

Chapter 2

2.1 The five elements of the Hierarchy of Process Design are:

- a. Batch or continuous process
- b. Input – output structure of process
- c. Recycle structure of process
- d. General separation structure of process
- e. Heat-exchanger network/process energy recovery

2.2

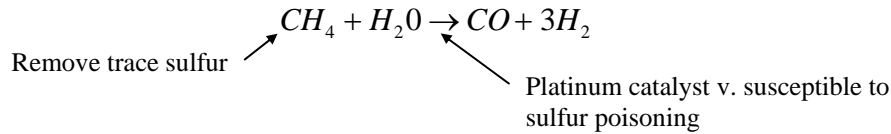
- a. Separate/purify unreacted feed and recycle – use when separation is feasible.
- b. Recycle without separation but with purge – when separation of unused reactants is infeasible/uneconomic. Purge is needed to stop build up of product or inerts.
- c. Recycle without separation or purge – product/byproduct must react further through equilibrium reaction.

2.3 Batch preferred over continuous when: small quantities required, batch-to-batch accountabilities required, seasonal demand for product or feed stock availability, need to produce multiple products using the same equipment, very slow reactions, and high equipment fouling.

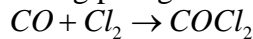
2.4 One example is the addition of steam to a catalytic reaction using hydrocarbon feeds. Examples are given in Appendix B (styrene, acrylic acid.) In the styrene process, superheated steam is added to provide energy for the desired endothermic reaction and to force the equilibrium towards styrene product. In the acrylic acid example, steam is added to the feed of propylene and air to act as thermal ballast (absorb the heat of reaction and regulate the temperature), and it also serves as an anti-coking agent – preventing coking reactions that deactivate the catalyst.

2.5 Reasons for purifying a feed material prior to feeding it to a process include:

- a. If impurity foul or poison a catalyst used in the process.
 e.g. Remove trace sulfur compounds in natural gas prior to sending to the steam reforming reactor to produce hydrogen.

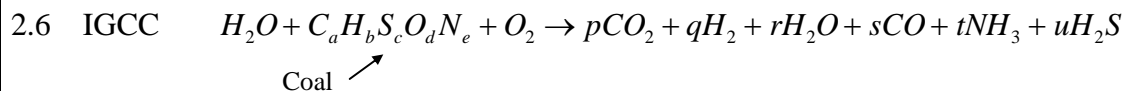


- b. If impurities react to form difficult-to-separate or hazardous products/byproducts.
 e.g. Production of isocyanates using phosgene. Production of phosgene is



The carbon monoxide is formed via steam reforming of CH_4 to give $\text{CO} + \text{H}_2$. H_2 must be removed from CO prior to reaction with Cl_2 to form HCl , which is highly corrosive and causes many problems in the downstream processes.

- c. If the impurity is present in large quantities then it may be better to remove the impurity rather than having to size all the down stream equipment to handle the large flow of inert material.
 e.g. One example is using oxygen rather than air to fire a combustion or gasification processes. Removing nitrogen reduces equipment size and makes the removal of CO_2 and H_2S much easier because these species are more concentrated.



In modern IGCC plants, coal is partially oxidized (gasified) to produce synthesis gas $\text{CO} + \text{H}_2$ and other compounds. Prior to combusting the synthesis gas in a turbine, it must be "cleaned" or H_2S and CO_2 (if carbon capture is to be employed.) Both H_2S and CO_2 are acid gases that are removed by one of a variety of physical or chemical absorption schemes. By removing nitrogen from the air, the raw synthesis gas stream is much smaller making the acid gas removal much easier. In fact, when CO_2 removal is required IGCC is the preferred technology, i.e. the cheapest.

