Material Balance

- Key feature of process design
  - Determine amount of raw materials needed
  - Determine amount of product output
  - Balances over units set process stream flows and compositions
  - Provide information for equipment sizing
- Process simulators help, but appreciation of material balances needed
  - Give better initial estimates to simulators which speed up convergence
  - Should check simulator output for important processes

General Procedure

- Draw block diagram of process
- List available data
- List information required of balance
- Write out chemical reactions
- Decide system boundaries (for part or all or process)
- Note other constraints (phase or reaction equilibria, tie components…)
- Check number of equations and number of unknowns
- Decide the basis of the calculation

Choice of Units

- Flows can be expressed by weight (really mass), moles, or volumes
- w/w, wt%, %wt all used for weight
- Vol%, LV%, v/v used for volume
- Example: technical grade hydrochloric acid has a strength of 28% w/w. Express this as a mole fraction
  - Molecular masses; water 18, HCl 36.5
  - In 100kg's, 28kg's are HCl
  - This is 28/36.5 = 0.77kmol's
  - In 100kg's, 72kg's are H_2O
  - This is 72/18 = 4 kmol's
  - Total is 0.77 + 4 =4.77kmol's
  - Percentage of HCl is 0.77/4.77 = 0.16 = 16%
  - Percentage of H_2O is 4/4.77 = 0.84 = 84%

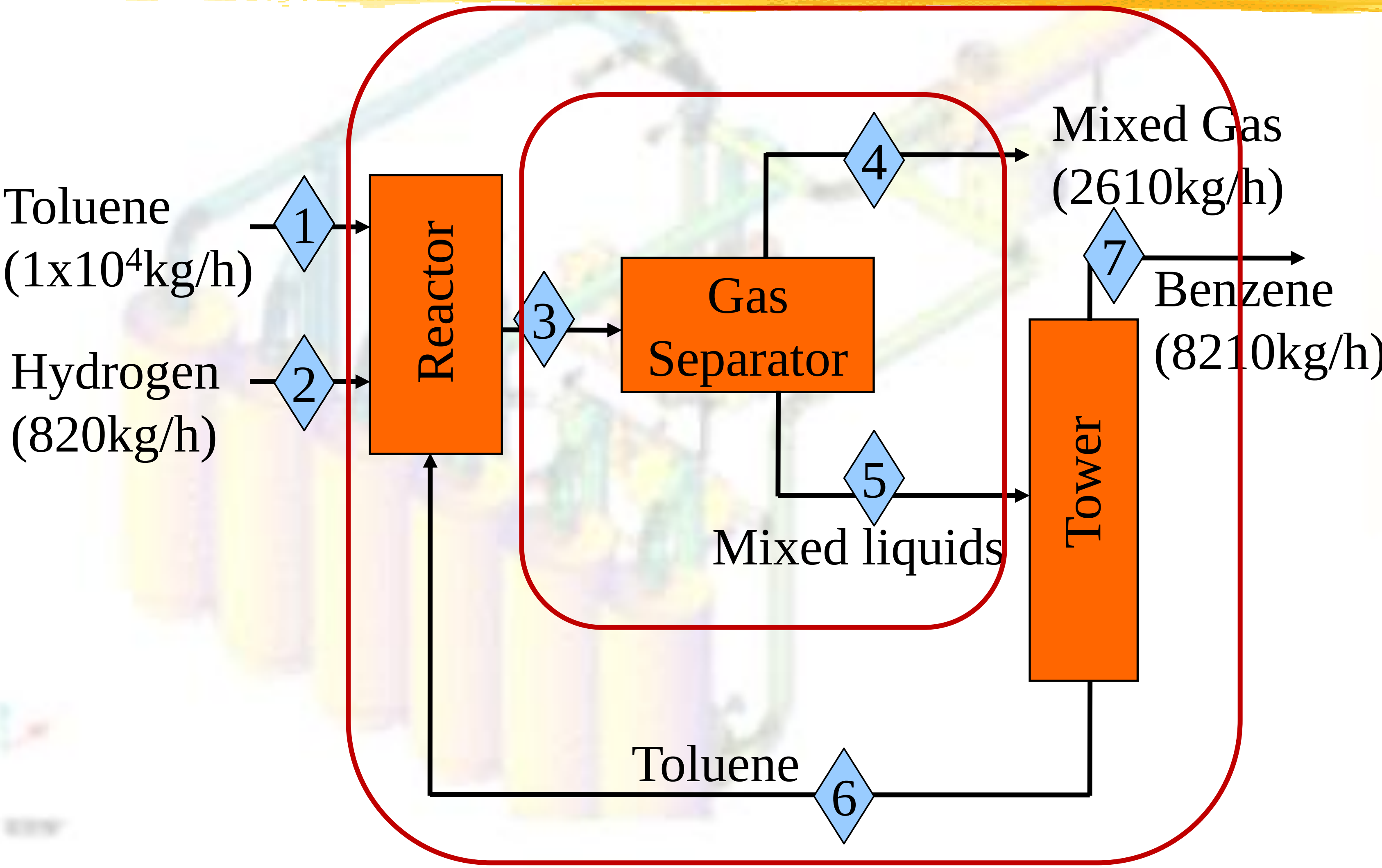
Stoichiometry

- Stoichiometric equation states how many moles of reactants and products are involved
- Equation must balance
- Look at each species in turn and solve the simultaneous equations
- Example
  - $\alpha(C_2H_4)+\beta(Cl_2)+\gamma(O_2)=>\delta(C_2H_3Cl)+\varepsilon(H_2O)$
  - Analysis gives $4C_2H_4+2Cl_2+O_2=>4C_2H_3Cl+2H_2O$

