Chapter 3

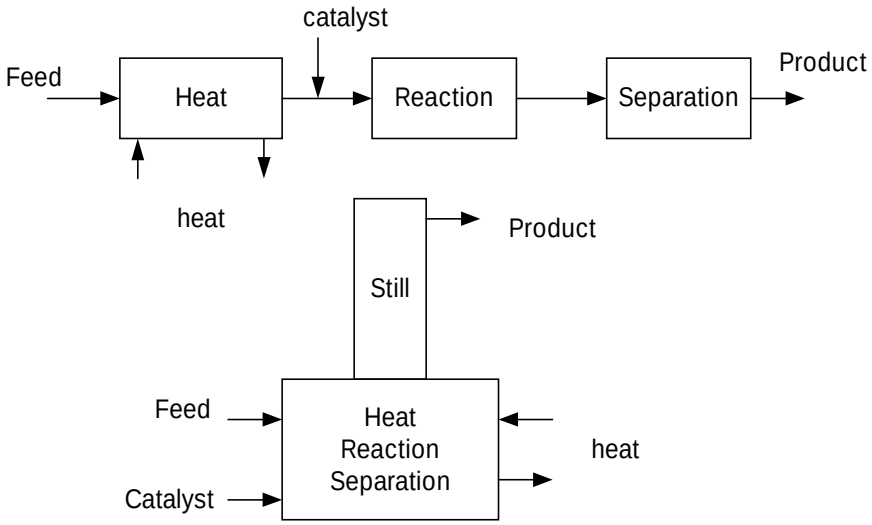
REACTION SYSTEM

3.1 Batch versus Continuous

Batch/Semi-Batch Reactor
PFR
CFSTR

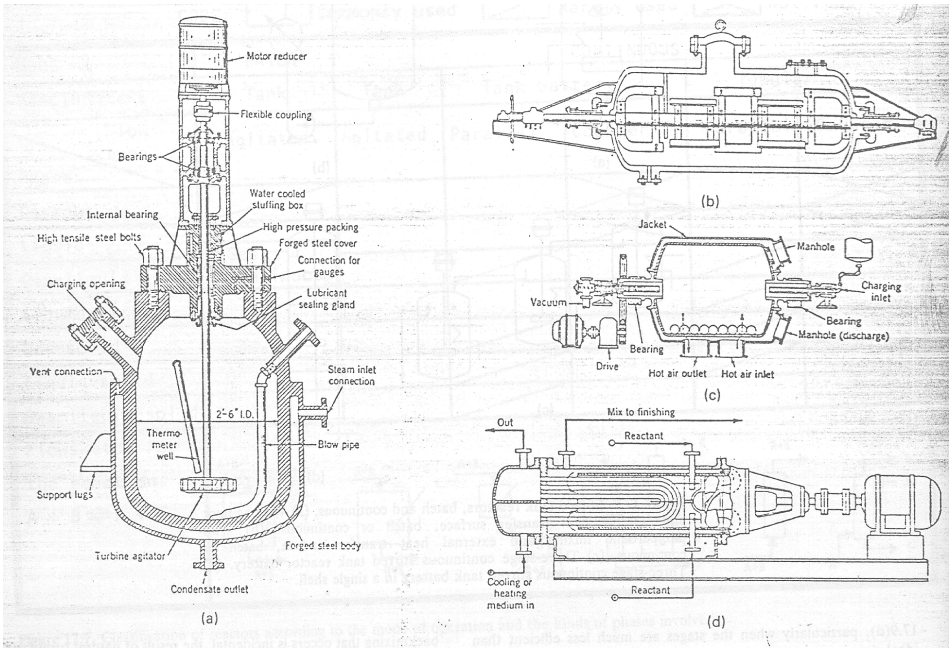
- Batch processes are generally for multi-purpose and multi-products
- Production rate
  - Usually batch if less than 500 ton/yr
  - Usually continuous if more than 5000 ton/yr
- Market forces
  - Usually batch for seasonal production
  - Usually batch for products with short life time
- Operational problem
  - Batch for very long reaction time
  - Batch for slurries at low flow rates
  - Batch for rapidly fouling products

Multiple operations can be carried out in a single vessel batch reactor.