2.7 Ethylbenzene Process

- a. Single pass conversion of benzene

$$\text{Benzene in reactor feed (stream 3)} = 226.51 \frac{\text{kmol}}{\text{h}}$$

$$\text{Benzene in reactor effluent (stream 14)} = 177.85 \frac{\text{kmol}}{\text{h}}$$

$$X_{sp} = 1 - \frac{177.85 \frac{\text{kmol}}{\text{h}}}{226.51 \frac{\text{kmol}}{\text{h}}} = 21.5\%$$

- b. Single pass conversion of ethylene

$$\text{Ethylene in reactor feed (stream 2)} = 93.0 \frac{\text{kmol}}{\text{h}}$$

$$\text{Ethylene in reactor effluent (stream 14)} = 0.54 \frac{\text{kmol}}{\text{h}}$$

$$X_{sp} = 1 - \frac{0.54 \frac{\text{kmol}}{\text{h}}}{93.0 \frac{\text{kmol}}{\text{h}}} = 99.4\%$$

- c. Overall conversion of benzene

$$\text{Benzene entering process (stream 1)} = 97.0 \frac{\text{kmol}}{\text{h}}$$

$$\text{Benzene leaving process (stream 15 and 19)} = 8.38 + 0.17 \frac{\text{kmol}}{\text{h}}$$

$$X_{ov} = 1 - \frac{8.55 \frac{\text{kmol}}{\text{h}}}{97.0 \frac{\text{kmol}}{\text{h}}} = 91.2\%$$

- d. Overall conversion of ethylene

$$\text{Ethylene entering process (stream 2)} = 93.0 \frac{\text{kmol}}{\text{h}}$$

$$\text{Ethylene leaving process (stream 15 and 19)} = 0.54 + 0 \frac{\text{kmol}}{\text{h}}$$

$$X_{ov} = 1 - \frac{0.54 \frac{\text{kmol}}{\text{h}}}{93.0 \frac{\text{kmol}}{\text{h}}} = 99.4\%$$

2.8 Separation of G from reactor effluent may or may not be difficult. (a) If G reacts to form a heavier (higher molecular weight) compound then separation may be relatively easy using a flash absorber or distillation and recycle can be achieved easily. (b) If process is to be viable then G must be separable from the product. If inerts enter with G or gaseous by-products are formed then separation of G may not be possible but recycling with a purge should be tried. In either case the statement is not true.

2.9 Pharmaceutical products are manufactured using batch process because:

- they are usually required in small quantities
- batch-to-batch accountability and tracking are required by the Food & Drug Administration (FDA)
- usually standardized equipment is used for many pharmaceutical products and campaigns are run to produce each product – this lends itself to batch operation.

2.10 a. Single pass conversion of ethylbenzene

$$\text{Ethylbenzene in reactor feed (stream 9)} = 512.7 \frac{\text{kmol}}{\text{h}}$$

$$\text{Ethylbenzene in reactor effluent (stream 12)} = 336.36 \frac{\text{kmol}}{\text{h}}$$

$$\text{Single pass conversion} = 1 - \frac{336.36 \frac{\text{kmol}}{\text{h}}}{512.7 \frac{\text{kmol}}{\text{h}}} = 34.4\%$$

b. Overall conversion of ethylbenzene

$$\text{Ethylbenzene entering process (stream 1)} = 180 \frac{\text{kmol}}{\text{h}}$$

$$\text{Ethylbenzene leaving process (stream 19, 26, 27 \& 28)} = 3.36 + 0.34 = 3.70 \frac{\text{kmol}}{\text{h}}$$

$$\text{Overall conversion} = 1 - \frac{3.70 \frac{\text{kmol}}{\text{h}}}{180 \frac{\text{kmol}}{\text{h}}} = 97.9\%$$

