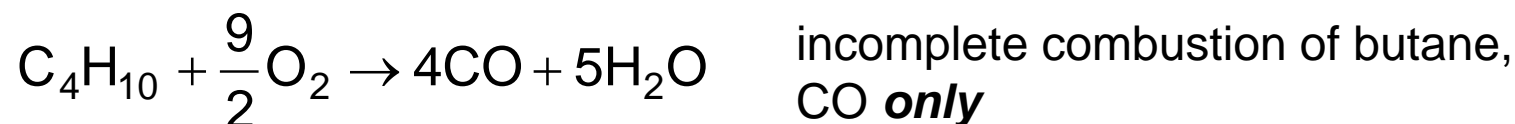
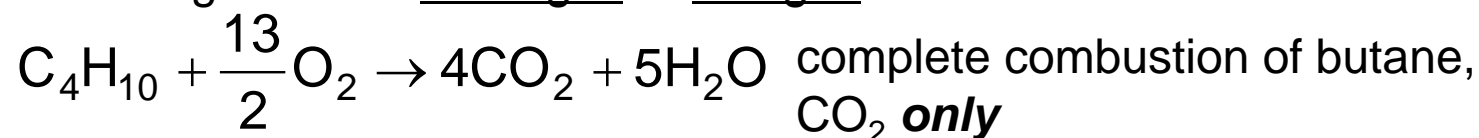


Combustion Reactions

Combustion – the rapid reaction of a fuel with **oxygen** to produce energy

- ❖ Fuels include: coal (C, H, some S), fuel oil (high molecular weight hydrocarbons and some S), gaseous fuel (natural gas – mostly methane), liquefied petroleum gas (propane and/or butane), or hydrogen.
- ❖ Maximum energy produced when fuel undergoes **complete combustion**
- ❖ Complete combustion: **all** C oxidized to CO₂, **all** H oxidized to H₂O.
- ❖ Incomplete combustion: Some C is oxidized to CO
- ❖ Product gas called stack gas or flue gas



*****If you know that incomplete combustion has occurred, you must write both rxn equations*****

Theoretical and Excess Air

For obvious economic reasons, air (**79% N₂, 21% O₂**) is the source of oxygen in most combustion reactions. Combustion reactions always use excess air, thus ensuring good conversion of the expensive fuel.

Theoretical Oxygen – moles or molar flow rate of O₂ required **for complete combustion** of all the fuel **based on stoichiometry to produce CO₂**.

Theoretical Air – quantity of air that contains the theoretical oxygen

$$\text{Theoretical Air} = 4.76 \times \text{Theoretical O}_2$$

Excess Air – amount by which the air fed to the reactor exceeds the theoretical air

$$\text{Percent Excess Air} = \frac{(\text{moles air})_{\text{fed}} - (\text{moles air})_{\text{theoretical}}}{(\text{moles air})_{\text{theoretical}}} \times 100\%$$

Material Balances on Combustion Reactions

The procedure for solving material balance problems on combustion problems is the same as that for other reactive systems.

1. Write and balance the rxn equations required, one if combustion is complete, two if not. Note for now no SO_2 or NO_x reactions are considered.
2. Calculate the inlet flow of O_2 and air required
3. Specify on the PFD what is contained in the product stream
 - This includes: unreacted fuel, O_2 , H_2O , CO_2 , CO and N_2
 - It is usually better (easier algebra) to specify unknown flowrates for each component, instead of total flow rate and stream composition
4. Translate the conversion and selectivity information into (PC) equations
5. Solve the problem
 - Combustion problems are most easily solved using atomic balance or extent of reaction methods

Combustion Reactions – Notes

Combustion problems often refer to the stack gas composition as being either on a wet or dry basis.

- ❖ Composition on a wet basis – stack gas component mole fractions that include water
- ❖ Composition on a dry basis – stack gas component mole fractions ***without*** water
- Example: a gas that contains 33.3 mole% CO_2 , 33.3% N_2 and 33.3 H_2O (wet basis) contains 50% CO_2 and 50% N_2 on a dry basis.

If a fuel of unknown composition is burned, you can deduce something about its composition by analyzing the stack gas and writing and solving atomic species balances (See F&R; not covered in lectures).

Example

Butane is fed at a rate of 100 moles/s to a boiler with 50% excess air. 70% of the butane is consumed, and the product gas contains 10 moles CO_2 per mole CO . Calculate the molar composition of the stack gas.

Comment: Note that “excess air” does not mean “complete combustion”. How do you know whether complete combustion has occurred or not?

