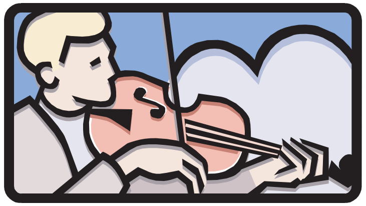
The Synthesis Step: From Ill-posed Problems to PFD



For every complicated problem, there is an answer that is short, simple and wrong

H.L. Mencken

Given: An ill-posed "word" problem

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This information is necessary for

- Feasibility analysis
- Detailed profitability analysis
- Generating P&IDs for construction

Basic Steps in Flowsheet Synthesis

- Gather information about the process chemistry

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Trace amounts of croton aldehyde are formed.

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Equilibrium considerations: Excess water will push the equilibrium towards ethanol.

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- Propylene has a vapor pressure of $15\ atm$ at $310K$.
  $=>$ expensive distillation

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- Estimate equipment size based on flow rates from previous step
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This procedure works for a large number of chemical, bio-chemical, environmental, and materials processes.

Step 1: Batch vs. Continuous Process

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When is continuous process preferred?

- Large quantity ($> 500\ tonnes/yr$)
- Well defined process
- Small variation in feed, product and operating conditions

Step 2: Input-Output Structure

Process Concept Diagram

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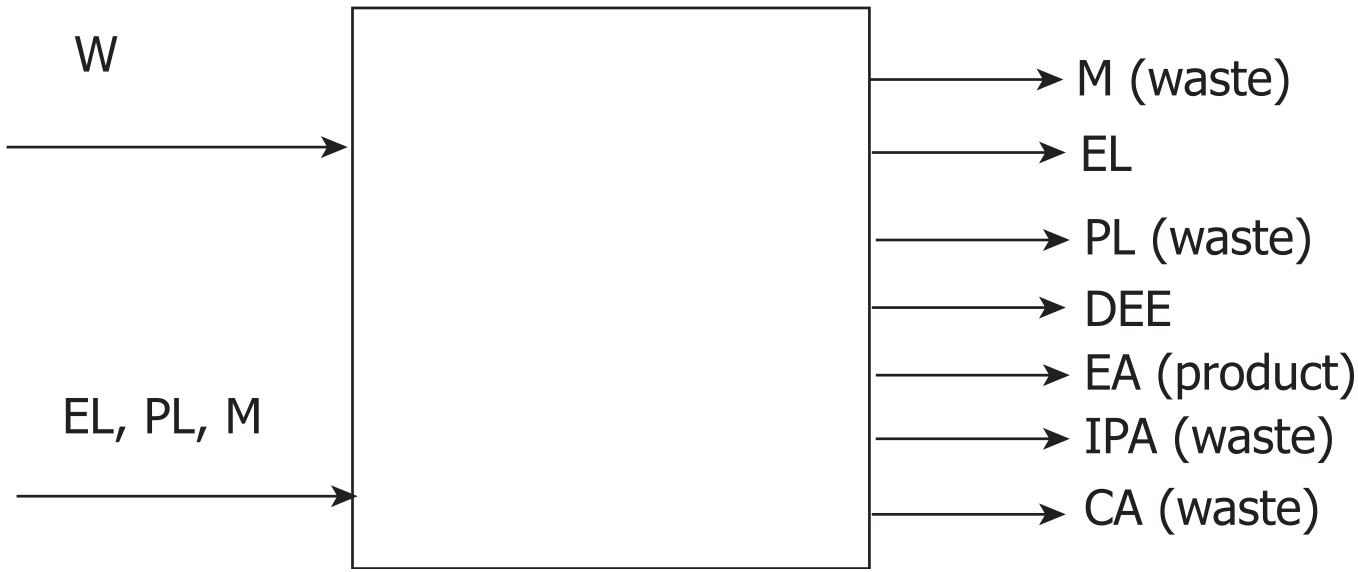
Process Concept Diagram



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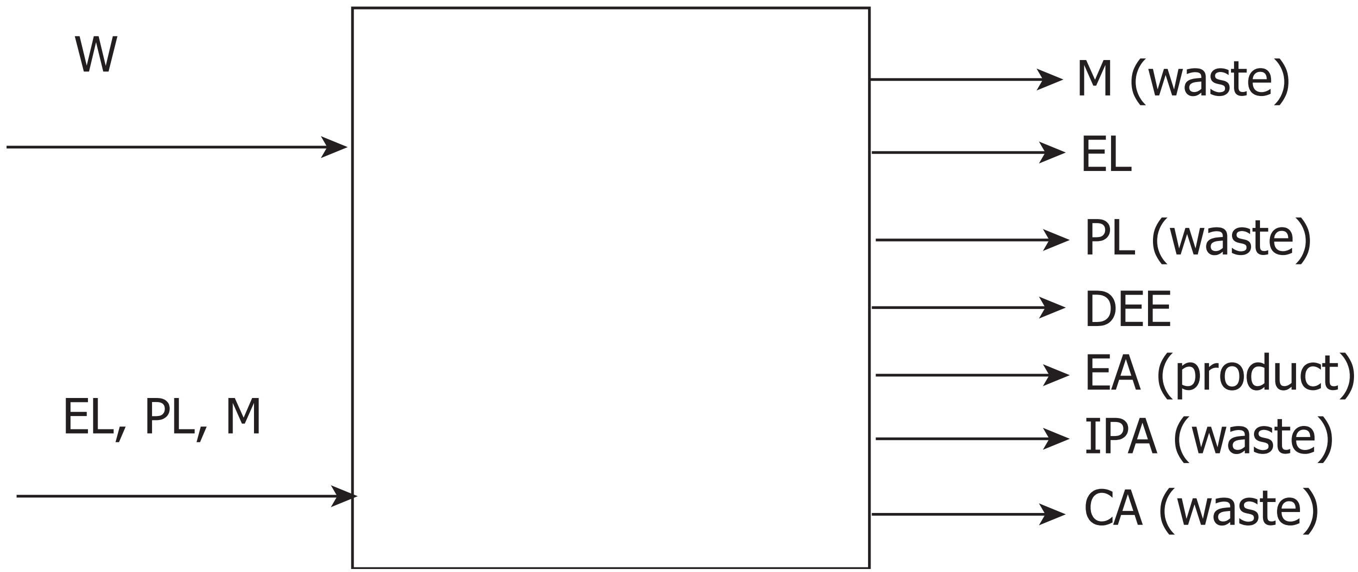
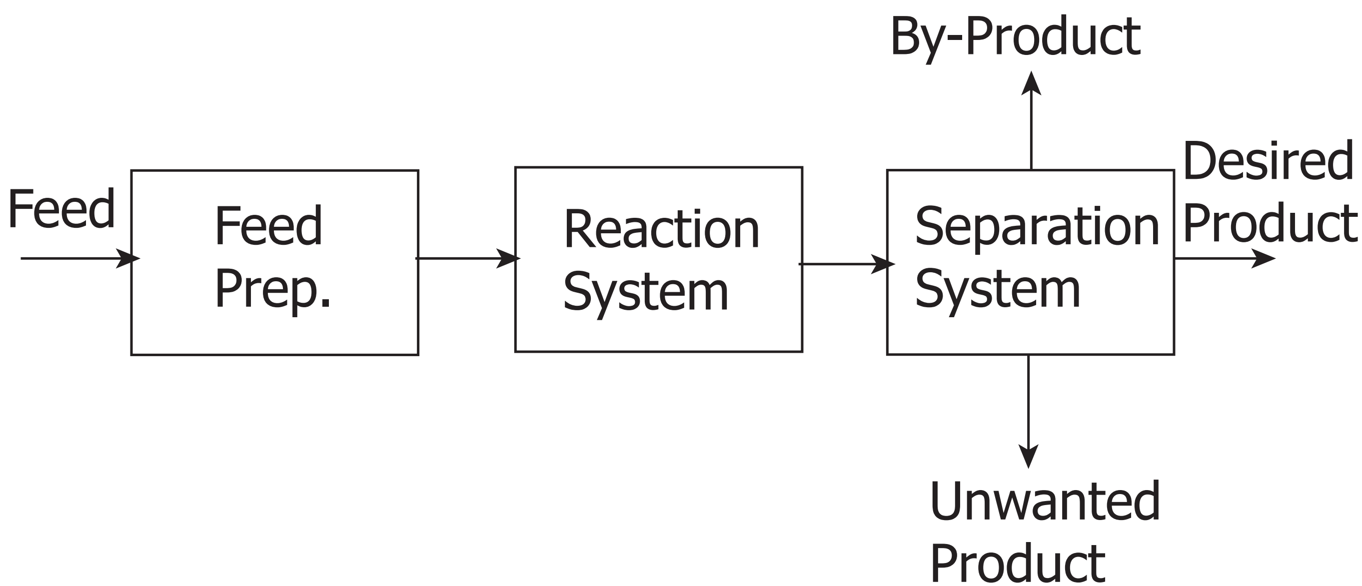


