Integration of Reaction and Separation Processes

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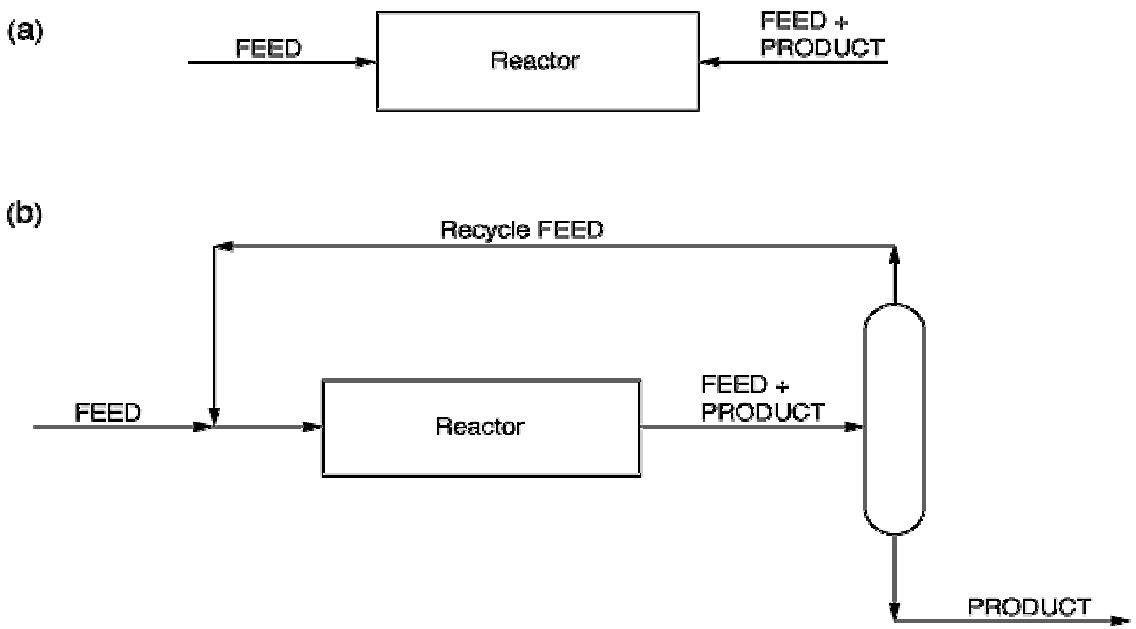
Chap. 4. Synthesis of Reaction-Separation Systems

- Interaction btn the reactor design and the separation system design will be discussed.
  - Function of process recycles
  - Vapor recycles and purges
  - Vapor *v.s.* liquid recycles