System Boundaries

- Material balance can be over entire process or any subset
- Look at flows into and out of boundary
- Clever choice of boundaries can simplify calculations
- Any streams that are poorly known can be fully wrapped inside boundary
- Recycle streams fully wrapped inside boundary

System Boundaries



Conversion, Selectivity, Yield

- **Conversion** = (amount of reagent consumed) / (amount supplied)
- Example: production of vinyl chloride by pyrolysis of dichlororethane. Conversion limited to 55% to reduce carbon formation. How much DCE fed to produce 5000kg/hr of VC? (molar weights are DCE=99 and VC=62.5)

[14405kg/hr]

Conversion, Selectivity, Yield

- **Selectivity** = (moles of product formed) / (moles of product that could have been formed had all reacted feed been used to make product)
- Addresses issues of side products
- Selectivity better at low conversion rates

Conversion, Selectivity, Yield

- **Yield** = (moles of product formed) / (moles of product that could have been formed had all feed been used to make product)

$$\text{Yield} = \frac{\text{moles of product formed}}{(\text{moles of reagent used}) \times \text{stoichiometry}}$$

- Yield = conversion x selectivity

Conversion, Selectivity, Yield

- In the production of ethanol by the hydrolysis of ethylene, diethyl ether is produced as a by-product. The feed stream composition is 55% ethylene, 5% inerts, 40% water. The composition of the product stream is 52.26% ethylene, 5.49% ethanol, 0.16% ether, 36.81% water, 5.28% inerts. All percentages are by mole. Calculate the selectivity of ethylene for ethanol and for ether and also the conversion of ethylene. The reactions are:

$$C_2H_4 + H_2O \rightarrow C_2H_5OH$$

$$2C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O$$

[selectivity for ethanol = 94.4%, for ether = 5.44%, conversion = 10%]

Conversion, Selectivity, Yield

⌘Yield Example

- In the chlorination of ethylene to produce DCE, the conversion of ethylene is 99%. If 94mol of DCE is produced from 100mol of ethylene reacted, calculate the selectivity and yield.

[94% and 93.1%]

Constraints on Flows and Compositions

- Total flow rate of a stream = sum of flow rates of individual components
- Stream specified by one of the following:
  - Flow rate of each component
  - Total flow rate plus composition
  - Flow rate of one component plus composition
- Example:
  - Flow rate to a reactor consists of w/w 16% ethylene, 9% oxygen, 31% nitrogen, 44% hydrogen chloride. The ethylene flow is 5000kg/hr. Calculate individual component flows and the total stream flow.

[total=31,250kg/hr, O_2 =2813kg/hr, N_2 = 9687kg/hr, HCl=13,750kg/hr]

Tie Components

- Components that pass unreacted through a process can be madly useful for calculations
- Used to relate input and output compositions
- These are called **Tie Components**
- Example:
  - CO_2 at a rate of 10kg/hr is added to an air stream. After mixing the stream has 0.45% v/v CO_2. Normal air has 0.03% CO_2 by mol. Calculate the flow rate of the air stream

[1560kg/h]

Excess Reagent

- In industrial reactions, and excess of one component is usually added
  - Components not added in their stoichiometric ratios
- The per cent excess is given by:

$$\text{Per cent excess} = \frac{\text{quantity supplied - stoichiometric}}{\text{stoichiometric}} \times 100$$

- example:
  - To ensure complete combustion, 20% excess air is supplied to a furnace burning 95% v/v methane, 5% ethane. Calculate the number of moles of air per mole of fuel. The reactions are:

$CH_4 + 2O_2 => CO_2 + 2H_2O$

$2C_2H_6 + 7O_2 => 4CO_2 + 6H_2O$

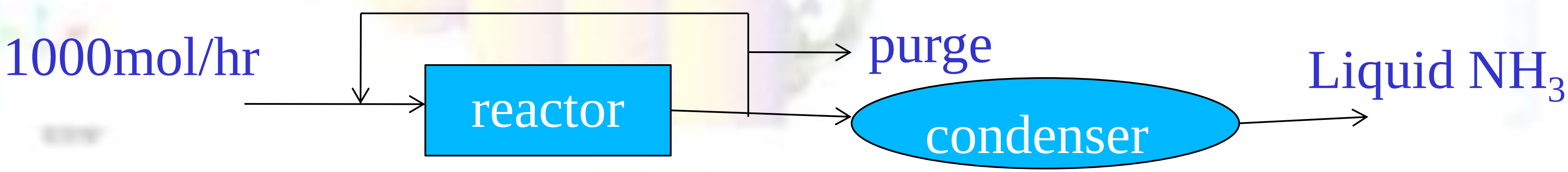
[11.86 moles per mole of fuel]

Recycle Processes

- Material from a latter point in a process is fed back to an upstream unit
- Examples:
  - a reaction with appreciably less than 100% conversion, feed unreacted components back to reactor
  - the reflux at the top of a distillation column
- Greatly complicates mass balance calculations
- Solutions:
  - Used tear streams and iterate until consistent within tolerances
  - Solve simultaneous equations

Purge

- Recycle streams means there can be a build up of inert components within a process
- Need to bleed these off somehow
- Use purge streams
- In steady state, rate of flow of inerts in purge stream equals rate of flow in feed stream
- Example:
  - 1000mol/hr feed of stoichiometric nitrogen and hydrogen is reacted to produce ammonia. Because the reaction conversion rate is low (~15%) the unreacted components are recycled. The feed stream contains 0.2% argon by mole. Calculate the purge rate required to keep the argon content of the recycle stream under 5% by mole.



[40mol/hr]