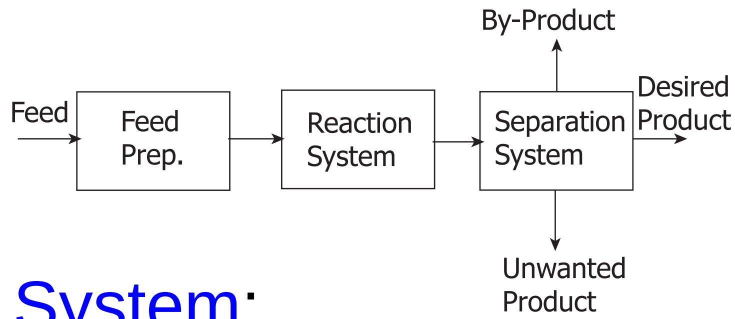
- Basic economic analysis on profit margin.
- What chemical components enter as feed and leave as product.
- All reactions, desired and undesired.

Generic Block Flow Diagram

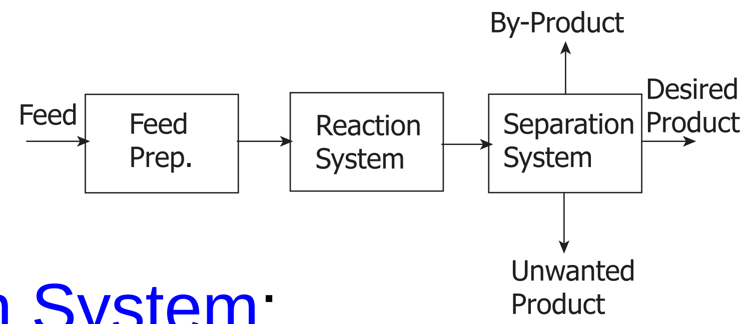
Generic Block Flow Diagram

A vast majority of processes can be represented by this generic BFD





Feed Preparation System:
This system is required to adjust T, P, and composition in preparation for the reactor.



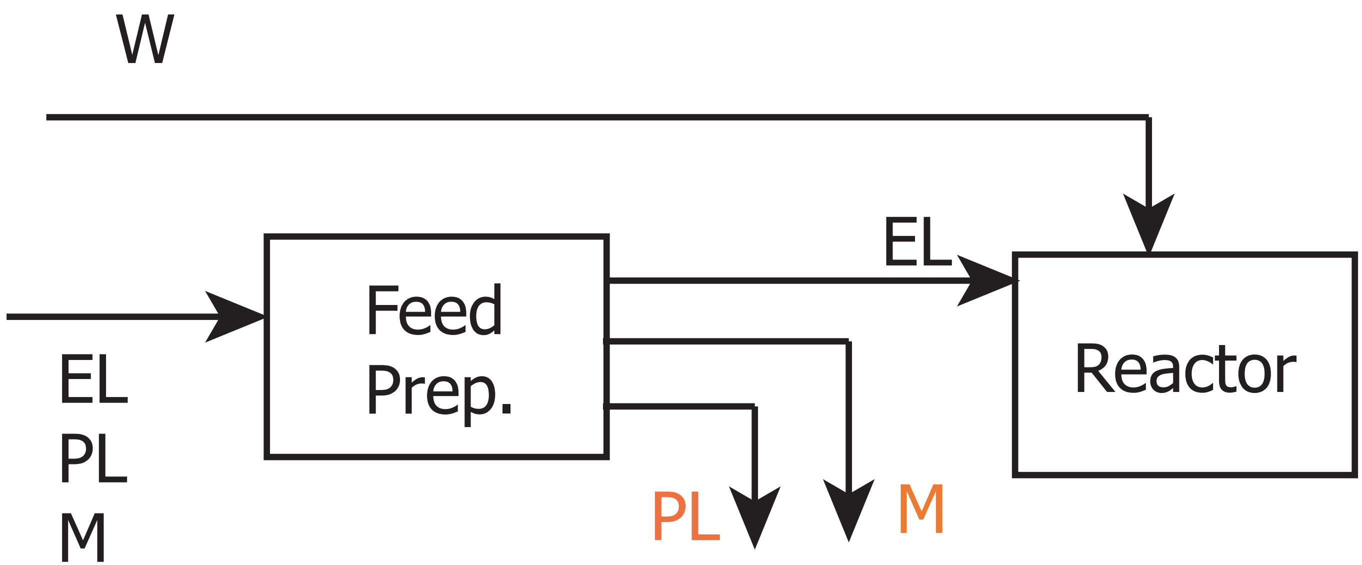
Feed Preparation System:

This system is required to adjust T, P, and composition in preparation for the reactor.

- If impurities are less than 10-20%, and these impurities do not react to form by-products, do not purify the feed.
- If separation of feed impurities is difficult (e.g. azeotropes are formed), do not purify the feed.
- If impurities foul the reactor catalyst or form hard-to-separate unwanted products, purify the feed.
- Add inert material to feed to control exothermic rxn.
- Add inert material to feed for favorable equilibrium rxn.

