Chemical Reactor Design

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CHAP. 1
MOLE BALANCE

Chemical Reactor Design

化學反應裝置設計

Chapter 1. Mole Balance

Objectives

After completing Chapter 1, the reader will be able to:

- **Define the rate of chemical reaction.**
- **Apply the mole balance equations to a batch reactor, CSTR, PFR, and PBR.**
- **Describe two industrial reaction engineering systems.**
- **Describe photos of real reactors.**

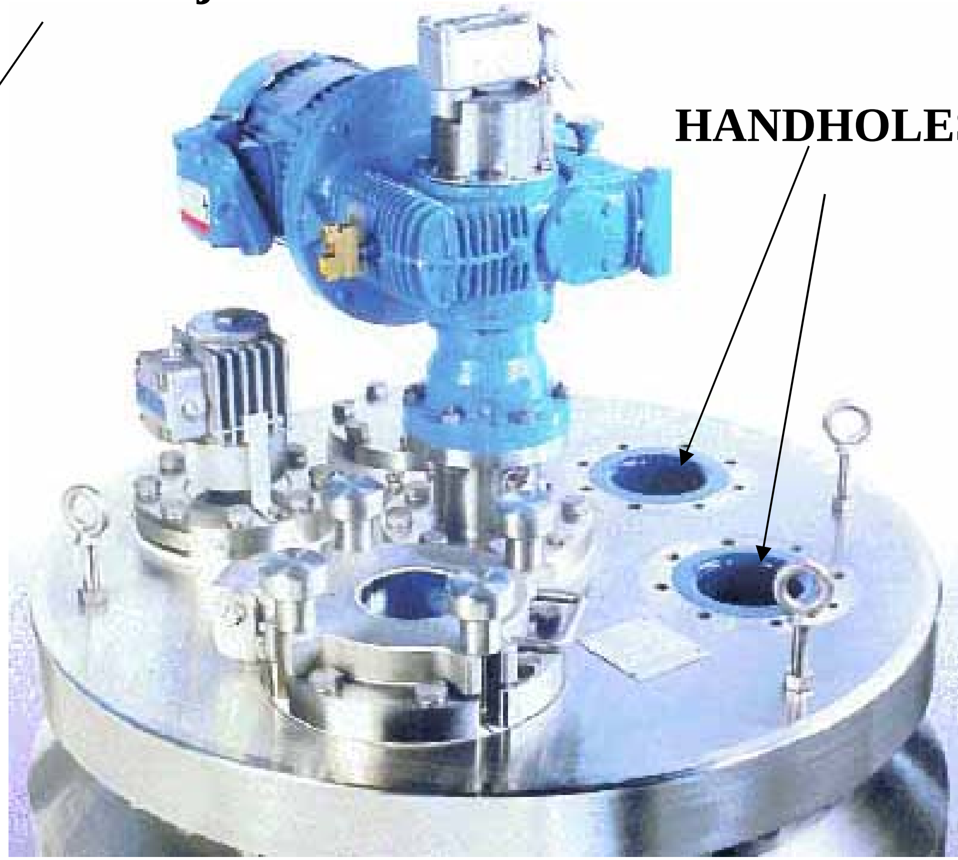
Chapter 1. Mole Balance

Industrial Reactors

Batch Reactor Stirring Apparatus

Conventional jacket

HANDHOLES

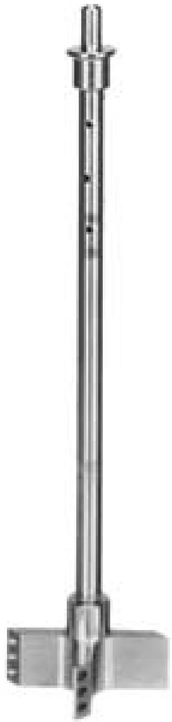


攪拌槽型 反應裝置

Cutaway View of CSTR

http://www.jeiopi.co.kr/english/prd/impeller.htm

Gas Entrainment Impeller



Turbine Type Impeller

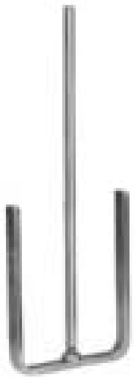
Spiral Agitator

pitched blade turbine

flat blade radial turbine

Helix Impeller

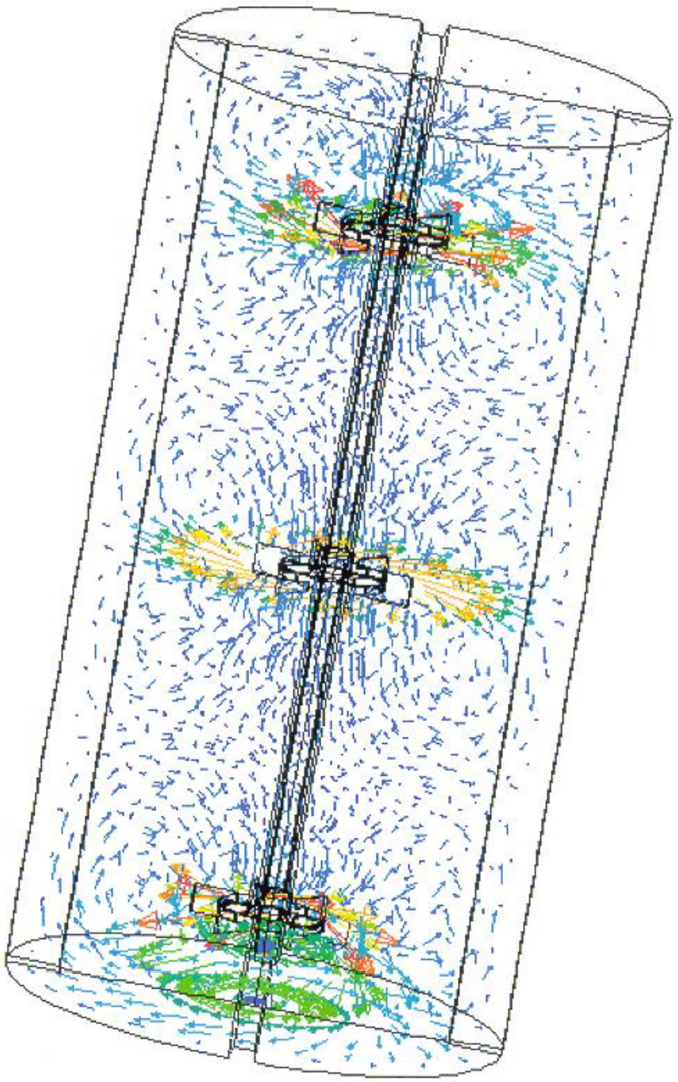
Anchor Stirrer

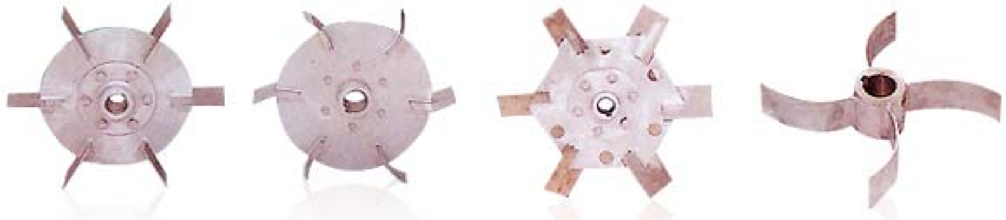


Hydrofoil

Marine Type Propeller

CSTR/batch Reactor





▪ RIGHT TUBBINE
: 중, 고속용, 중점도의 혼합, 용해, 가스흡입

▪ BEND TUBBINE

▪ PITCHED TUBBINE

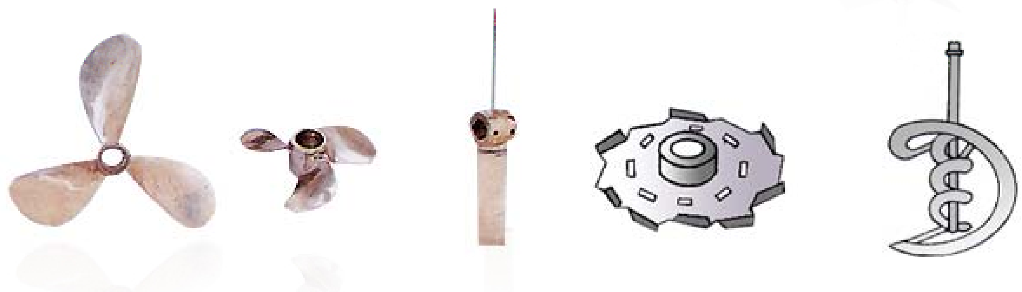
▪ BEND PADDLE

▪ 4 BLADE PITCHED PADDLE

▪ 3 BLADE PITCHED PADDLE

▪ HORSE ANCHOR
: 저속용, 고점도 분체의 용해 침강 방지

▪ PITCHED PADDLE
: 저, 중속용, 중점도의 혼합, 용해



▪ PROPELLER
: 중,고속용, 저점도의 혼합, 용해, 전열

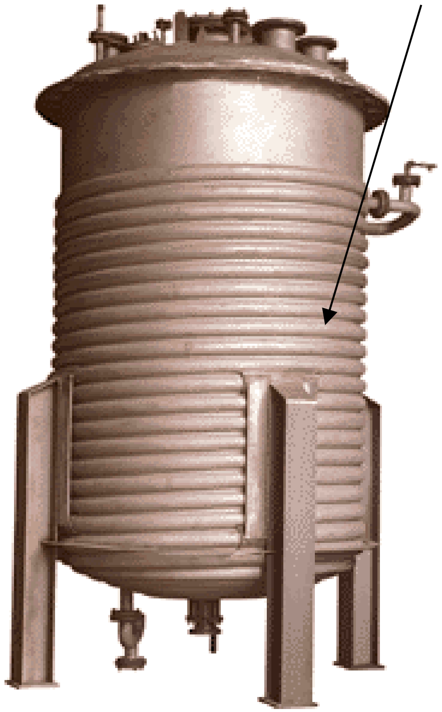
▪ 2 BLADE PITCHED PADDLE
: 저, 중속용, 중점도의 혼합, 용해

▪ DISPERSED TUBBINE
: 고속용, 고점도의 분체, 애멀젼화

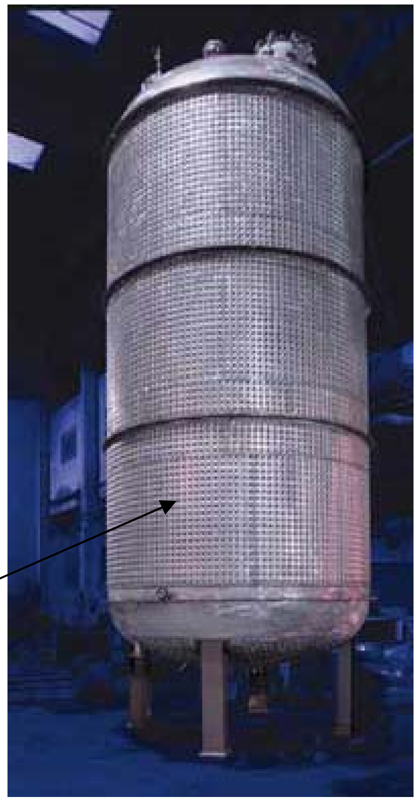
▪ RIBBON
: 저속용, 고점도의 혼합, 용해

Type of Jacket

Half pipe jacket



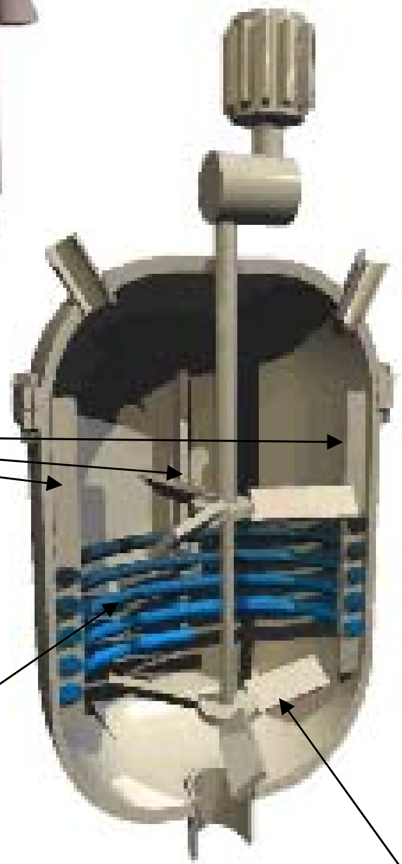
Dimpled Jacket



Conventional jacket

Baffles

Inner coil type
Heat exchange



impeller

www.centralfabricators.com/hpipej.htm

Stirred Tank Reactor

攪拌槽型 反應裝置

polymerization reactor

M.O.C	Dimensions	Weight	Surface
SA 515 Gr 70 + SA 240 316 L	I/D:2700 mm Thk: (24+3) mm Ht.: 4600 mm	12500 Kgs	Electropolished 500 Grit

Equipment : POLYMERIZATION REACTOR

Client : DCW

Year Of Mfg : 1992

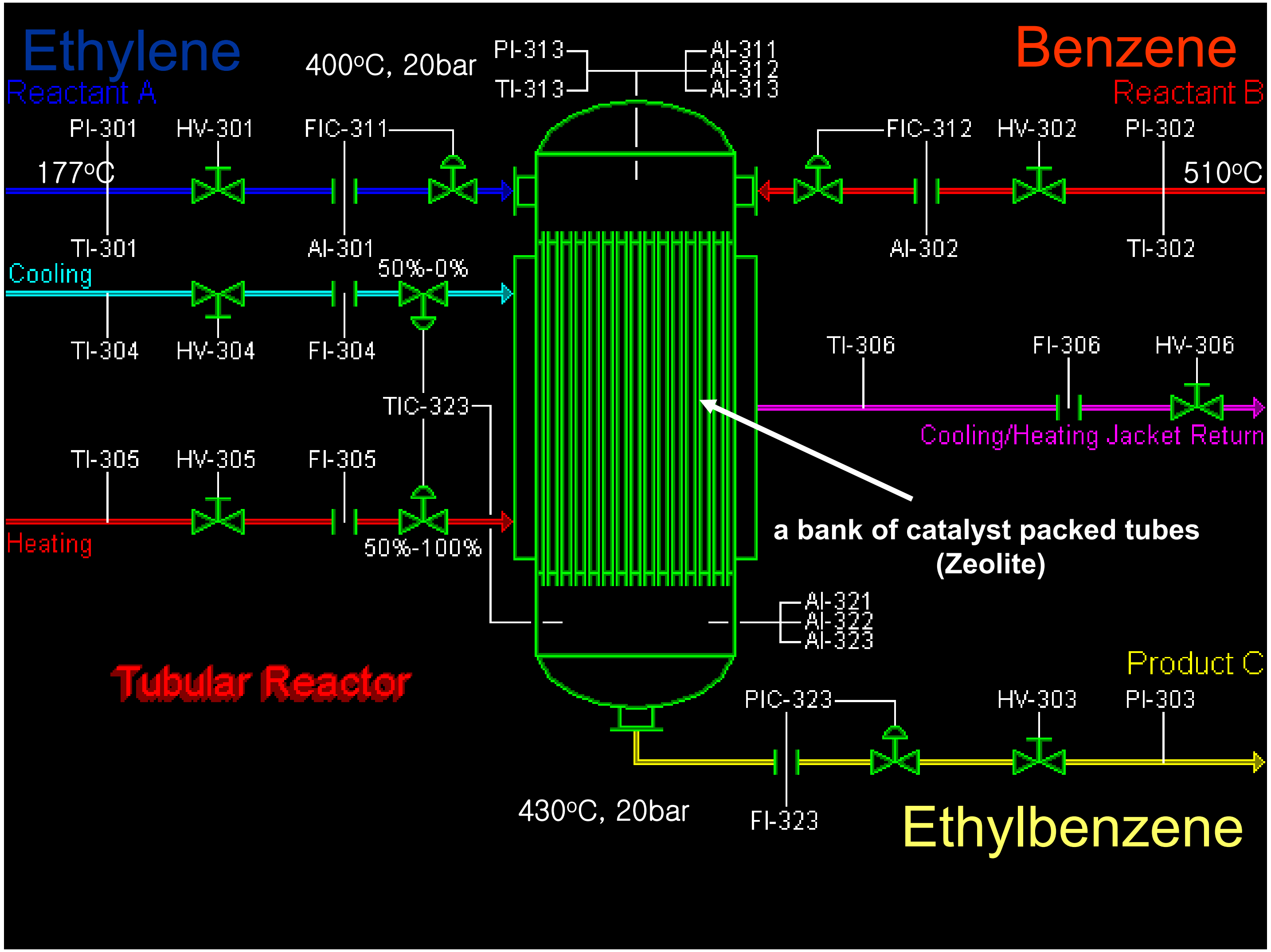
High Pressure Tubular Reactor for LDPE (Low Density PolyEthylene) plant

ExxonMobil's tubular process technology for Sasol's new high-pressure low density polyethylene (LDPE) plant in Sasolburg, South Africa. The new 220,000 ton-per-year plant is expected to be completed in 2005.