c. Yield of styrene

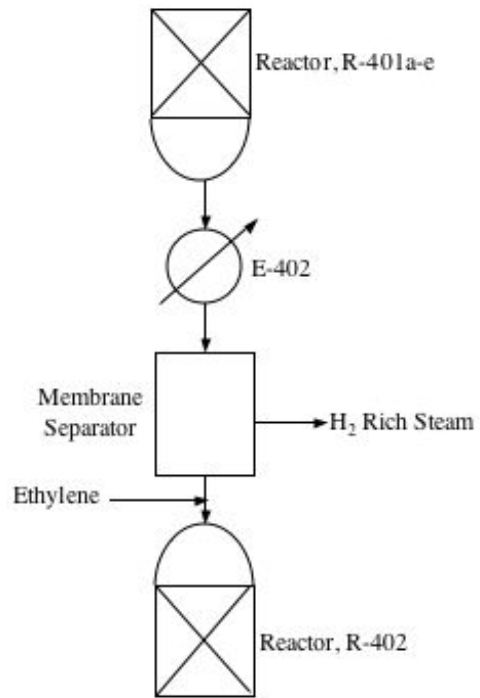
$$\text{Moles of ethylbenzene required to produce styrene} = 119.3 \frac{\text{kmol}}{\text{h}}$$

$$\text{Moles of ethylbenzene fed to process (stream 1)} = 180 \frac{\text{kmol}}{\text{h}}$$

$$\text{Yield} = \frac{119.3 \frac{\text{kmol}}{\text{h}}}{180 \frac{\text{kmol}}{\text{h}}} = 66.3\%$$

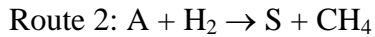
Possible strategies to increase the yield of styrene are

- (i) Increase steam content of reactor feed – this pushes the desired equilibrium reaction to the right.
- (ii) Increasing the temperature also pushes the equilibrium to right but increases benzene and toluene production.
- (iii) Remove hydrogen in effluent from each reactor – this will push the equilibrium of the desired reaction to the right and reduce the production of toluene from the third reaction – use a membrane separator, shown on following page.



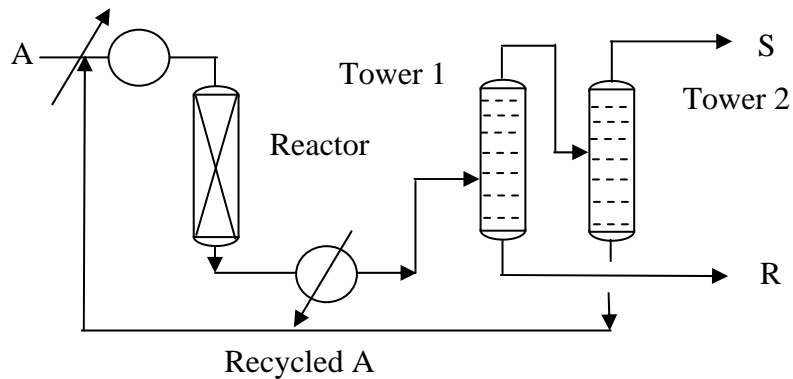
2.11 Route 1: $2A \rightarrow S + R$

Key features are that no light components (non-condensables) are formed and only one reactant is used. Therefore, separation of A, R, and S can take place using distillation columns.