The Function of Process Recycles

- **Reactor Conversion**

Feed → Product



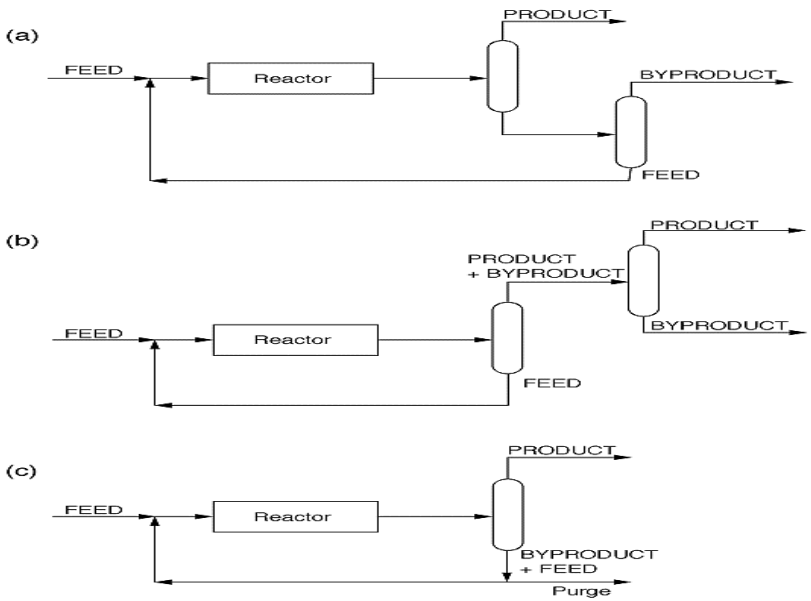
The Function of Process Recycles

- **Byproduct formation**

Feed → Product + Byproduct

or

Feed → Product
Product → Byproduct



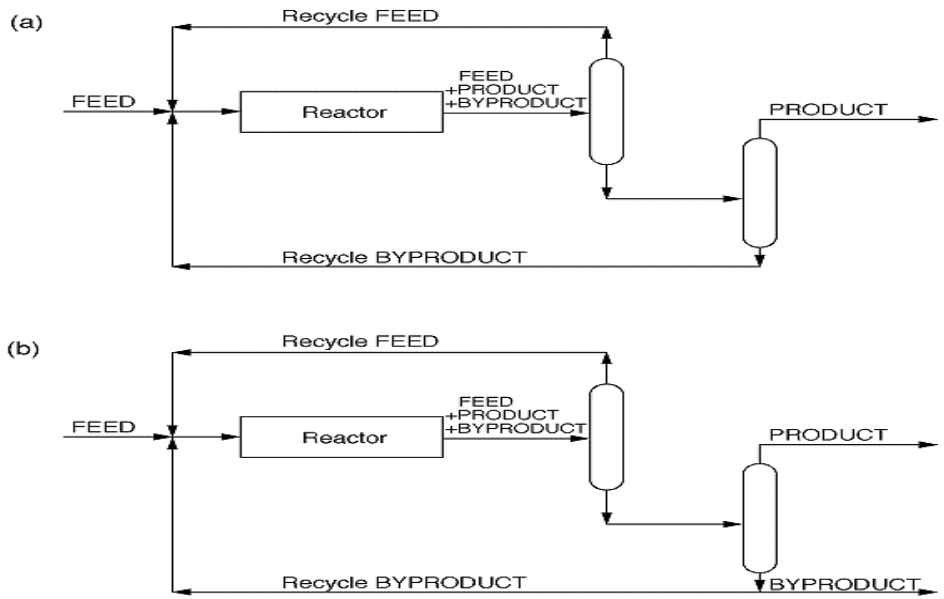
⇐ **two different sequences**

⇐ **separator cost *vs.***
raw materials losses
disposal cost

The Function of Process Recycles

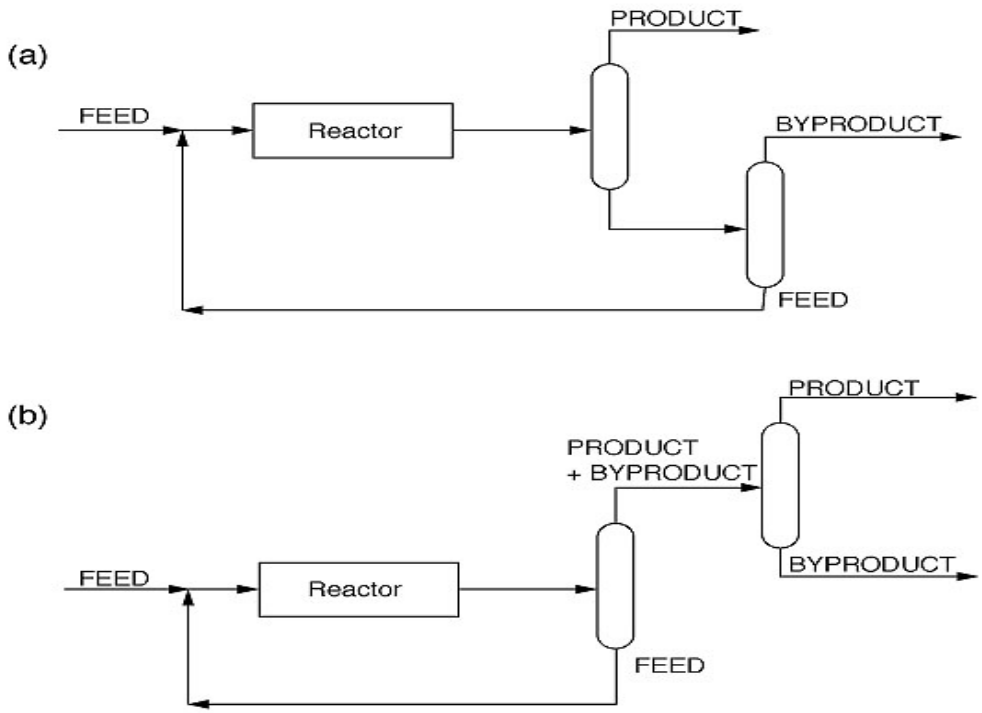
- **Recycling byproduct for selectivity**

Feed → Product
Feed ⇄ Byproduct



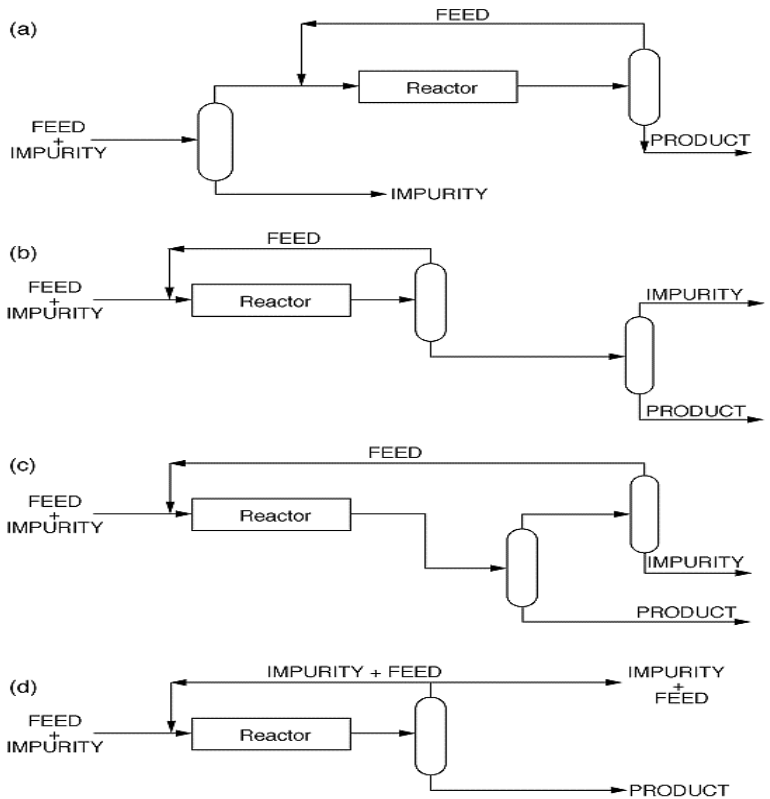
The Function of Process Recycles

- Recycling byproducts or contaminants damage the reactor



The Function of Process Recycles

- **Feed impurities**



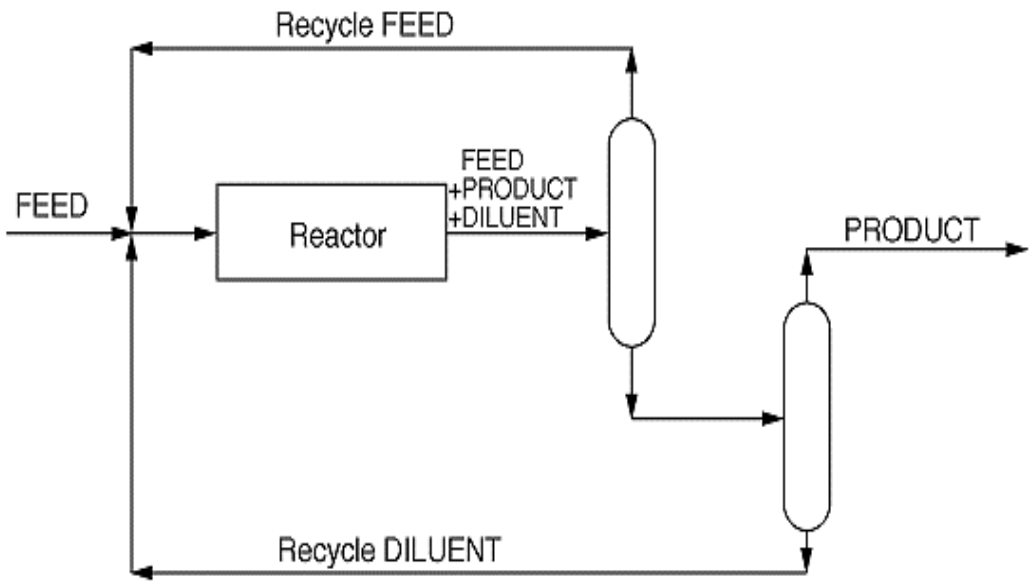
Impurity has an adverse effect on the reactor