Tubular Reactor for SCWO

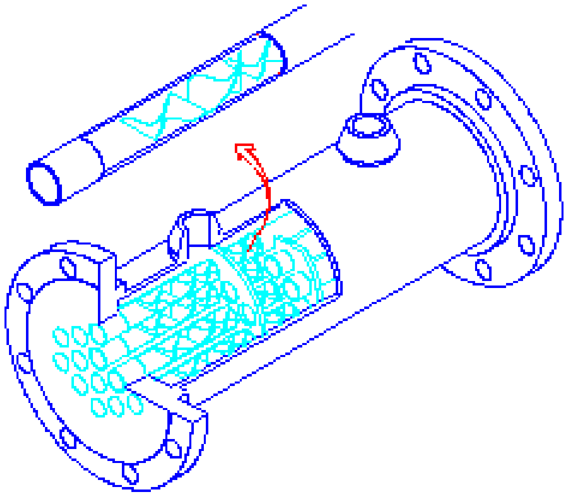
The Shinko Pantec Plant, Capacity: 1100 kg/h

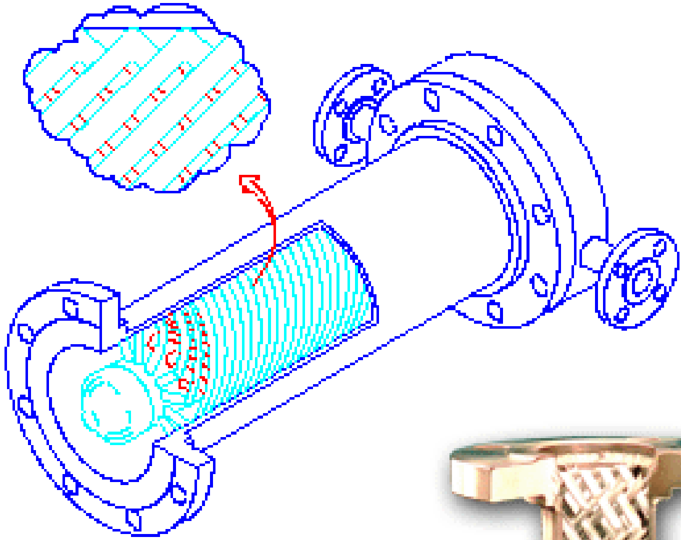
Tubular Reactor for production of ethylbenzene

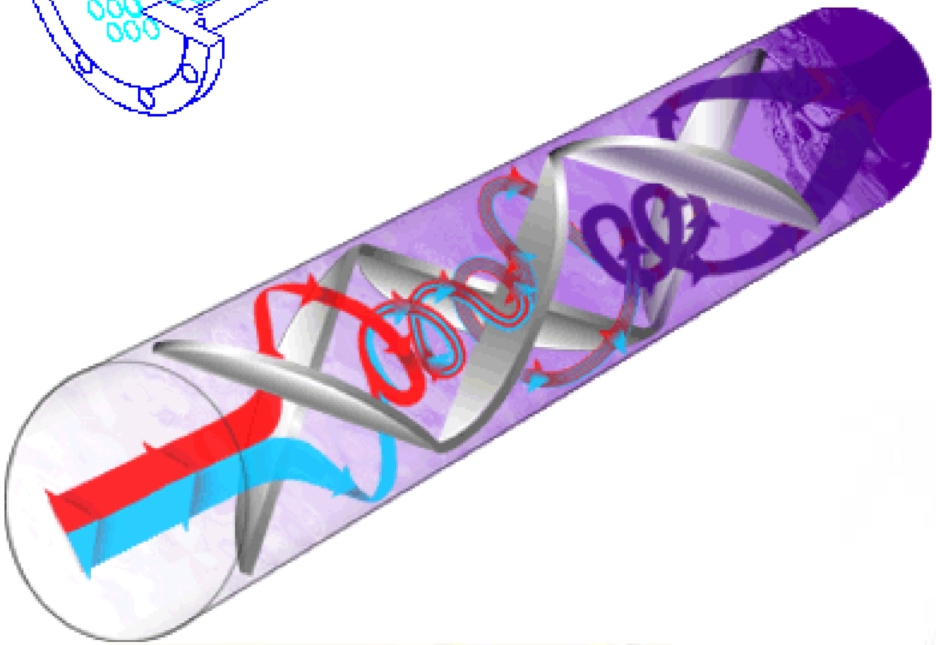


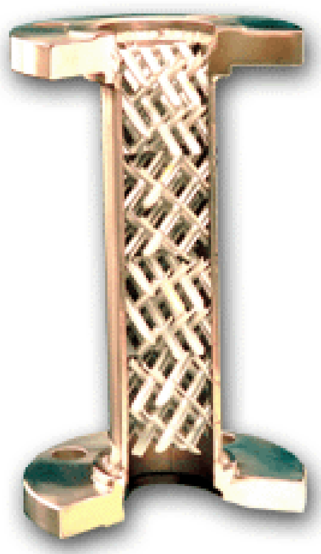
The default configuration catalytically reacts ethylene (reactant A) with benzene (reactant B), an exothermic reaction, to produce ethylbenzene (product C), an intermediate chemical used in the manufacture of styrene monomer. *(http://www.simtronics.com/catalog/spm/spm2200a.htm)*

Static Mixer in Tubular Reactor





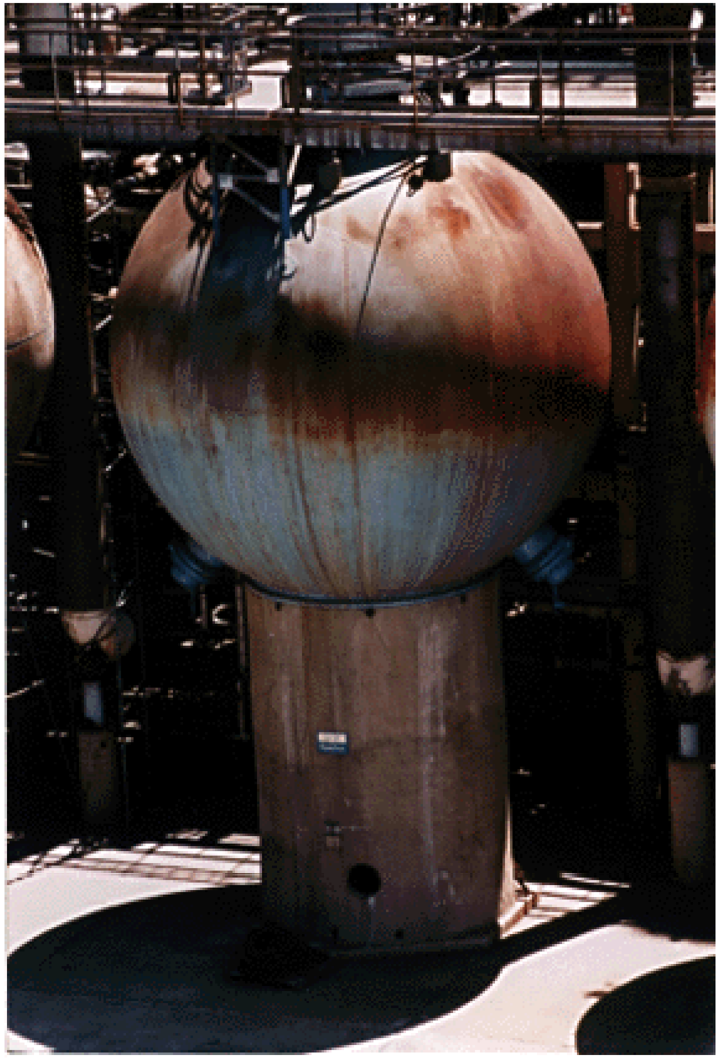




Industrial Reactor Photos

Reactor System Used at Amoco

“Ultraformer Reactor”-Reforming Petroleum Naphtha



Spherical Reactor at AMOCO

Spherical Reactors Connected in Series

Hydrotreating Unit

Catalytic hydrotreating is a hydrogenation process used to remove about 90% of contaminants such as nitrogen, sulfur, oxygen, and metals from liquid petroleum fractions. These contaminants, if not removed from the petroleum fractions as they travel through the refinery processing units, can have detrimental effects on the equipment, the catalysts, and the quality of the finished product. Typically, hydrotreating is done prior to processes such as catalytic reforming so that the catalyst is not contaminated by untreated feedstock. Hydrotreating is also used prior to catalytic cracking to reduce sulfur and improve product yields, and to upgrade middle-distillate petroleum fractions into finished kerosene, diesel fuel, and heating fuel oils. In addition, hydrotreating converts olefins and aromatics to saturated compounds.

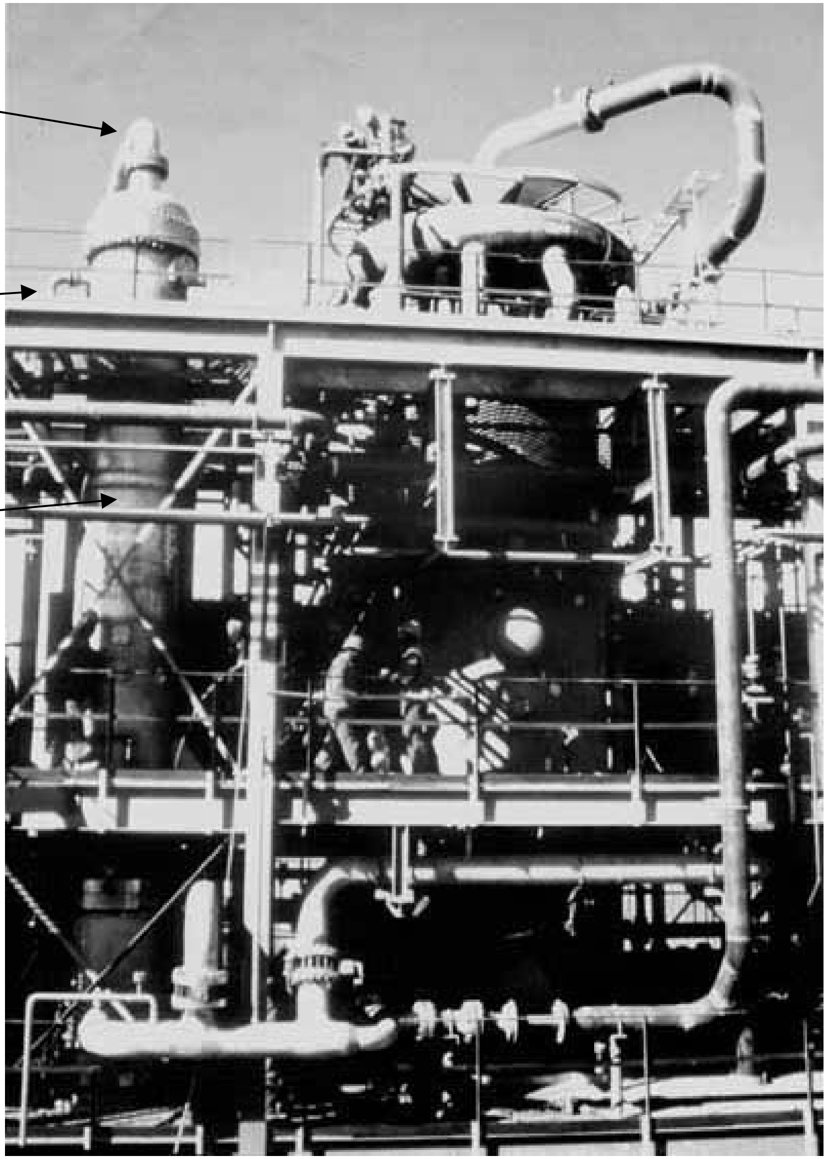
Packed Bed Reactor

Fisher-Tropsch synthesis reaction at Sasol Limited Chemical

Gas inlet
(50% conversion)

Steam injector

Tube bundle
(2050 tubes)
5cm ID X 12 m H



Catalyst

K_2O/SiO_2 on Fe
BET=200m^2/g

Product
= Light hydrocarbon
+ wax (candle &
printing inks)

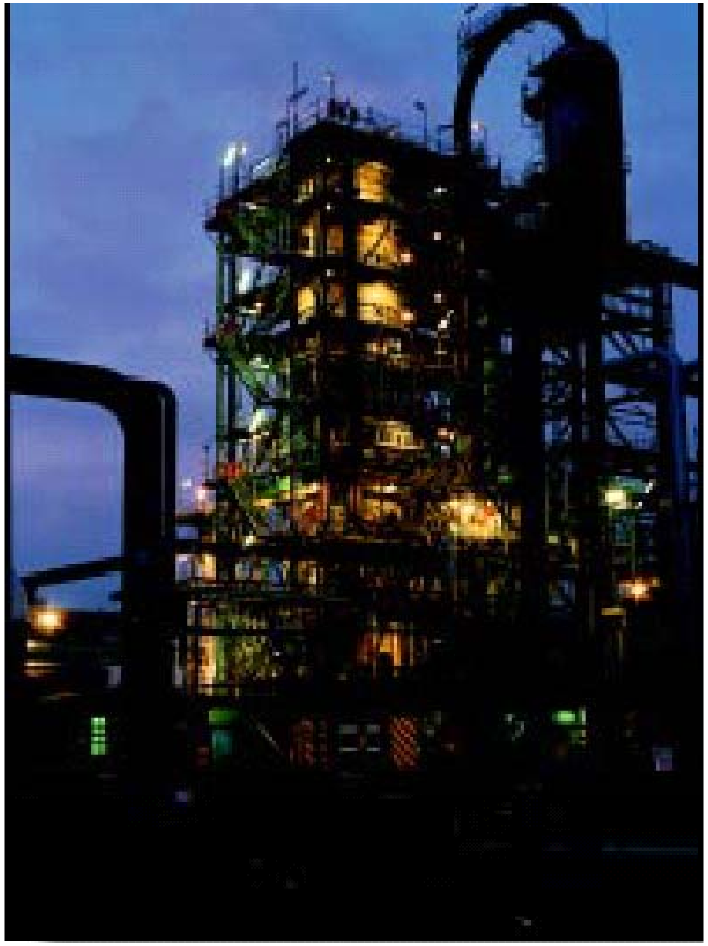
Straight Though Transport Reactor

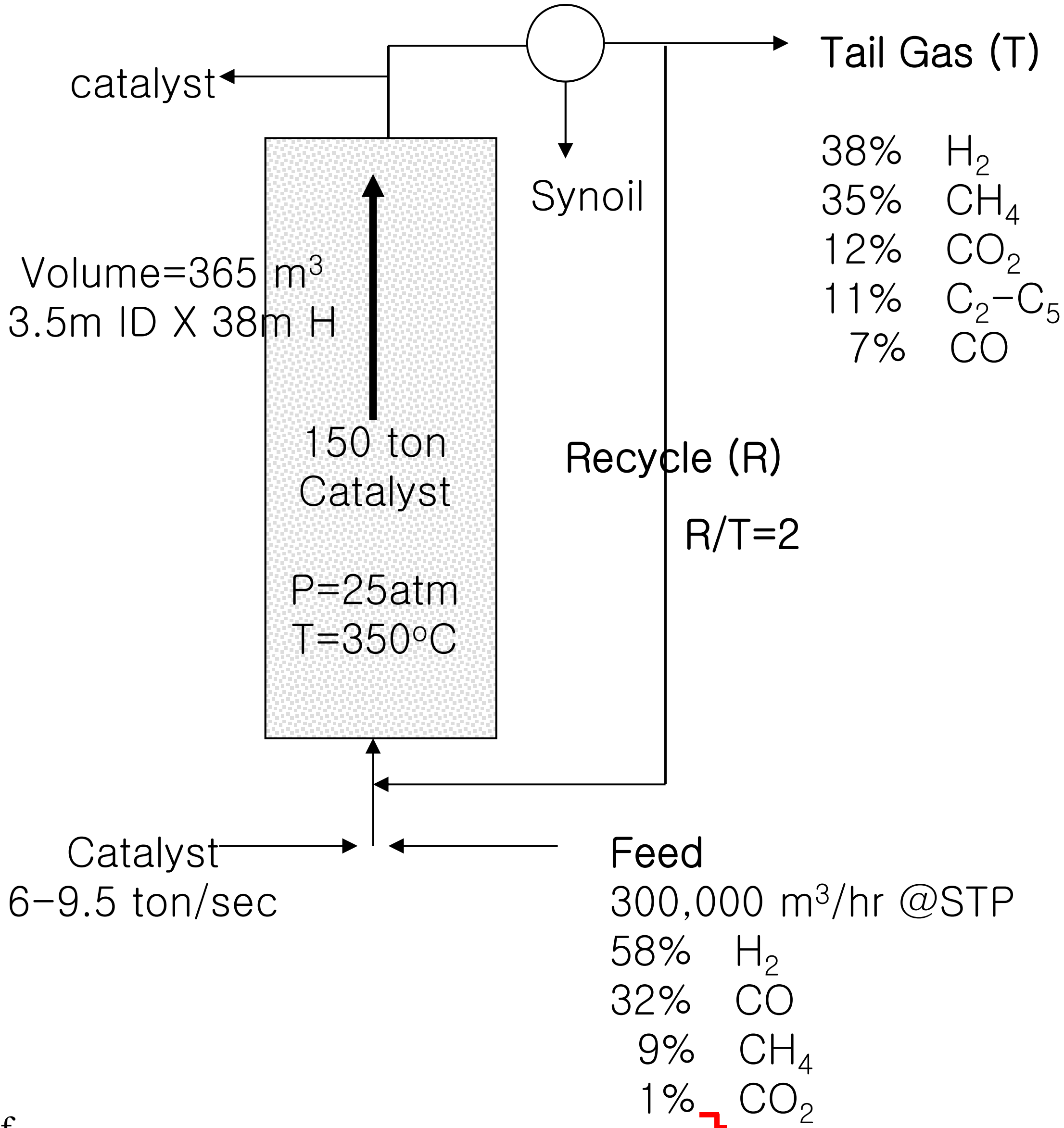
Fisher-Tropsch synthesis reaction at Sasol Limited Chemical