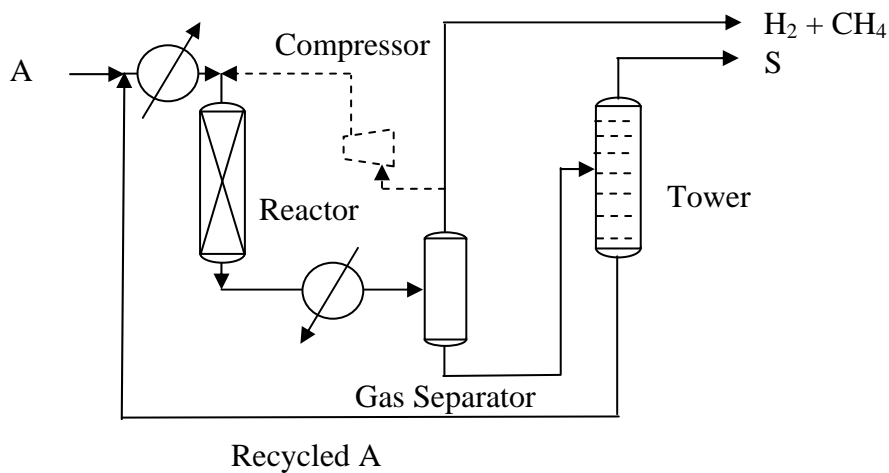


Unlike Route 1, this process route requires separation of the non-condensables from A and S. If hydrogen is used in great excess (as with the toluene HDA process), then a recycle and purge of the light gas stream will be required. Otherwise, if hydrogen conversion is high, the unreacted hydrogen along with the methane may be vented directly to fuel gas.

Route 1 – PFD sketch



Route 2 – PFD sketch – gas recycle shown dotted since it is only needed if H_2 is used in (considerable) excess and must be recycled.

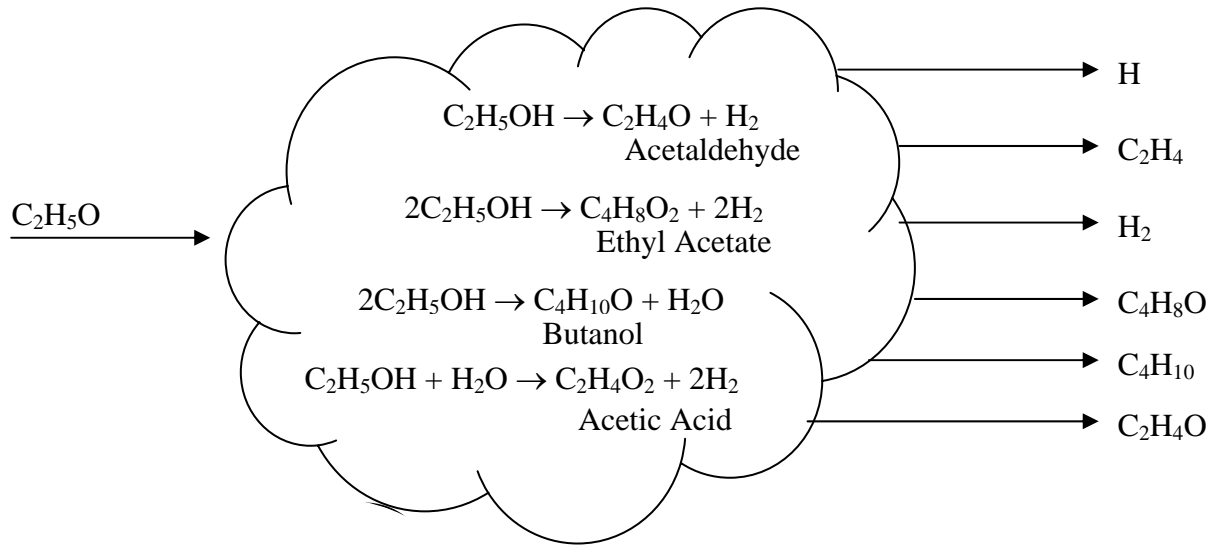


Route 1 is better since:

- Simpler PFD
- No gas recycle (no recycle compressor)
- No build up of inerts (CH_4) so recycle stream is not as large
- All products are valuable – fuel gas in Route 2 has a low value

- 2.12
- a. Good when product(s) and reactant(s) are easily separated and purified (most often by distillation.) Any inerts in the feed or byproducts can be removed by some unit operation and thus recycle does not require a purge.
 - b. When unused reactant(s) and product(s) are not easily separated (for example when both are low boiling point gases) and single pass conversion of reactant is low.
 - c. This is only possible when no significant inerts are present and any byproducts formed will react further or can reach equilibrium.