Impurity has an insignificant effect

Separator cost *vs.* raw material costs

The Function of Process Recycles

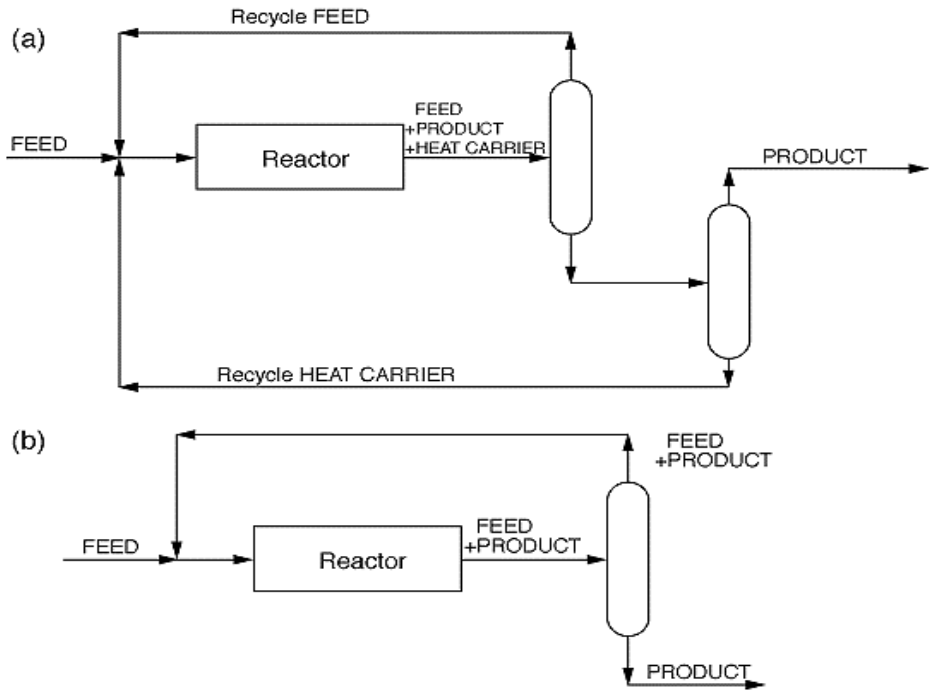
- Reactor diluents and solvents



The Function of Process Recycles

- **Reactor heat carrier**

  - Extraneous component *vs.* product as a heat carrier



The Function of Process Recycles

Example : MCD production from DEC & Cl_2

$$C_{10}H_{22} + Cl_2 \rightarrow C_{10}H_{21}Cl + HCl$$

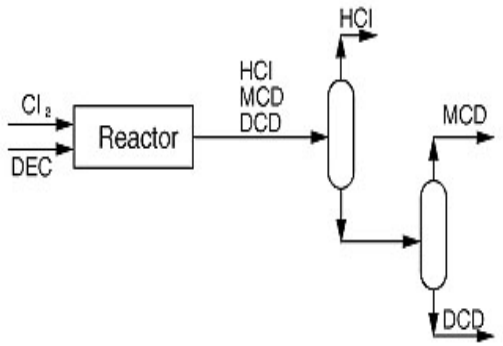
DEC MCD

$$C_{10}H_{21}Cl + Cl_2 \rightarrow C_{10}H_{20}Cl_2 + HCl$$

MCD DCD

The Function of Process Recycles

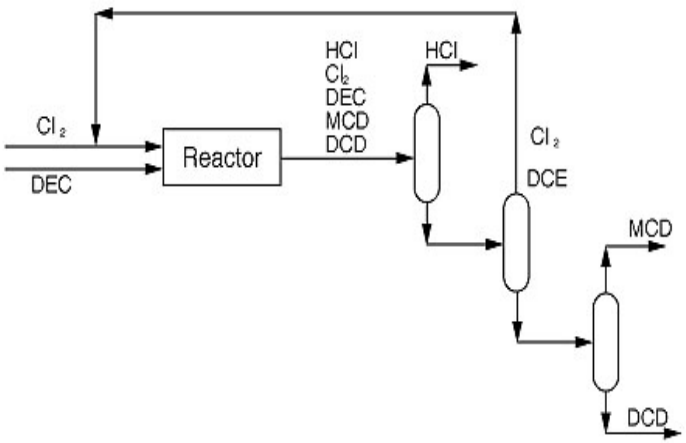
(a)



- Complete conversion of both feeds

→ Attractive but impractical

(b)

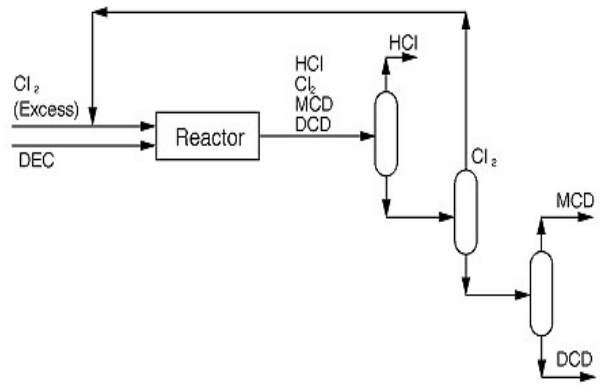


- Incomplete conversion of both feeds

→ No effect on selectivity

The Function of Process Recycles

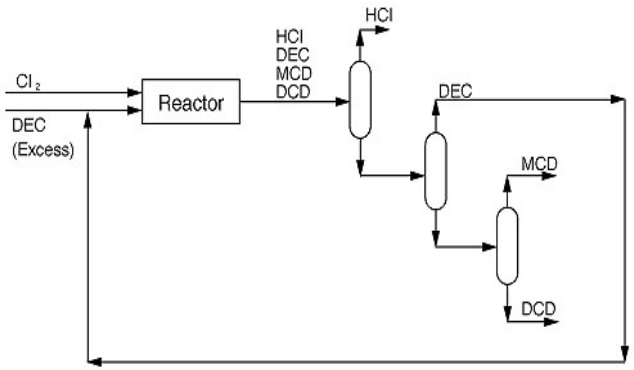
(c)



- **Excess chlorine**

→ **force DEC to complete conversion**
→ **force MCD to byproduct DCD**

(d)



- **Excess DEC**

→ **force Cl_2 to complete conversion**
→ **suppress the side reaction**

Vapor Recycles and Purges

- **Reactor effluent with a wide range of volatilities**

  → **partial condensation or vaporization followed by a simple phase split**

- **Vapor is difficult to condense**

  → **further separation such as membrane, adsorption, absorption, refrigerated condensation.**

- **Purge instead of vapor separation**

- **Combination of purge with separator**

Synthesis of Reaction-Separation Systems-Summary

- The use of excess reactants, diluents, or heat carriers has a significant effect on the flowsheet recycle structure.