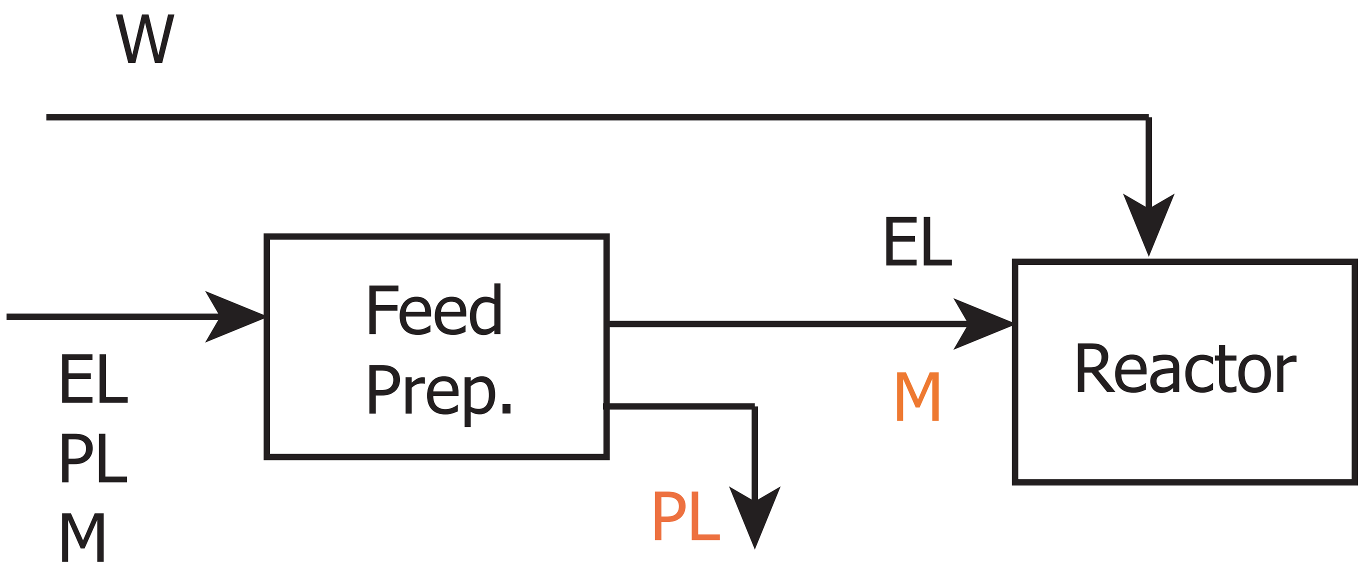
Case Study: Ethanol Synthesis

Alternative 1



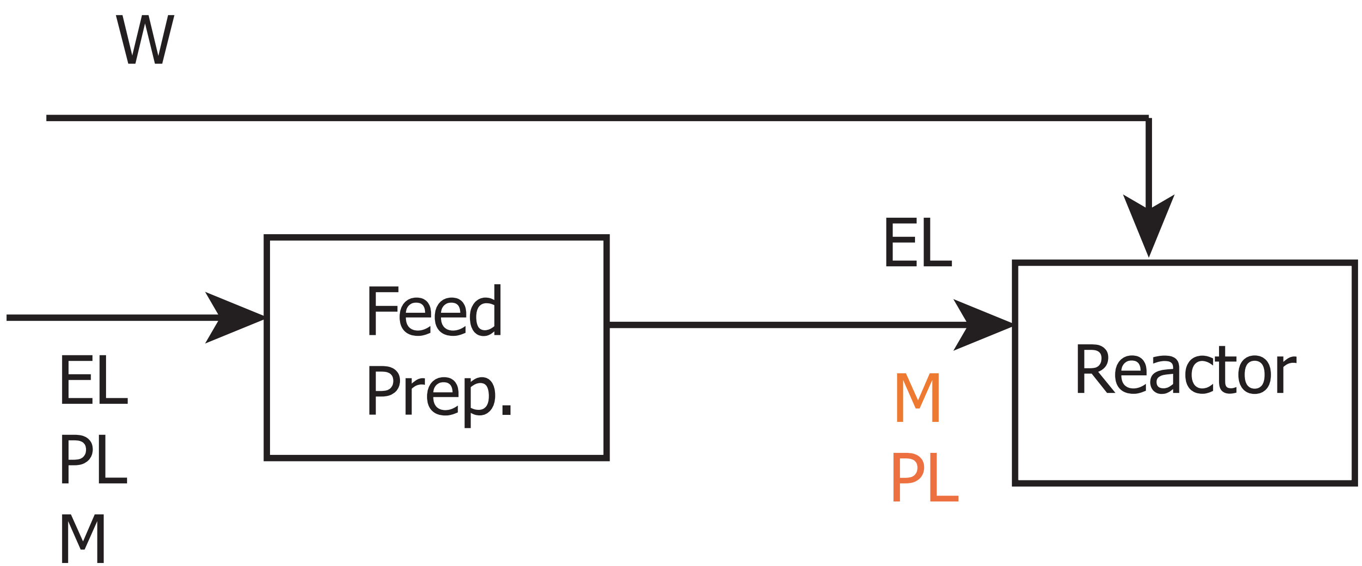
Case Study: Ethanol Synthesis

Alternative 2

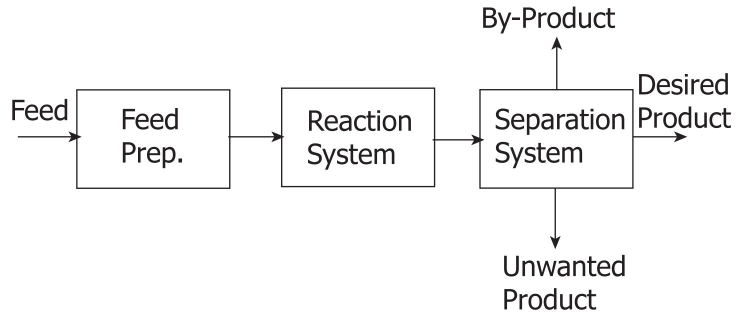


Case Study: Ethanol Synthesis

Alternative 3

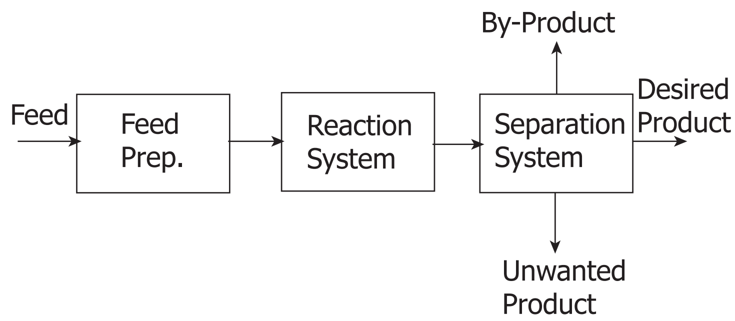


Which alternative would you choose?



Reaction System:

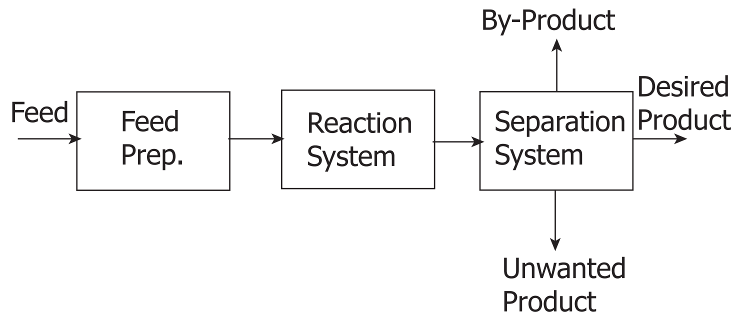
In this system, composition changes due to chemical reaction.



Reaction System:

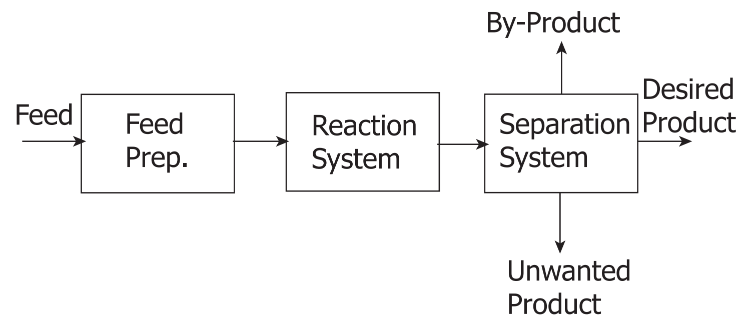
In this system, composition changes due to chemical reaction.

- Temperature and pressure ranges are set by reaction chemistry.
- Catalyst used is set by reaction chemistry.
- Reaction type (e.g. packed bed, fluidized bed, CSTR) are set by reactions occuring and reactor conditions (e.g. exothermic, endothermic)



Separation System:

In this system, the desired products are separated from by-products and unwanted products. The product stream may be further processed due to environmental, safety, or economic considerations.



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This system is analyzed in detail in Step 4

Step 3: Recycle Structure

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- Raw material costs form a significant portion of operating costs.
- Unused reactants are easy to separate.
- Reactants are environmentally unfriendly.

Three ways to recycle unused reactants

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- Recycle feed and product together and do not use purge stream.

Recycle in Ethanol Synthesis

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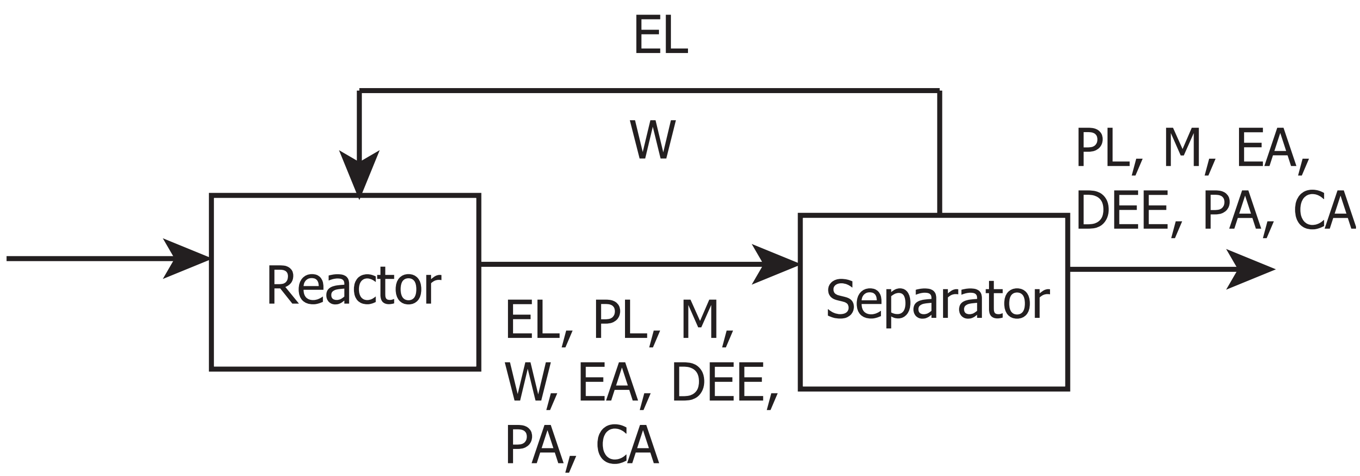