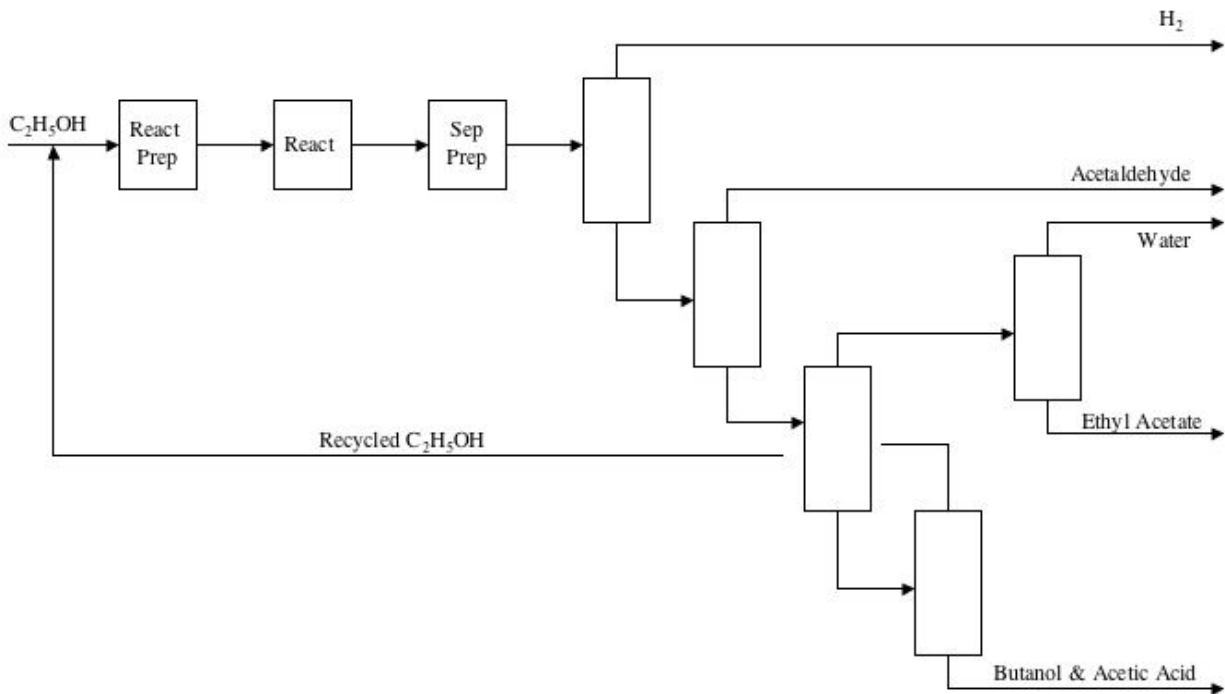
2.13 a.



Order of volatility is acetaldehyde, water, ethyl acetate, ethanol, isobutanol, acetic acid.