- Recycling of unwanted byproduct
  - -improves the overall use of raw materials
  - -eliminate effluent disposal problems
  - -but raise some of other costs.(tradeoffs exist)

- Mixture with wide range of volatilities $\rightarrow$ partial condensation or vaporization with simple phase split

- Further separation such as membrane is needed to non-condensable vapor

Chapter 5. Distillation Sequencing

- **Choice of the order in which components are separated will be discussed.**

  - Selection of the sequence for simple, nonintegrated columns

  - Heat integration of sequences of simple columns

  - Internal mass flows in sequences of simple columns

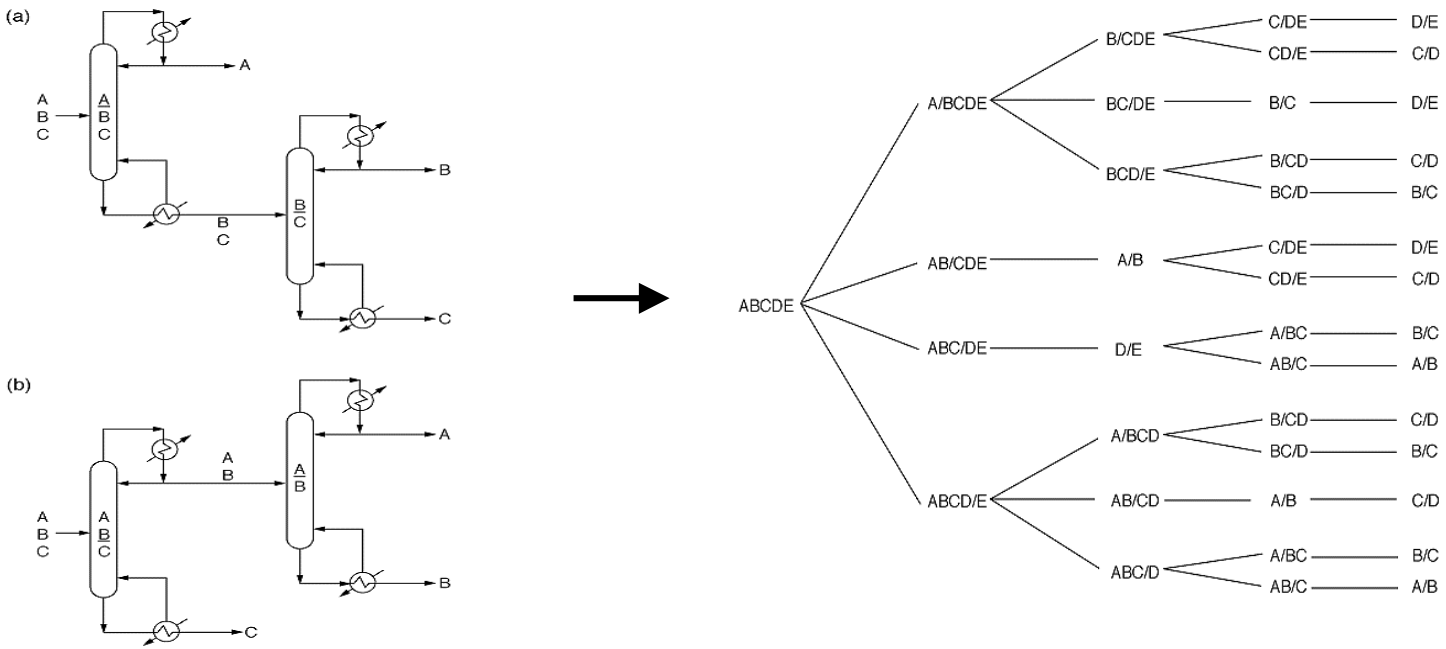
  - Sequencing using columns with more than two products

  - Sequencing using thermal coupling

Distillation Sequencing Using Simple Columns

- **Complexity in sequence increases dramatically as the number of component increases**

$$\frac{2(N-1)!}{N!(N-1)!}$$



Practical Constraints that Restrict Options

- **Process constraints often reduce the number of options**
  - **Hazardous component must be removed as early as possible**
  - **Reactive and heat sensitive component must be removed**
  - **Corrosive component must be removed early**
  - **Finished products might not be taken from bottoms**
  - **Light components might be removed from the top of 1st column**

Selection of the Sequences for Simple Columns

- **Typical heuristics for sequence selection are :**
  - **Do the most difficult separator last**
  - **Favor the direct sequence**
  - **Remove component with a large fraction first**
  - **Favor near-equimolar splits**

⇨ **The heuristics are often in conflict with each other**

Selection of the Sequences for Simple Columns

- **Vapor flow rate up the column is a good measure of both capital & operating costs.**

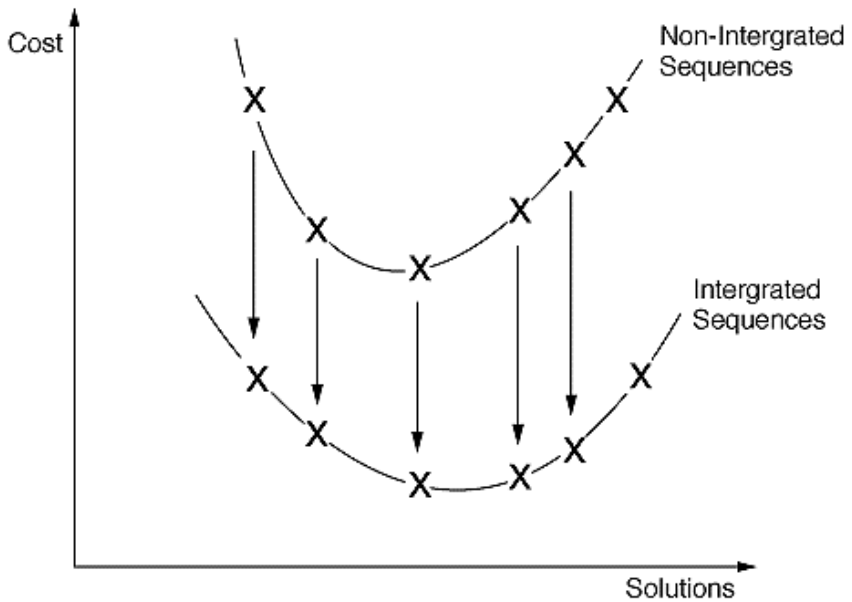
- **How is the total vapor load predicted ?**

$$\Rightarrow \quad V = (F_A + F_B + \cdots + F_{LK}) + (F_A + F_B + \cdots + F_{LK} + F_{HK} + \cdots + F_{NC}) \frac{R_F}{\alpha - 1}$$