Recycle in Ethanol Synthesis

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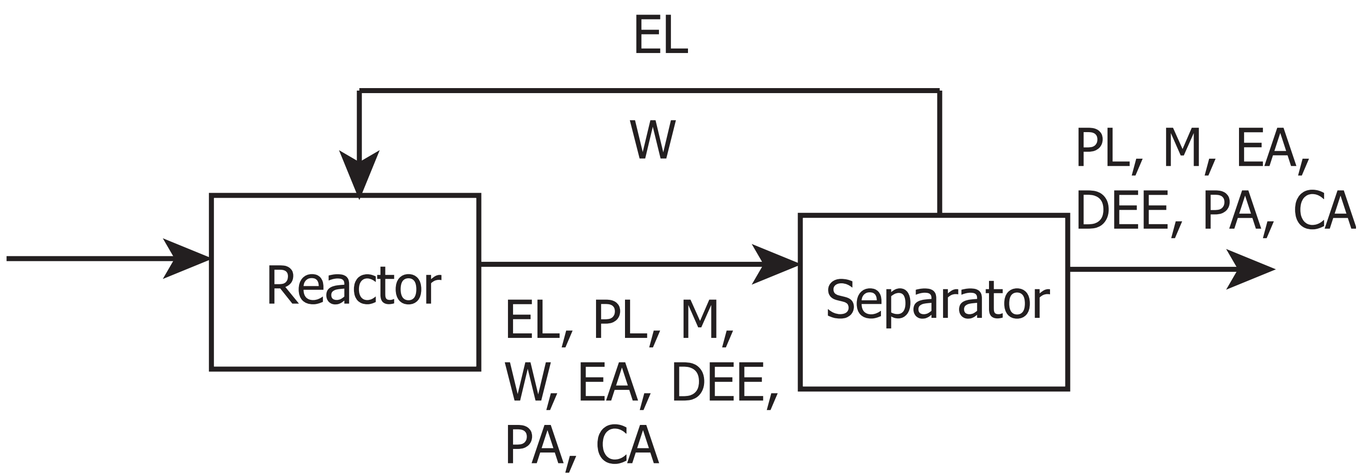
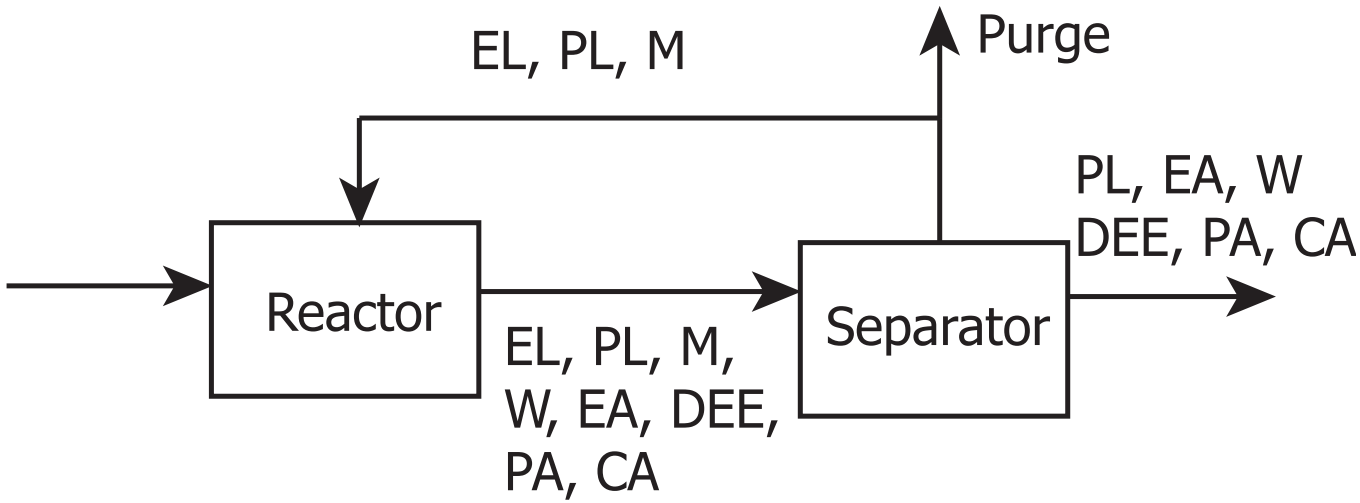


How to separate EL and W from the reactor outlet?

Recycle in Ethanol Synthesis

Recycle in Ethanol Synthesis

Alternative 2



Recycle in Ethanol Synthesis

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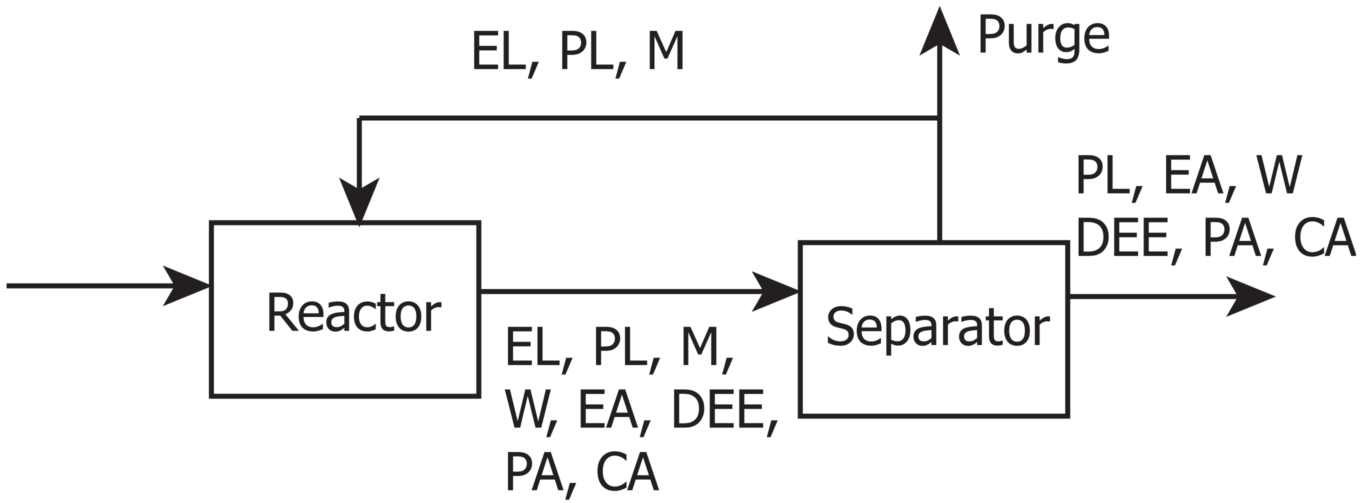
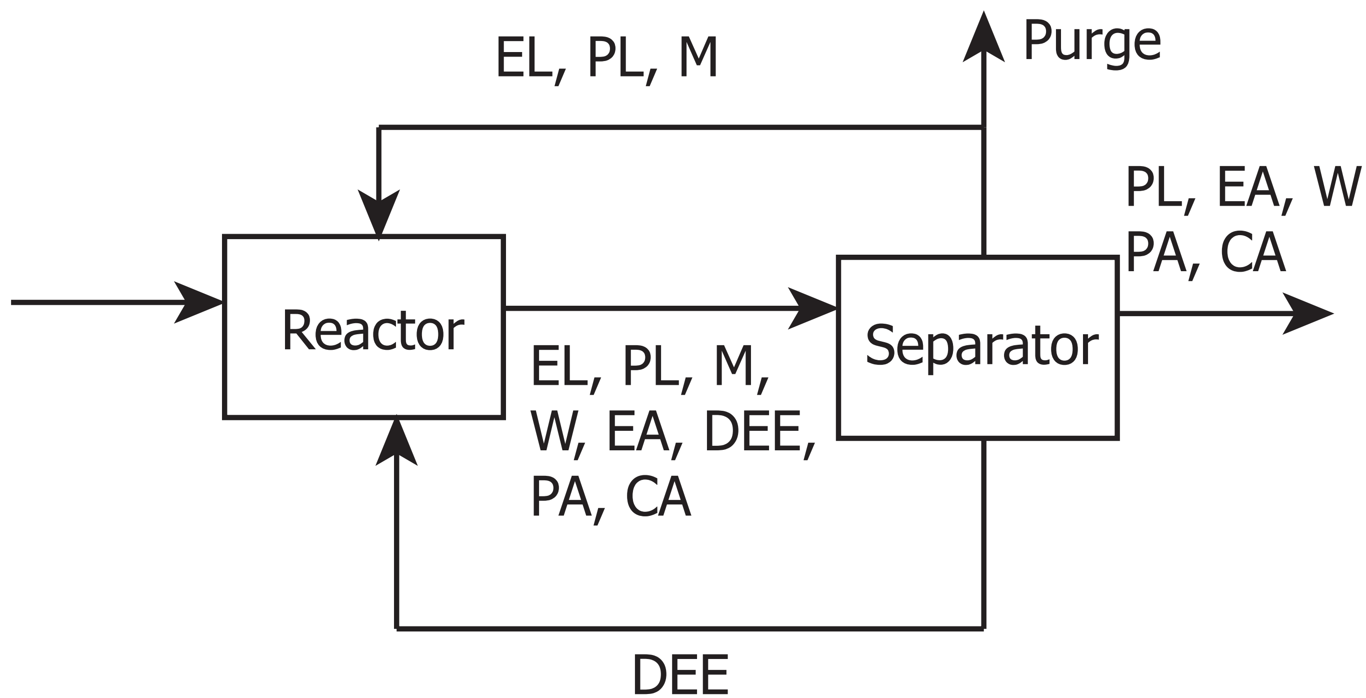


What should be the purge fraction?
What happens to the DEE reaction which is an equilibrium reaction?