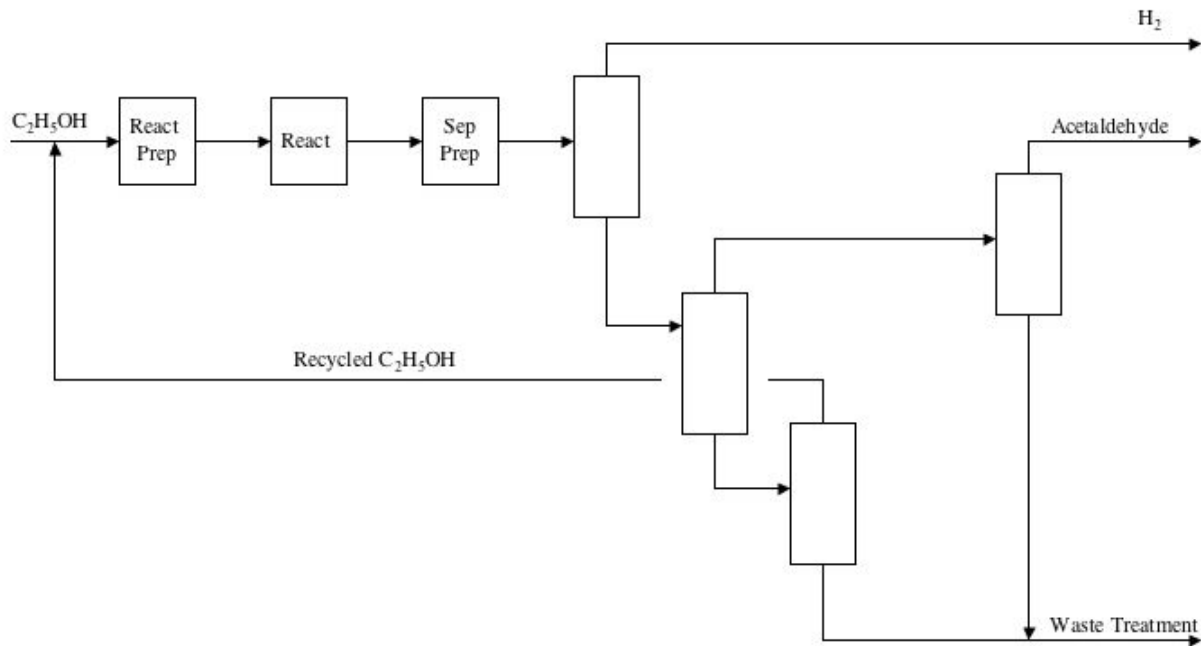
b.

Alternative 1



Alternative 1 assumes butanol and acetic acid can be sold as a mixed product \Rightarrow very unlikely so probably have to add another column to separate.