Reaction with Product Separation and Recycle

Because reactions seldom go to completion, a recycle stream is often introduced to recover and reuse unreacted reactants. Two definitions of reactant conversion are used in the analysis of chemical reactors with product separation and recycle of unconsumed reactants:

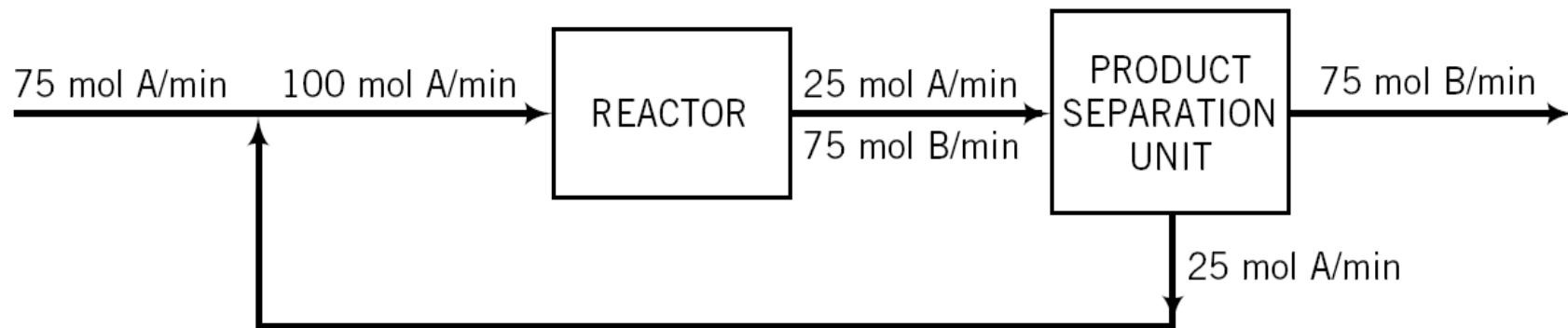
$$\text{Overall Conversion} = \frac{\text{reactant input to } \textit{process} - \text{reactant output from } \textit{process}}{\text{reactant input to } \textit{process}} (\times 100\%)$$

$$\text{Single-Pass Conversion} = \frac{\text{reactant input to } \textit{reactor} - \text{reactant output from } \textit{reactor}}{\text{reactant input to } \textit{reactor}} (\times 100\%)$$

The recycle stream allows operation of the reactor at low single-pass conversion, while still achieving high overall conversion for the system. Know the difference between fresh feed and reactor feed

Reaction with Product Separation and Recycle

Consider the Reaction $A \rightarrow B$, with the process scheme shown below:



From Previous Equations, Overall Conversion = 100%
and Single Pass Conversion = 75%. What is the Fresh Feed
and what is the Reactor Feed?

The advantage gained by obtaining 100% conversion (and thus not wasting costly reactants) may be offset by the additional costs of separation and recycle equipment. This is an optimization problem.