Recycle in Ethanol Synthesis

Recycle in Ethanol Synthesis

Alternative 3



Recycle in Ethanol Synthesis

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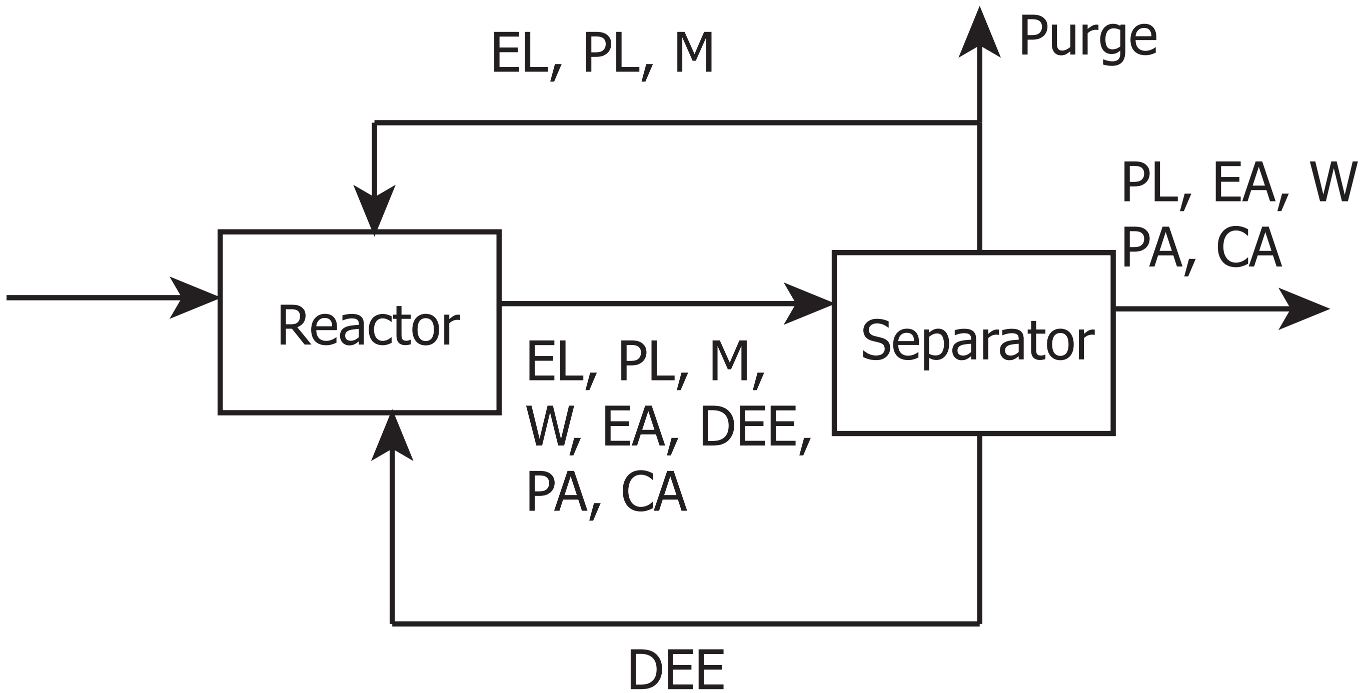

At steady state, DEE is at equilibrium and no reactant is consumed.

Step 4: Separation System Synthesis

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Flash

Distillation

Gas Absorption

Extraction

Step 4: Separation System Synthesis

Flash	Filtration
Distillation	Chromatography
Gas Absorption	Centrifugation
Extraction	Membrane Separation

Step 4: Separation System Synthesis

Flash	Filtration	Crystalization
Distillation	Chromatography	Drying
Gas Absorption	Centrifugation	.
Extraction	Membrane Separation	.

Guidelines for Choosing Separation Units

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Please see Table 10.1 (page 360, TBWS)

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Separation System for Ethanol Synthesis

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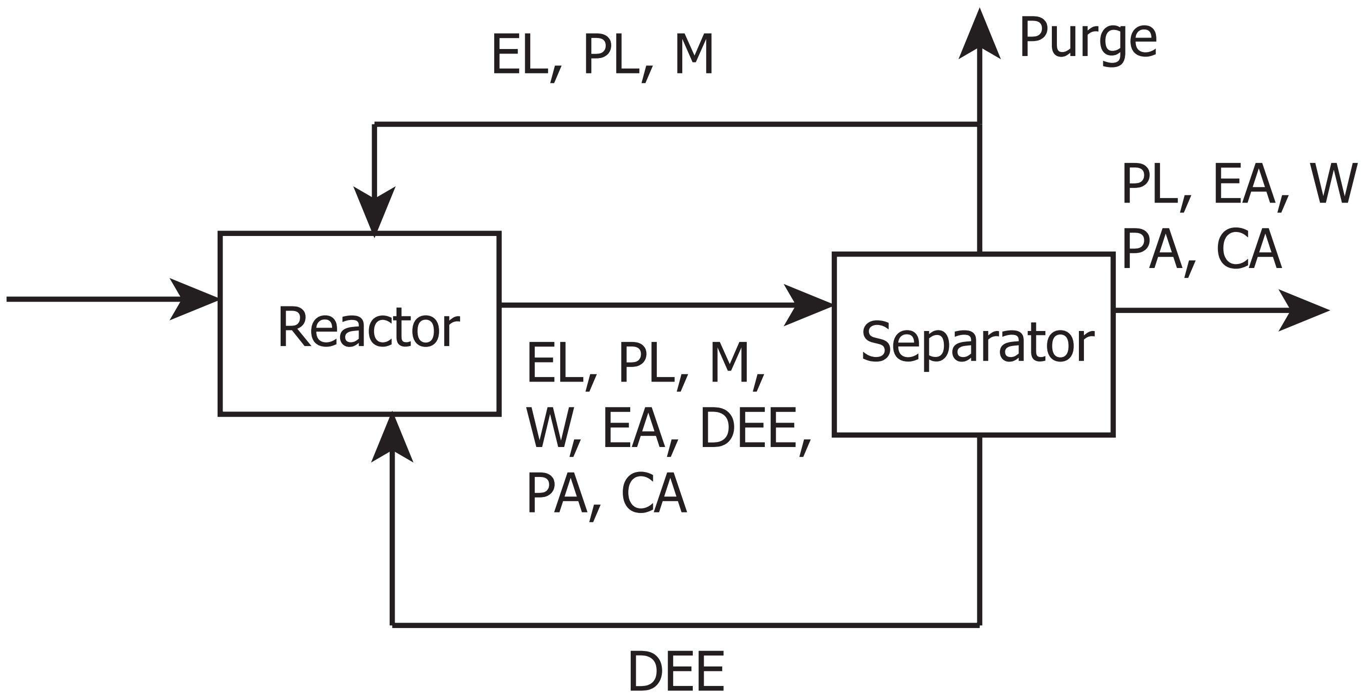