Reactor
3.5 m ID x 38 m H

Straight Though Transport Reactor

waxes and distillate fuels

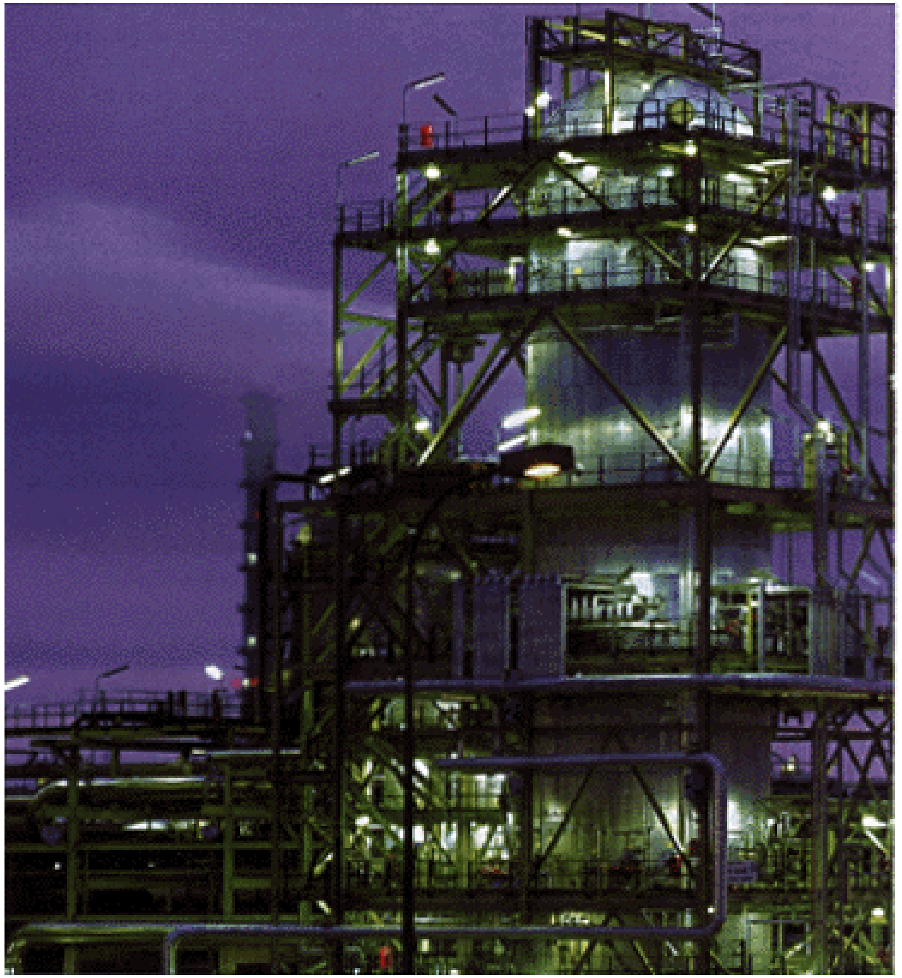




http://www.hcasia.safan.com/mag/hnov02/it60.pdf

Sasol Advanced Synthol (SAS) Reactor

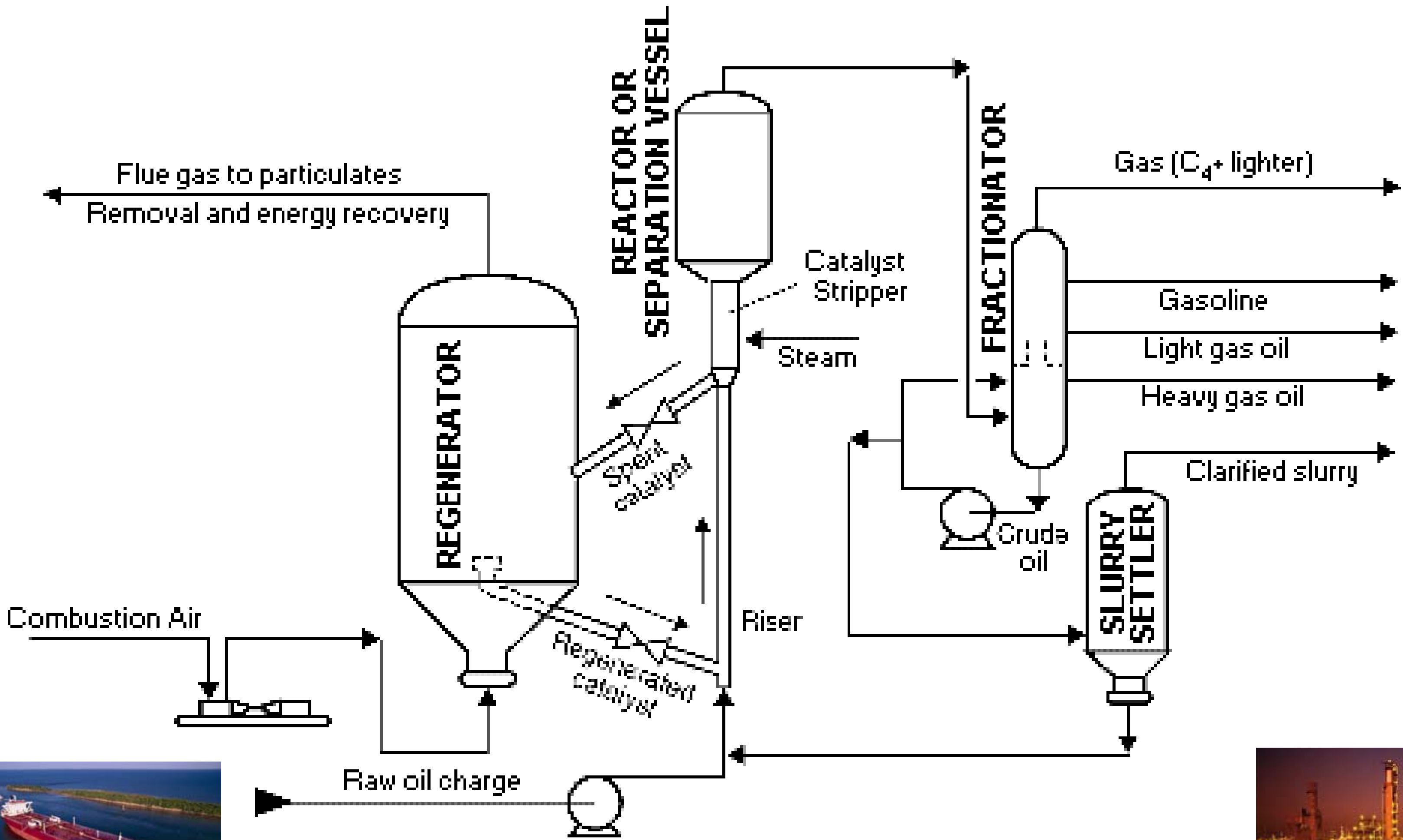
light olefins and gasoline fractions



流動層型 反應裝置

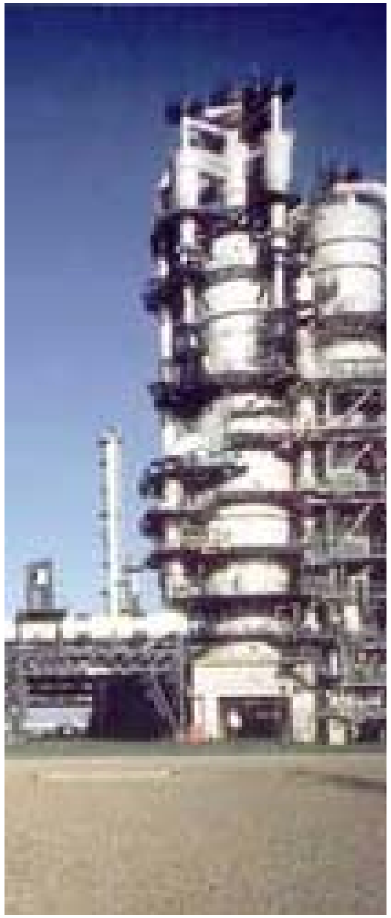
Fluidized Catalytic Cracking Unit

in the petroleum refining industry



Fluidized Catalytic Cracking Reactor

流動層型 反應裝置



Stone & Webster's

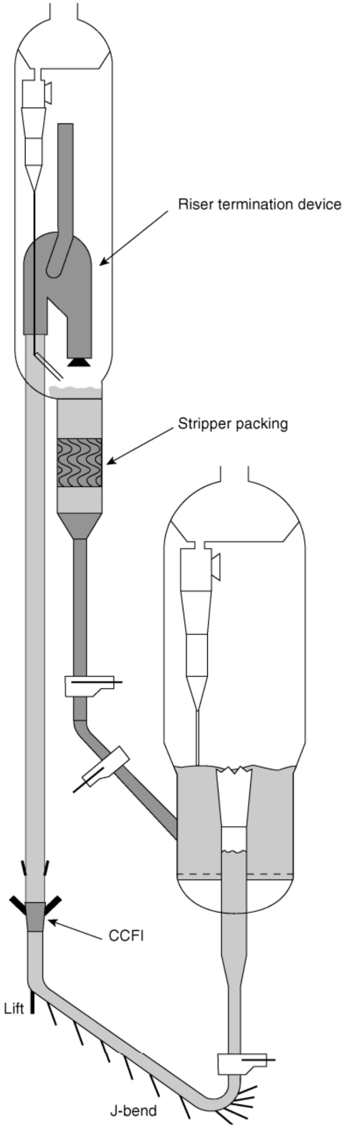
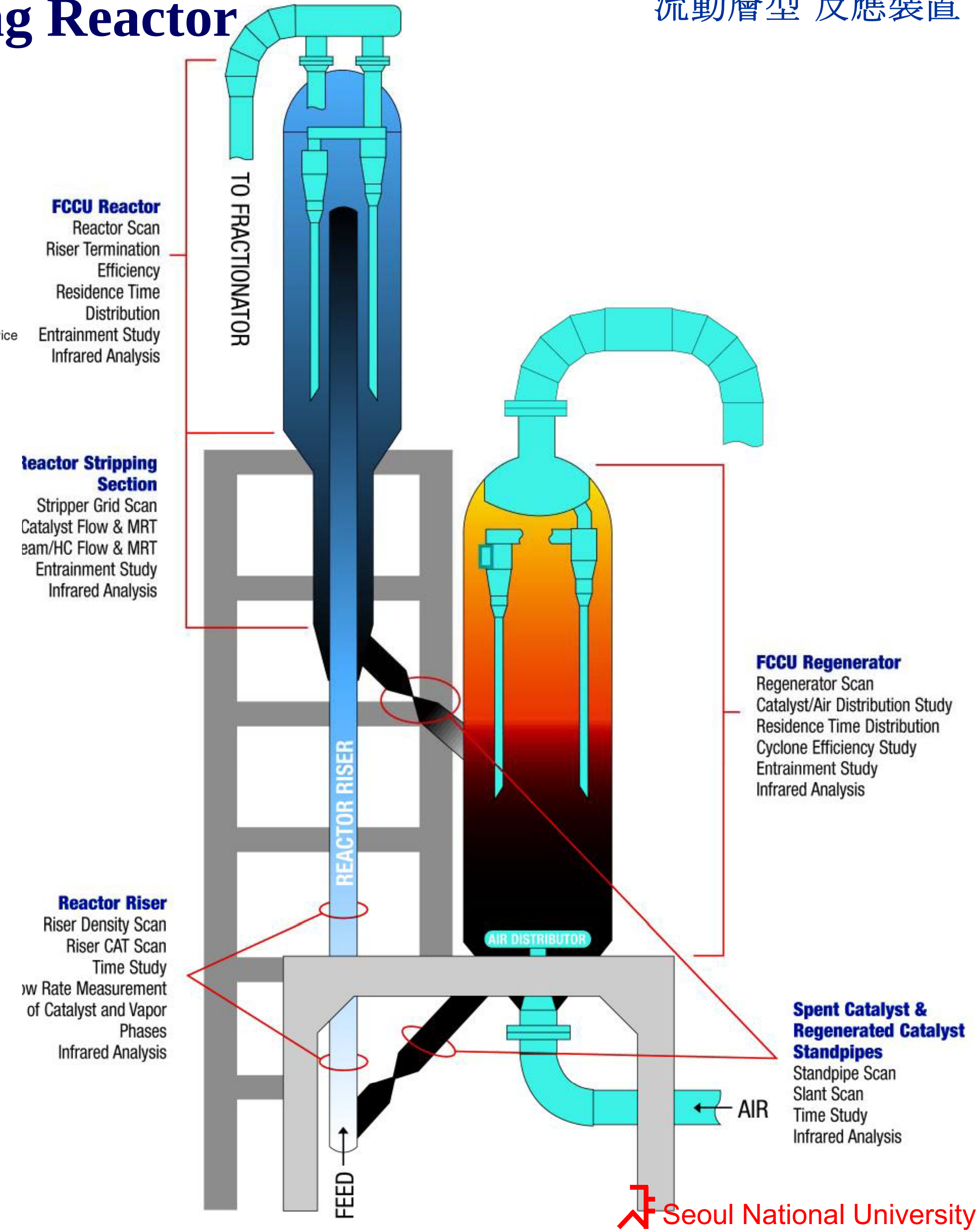


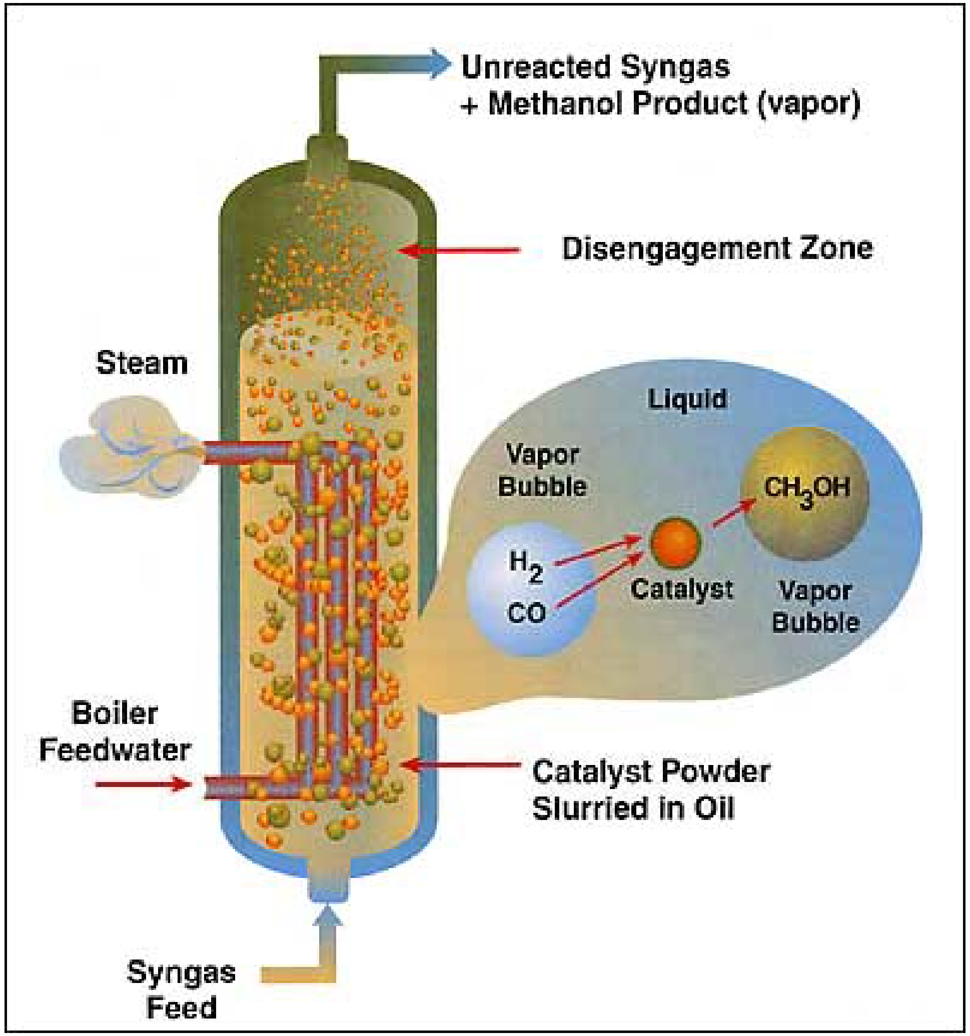
Figure 1
Dunkerque FCC unit configuration.



