagrams



Generic Structure of Process Flow Diagrams



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

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]

- Five step process to tackle a conceptual process design
  - Batch vs. continuous
  - Input-output structure
  - Identify and define recycle structure of process
  - Identify and design general structure of separation system
  - Identify and design 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 tonne/yr ~ 1.5 tonne/day
    (< 2 m^3 of liquid or solid per day)
  - Continuous > 5000 tonne/yr

Batch vs. Continuous(cont.)

- 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.)

Continuous allows the process to benefit from the “Economy of Scale,” but the price is less flexibility

Batch vs. Continuous(cont.)

- Other Issues
  - Accountability and quality control – FDA requires batch accountability
  - Safety – batch is more accident prone
  - Scheduling of equipment – may be most important issue
  - Seasonal demands – *e.g.*, antifreeze, food products

Input – Output Structure

(Process Concept Diagram)

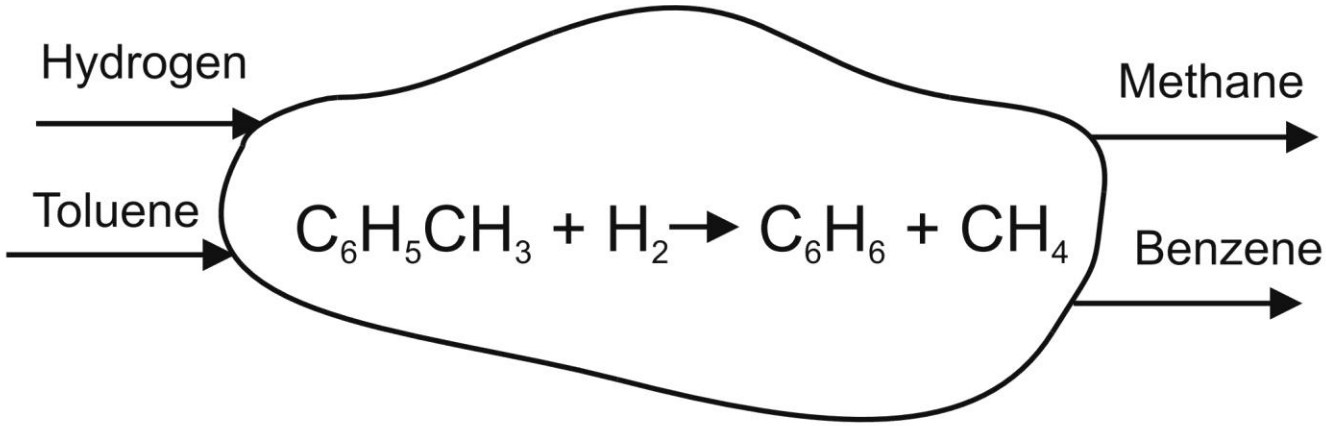


Figure 2.1: Input-Output Structure of Process Concept Diagram for the Toluene Hydrodealkylation Process