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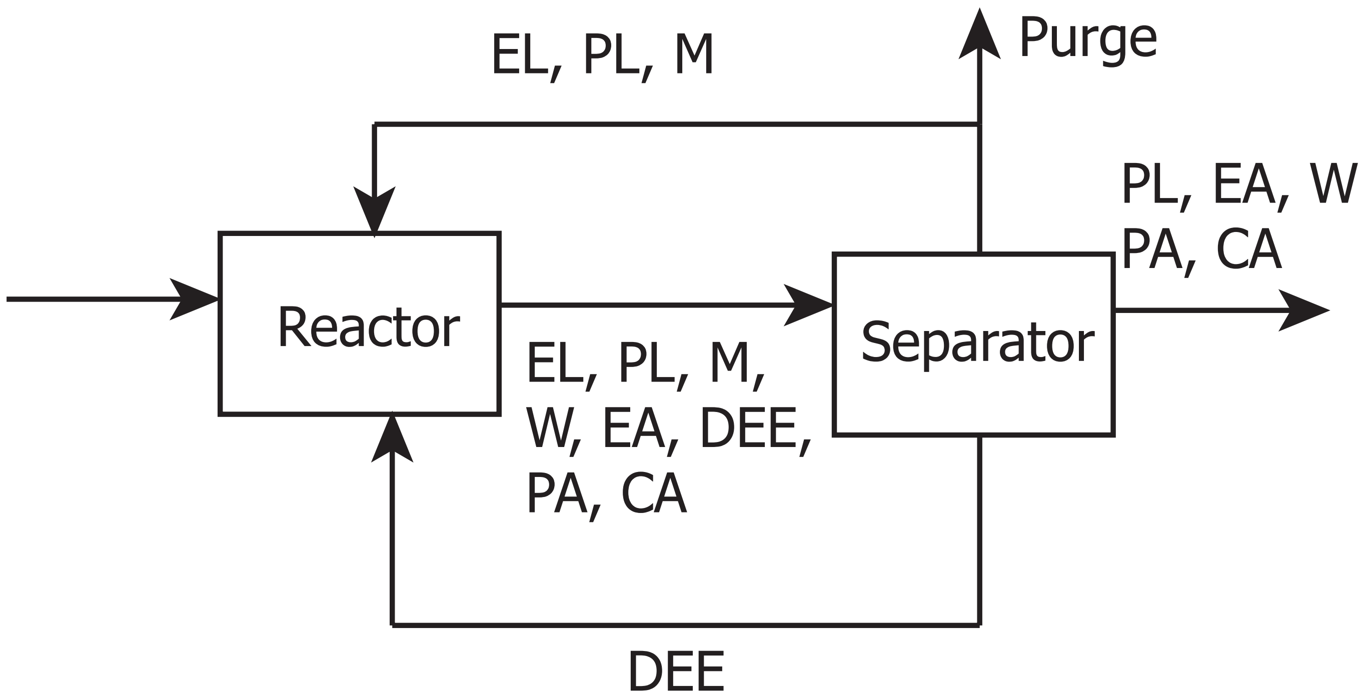
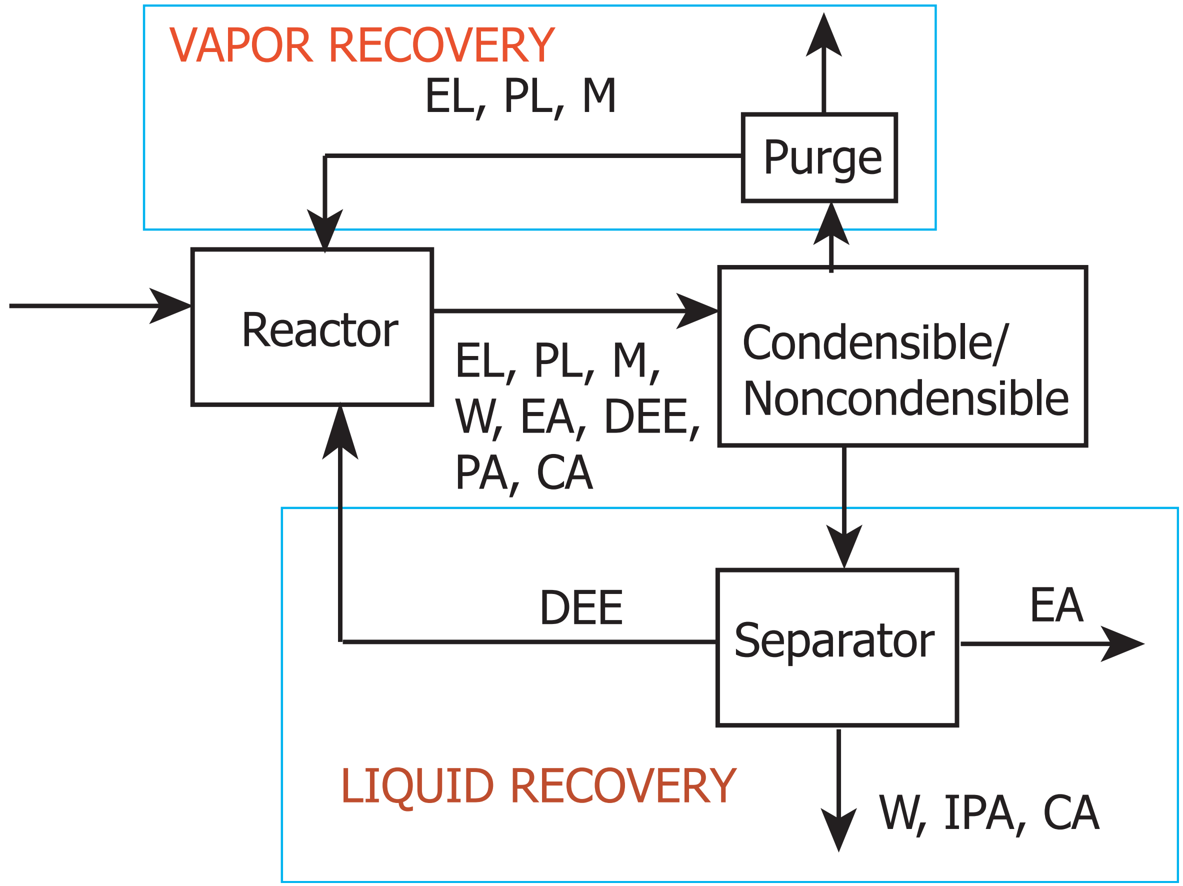
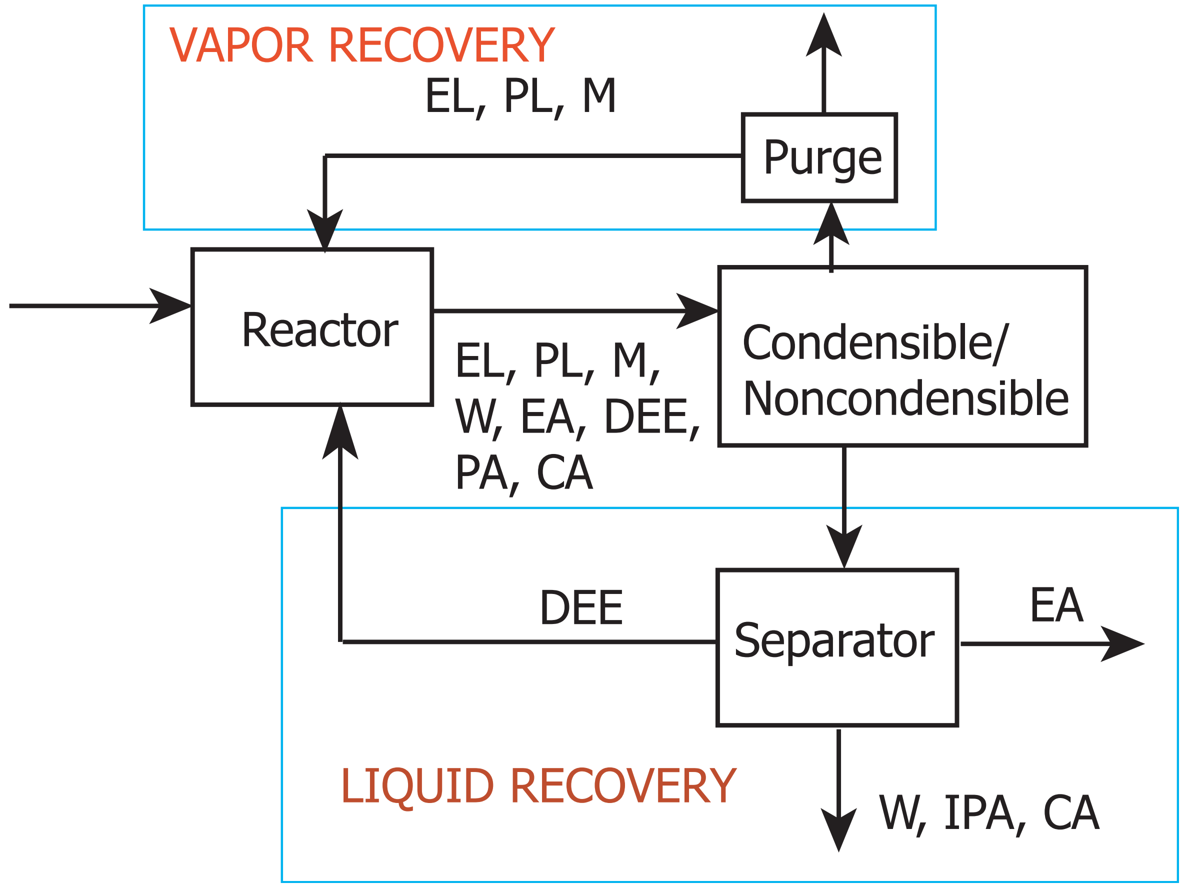