Slurry Phase Distillate Reactor

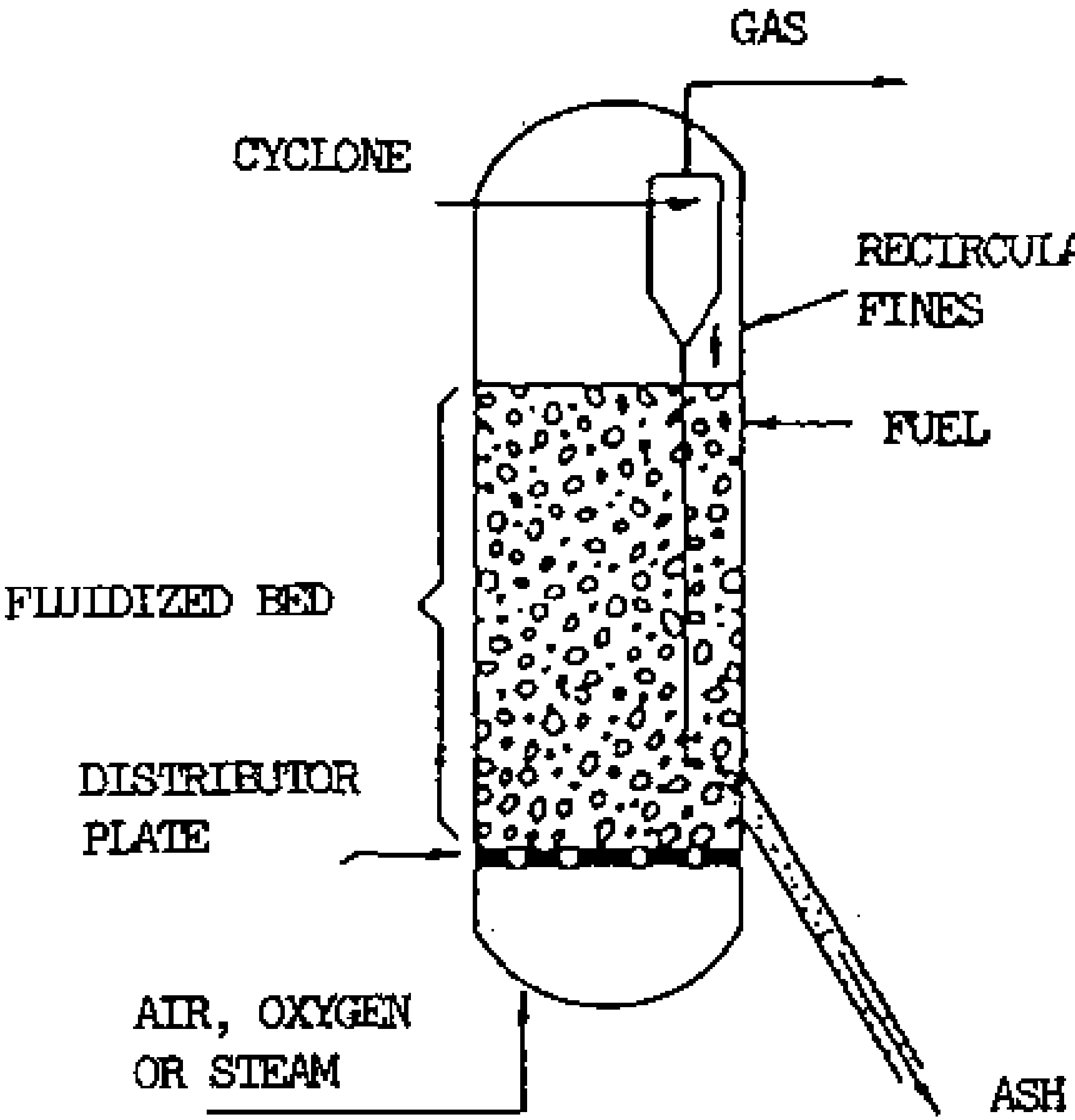
氣泡塔型 反應裝置

Bubble Column Reactor
For Fischer-Tropsch Reaction



www.fe.doe.gov/programs/.../tl_liqphase_schematic.html

Fluidized Bed Gasification Reactor

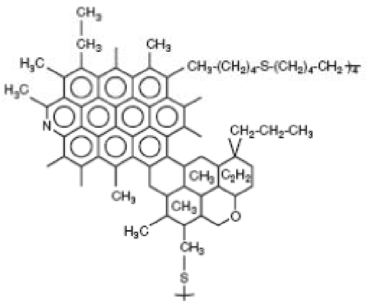


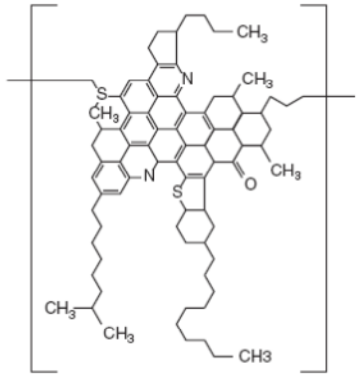
www.fao.org/DOCREP/T0512E/
T0512e0a.htm

GTL reactor for Sasol
coal-gasified gas into synthetic oil

Residual Oil Fluidized-Bed Catalytic Cracking reactor

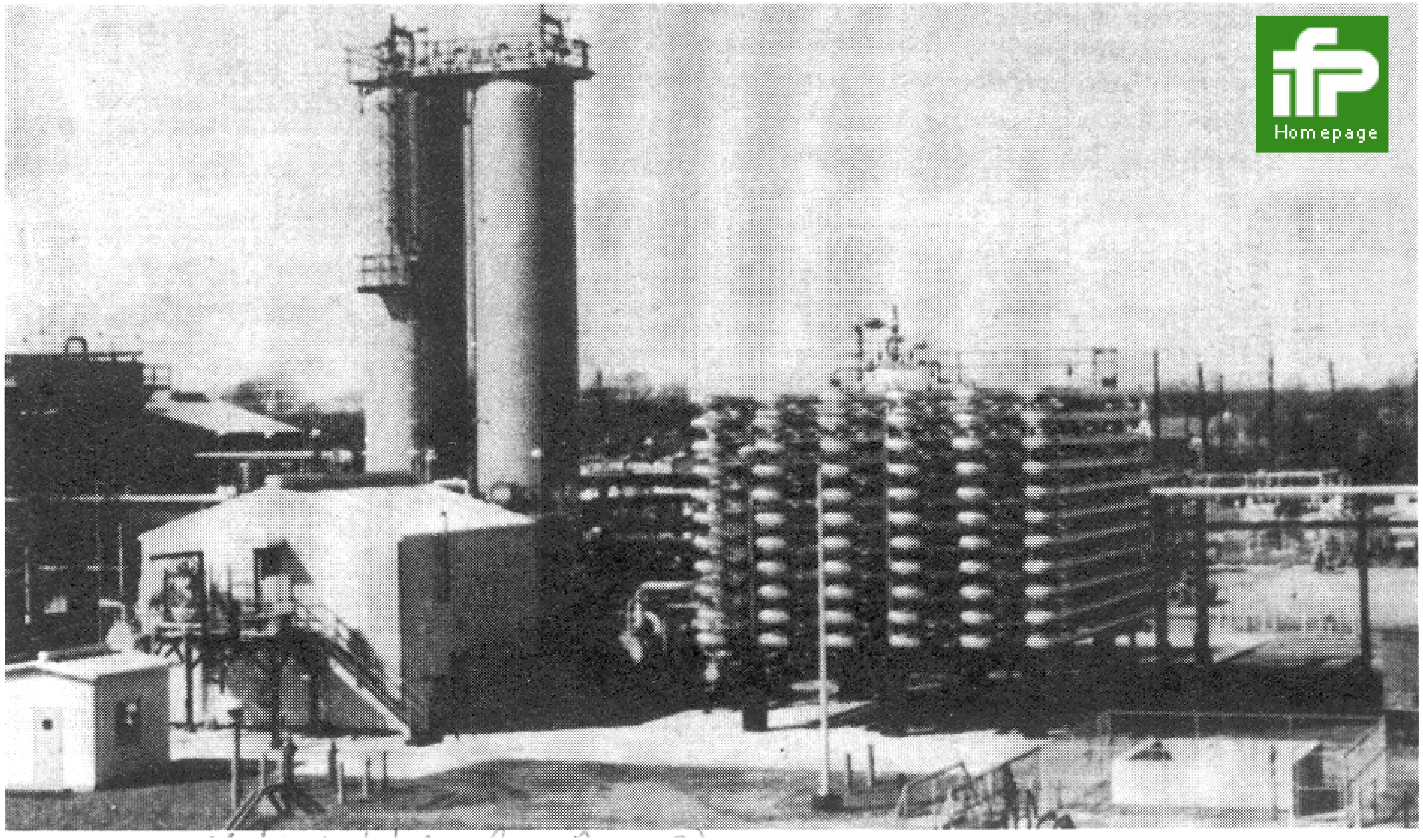
Asphaltene molecules
MW = 500 - 1000 g/mol





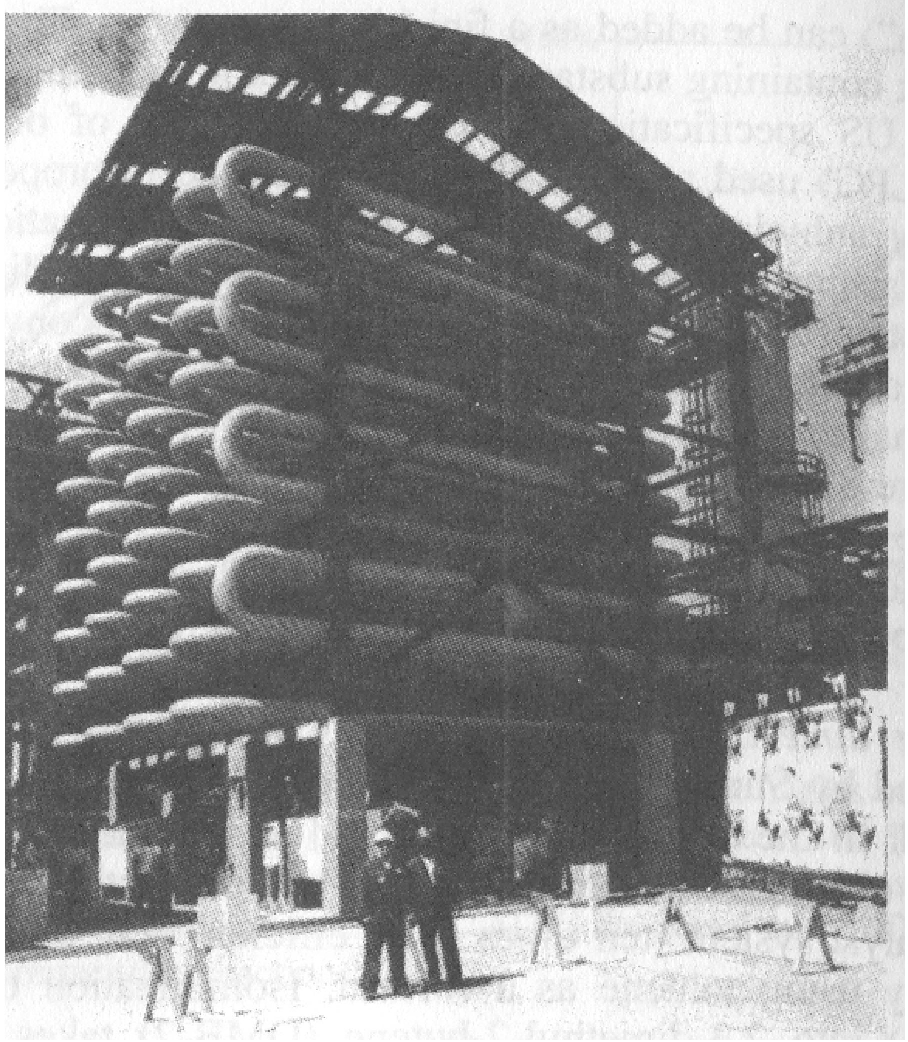
Dimersol G unit (Two –CSTR and one PFR in series)

Institute Français du Petróle Process



http://www.ifp.fr/ **Dimerization propylene into isohexanes**

Plug-flow reactor for Dimersol™ process



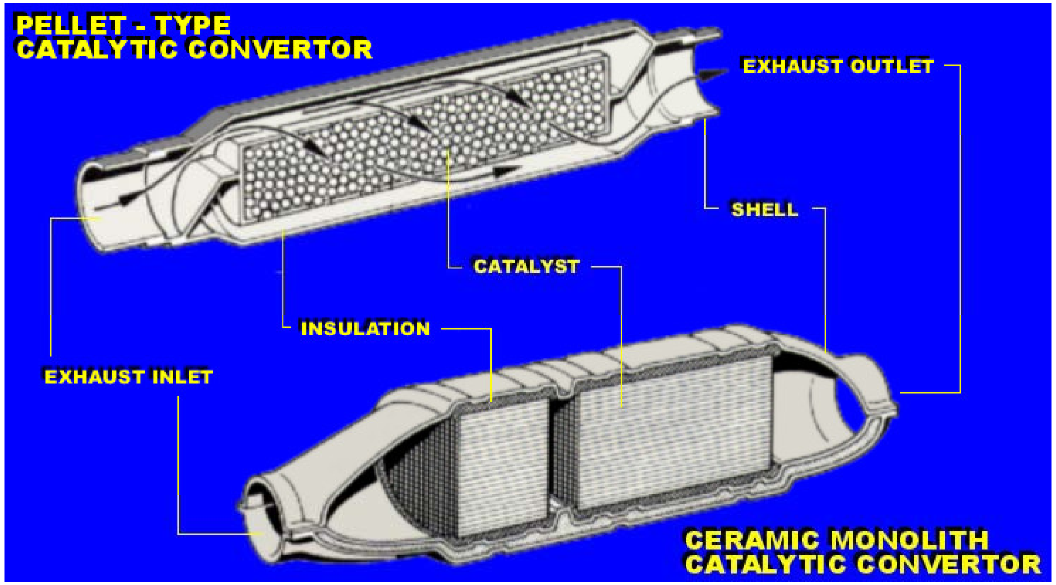
The finishing reactor ("the snake") to comply with LPG specification in the USA (less than 5% olefins)