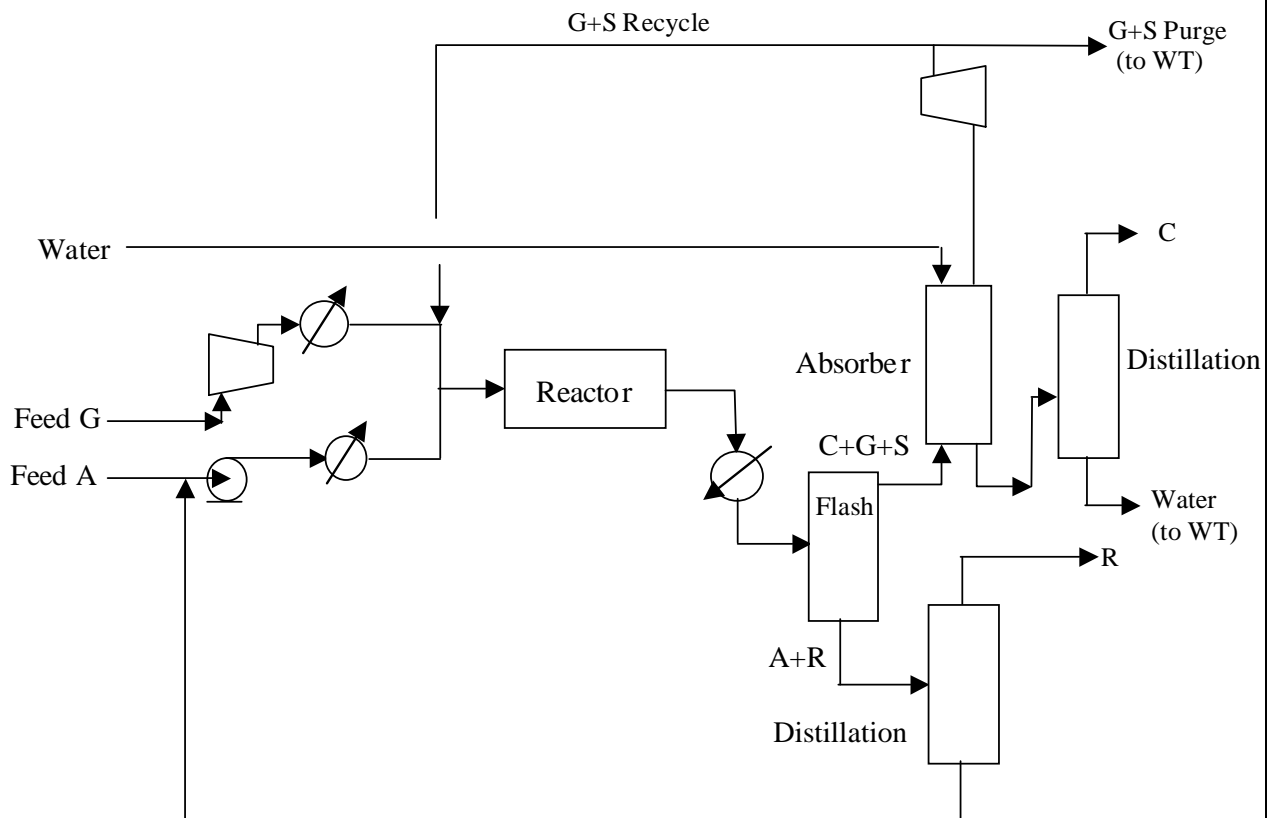
Alternative 2



This alternative recycles C_2H_5OH and produces “pure” acetaldehyde – the remaining streams are considered waste – incineration of organics or wastewater treatment are possible ways to remove organics.

2.14

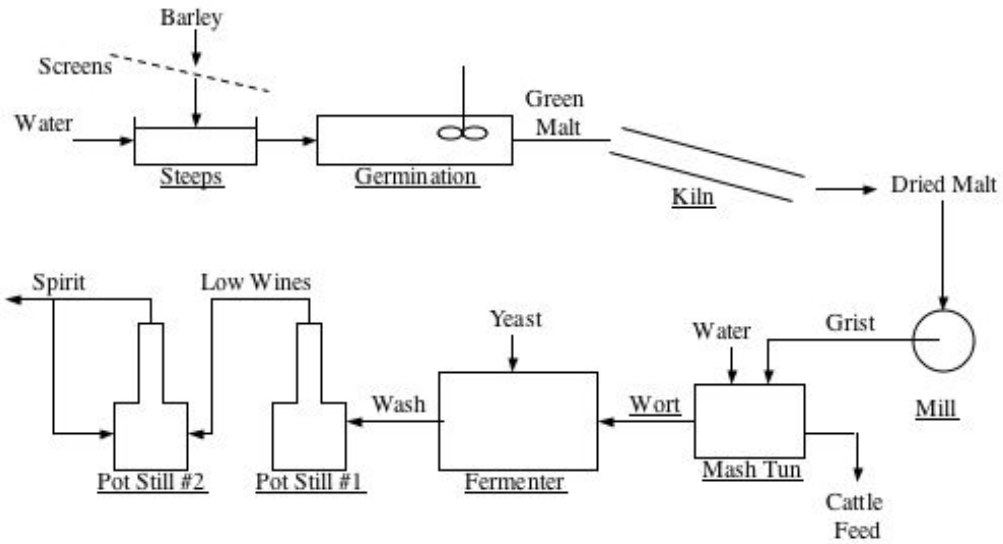
- A and R are both condensable and may be separated via distillation
- C may be separated by absorption into water
- R will be absorbed into water
- G and S cannot be separated except at very high pressure or low temperature
- After reaction, cool and condense A and R from other components.
- Separate A from R using distillation and recycle purified liquid A to the front end of the process
- Treat remaining gas stream in a water absorber to remove product C
- Separate C and from water via distillation
- Recycle unused G containing S – since S does not react further – we must add a purge to prevent accumulation of S in the system. This stream must be recycled as a gas using a recycle gas compressor.



If the value of G was very low, then consider not recycling G (and S.)

2.15

Malt Whiskey Process



Grain Whisky Process