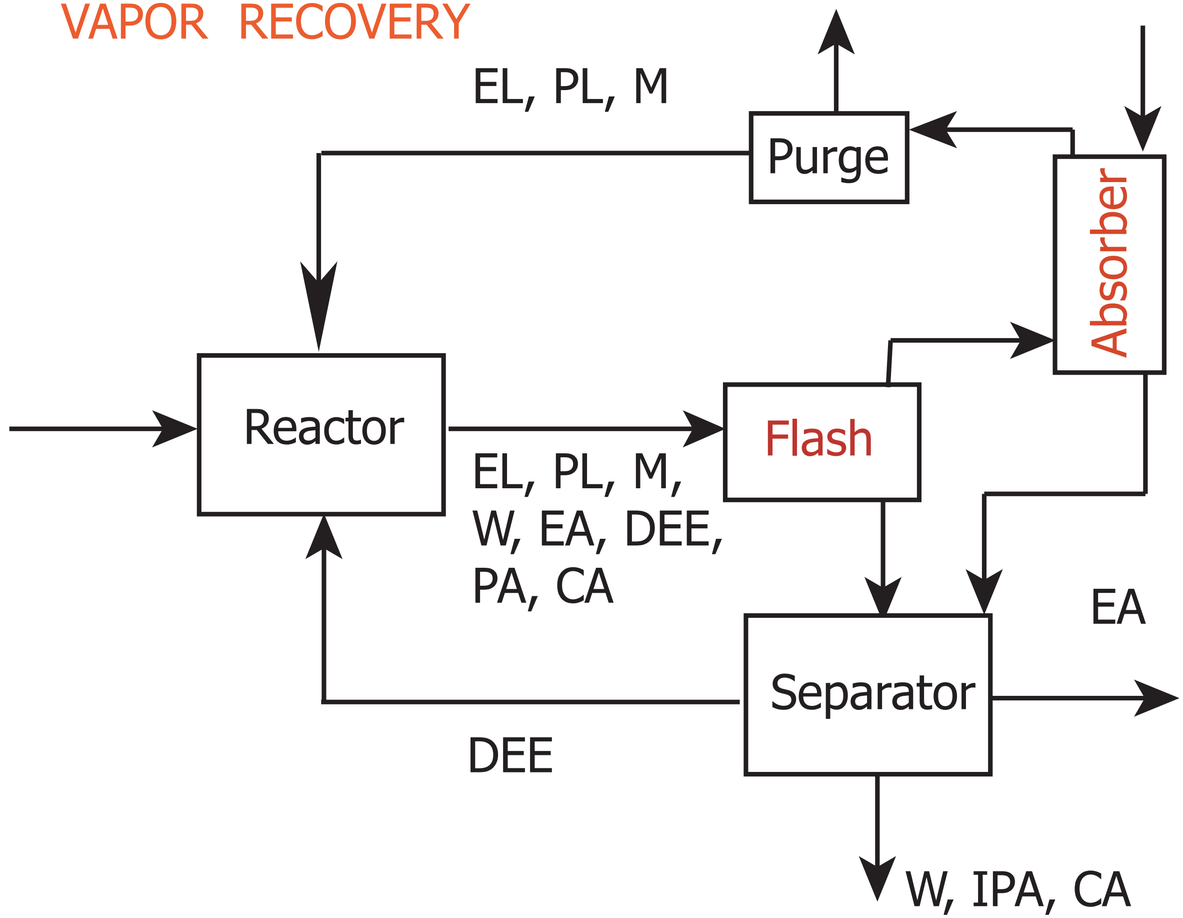
- Separate the reactor products into a liquid phase and vapor phase.
- Design vapor recovery system and liquid recovery system separately.

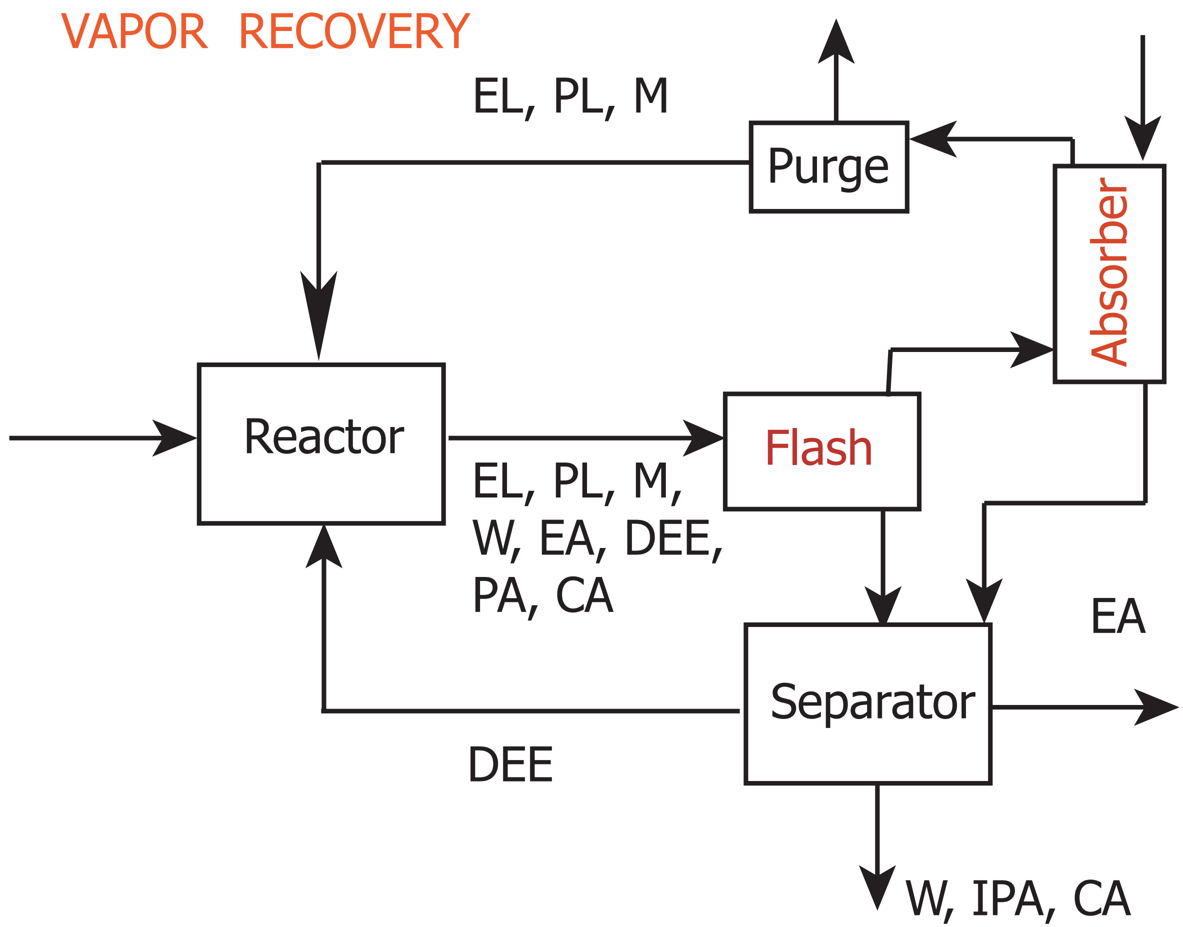

VAPOR RECOVERY
EL, PL, M
Purge
Reactor
Condensible/
Noncondensible
EL, PL, M,
W, EA, DEE,
PA, CA
DEE
Separator
EA
LIQUID RECOVERY
W, IPA, CA



- Flash the reactor products to get a vapor stream and liquid stream.
- The vapor stream is mainly EL, PL, and M and is recycled back.
- Some EL will leave in the vapor stream which can be recovered via an absorber.