Automotive Catalytic Converter

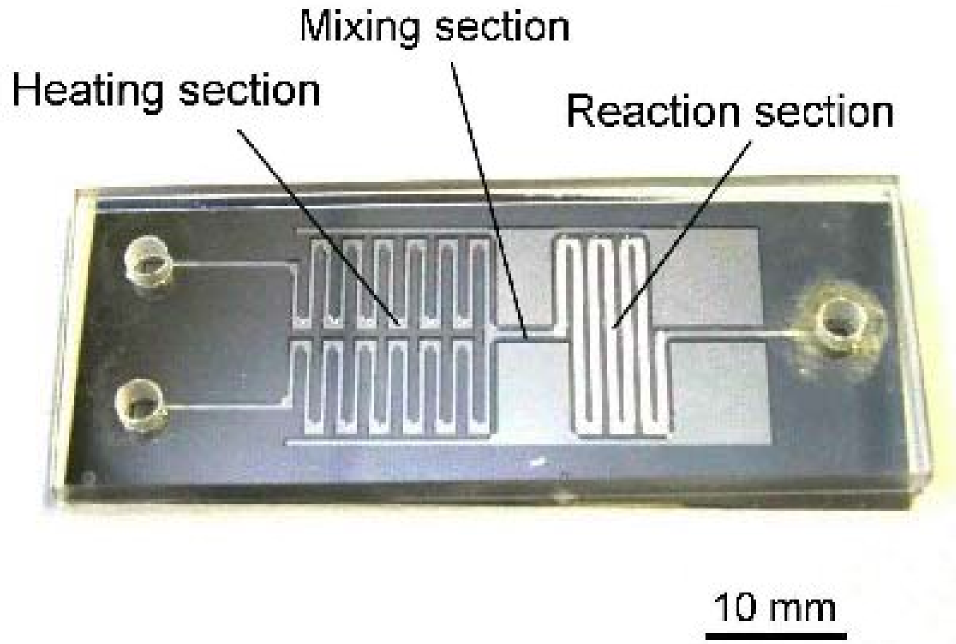
$$2NO \rightarrow N_2 + O_2$$

$$2NO_2 \rightarrow N_2 + 2O_2$$

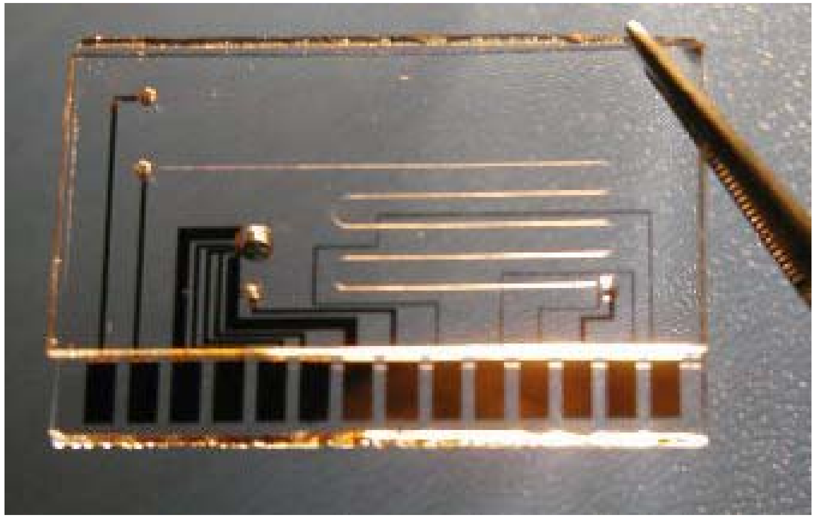
$$2CO + O_2 \rightarrow 2CO_2$$



Microreactor and Lab-on-Chip



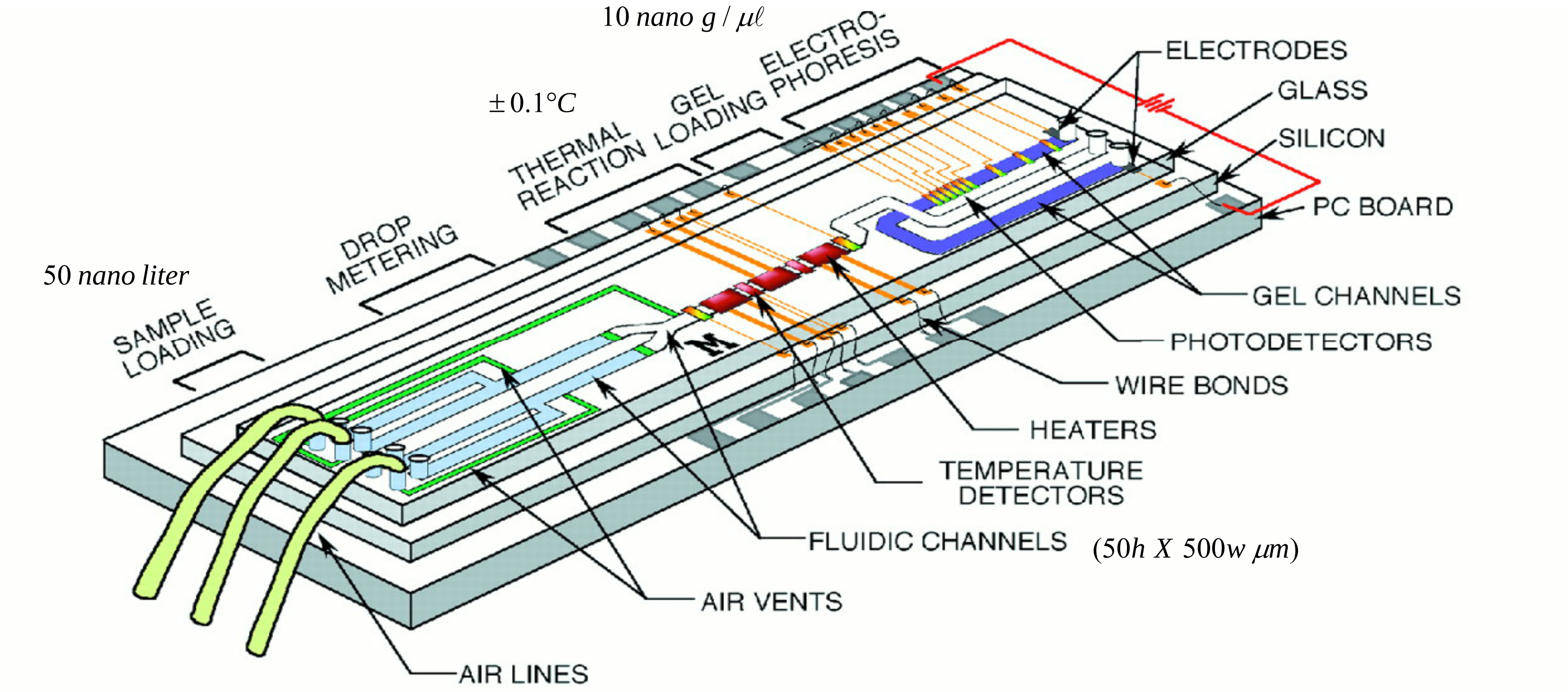
Microreactor made of silicon anodically bonded with glass

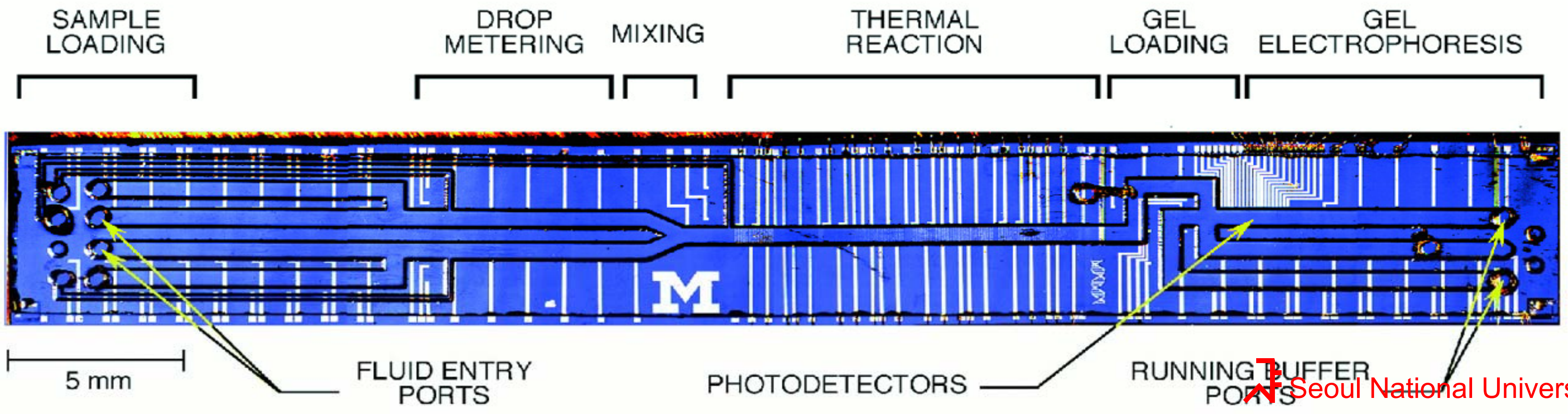


Lab-on-Chip made of glass and polymer for DNA amplification and detection

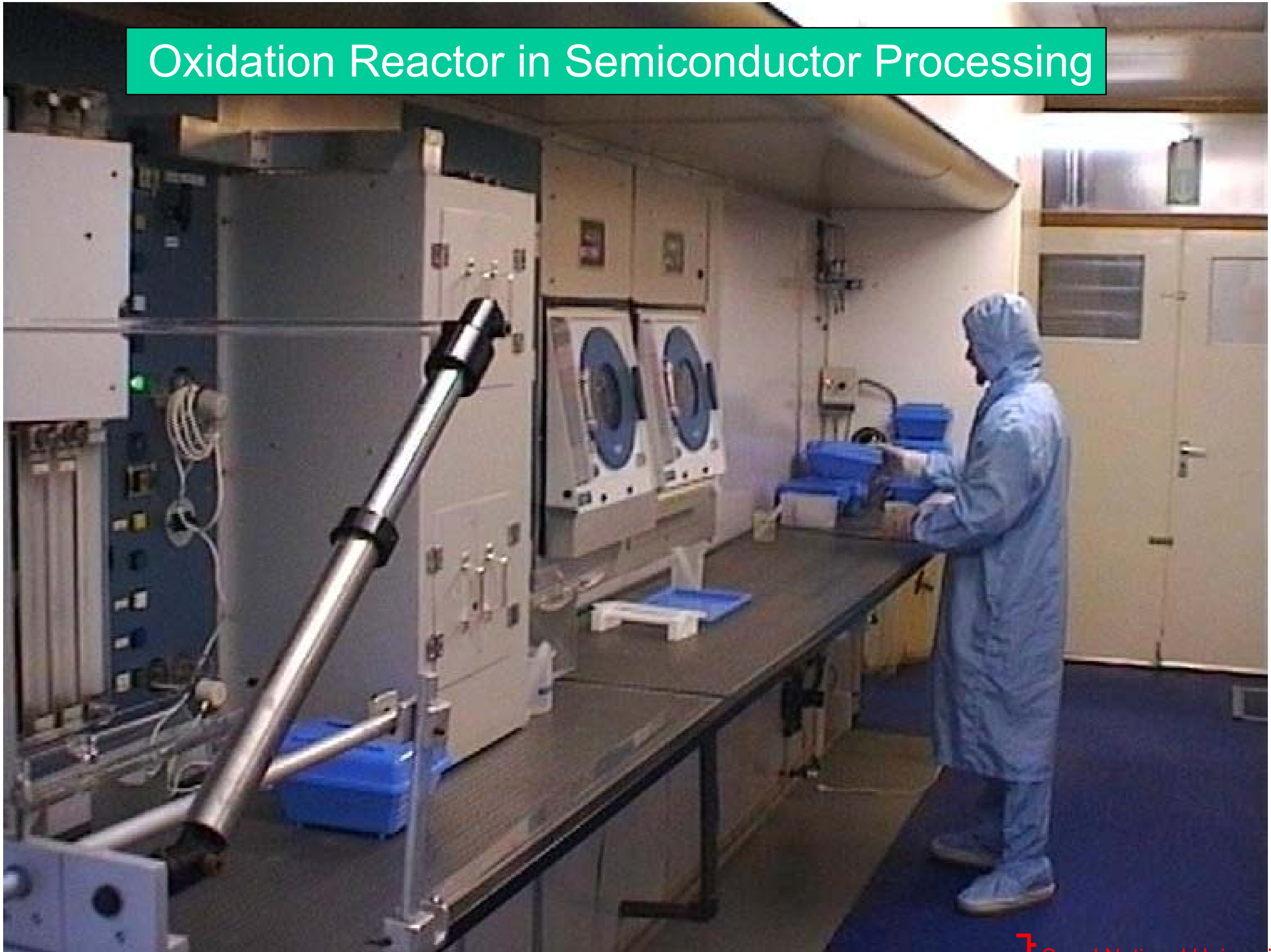
Rutherford Appleton Laboratory (RAL) in the UK

Microreactor for DNA analysis

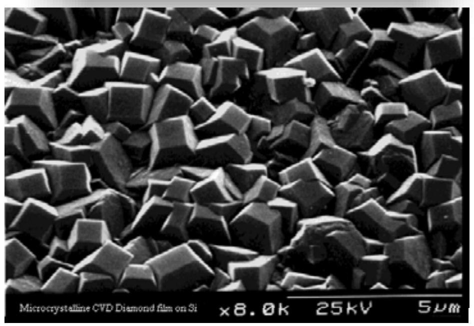




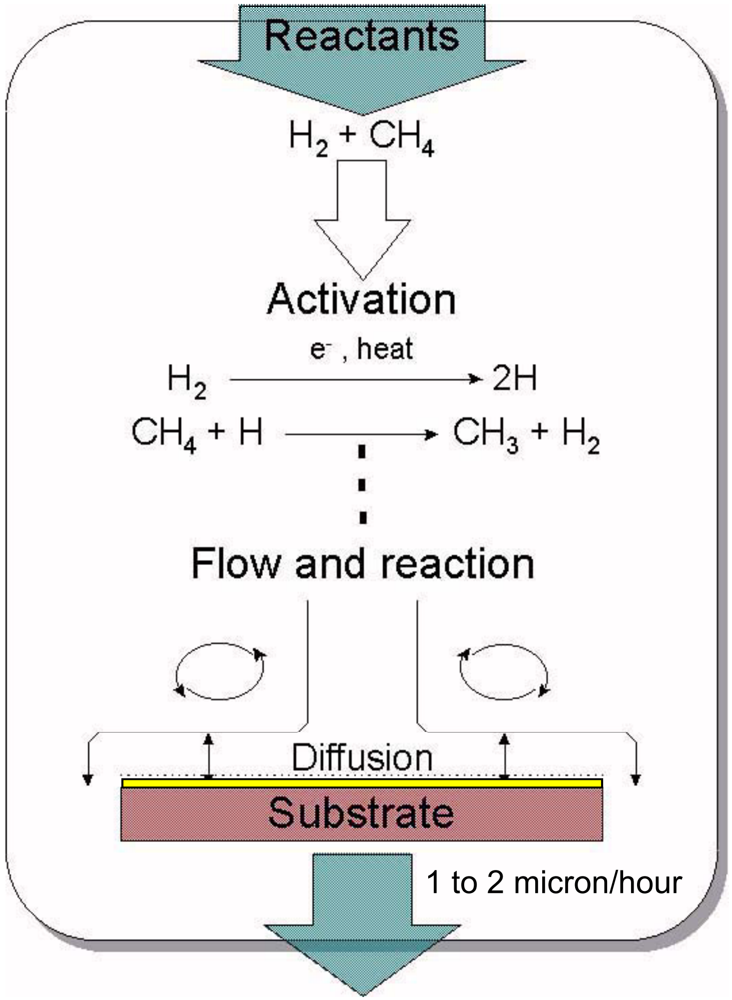
Oxidation Reactor in Semiconductor Processing



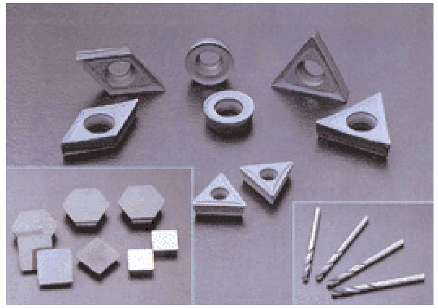
Diamond film is synthesized through CVD (Chemical Vapor Deposition)

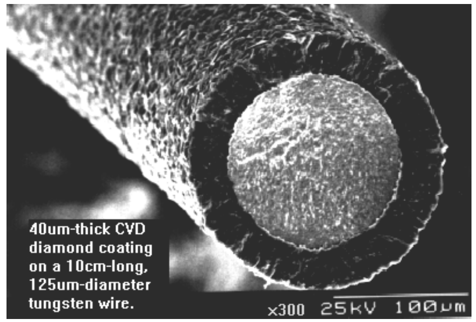


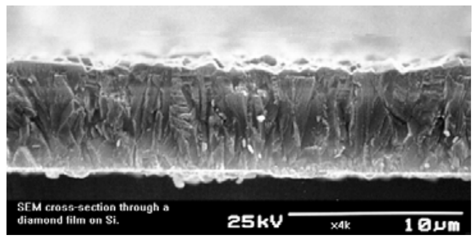
SEM of Diamond Films on
Si-wafer substrate



CVD Diamond coated tools

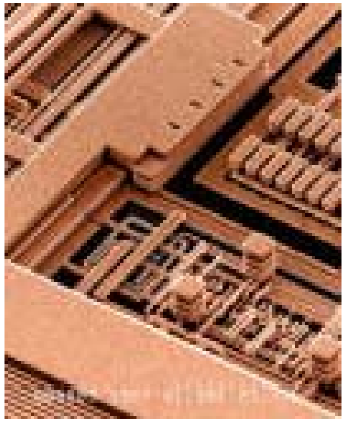


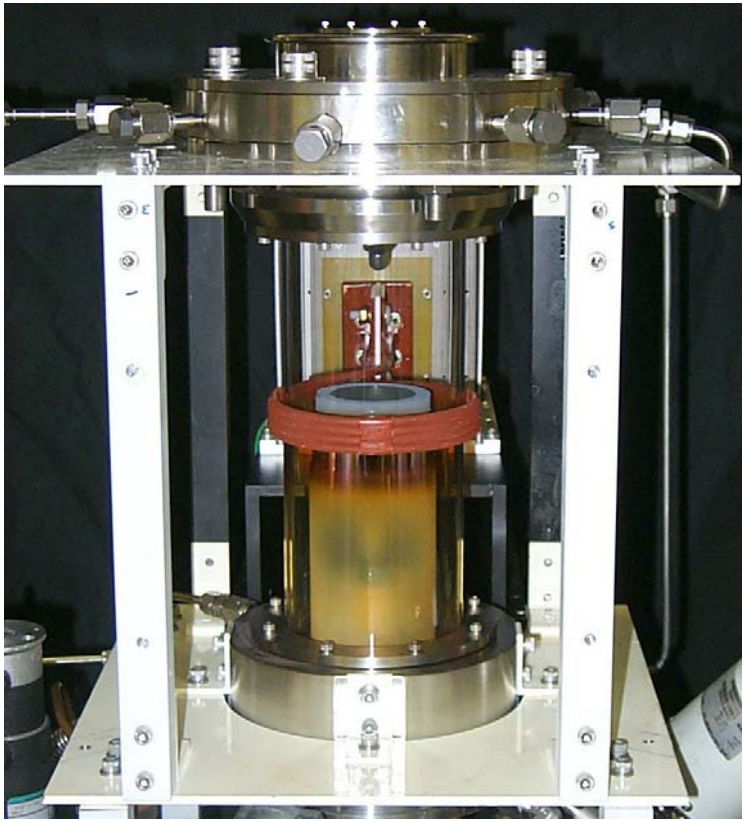


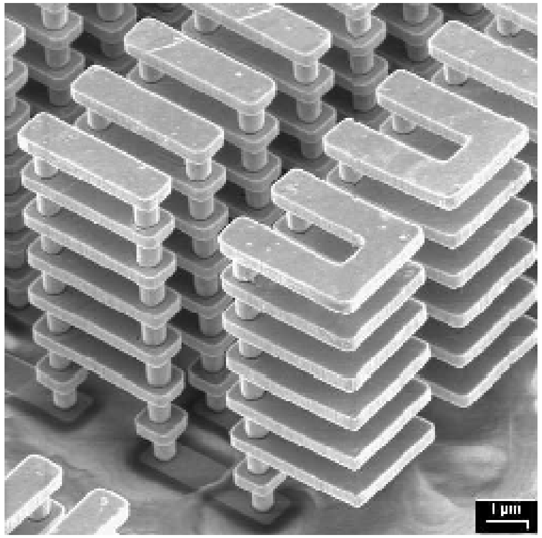


Metallization

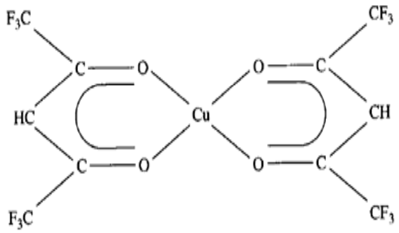
$$Cu(hfac)_2 + H_2 \rightarrow Cu + 2H(hfac)$$

