458.401 Process & Product Design

03

Structure and Synthesis of Process Flow Diagram

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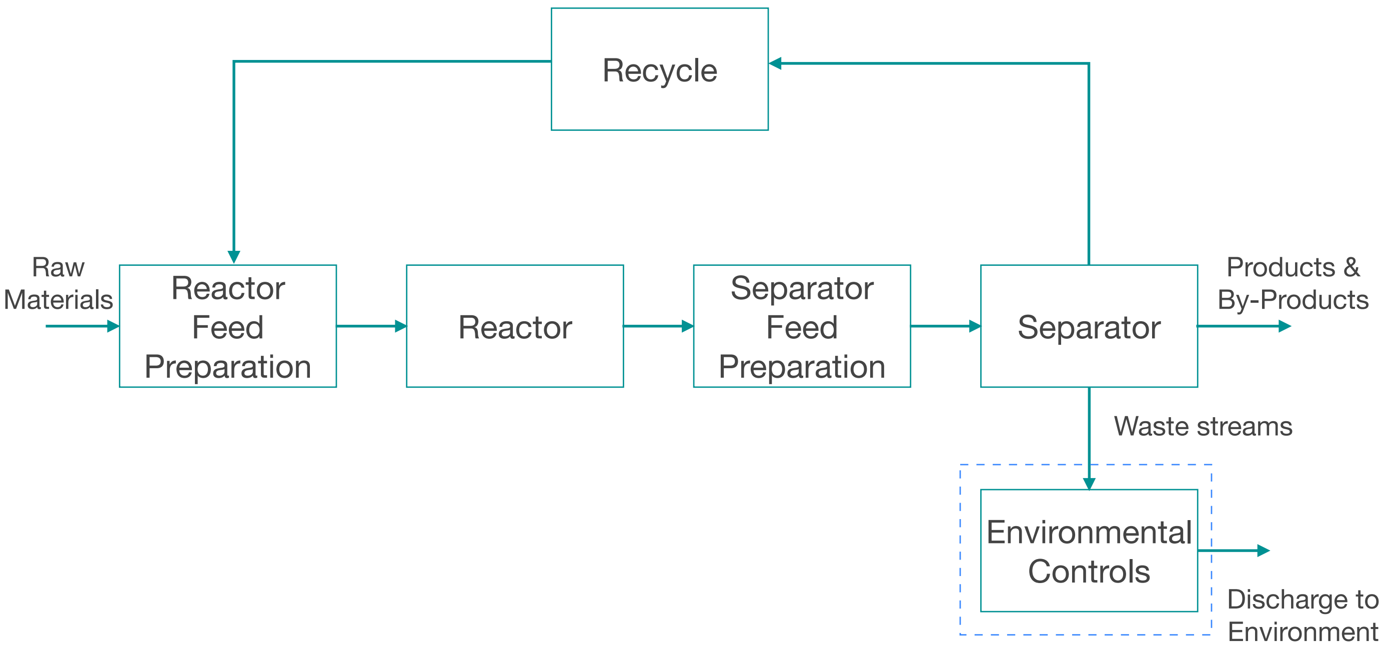
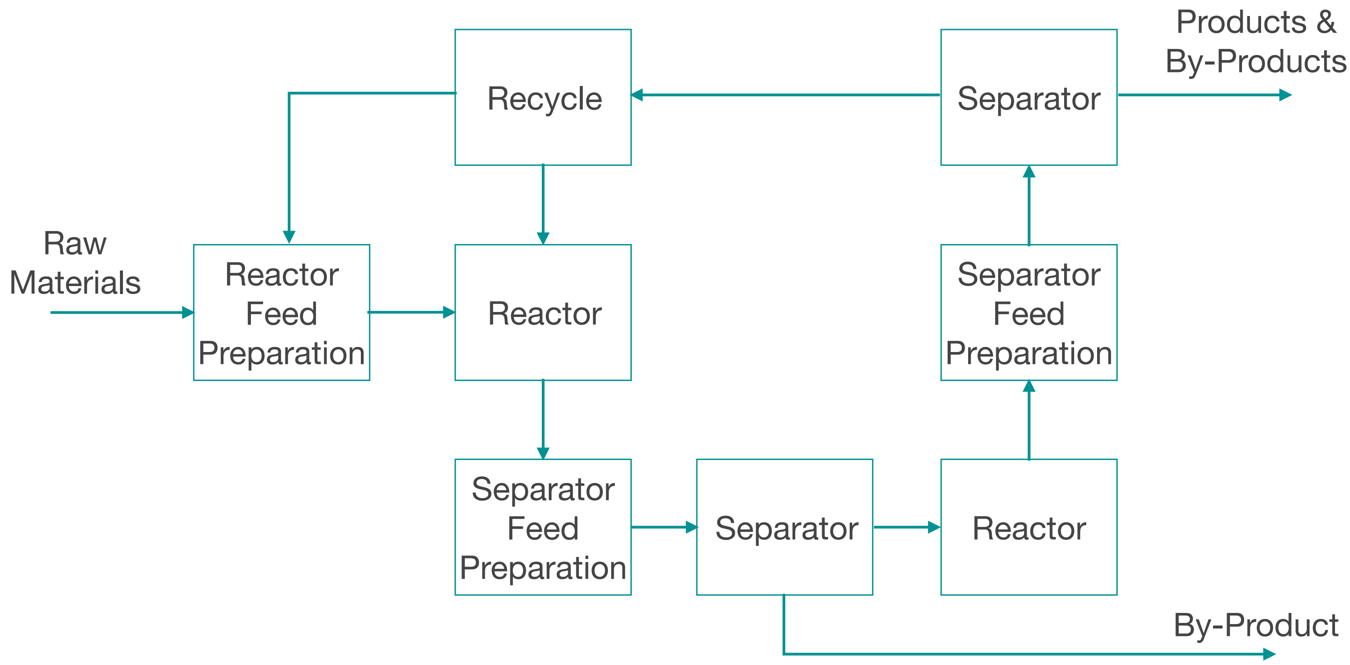
Generic Structure of Process Flow Diagrams