Input-Output on PFD

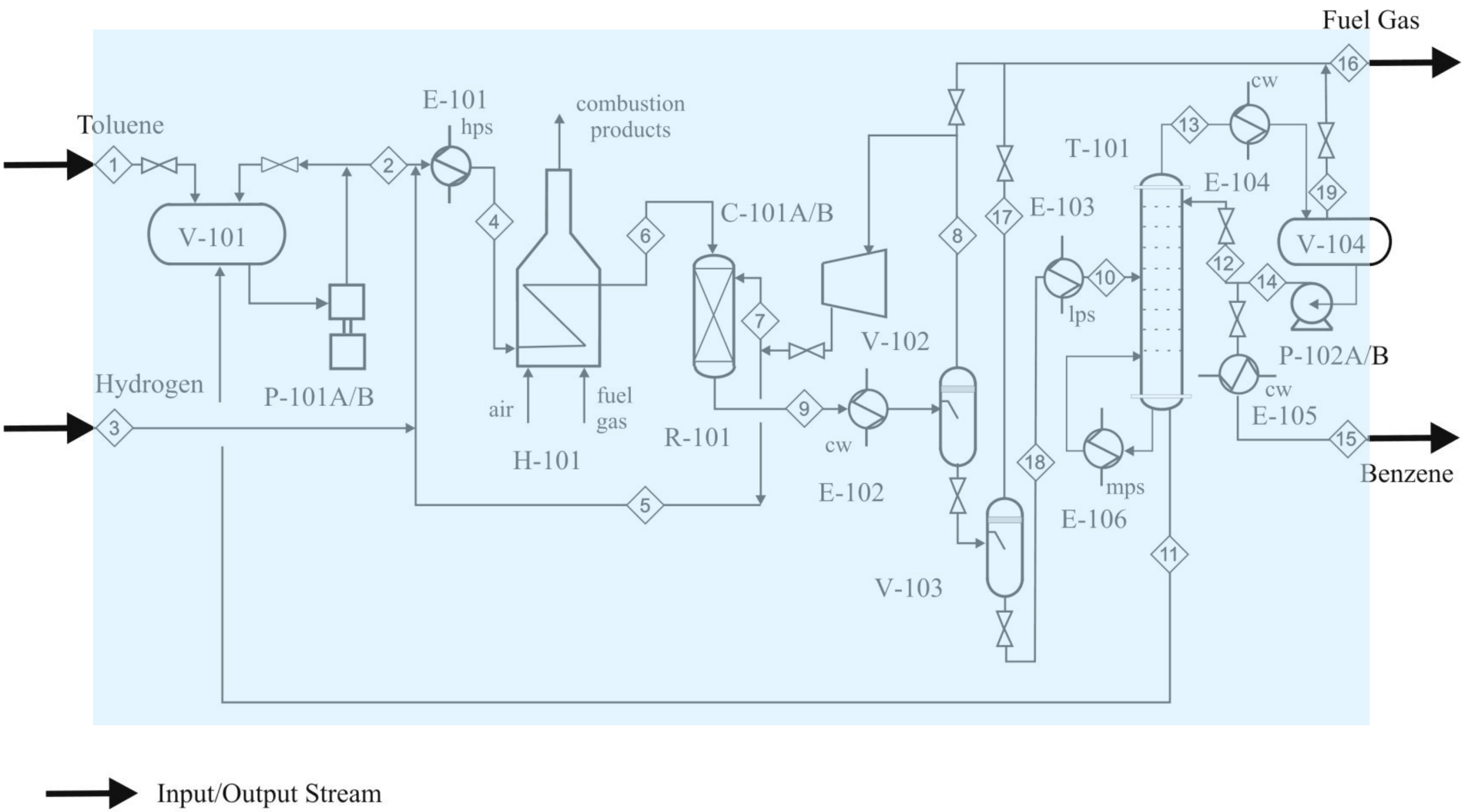


Figure 2.2 Input Output Streams on Toluene Hydrodealkylation PFD

Input-Output – Utility Streams

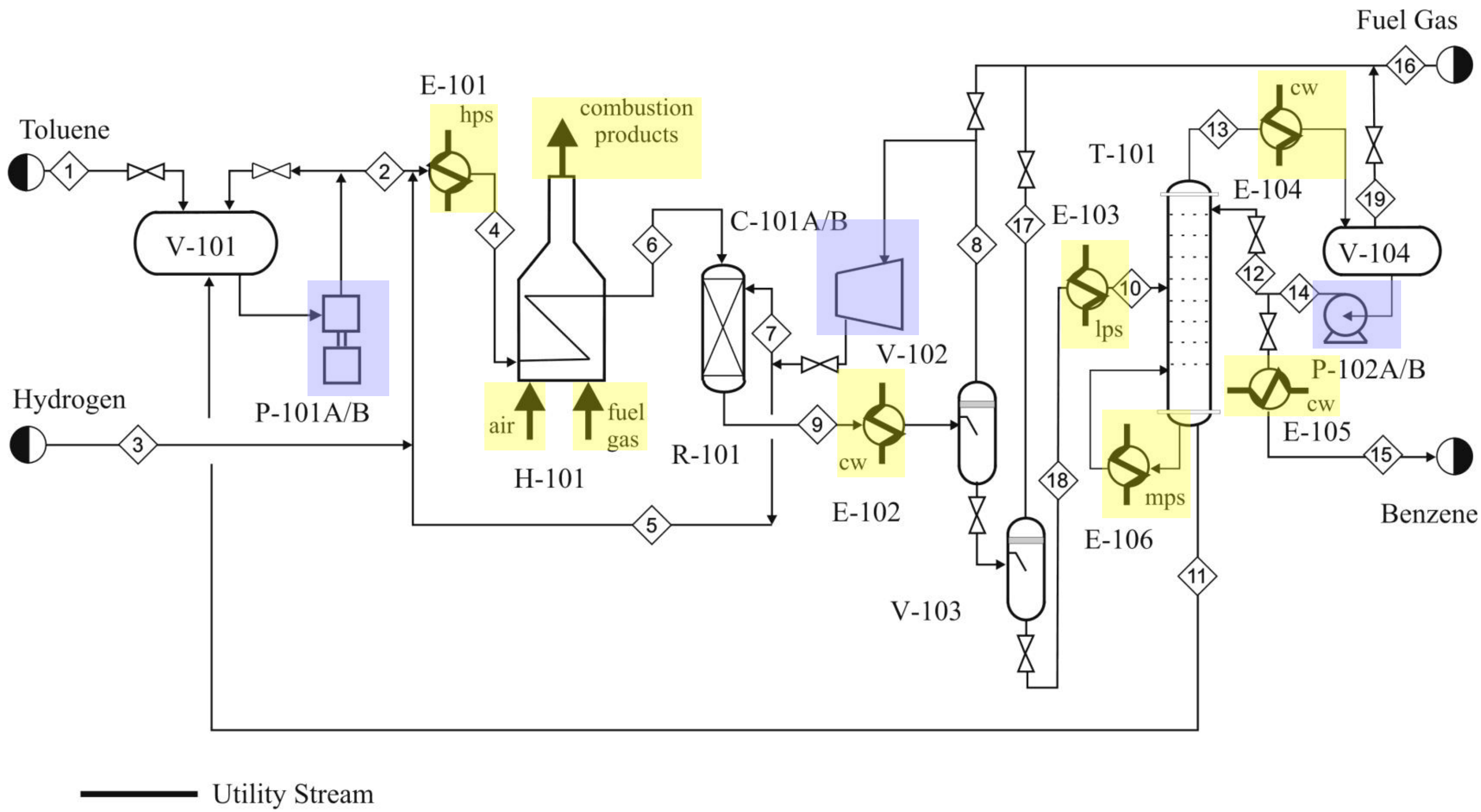


Figure 2.3: Identification of Utility Streams on the Toluene HDA PFD

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 then ***<u>separate</u>***
  - 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

$$CH_4 + H_2O \longrightarrow CO + 3H_2$$

$$CO + Cl_2 \longrightarrow COCl_2$$

$$\text{Any } H_2 \longrightarrow HCl$$

Other Input – Output Issues (cont)

- Impurity in large quantities then ***purify*** – why?

A notable exception is air

Add Materials to Feed

- Stabilize products
- Enable separation/minimize side reactions
  - Anti-oxidants and scavengers
  - Solvents and catalysts

Inert Feeds

- Control exothermic reactions
  - Steam for oxidation reactions (e›
  - Reduces coke formation on catalyst
- Control equilibrium
  - Adding inerts shifts equilibrium to the right

    e.g., styrene reaction

$$C_6H_5CH_2CH_3 \rightleftharpoons C_6H_5CHCH_2 + H_2$$

Profit Margin

- If $ Products - $ Raw Material < 0,

  then do not bother to pursue this process, but start looking for an alternate route