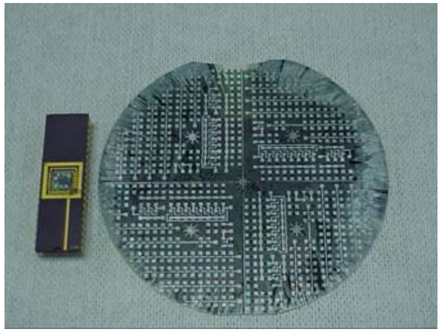






Copper Stacked Via structures





Integrated Circuit Wafer and Packaged Device

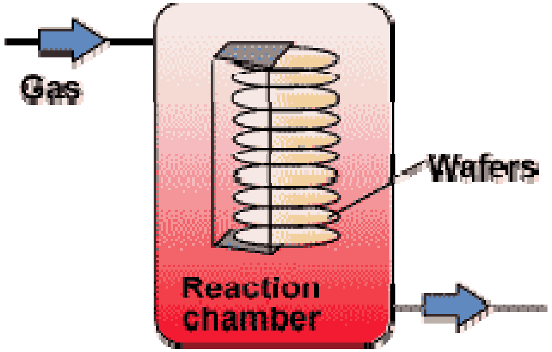
bis-hexafluoroacetyl-acetonate-Cu^{II}

$(CF^3COCHCF^3CO)^2Cu$

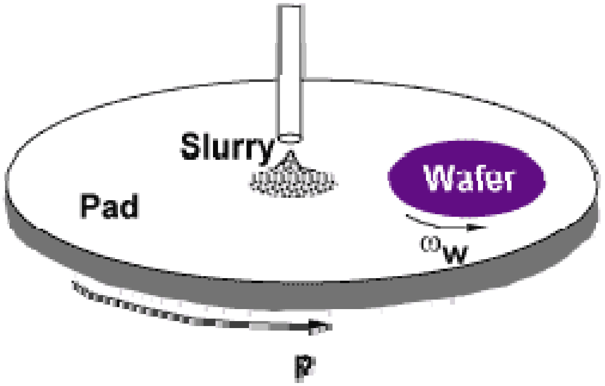
$Cu^{II}(hfac)_2$

Chemical Reactions in Microelectronics Processing

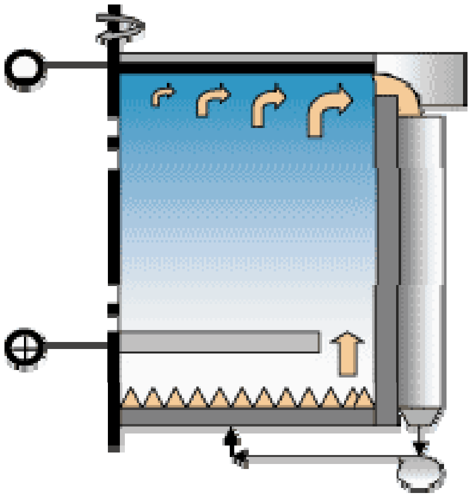
Chemical Vapor Deposition



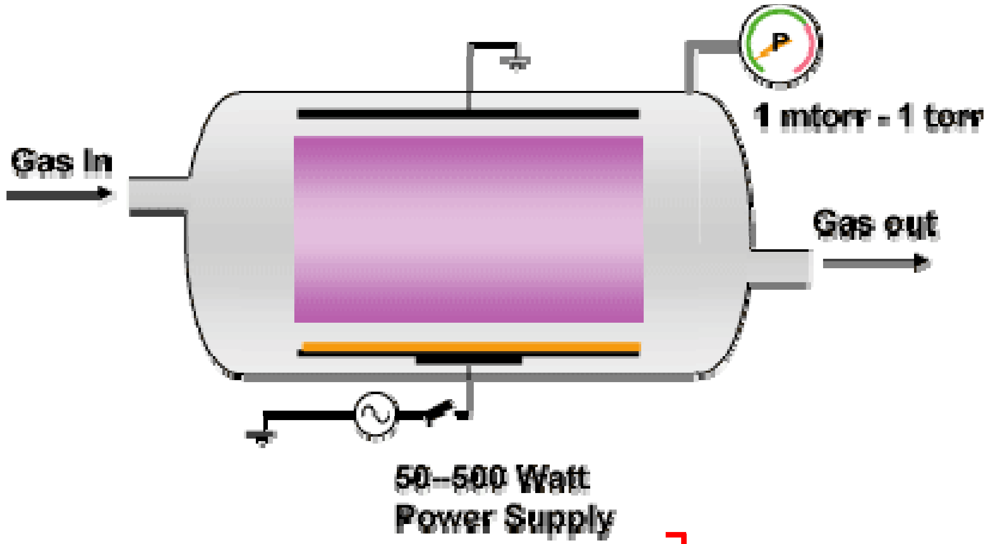
Chemical Mechanical Polishing



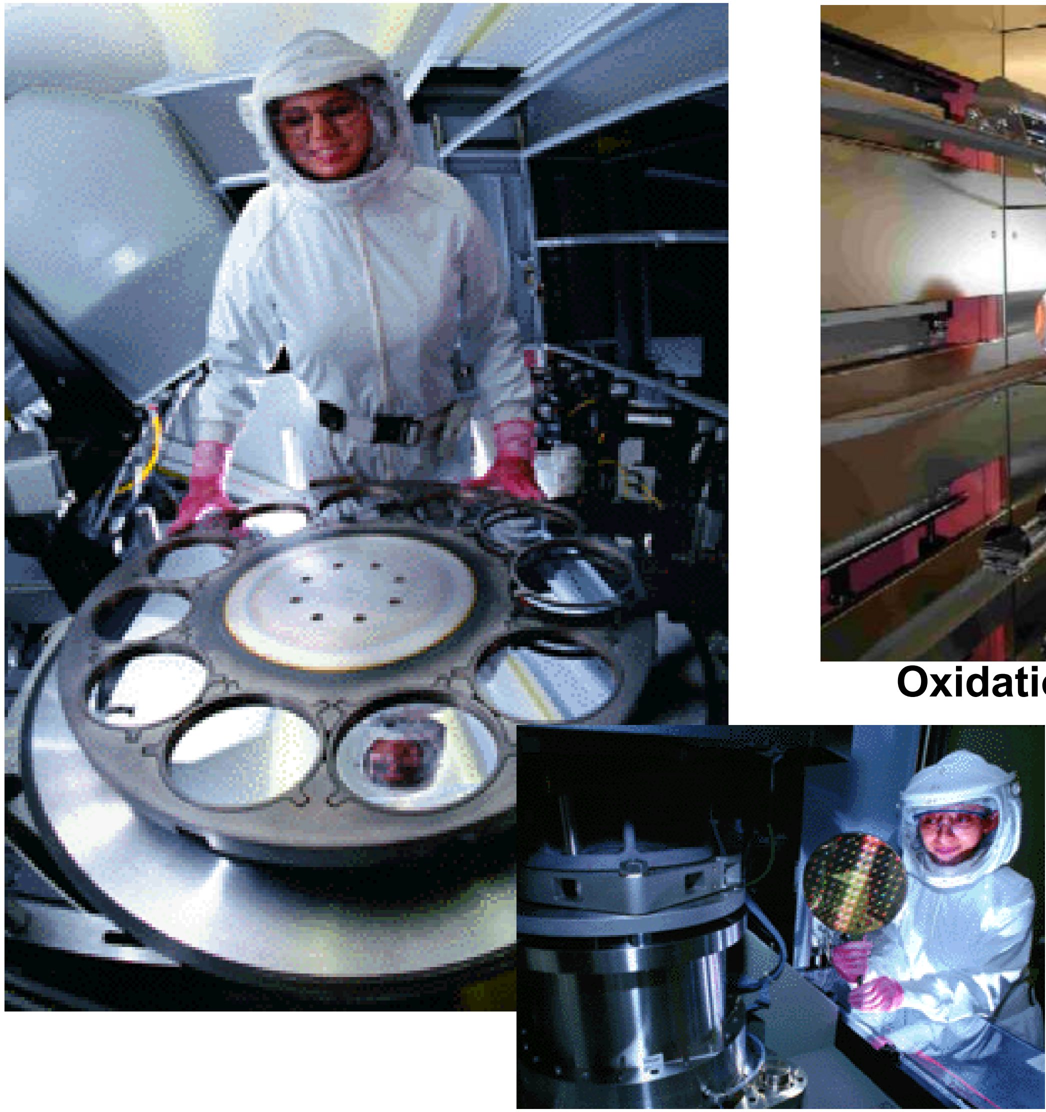
Electrochemical Deposition



Plasma Etching

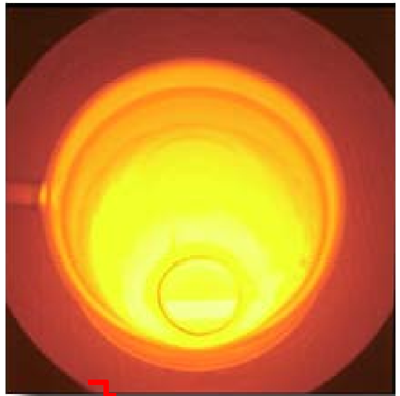


Metal Deposition in Microelectronics Processing



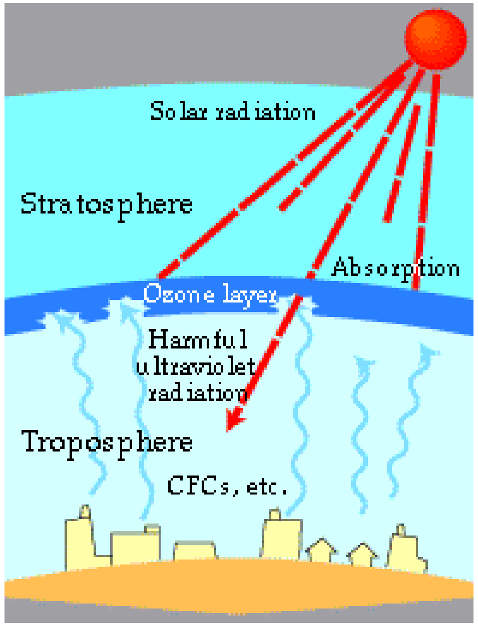
$$Si + 2H_2O \rightarrow SiO_2 + 2H_{2\ (g)}$$
$$Si + O_2 \rightarrow SiO_2$$

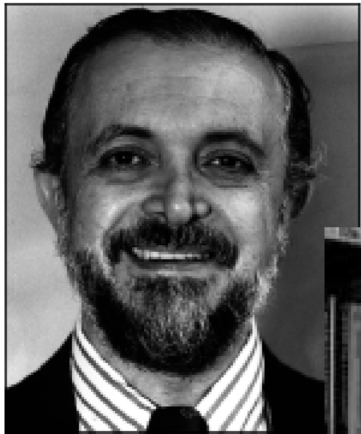
Oxidation reactor silicon-diffusion furnace



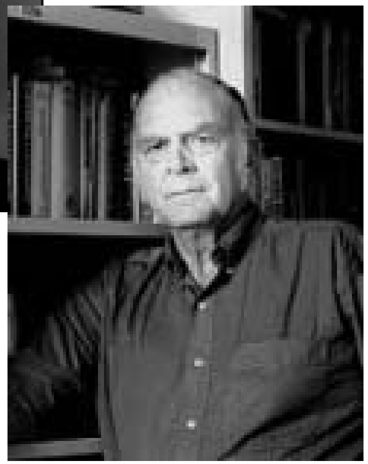
Metal Deposition Reactor

Ozone Depletion Reaction in Stratosphere



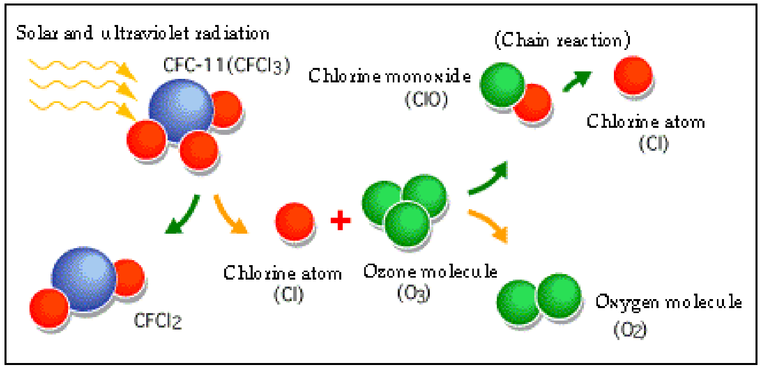


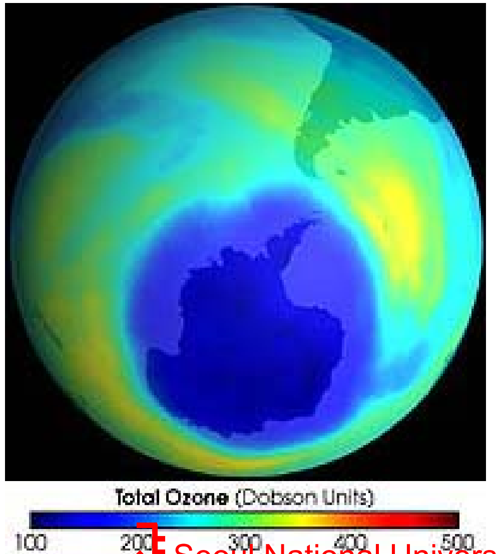
Mario Molina
(MIT)



F. Sherwood Rowland
(U. C. Irvine)

Paul Crutzen
(Seoul National University)

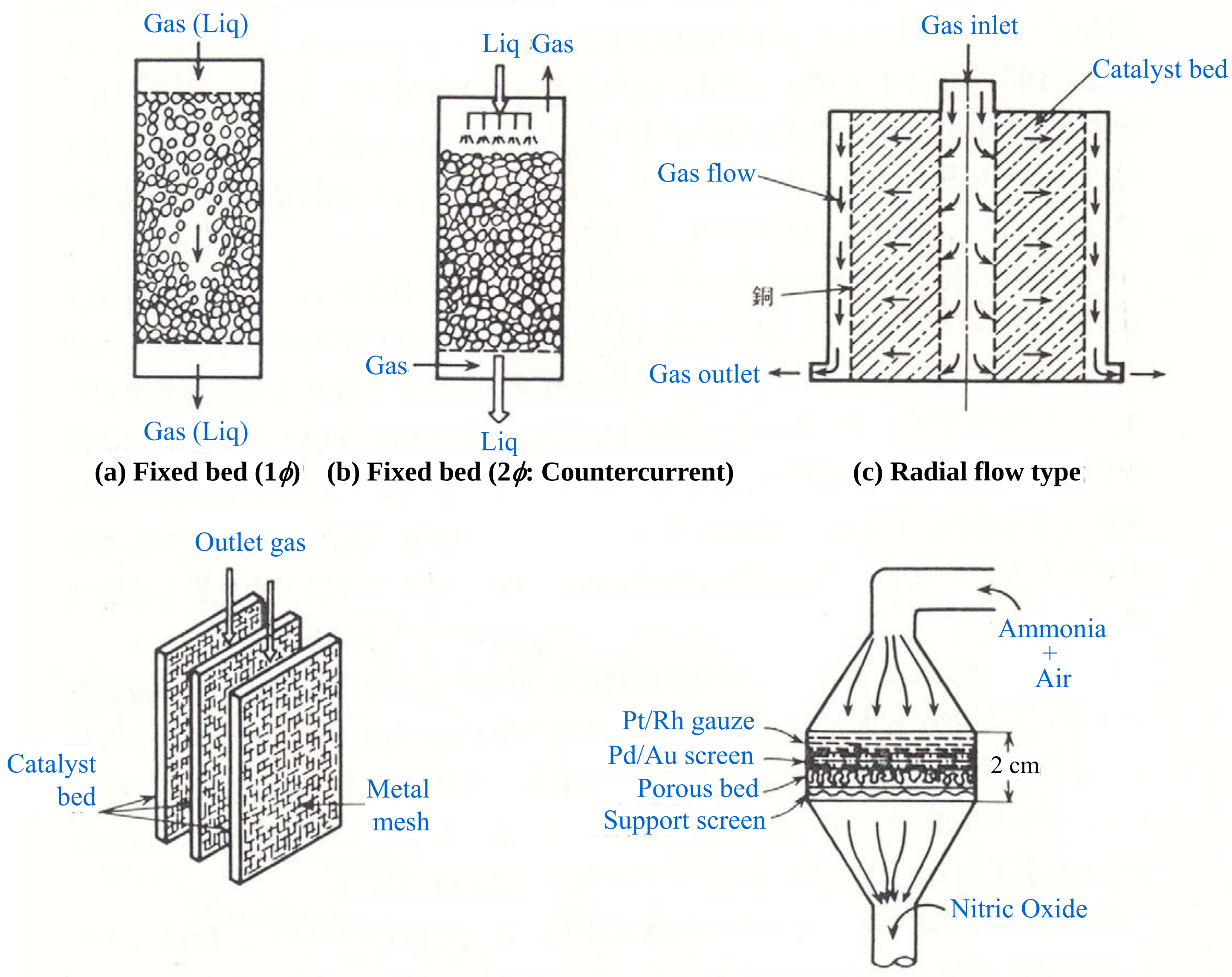




工業反應裝置 分類

1. 固定層型 反應裝置 (Fixed bed)
2. 移動層型 反應裝置 (Moving bed)
3. 流動層型 反應裝置 (Fluidized bed)
4. 攪拌槽型 反應裝置 (Stirred Tank)
5. 氣泡塔型 反應裝置 (Bubble cap tower)
6. 管型 反應裝置 (Tubular)
7. 火炎型 反應裝置 (Flammed)
8. 氣流型 反應裝置 (Pneumatic conveying)
9. 段塔型 反應裝置 (Multi-staged)
10. 回轉圓板型 反應裝置 (Rotary)