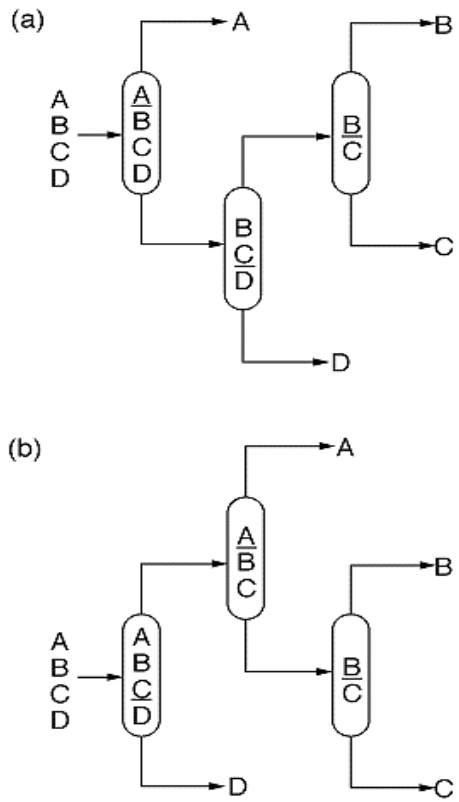
$$\Rightarrow \quad \min_{sequence} \sum V$$

Heat Integration of Sequences of Simple Columns

- **Separation sequencing and heat integration can be decoupled**



Internal Mass Flows in Sequences of Simple Columns



Total flow of keys is the same

$$\sum_{keys}(m) = m_A + 2(m_B + m_C) + m_D$$

Total flow of nonkeys is different

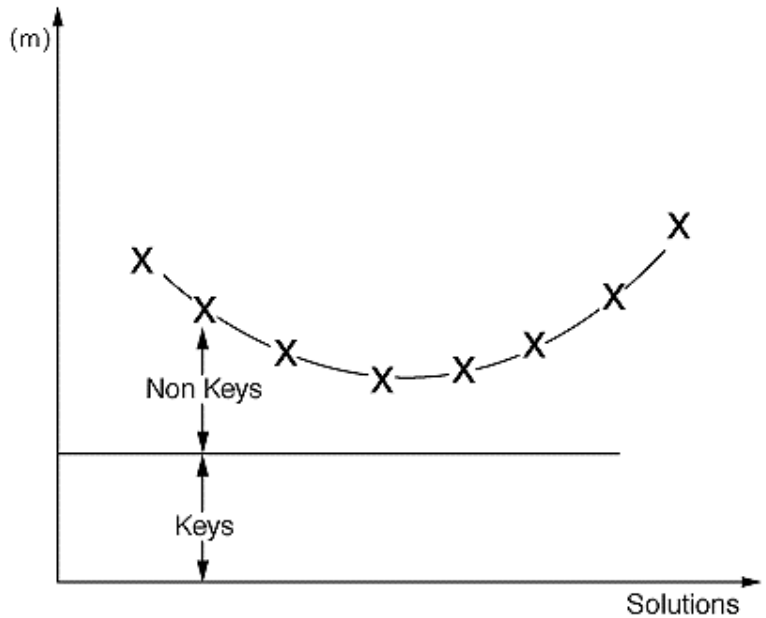
$$(a) \rightarrow \sum_{NonKeys}(m) = m_B + m_C + m_D$$

$$(b) \rightarrow \sum_{NonKeys}(m) = m_A + m_B + m_C$$

Internal Mass Flows in Sequences of Simple Columns

- F_{key} is constant and independent of the sequence ;

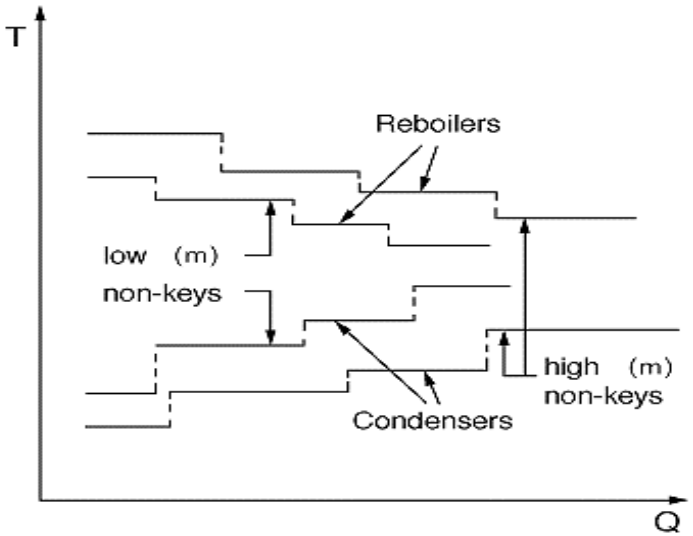
  F_{nonkey} varies according to the choice of sequences



Internal Mass Flows in Sequences of Simple Columns

- **Integration always benefits from colder reboiler streams and hotter condenser streams**
- **Columns with small temperature differences are easier to integrate**
- **It is unlikely that a sequence has a small capital cost and a large operating cost, or vice versa**

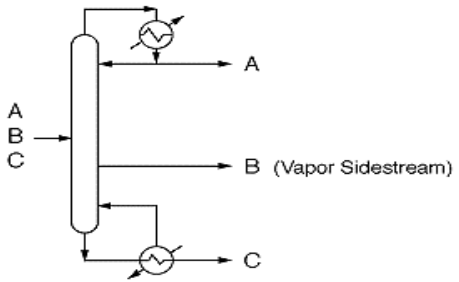
⇨ **Minimize F_{nonkey}**



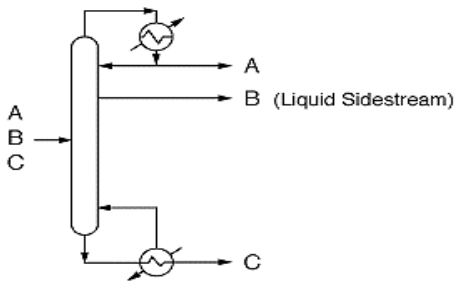
Distillation Sequences Using Multi-Product Columns