Toluene HDA vs. Toluene Disproportionation

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

Toluene benzene

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

Toluene benzene xylene

Toluene used more efficiently

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

3 Basic Recycle Structures

- Separate and purify unreacted feed from products and then recycle, *e.g*., toluene
- Recycle feed and products together and use a purge stream, *e.g*., hydrogen with purge as fuel gas
- Recycle feed and products together but do not use a purge stream - must come to Equilibrium

$$2C_6H_6 \rightleftharpoons C_{12}H_{10} + H_2$$

Recycle Structure in PFD

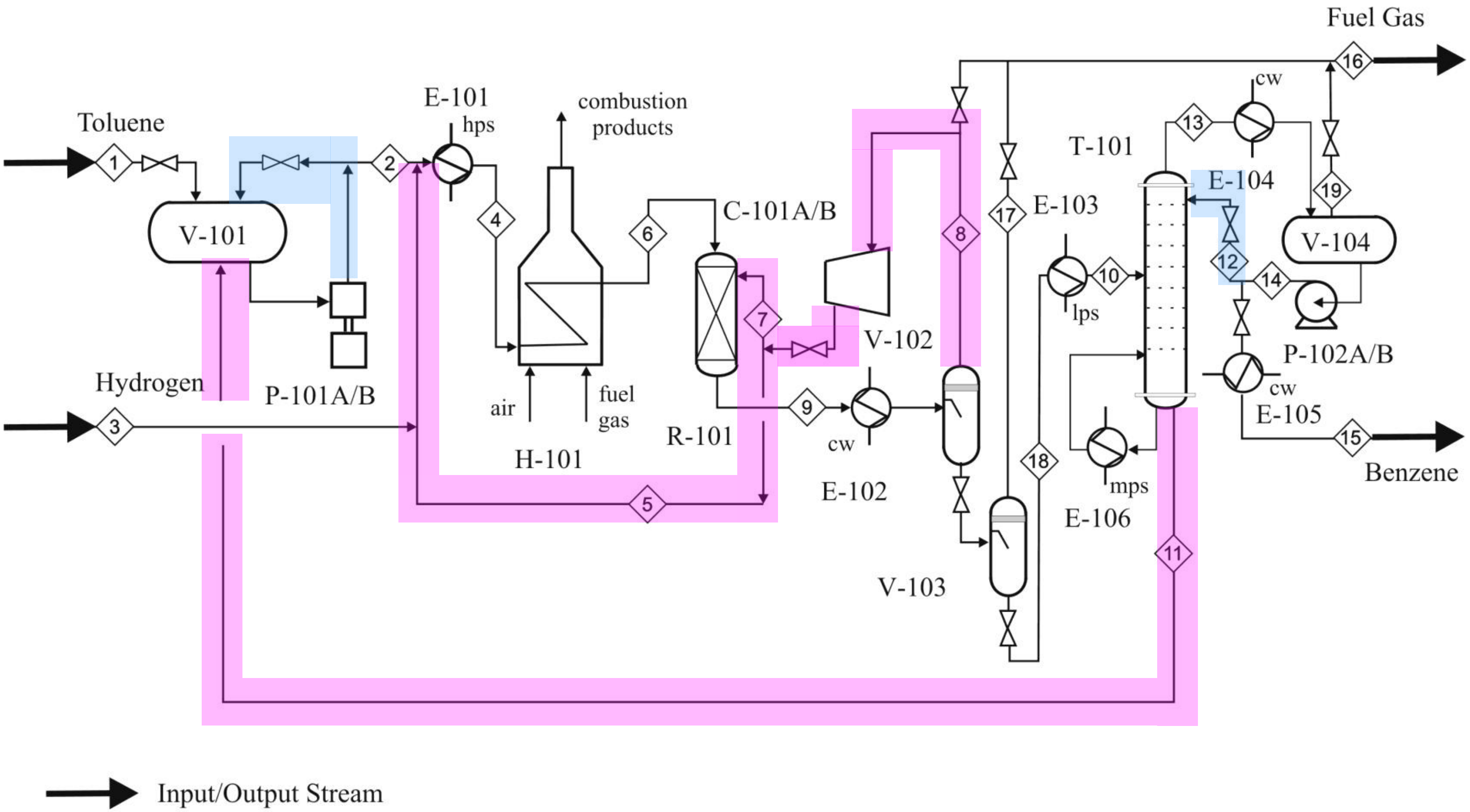
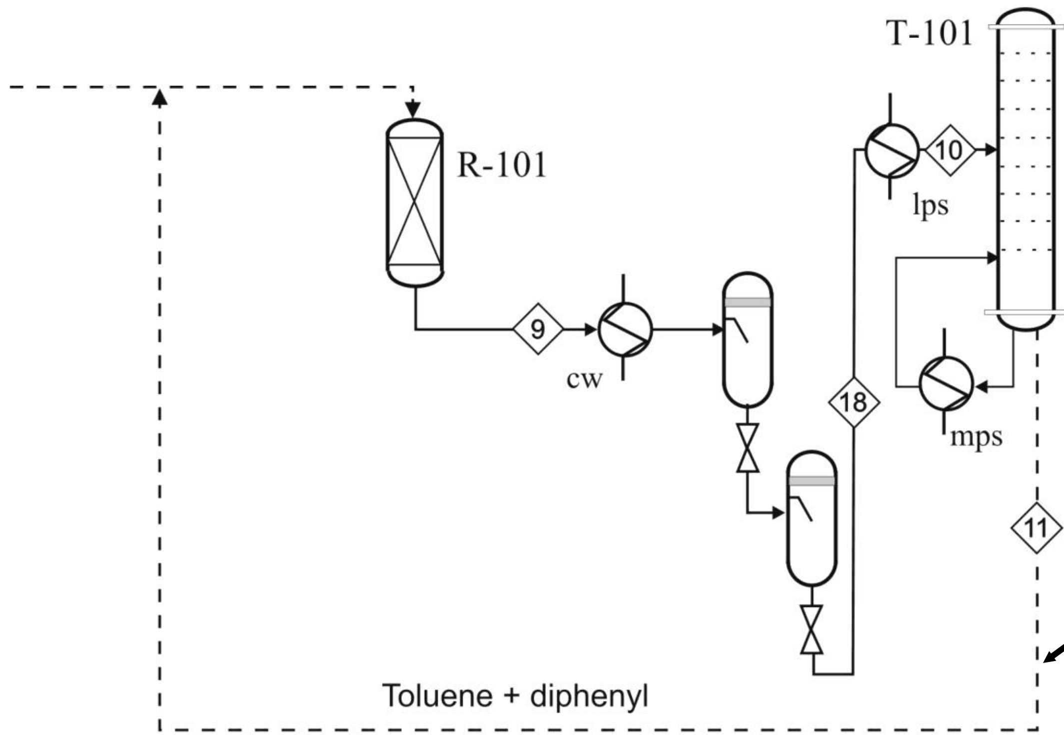