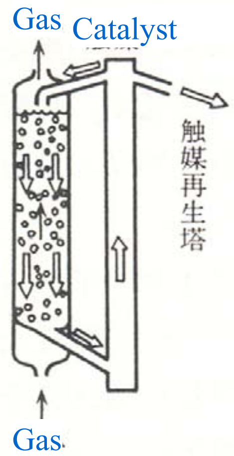
固定層型 反應裝置 (Fixed bed)



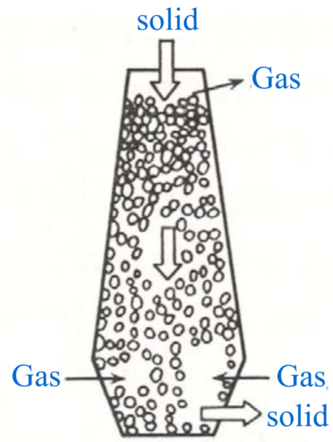
(a) Fixed bed (1ϕ) **(b) Fixed bed (2ϕ: Countercurrent)** **(c) Radial flow type**

(d) Parallel flow type **(e) Thin bed catalysis reactor (Ammonia Oxidation)**

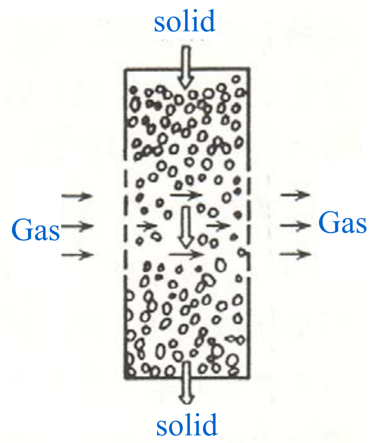
移動層型 反應裝置 (Moving bed)



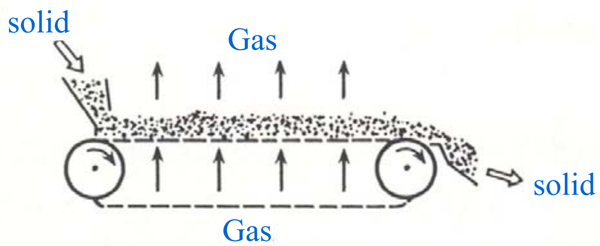
(a) Countercurrent (gas-solid cat. rxn)



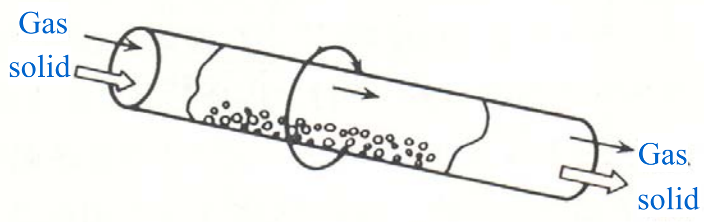
(b) Countercurrent (gas-solid rxn)



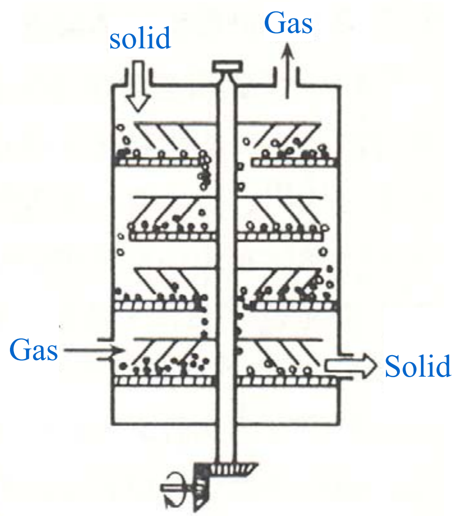
(c) Cross flow



(d) Moving grid

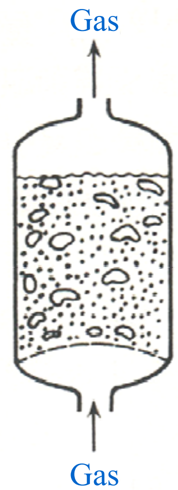


(e) Rotary kiln (rotated)

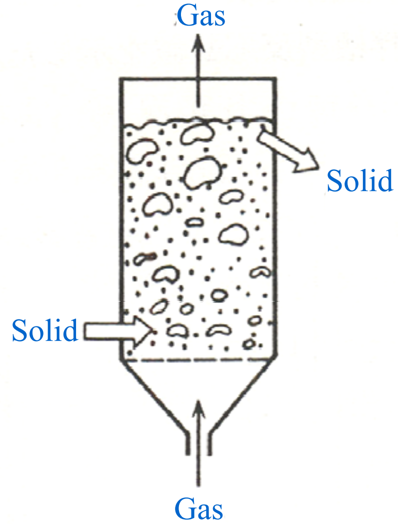


(f) Multistaged

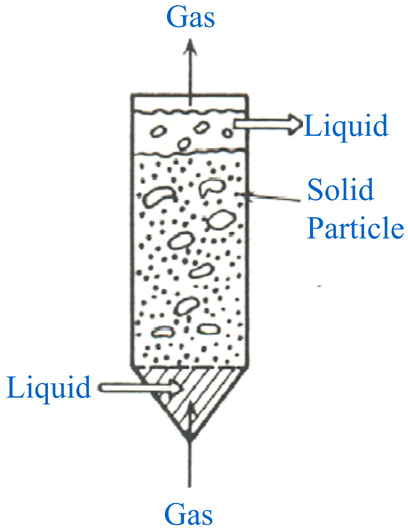
流動層型 反應裝置 (Fluidized bed)



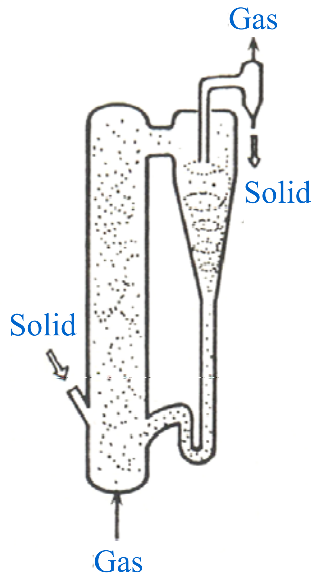
(a) Fluidized bed
(gas-solid cat.)



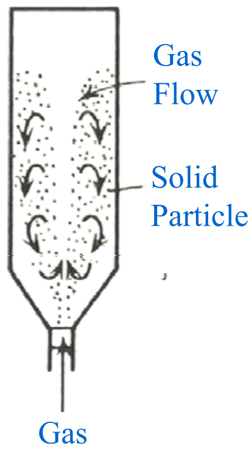
(b) Fluidized bed
(gas-solid rxn)



(c) 3ϕ Fluidized bed

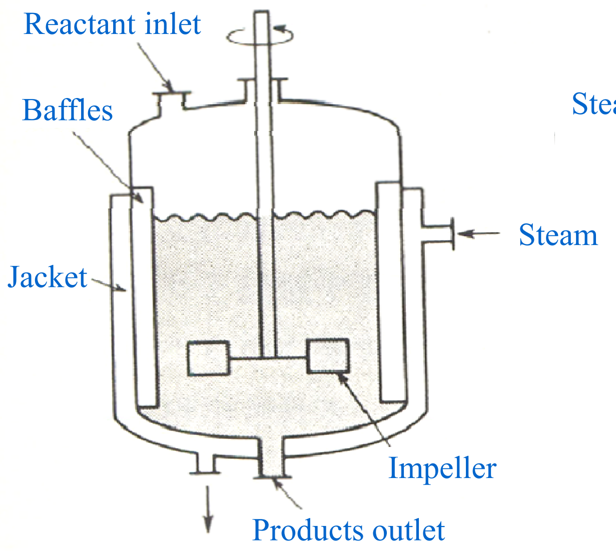


(d) High flow fluidized bed

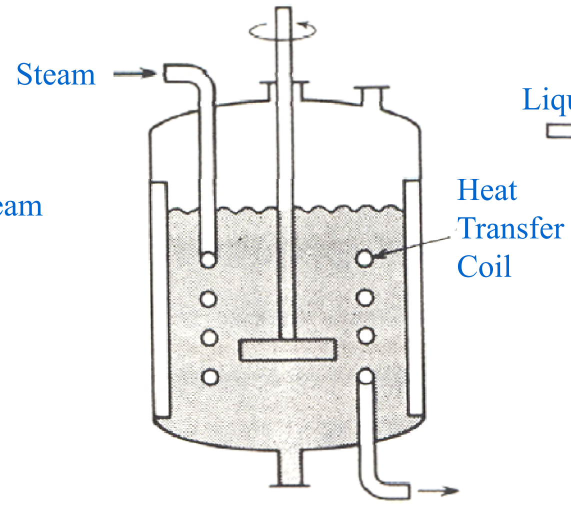


(e) Spray flow bed

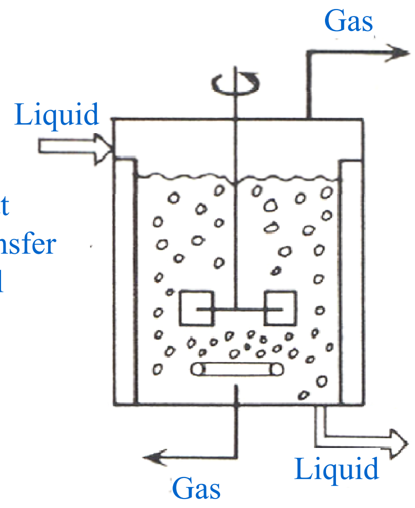
攪拌槽型 反應裝置 (Stirred Tank)



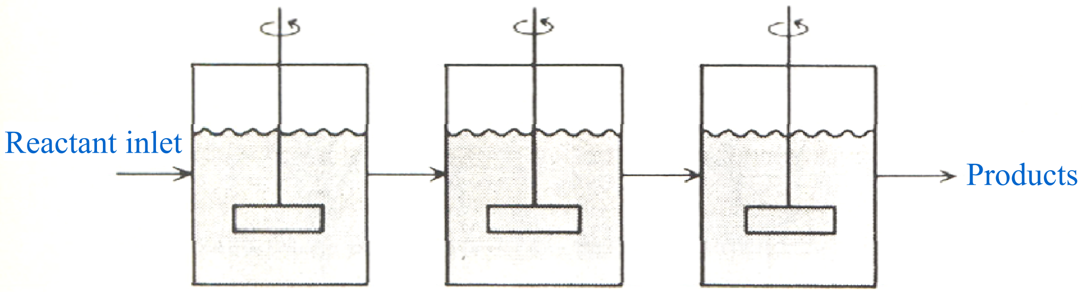
(a) CSTR (Jacket)



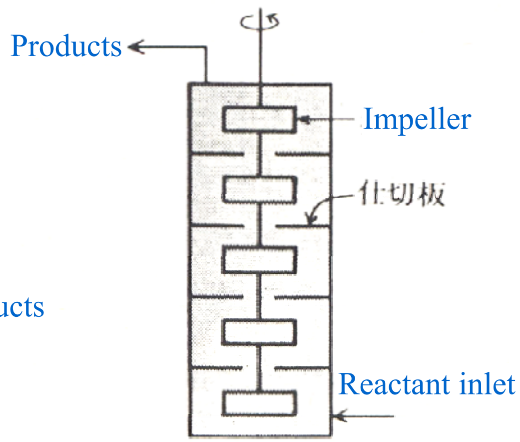
(a) CSTR (Coiled)



(c) CSTR (G-L)

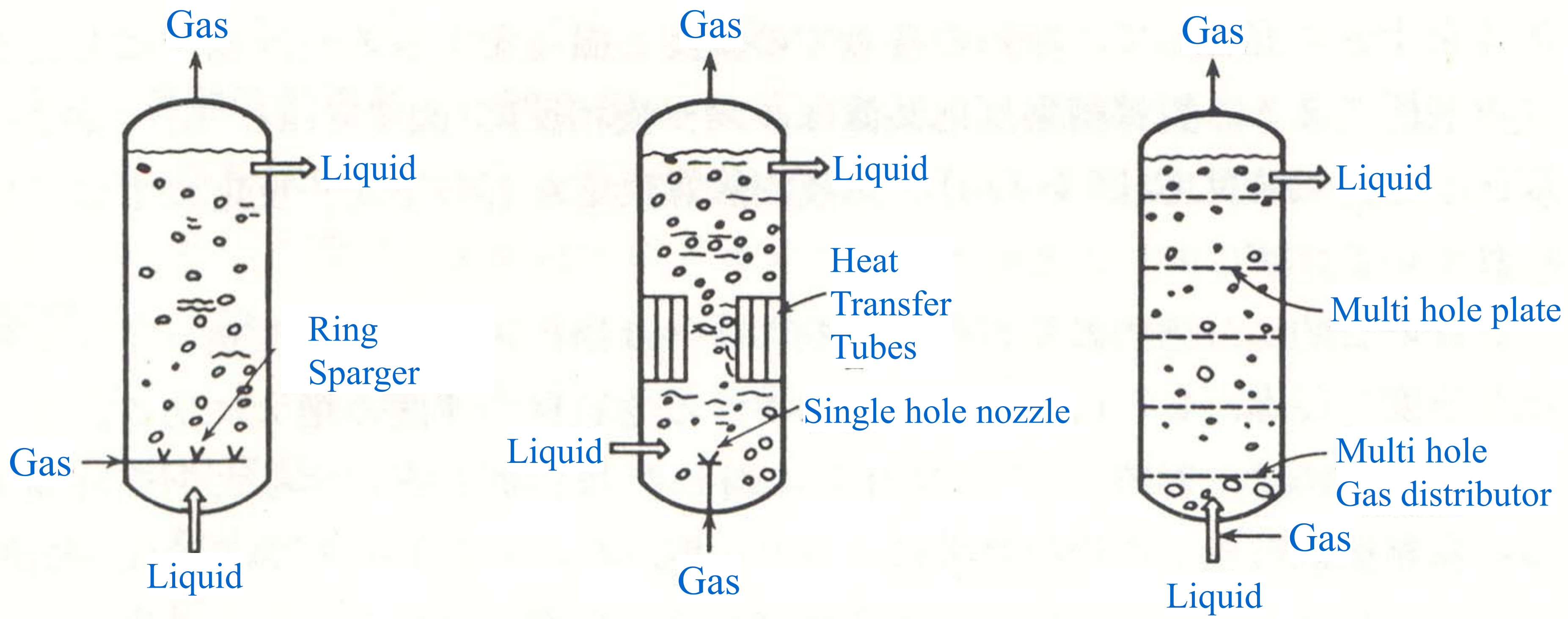


(d) Series CSTRs



(e) Multi-Staged CSTRs

氣泡塔型 反應裝置 (Bubble cap tower)

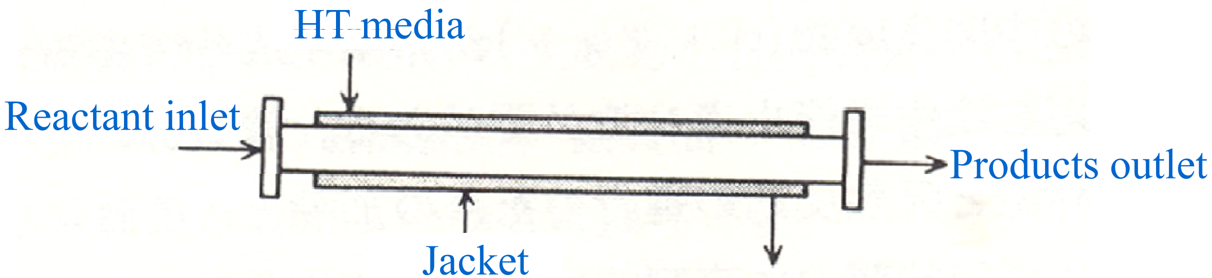


(a) Ring sparger type

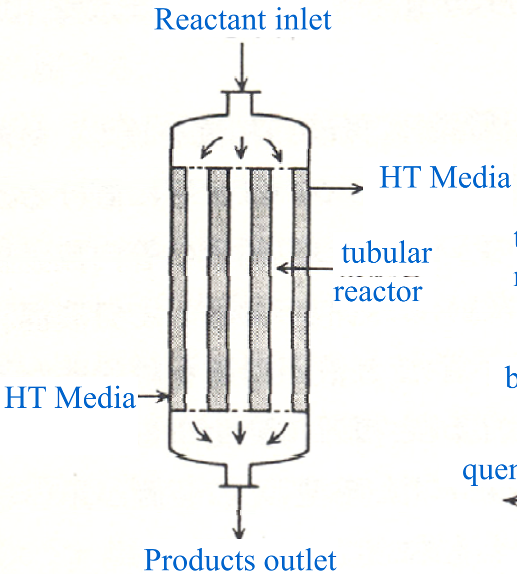
(b) Single nozzle gas distribution

(c) Multi hole gas distribution

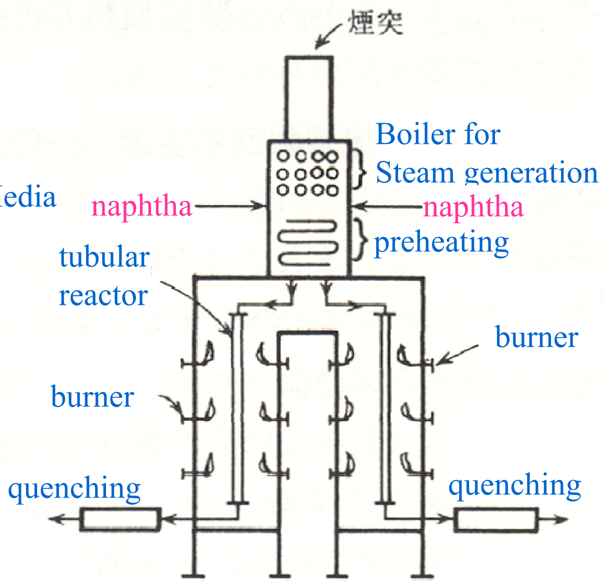
管型 反應裝置 (Tubular)