- **Single columns side stream arrangements can be attractive**

← middle product is in excess and the other product is minor

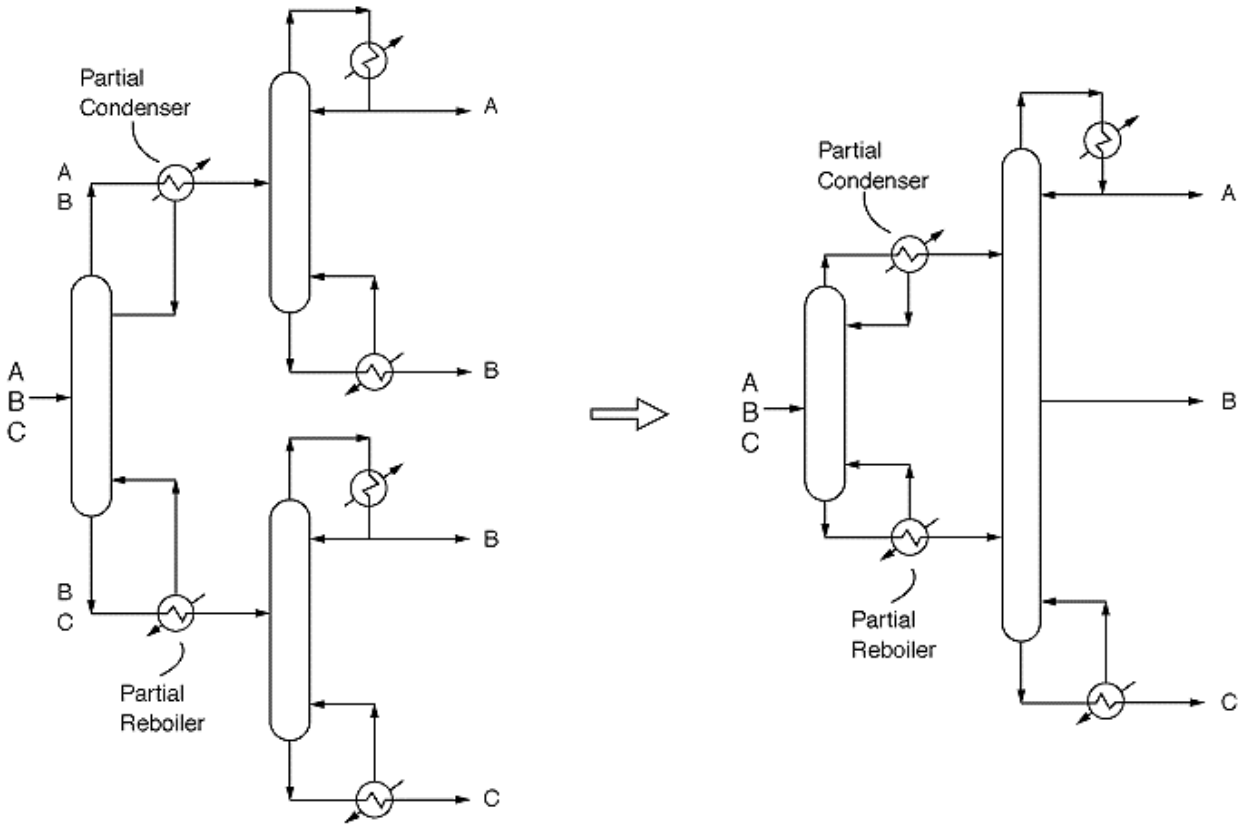


More then 50% middle component and less then 5% heaviest component



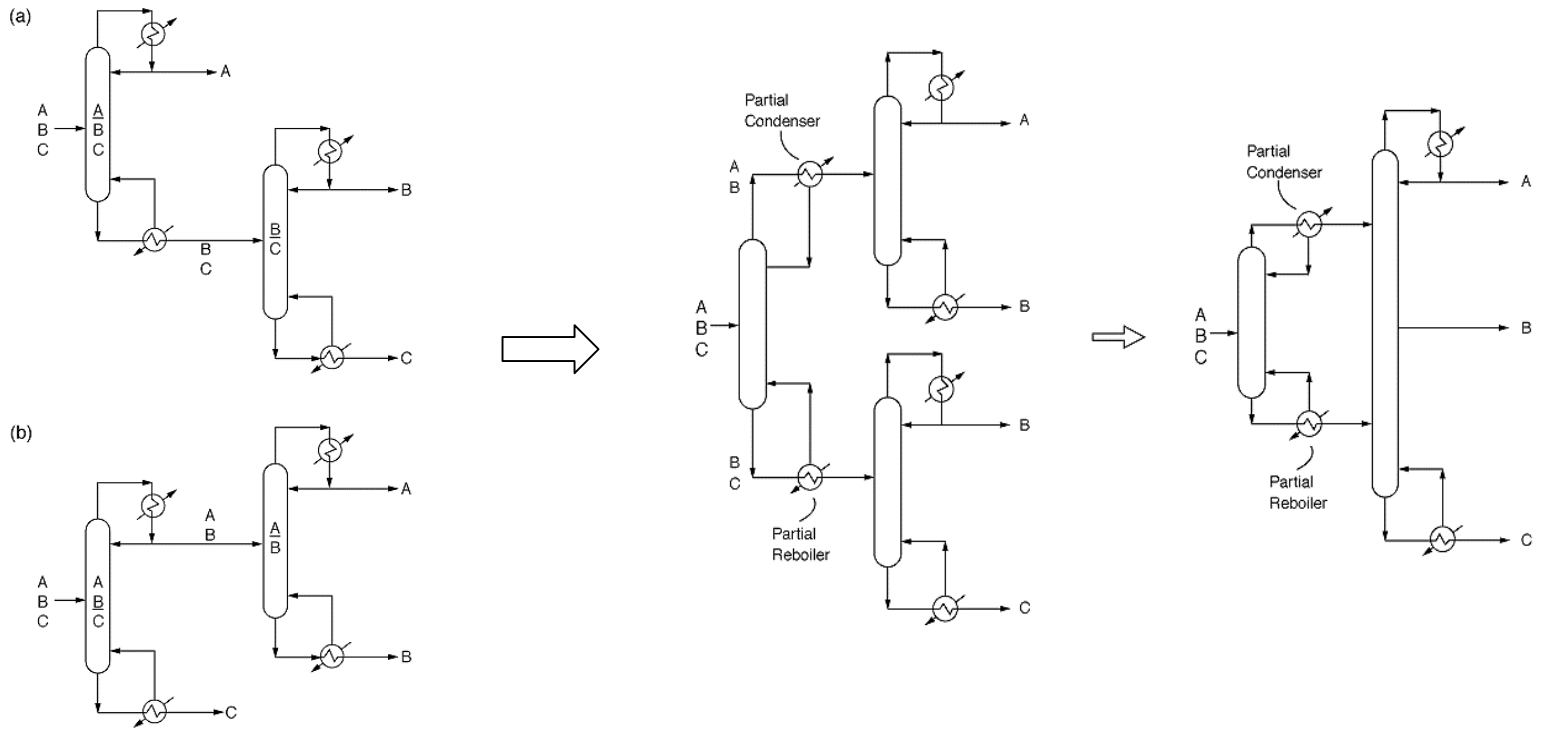
More then 50% middle component and less then 5% lightest component