VAPOR RECOVERY





- Increasing the purge stream results in loss of reactants but reduces the amount of methane going into the reactor (M has to less than 10% to prevent coking).
- The liquid recovery system is designed as a series of distillation columns.

Final Design

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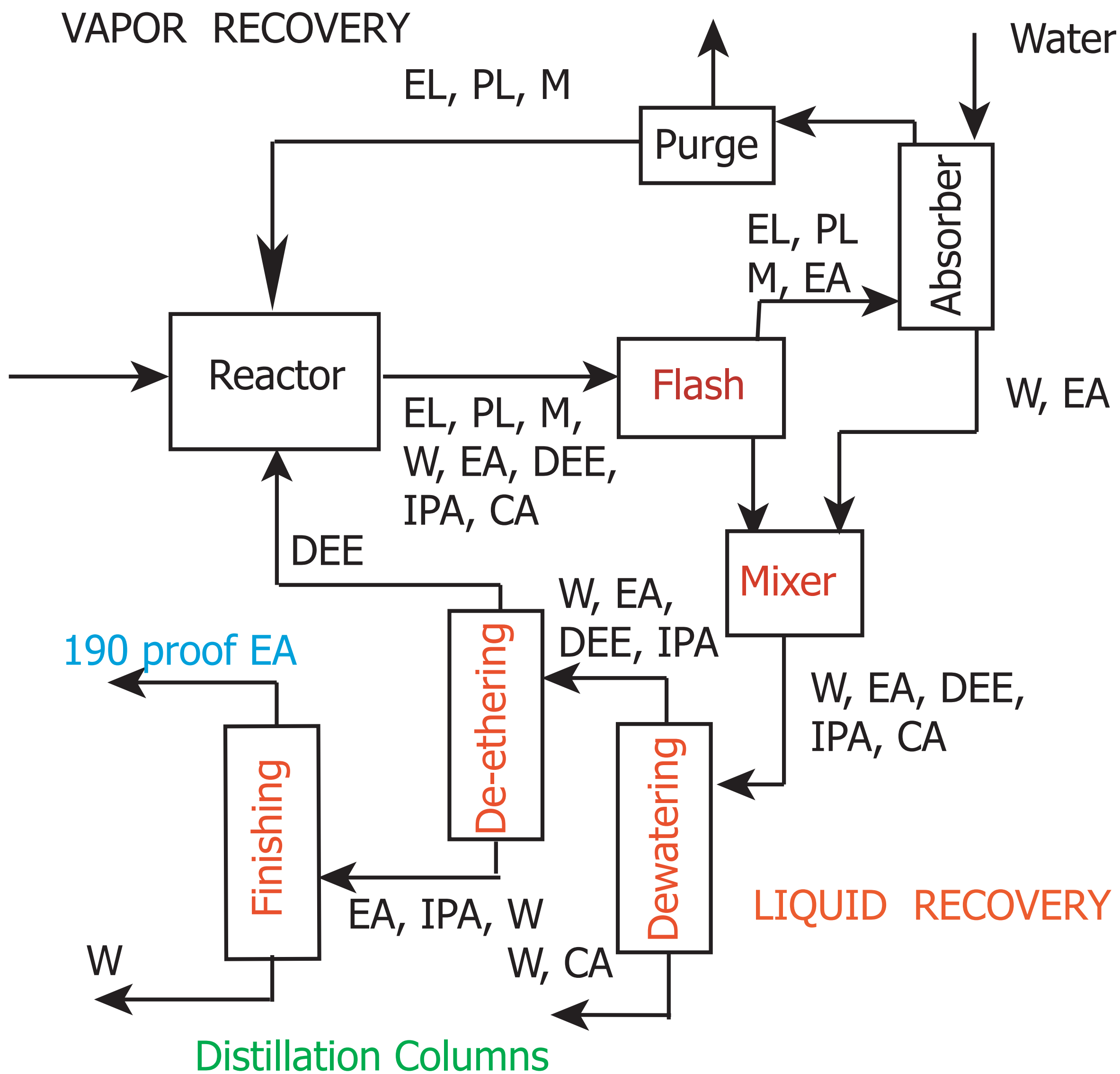

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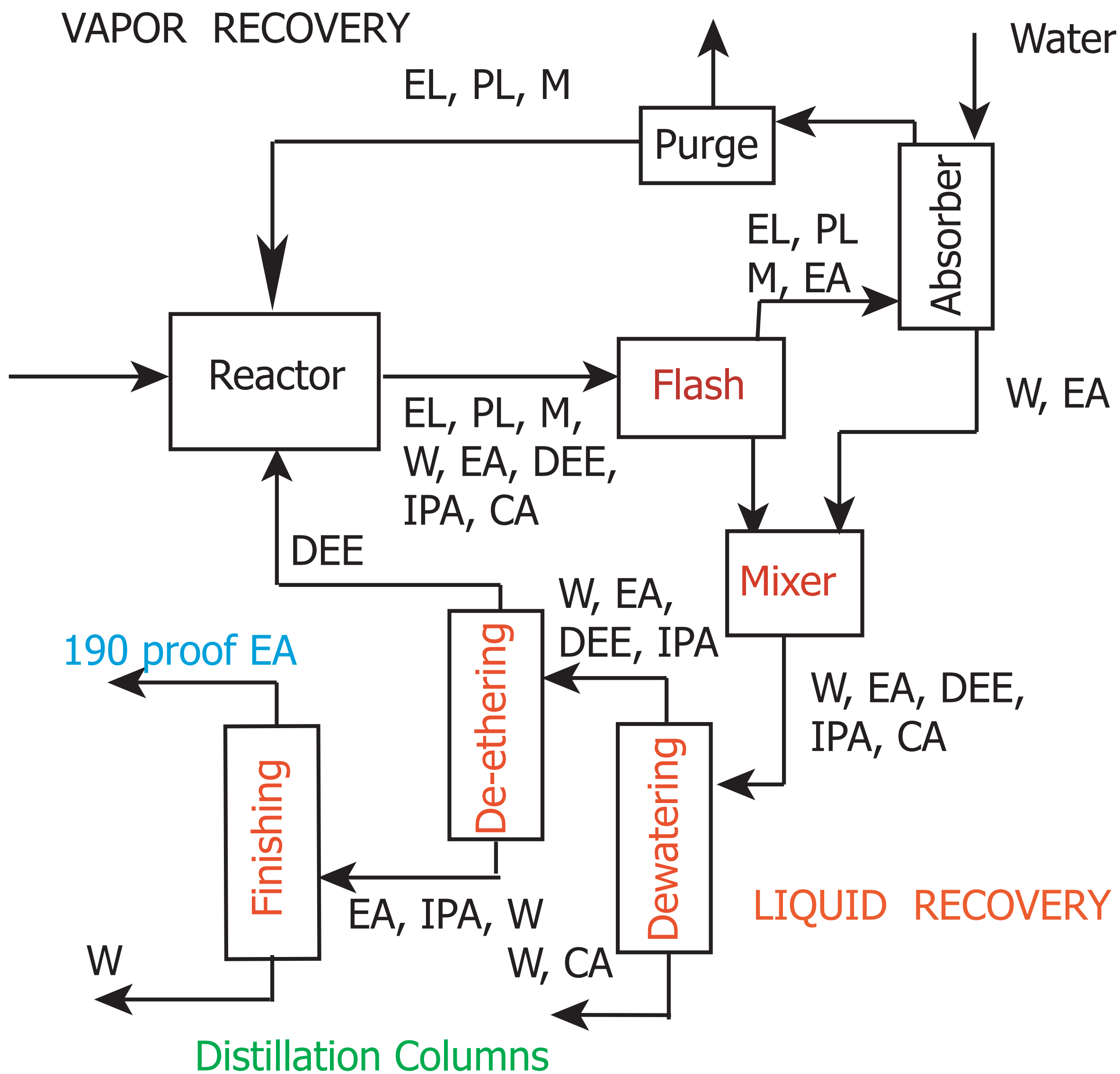

- Distillation is carried out in order of decreasing volatility of species.

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Which option to use depends on process economics.

Basic Steps in Flowsheet Synthesis

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- ✓Generate flow diagram based on Douglas Hierarchy
- Solve mass and energy balances
- Estimate equipment size based on flow rates from previous step
- Estimate equipment cost based on size from previous step
- Optimize process