Figure 2.2 Input Output Streams on Toluene Hydrodealkylation PFD

Recycle without separation or purge



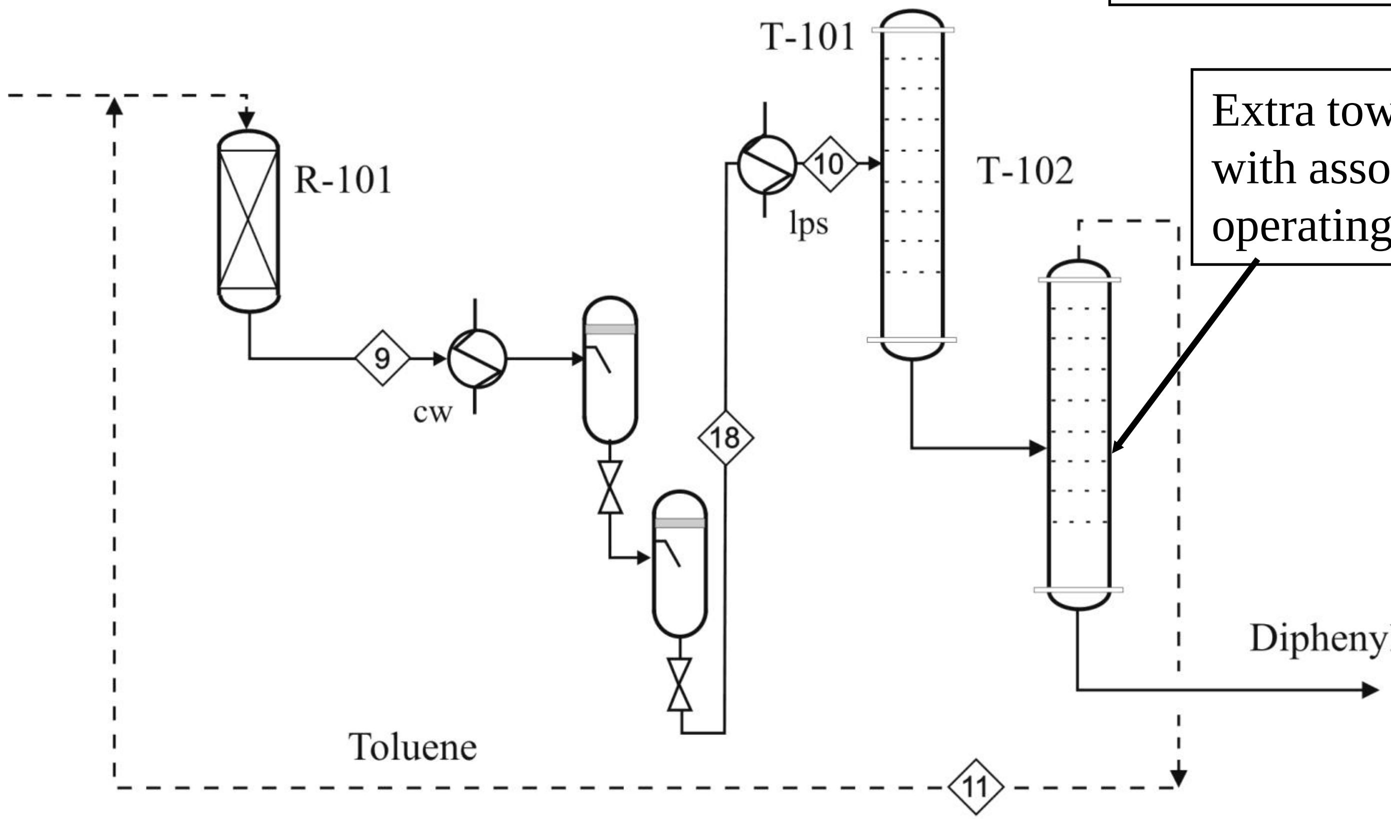
Recycle increases and equip. and op. costs increase

$$2C_6H_6 \rightleftharpoons C_{12}H_{10} + H_2$$

Figure E2.5A: PFD for Alternative A in Example 2.5 - Recycle of Diphenyl without Separation

Recycle with Separation (and Purge)

$$2C_6H_6 \rightleftharpoons C_{12}H_{10} + H_2$$



Extra tower with associated operating costs

Figure E2.5B: PFD for Alternative B in Example 2.5 - Separation of Diphenyl prior to Recycle of Toluene

Other Issues on Recycle

- Number of recycle streams
- Does excess reactant affect structure
  - Size of Recycle Loop

    H_2 : Toluene = 5 : 1
- Number of Reactors
  - Separate and recycle to different reactors

Other Issues on Recycle (cont.)

- Do we need to purify prior to recycling?
- Is recycling of inerts warranted?
- Can recycling an unwanted inert material push equilibrium to the right?
  - Gasification of coal – CO_2 recycle

Other Issues on Recycle (cont.)

- Can recycling an unwanted inert control reaction
  - CO_2 in Gasifier
- Phase of Recycle Stream?