Distillation Sequences Using Multi-Product Columns



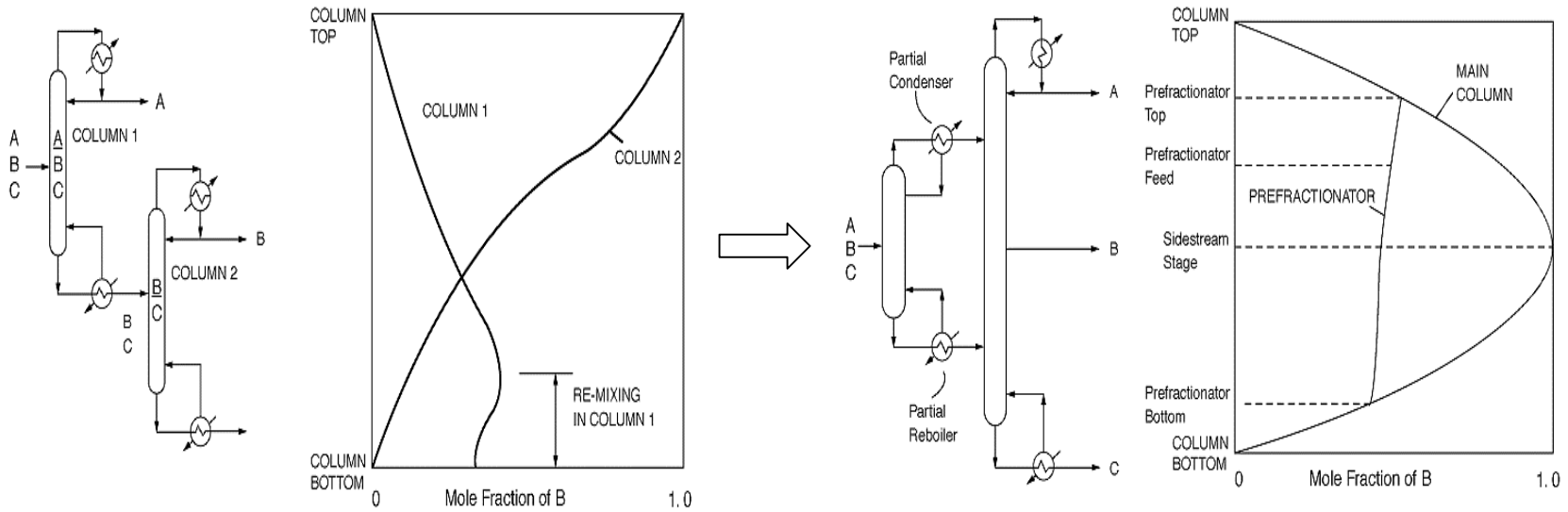
Distillation Sequences Using Multiple Products

- **Prefractionator arrangement requires 30% less energy**



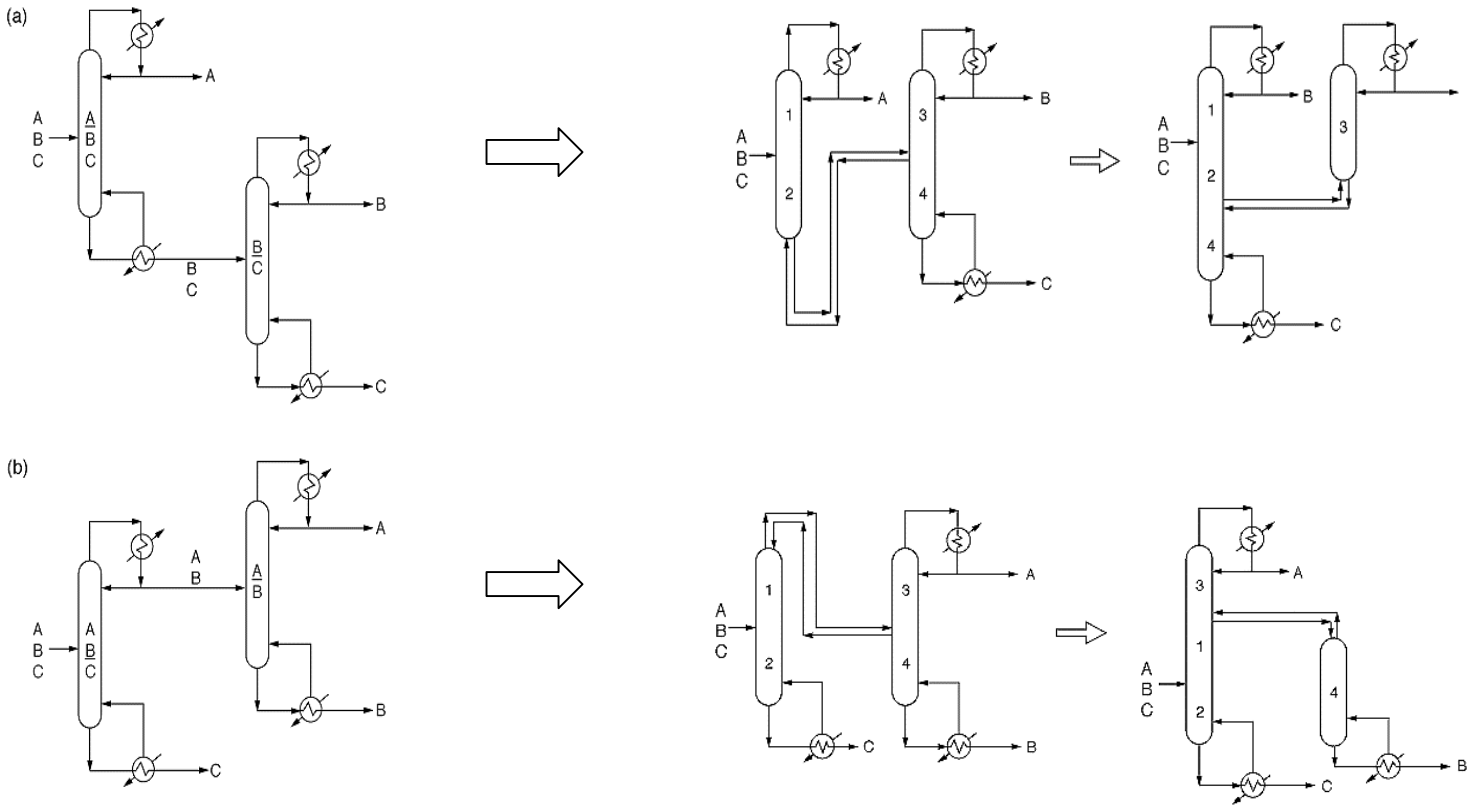
Distillation Sequences Using Multiple Products