6 Elements

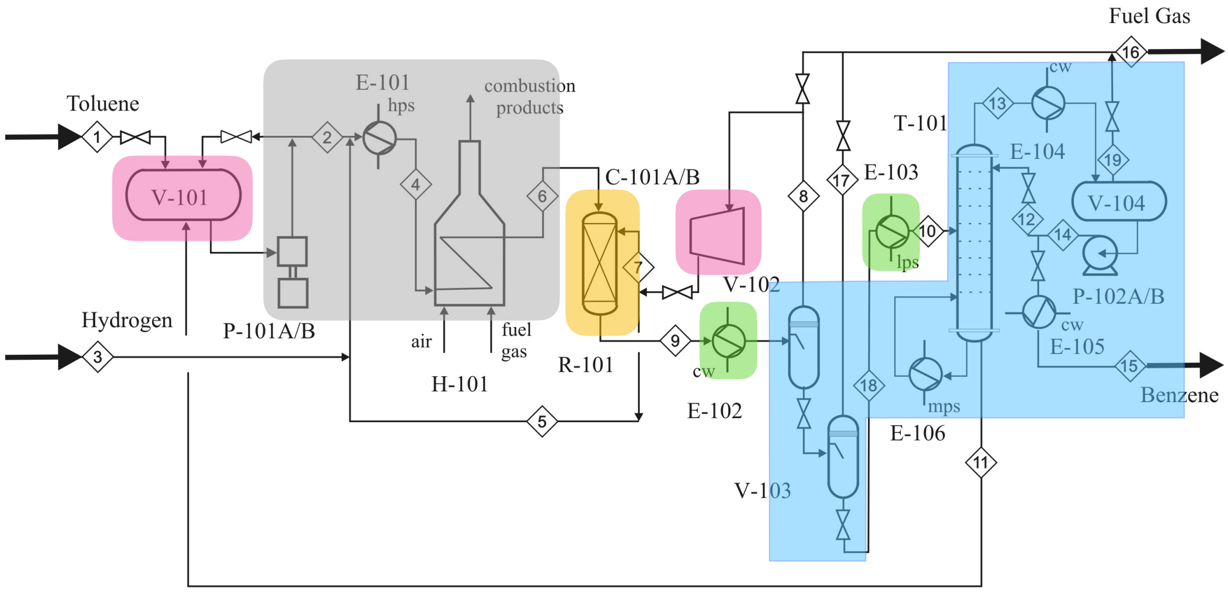


Generic Structure of Process Flow Diagrams

A process requiring multiple blocks



Generic Structure of Process Flow Diagrams



Input/Output Stream

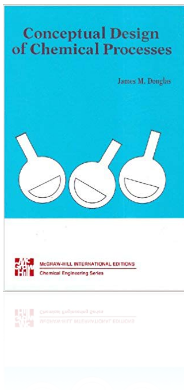
$$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$$

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, NOx control
  - Wastewater
    - Biological / sedimentation / filtration