3.1.1 Shapes of Industrial Reactors

Different types of batch reactors



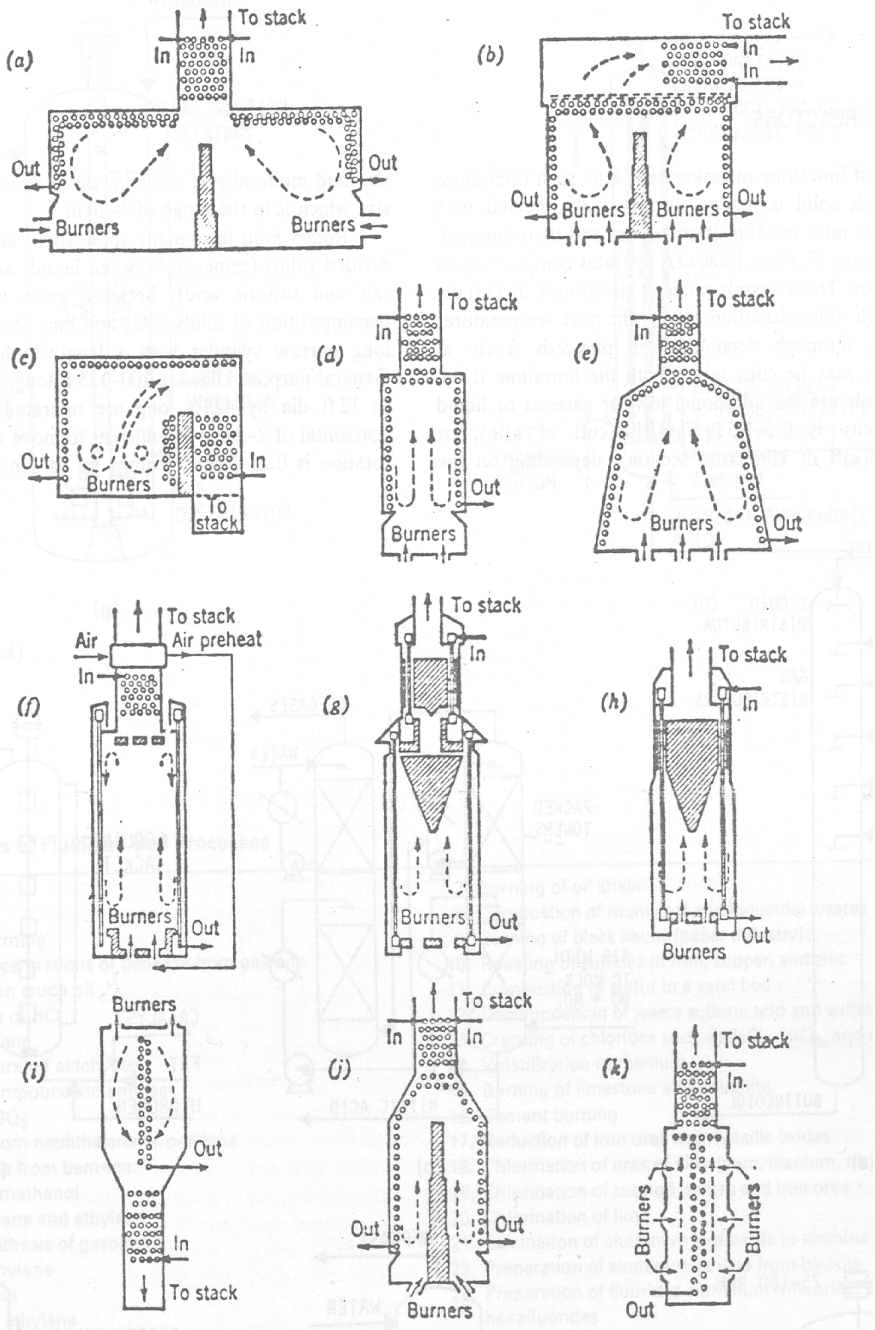


Figure 17.16. Basic types of tubular furnaces [*Nelson*, Petroleum Refinery Engineering, *McGraw-Hill, 1958. Courtesy McGraw-Hill, New York*].