- **Prefractionator arrangement avoids remixing**



Distillation Sequences Using Thermal Coupling

- **Reduced mixing losses reduce the energy consumption**



Distillation Sequences Using Thermal Coupling

- **Divided wall column gives**

No remixing

Reducing feed mismatch

Thermal efficiency benefit

Only one column

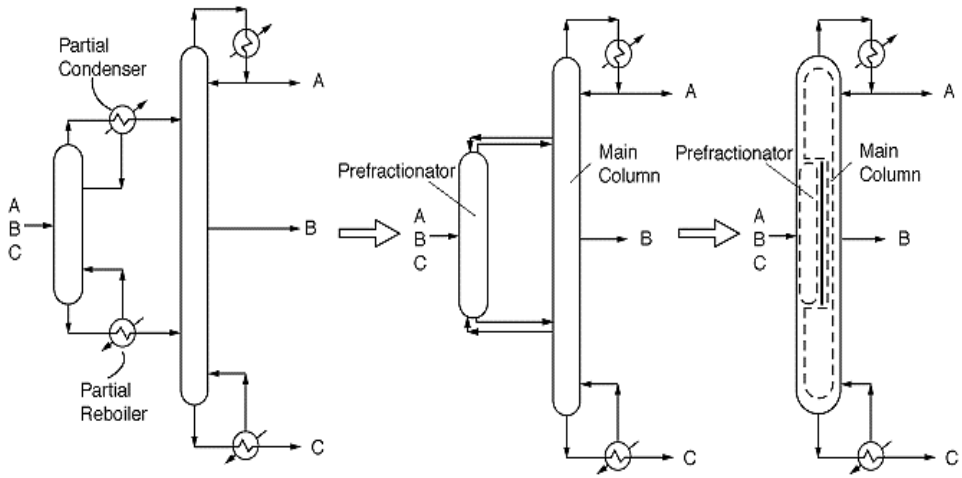
⇨

Reduced Energy

Capital Saving

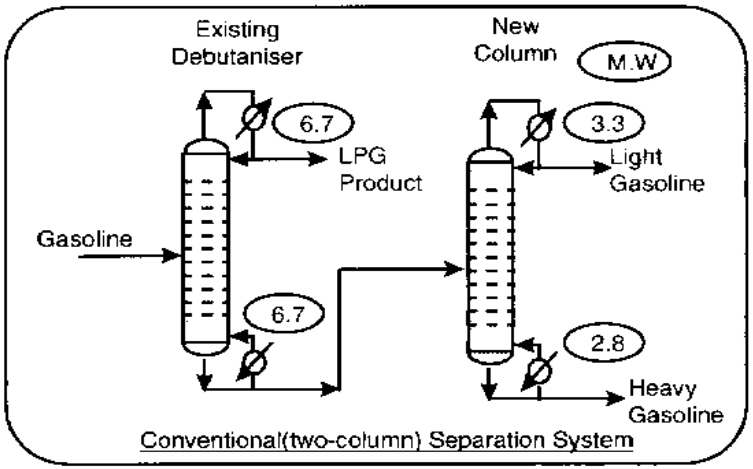
Improved Yield/Quality

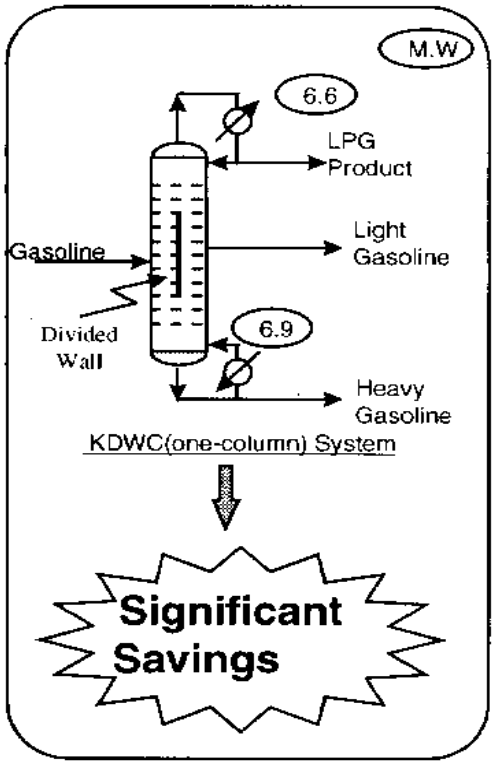
Smaller Plot Area



Distillation Sequences Using Thermal Coupling

Comparison between conventional two column system and KDWC





Utility Consumption

	Conventional Two Column (MW)	KDWC (MW)	SAVING (MW)	(%)
Condenser No.1	6.7	6.6		
Condenser No.2	3.3	–		
TOTAL:	10.0	6.6	3.4	34
Reboiler No.1	6.7	6.9		
Reboiler No.2	2.8	–		
TOTAL:	9.5	6.9	2.6	27

Distillation Sequencing - Summary

- Sequencing of simple columns are carried out by
  - considering constraints
  - identifying the best few nonintegrated sequences
  - then studying heat integration

- The best few nonintegrated sequences can be identified by
  - using the total vapor load as a criterion
  - using the shortcut techniques

- Once the complete design based on simple column is established, then thermally coupled arrangements can be evaluated in the context of the overall design.

Summary

- **Flowsheet recycle structure depends on**
  - → use of excess reactants, diluents, heat carriers in the reactor design
  - → unwanted byproduct formation
  - → range of volatilities of reactor effluent

- **Sequencing of simple columns are carried out**
  - → considering constraints
  - → identifying the best few nonintegrated sequences
  - → then studying heat integration