Approach of Douglas



- 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

Batch vs. Continuous

- Size
  - Batch
    - < 500 tonne/yr ~ 1.5 tonne/day
    - < $2m^3$ of liquid or solid per day
  - Continuous
    - > 5000 tonne/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

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

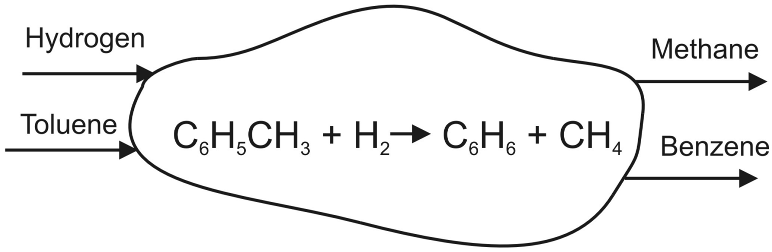
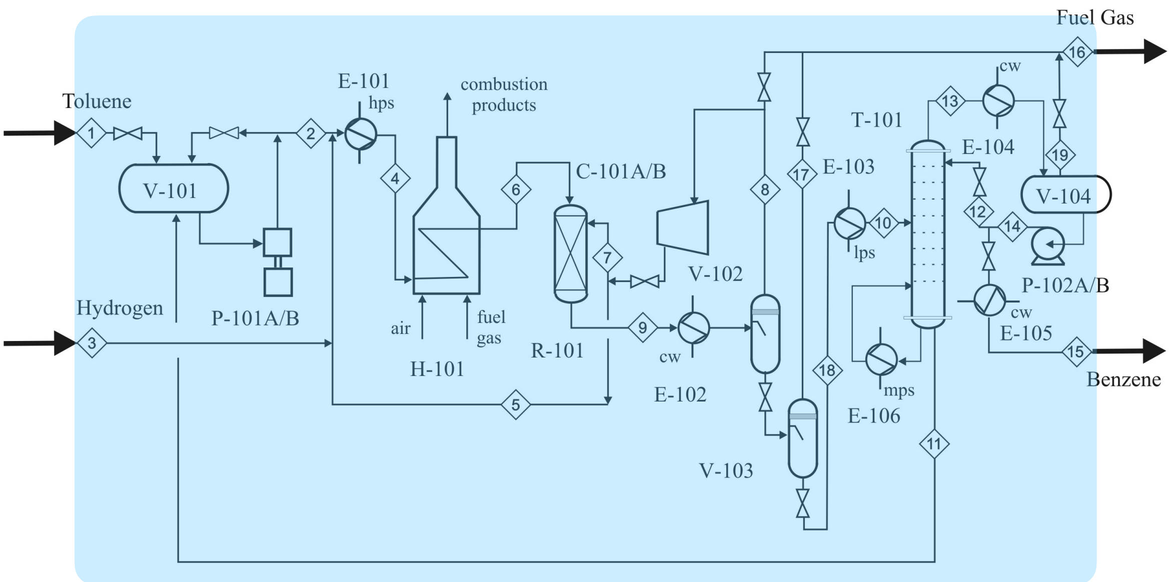


Figure 2.1: Input-Output Structure of Process Concept Diagram for the Toluene Hydrodealkylation Process