Reaction with Recycle and Purge

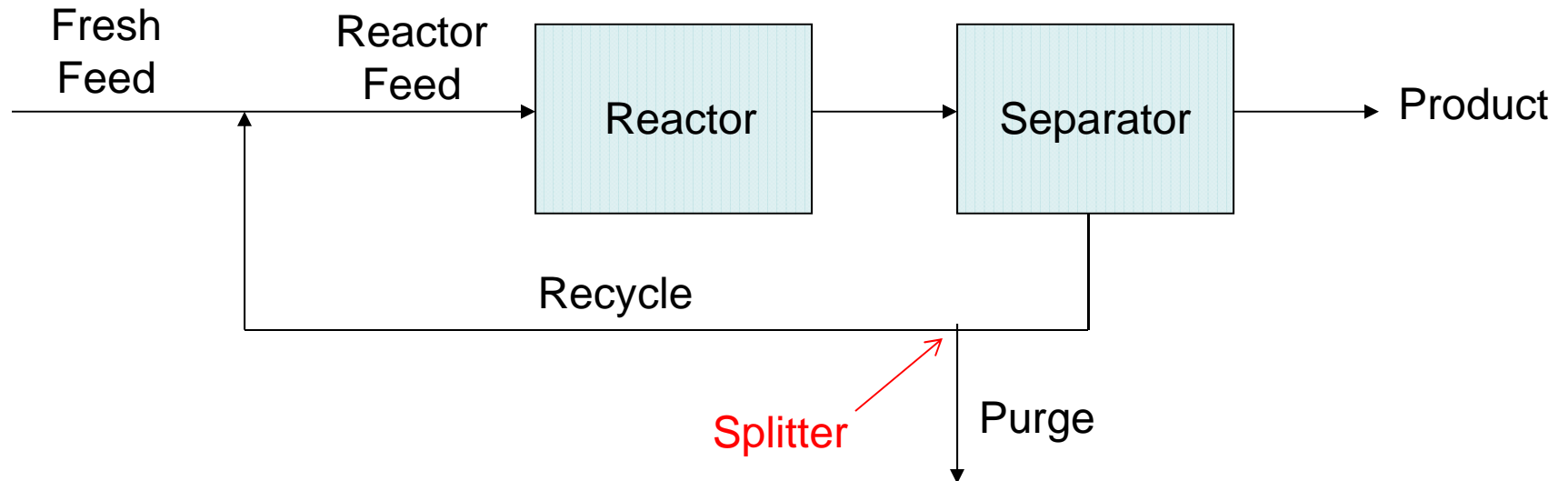
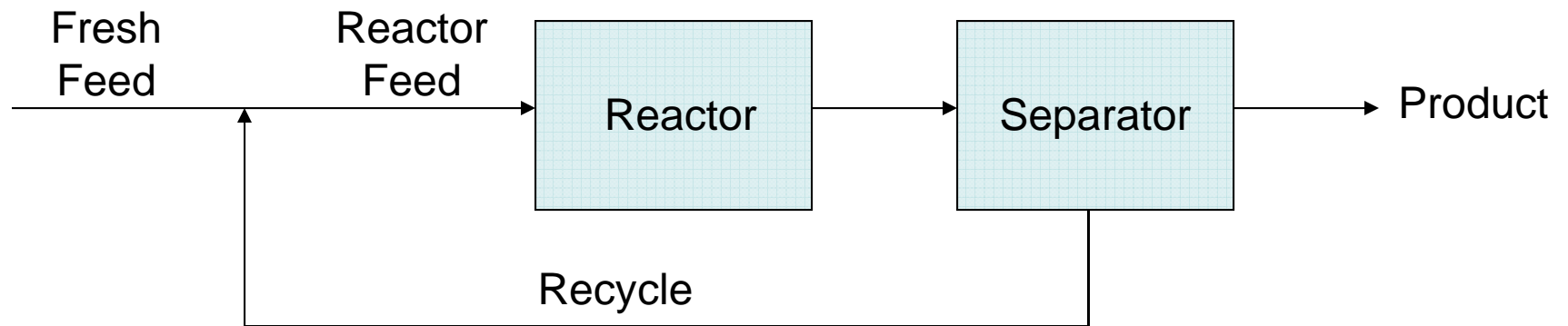
A problem that can occur in processes involving recycle is that a material that enters the process in the feed stream, or is generated in the reactor, may remain entirely in the process rather than being carried out in the product stream.

To prevent this buildup, a portion of the recycle stream is withdrawn as a purge stream. This is effective in eliminating the build-up of undesirable components, but also results in the loss of some reactants.

In the process flowchart, a purge point is a simple splitter

- the recycle stream before and after the purge point have the same composition
- only one independent material balance

Flowsheet for Reaction with Recycle and/or Purge



Reaction and Multiple-Unit Steady-State Processes

❖ Same procedures as before except that...

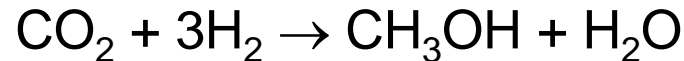
Some subsystems will contain reactions and some won't.

- Subsystems without reaction (mixer, splitter, separator)
 - Input=output (moles are conserved for individual species, and overall; no generation/consumption terms)
 - More flexibility as to stream specification (component flows or composition)
- Subsystems with reaction (generally reactor and the overall system)
 - If possible, use individual component flows around the reactor or overall system (not composition); this simplifies the math.
 - Include stoichiometry and generation/consumption for component balance method, chemical formulae, and no generation/consumption for atom balance method.

The key is setting up the flow diagram properly, and identifying the subsystem(s) that can be solved first (i.e. $DF = 0$)

Example: F&R 4.7-3

Methanol is produced in the reaction of carbon dioxide and hydrogen:



The fresh feed to the process contains hydrogen, carbon dioxide, and 0.400 mole% inerts (I). The reactor effluent passes to a condenser that removes all the methanol and water formed and none of the reactants or inerts. The latter substances are recycled to the reactor. To avoid buildup of the inerts in the system, a purge stream is withdrawn from the recycle.

The feed to the reactor (not the fresh feed to the process) contains 28.0 mole% CO_2 , 70.0 mole% H_2 , and 2.00 mole% inerts. The single-pass conversion of hydrogen is 60.0%. Calculate the molar flow rates and molar compositions of the fresh feed, the total feed to the reactor, the recycle stream, and the purge stream for a methanol production rate of 155 kmol $\text{CH}_3\text{OH}/\text{h}$.

Interactive Tutorial

Now is a good time to work through Interactive Tutorial 3...

END OF CHAPTER 4!!!