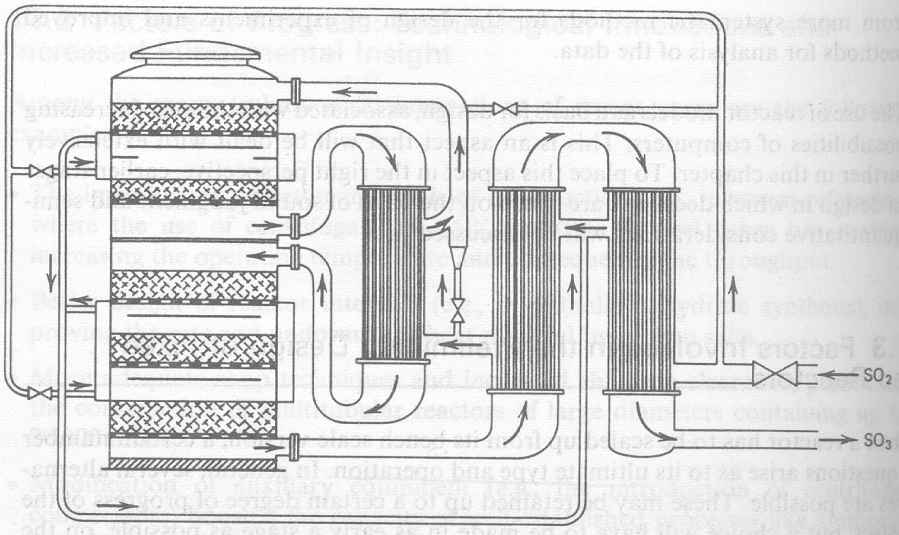


Figure 11.3-2 Multibed adiabatic reactor for SO_3 synthesis (after Winnacker and Kuechler [2], from Froment [148]).

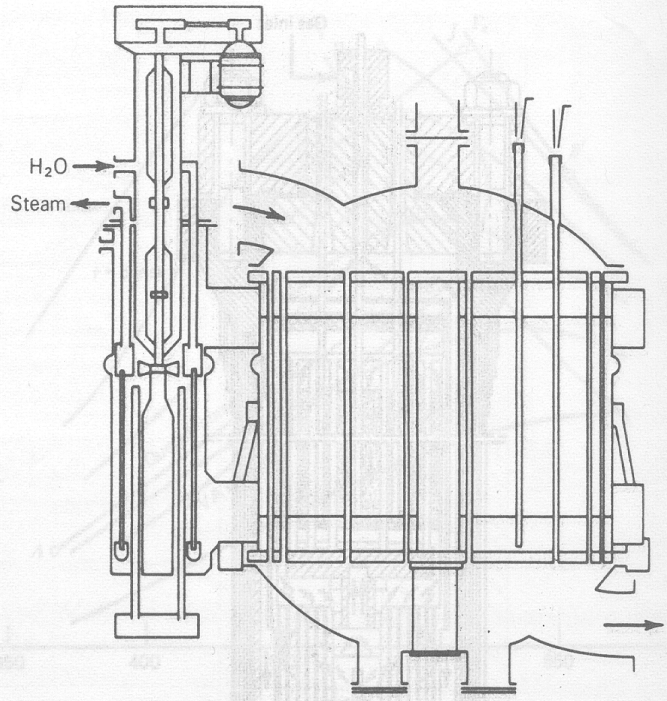


Figure 11.3-6 Multitubular reactor for phthalic anhydride thesis by o-xylene oxidation (from Suter [6]).