Input-Output on PFD



Input/Output Stream

Figure 2.2 Input Output Streams on Toluene Hydrodealkylation PFD

Input-Output: Utility Streams

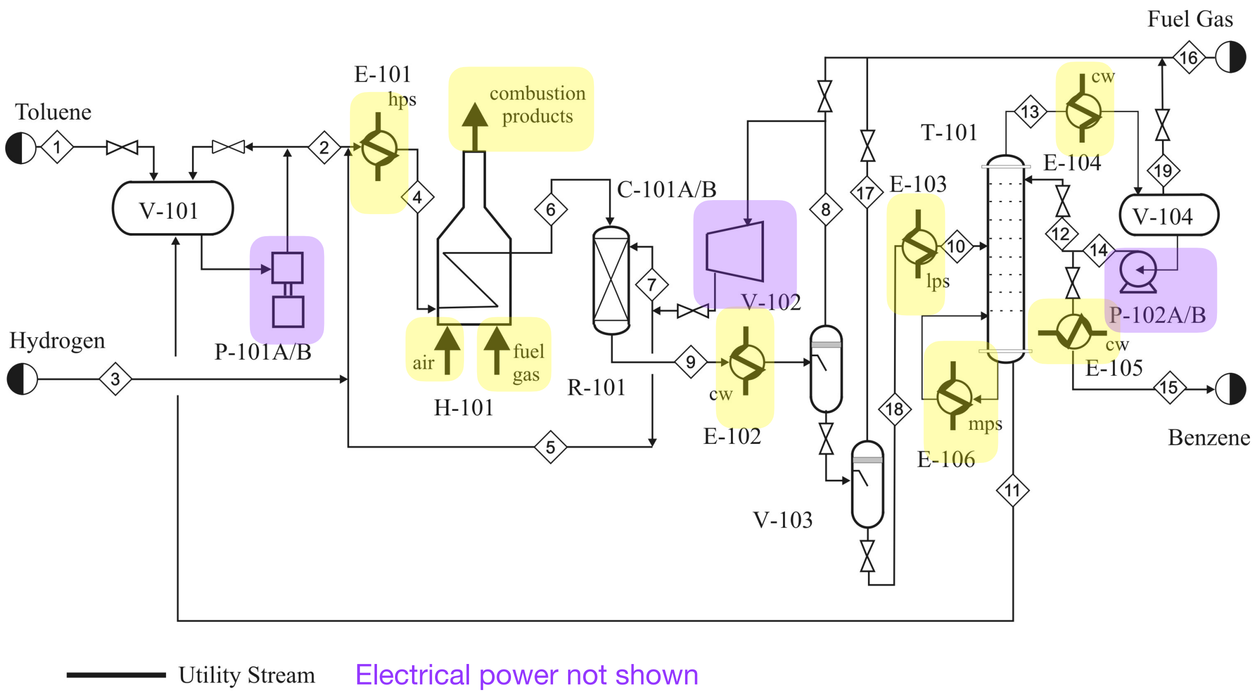


Figure 2.3: Identification of Utility Streams on the Toluene HDA PFD

Other Input-Output Issues

Purify Feed?

Feed purity and trace components

- Small quantities (say, < 10-20%) and inerts: do not separate

Examples) H_2 in feed contains CH_4 (5 mol%)
CH_4 does not react
so - do not remove

Other Input-Output Issues

- If separation of impurities is difficult, do NOT separate

  - Azeotrope: water and ethanol

  - Gases: requires high P and low T

Example-01

For the separation of methane and hydrogen, consider distillation given: normal b.p. of CH_4 = -161 °C, normal b.p. of H_2 = -252 °C and what about absorption of CH_4?

Requires low T and high P

Other Input-Output Issues

- If impurities foul or poison catalyst then 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)

- If impurity reacts to form difficult-to-separate material or hazardous product then separate

Phosgene Example

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

$$CO + Cl_2 \rightarrow COCl_2$$

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

Other Input-Output Issues

- 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 scavenger
  - Solvents and catalysts

Inert Feeds

- Control exothermic reactions
  - Steam for oxidation reactions (to reduce the potential for explosion)
  - Reduces coke formation on catalyst
- Control equilibrium
  - Adding inerts shifts equilibrium to the right
  - e.g., styrene reaction

$$C_6H_5CH_2CH_3 \longleftrightarrow C_6H_5CHCH_2 + H_2$$

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

$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$

$C_6H_5CH_3 \rightarrow C_6H_6 + C_6H_4(CH_3)_2$ Toluene used more efficiently

xylene

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; e.g., Air Separation

3 Basic Types of Recycle Structures

1. Separate and purify unreacted feed from products and then recycle, e.g., toluene
2. Recycle feed and products together and use a purge stream, e.g., hydrogen with purge as fuel gas (separation of unused reactants is infeasible/ uneconomic)
3. Recycle feed and products together but do not use a purge stream (must react further through equilibrium reaction)

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

Example-02

Calculate the single-pass conversion, overall conversion, and yield of most costly reactant, i.e., toluene

Figure 2.3

Solution-02

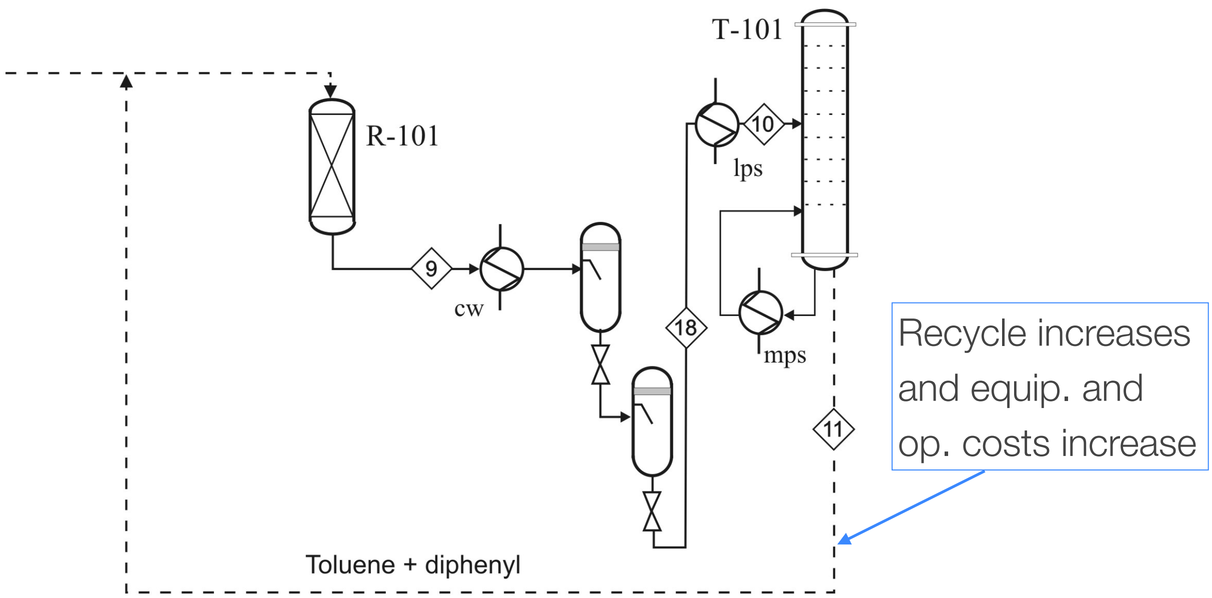
We refer to Table 1.5

Single-pass conv. = (144.0 - 36.0) / 144.0 = 0.75

Overall conv. = (108.7 - 0.4 - 0.31) / 108.7 = 0.993

Yield = Moles of reactant to produce desired product / Moles of limiting reactant reacted = (105.2 + 2.85) / (108.7 - 0.4 - 0.31) = 0.9995

Recycle without Separation or Purge



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

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

Recycle with Separation (and Purge)

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

Extra tower with associated operating costs

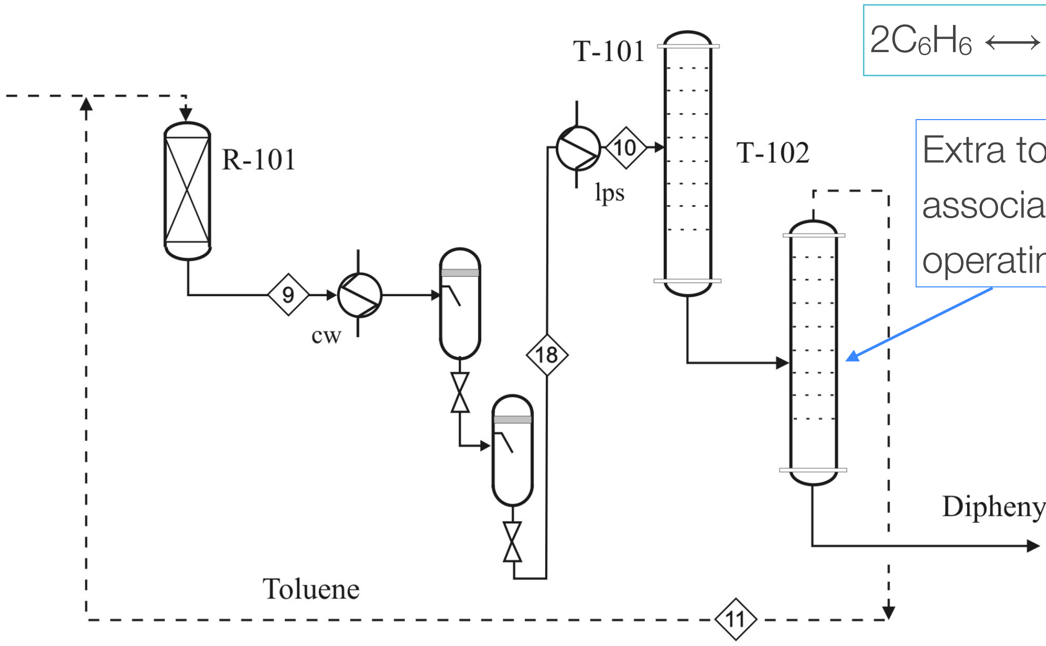


Figure E2.5B: PFD for Alternative B in Example 2.5 - Separation of Diphenyl prior to Recycle of Toluene

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