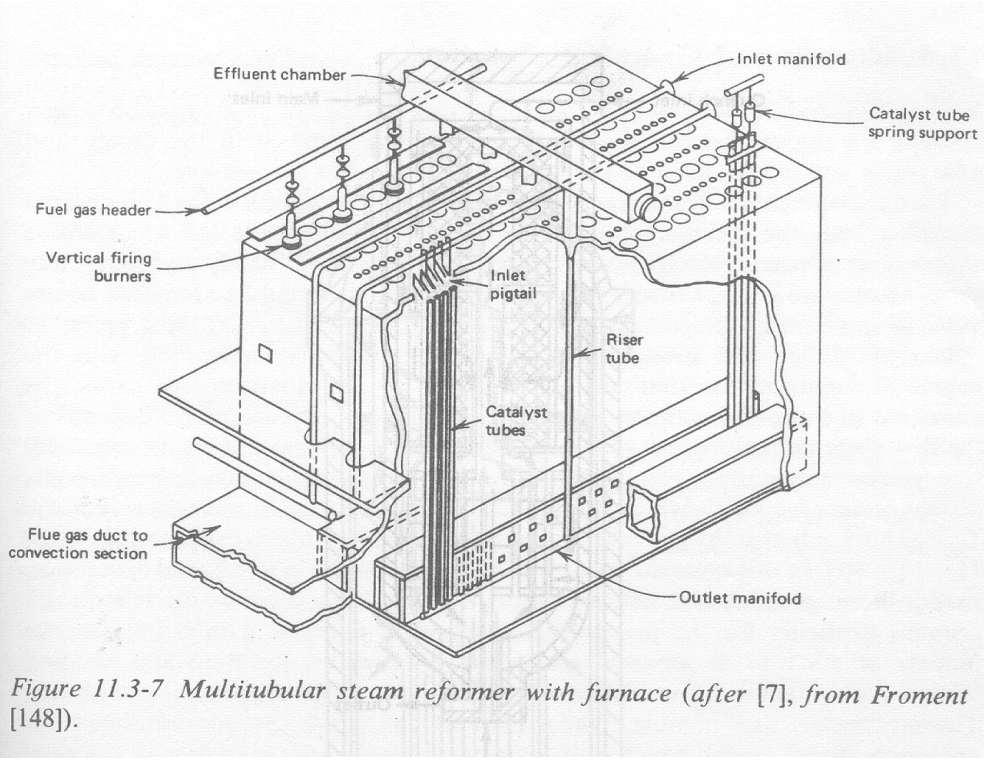


Figure 11.3-7 Multitubular steam reformer with furnace (after [7], *from Froment* [148]).

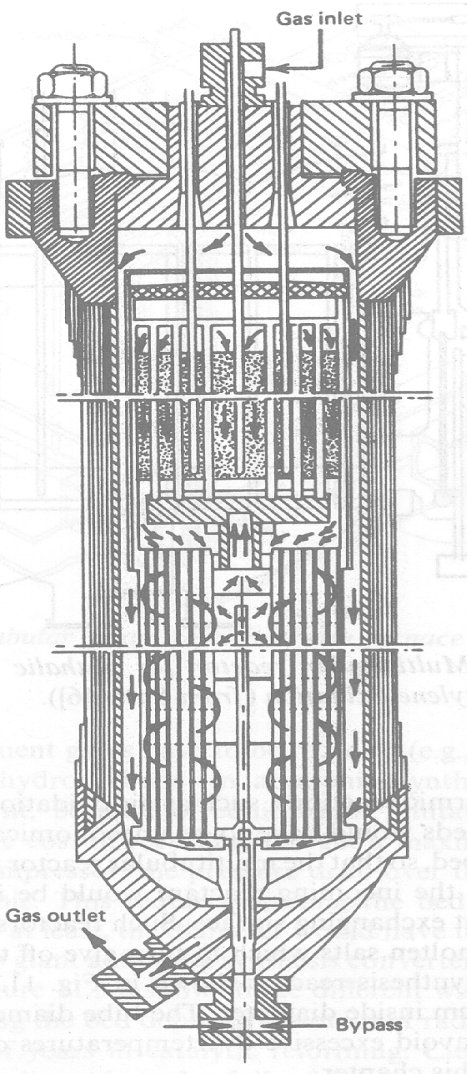
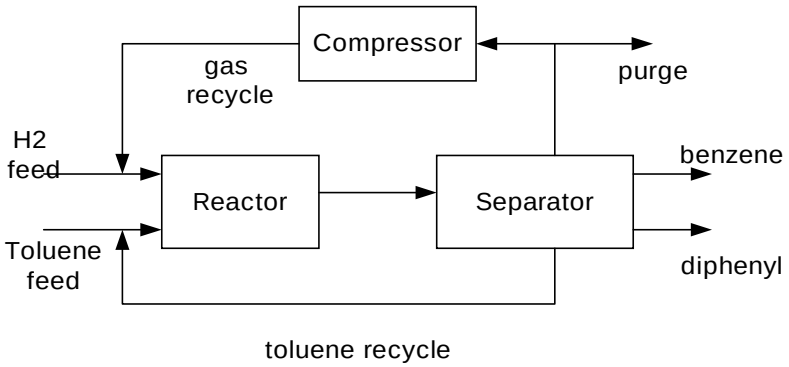


Figure 11.3-5 Ammonia synthesis reactor with tubular heat exchanger (from Vancini [4]).

3.2 Multiple Reactor System

Dependent on the reaction conditions (temperature and pressure...)

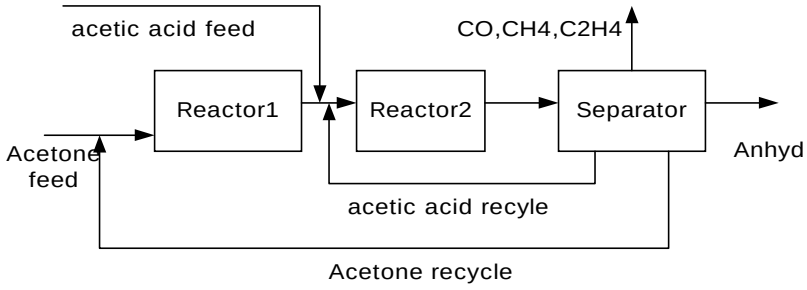
$$Toluene + H_2 \rightarrow Benzene + CH_4$$
$$2\ Benzene \leftrightarrow Diphenyl + H_2$$
at 1500^oF and 500 psia $\Rightarrow$ *Single reactor*



$$Acetone(CH_3COCH_3) \rightarrow Ketene(COCH_2) + CH_4$$
$$Ketene(COCH_2) \rightarrow CO + 0.5C_2H_4 \text{ at } 700^oC \text{ and 1 atm}$$

$$Ketene + Acetic\ Acid(CH_3COOH) \rightarrow Acetic\ Anhydride(CH_3COOCOCH_3)$$
at 80^oC and 1 atm

$\Rightarrow$ two reactors



Mild exo- or endo-thermic reactions $\Rightarrow$ Multiple reactors with interstage coolers or heaters

3.3 Excess Reactant

- To shift product distribution

$$Butene + \underline{Isobutane} \rightarrow Isooctane^{*}$$
$$Butene + Isooctane \rightarrow C_{12}$$

  The lareger the excess of i-C4, the greater the improvement in the selctivity of i-C8.

- To force a component to reach complete conversion.

$$CO + Cl_2 \rightarrow \underbrace{COCl_2(\text{diisocyanate})}_{\text{should be free of } Cl_2}$$

- To shift equilibrium conversion

$$Bz + 3H_2 \leftrightarrow \text{Cyclohexane}$$

  If Cyclohexane $\gg$ Bz, no need to do distillation.

- As the amount of excess reactant increases, recycle cost and reactor cost increase.

3.4 Effect of Heat of Reaction

Adiabatic, direct heating or cooling ? Use heat carrier ?

Adiabatic Temperature Rise

$$Q_R = FC_p(T_{R,out} - T_{R,in}) \rightarrow \Delta T_R = Q_R/FC_P$$

If ΔT_R is less than 15^oC, use an adiabatic reactor.
Otherwise,

- heat exchanger type reactor

- inter-stage cooling or heating
- heat carrier

Heat Carriers

inert and high C_p

$$CH_4 \ : \ C_p = 0.55\text{Btu/lb } {}^oF \text{ at } 60^oF,\ 1.0\text{Btu/lb } {}^oF \text{ at } 900^oF$$
$$N_2 \ : \ C_p = 0.25\text{Btu/lb } {}^oF \text{ at } 60^oF,\ 0.26\text{Btu/lb } {}^oF \text{ at } 900^oF$$

3.5 Equilibrium Limitations

[**Ex. 1**]

$$C_6H_6 \ + \ 3H_2 \ \leftrightarrow \ C_6H_6 \ \text{ exothermic}$$

$$K_e(T) = \frac{f_c}{f_B f_H^3} = \frac{\nu_c y_c}{P^3 \nu_B \nu_H^3 y_B y_H^3}$$

To reach complete conversion,
decrease T and/or increase H_2/C_6H_6 nd/or increase P.

[**Ex. 2**] At 1100^oF and $20psia$,

$$\begin{aligned} Ethylbenzene &\leftrightarrow Styrene \ + \ H_2 \\ Ethylbenzene &\rightarrow Benzene \ + \ Ethylene \\ Ethylbenzene &\rightarrow Toluene \ + \ Methane \end{aligned}$$

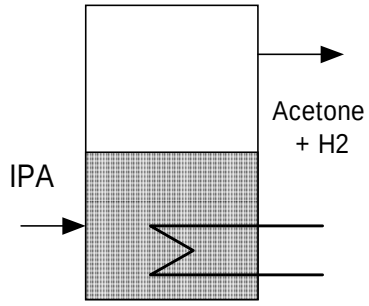
Steam is used as a diluent to shift equilibrium conversion.

3.6 Separator Reactors

Equilibrium-limited reaction can be forced to reach complete conversion if one of the products can be removed.

Ex. $IPA(82.5^oC) \rightarrow Acetone(56.5^oC) + H_2$

$X_e = 0.32$ at 300^oF, $\Delta H_r > 0$, liquid phase reaction



Ex. Acrylic Acid (141^oC) + Ethanol $(78.5^oC) \leftrightarrow$ Ethylacrylate$(99.4\ ^oC)$ + Water