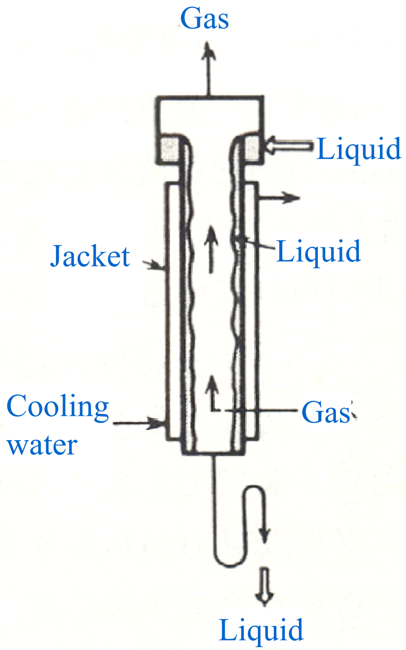
(a) Single tube type



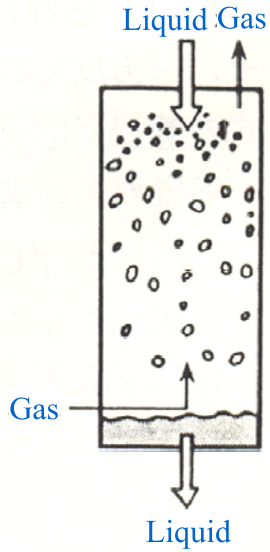
(b) Multi tube type



(c) Burner heated type

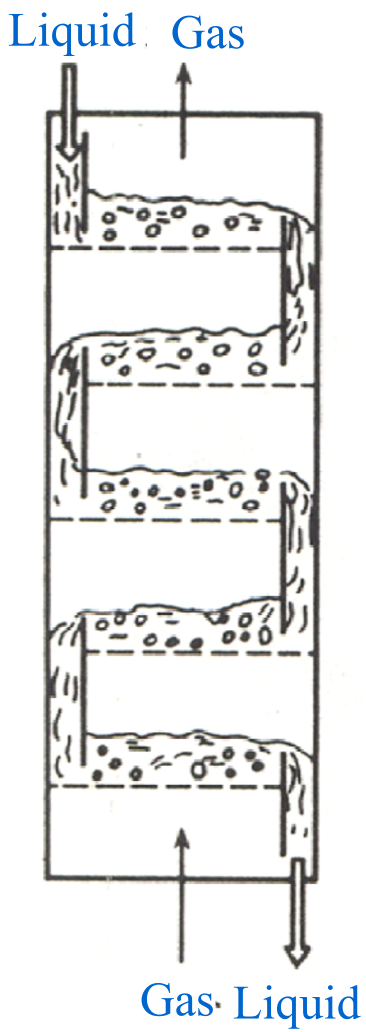


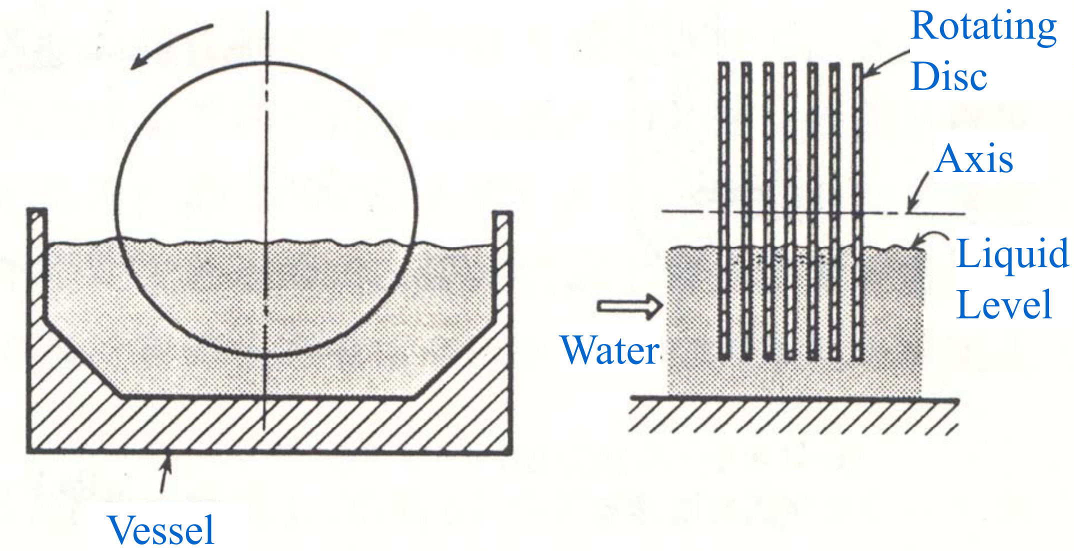
(d) Wetted wall type



(e) Spray tower

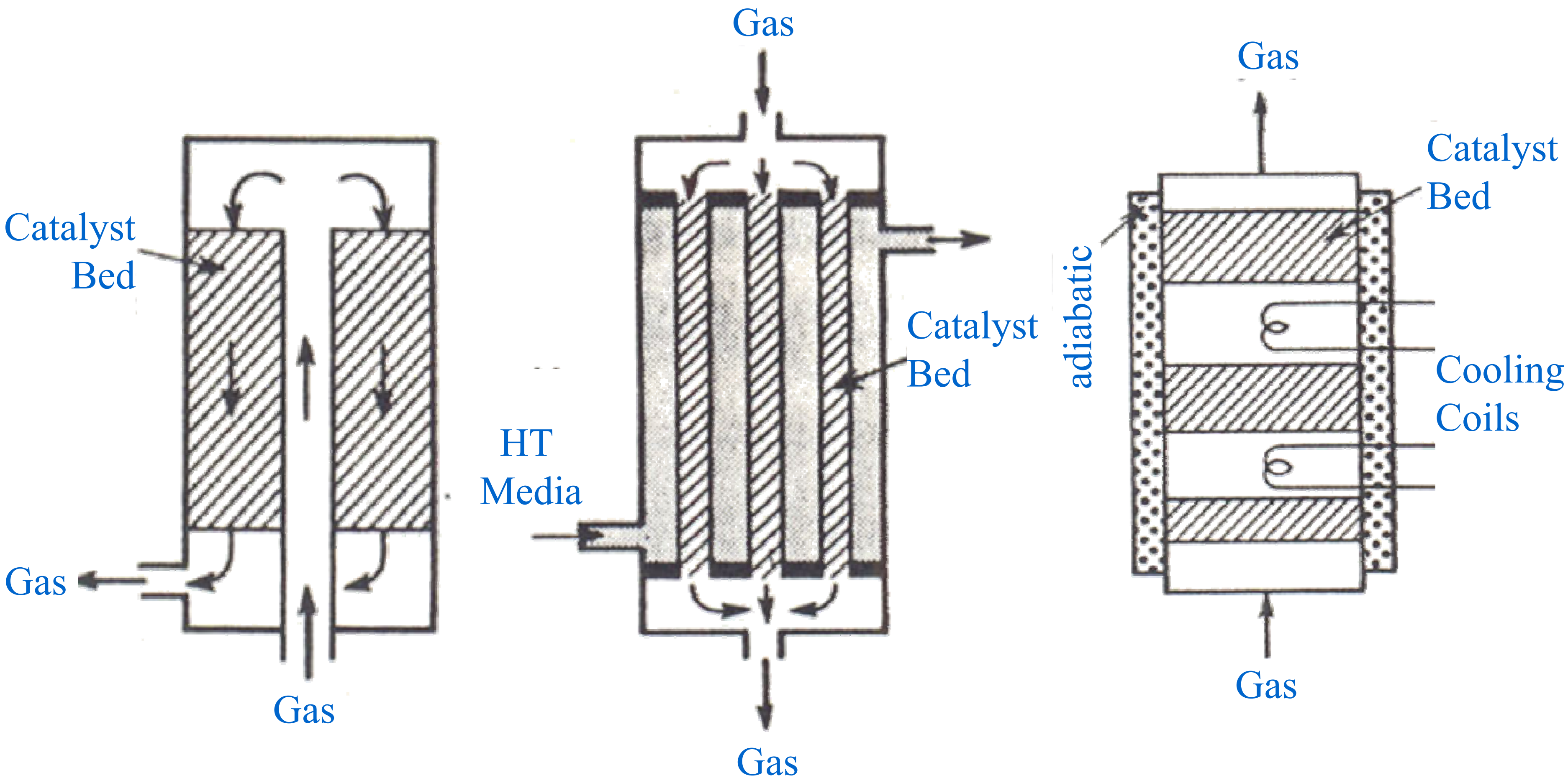
段塔型 反應裝置 (Multi-staged)





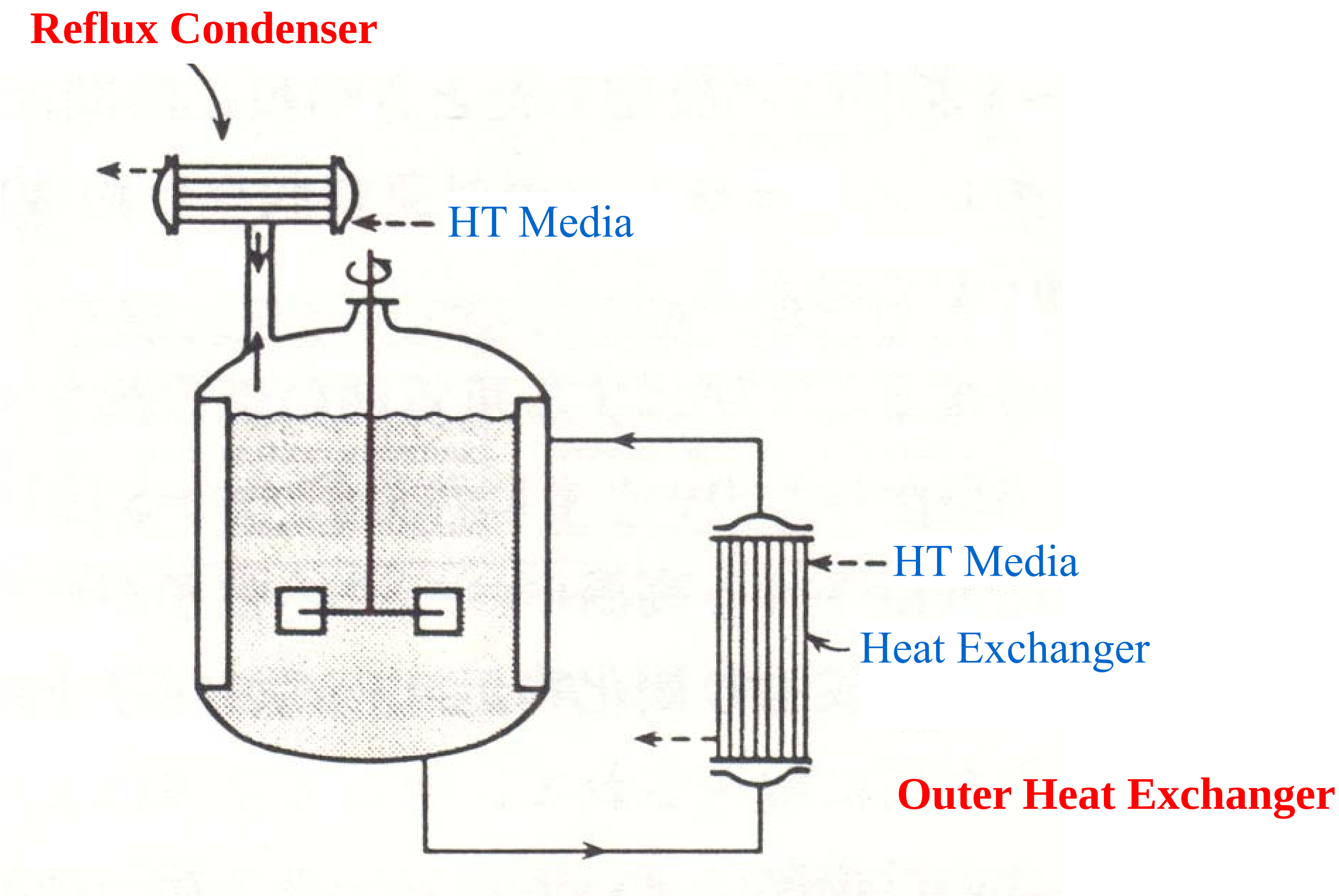
回轉圓板型 反應裝置 (Rotary)

Heat Transfer Mode in Fixed bed catalytic reactor



(a) Self-heat exchange (b) Multi-tube heat exchange (c) Internal cooler

Heat Transfer Mode in Stirred Tank Reactor



Selection of Reactor Type

Reactor \ Phase	G	L	SC	GS	GL	GLS	LL	LG	SS
Fixed bed		1				2		3	
Moving bed				4					
Fluidized bed			5	6					
Stirred tank		7			8	9	10	11	
Bubble cap					12				
Tubular	13								
Pneumatic				14					

G=Gas; phase, L= Liquid phase, SC=Solid catalyst, GS=Gas-Solid phase, GL=Gas-Liquid phase, GLS=Gas-Liquid-Solid phase, LL=Liquid-Liquid phase, LG=Liquid-Gas phase, LS=Liquid-Solid phase, SS=Solid-Solid phase

Selection of Reactor Type

1. Partial Oxidation of Propylene
   Ammonia Synthesis
   Naphtha Reforming Reaction
2. Hydrodesulphurization
3. Immobilized Enzyme Reaction
4. Production of Steel in Furnace
5. Sohio Process for Production of Acrylonitrile
   Fluidized Catalytic Cracking
6. Gas phase Polymerization of propylene
   Fluidized Coal Combustion
7. Bulk Polymerization of Styrene
8. Production of Antibiotics
9. Production of Terephthalic Acid
   Hydrogenation of Edible Oil
10. Emulsion Polymerization of SBR
11. Production of HDPE
12. Liquid phase Oxidation of Olefin
13. Production of Ethylene by Cracking of Naphtha
14. Production of Syngas

Batch Reactor

Characteristics	**No charge or discharge during reaction**
Phases	**Gas, Liquid, Liquid/Solid**
Application	**Small scale production** **Intermediate or one shot production** **Pharmaceutical** **Fermentation** **agricultural chemistry**
Advantages	**High conversion per unit volume for one pass** **Flexibility of operation** (same reactor can produce one product one time and a different product the next) **Easy to clean**
Disadvantages	**High operation cost** **Product quality can be changed batch to batch**

Semi-batch Reactor

Characteristics	**Either one reactant is charged and the other is led continuously (at small concentrations) or else one of the product can be removed continuously to avoid side reaction.**
Phases	**Gas/Liquid, Liquid/Solid**
Application	**Small scale production** **Competing reactions**
Advantages	**High conversion per unit volume for one run** **Good selectivity** **Flexibility of operation** (can be used with a reflux condenser for solvent recovery or in bubble type runs)
Disadvantages	**High operation cost** **Product quality more variable than with continuous operation**

Continuous-Stirred Tank Reactor (CSTR)

Characteristics	Run at steady state with continuous flow of reactants and products: the feed assumes a uniform composition through the reactor, exit stream has the same composition as in the tank
Phases	Liquid, Gas/Liquid, Liquid/Solid
Application	When agitation is required, Series configurations for different concentration streams
Advantages	Continuous operation Good temperature control Easily adapts to two phase runs Low operating (labor) cost Easy to clean
Disadvantages	Lowest conversion per unit volume By-passing and channeling possible with poor agitation

Plug Flow Reactor (PFR)

Characteristics	One long reactor or many short reactors in a tube bank No radial variation in reaction rate (concentration) Changes with length down the reactor
Phases	Gas
Application	Large scale production/Continuous Production Fast reaction High Temperature
Advantages	High conversion per unit volume Low operating (labor) cost Continuous operation Good heat transfer
Disadvantages	Undesired thermal gradients Poor temperature control (hot spot) Shutdown and cleaning may be expensive

Packed-Bed Reactor (PBR)

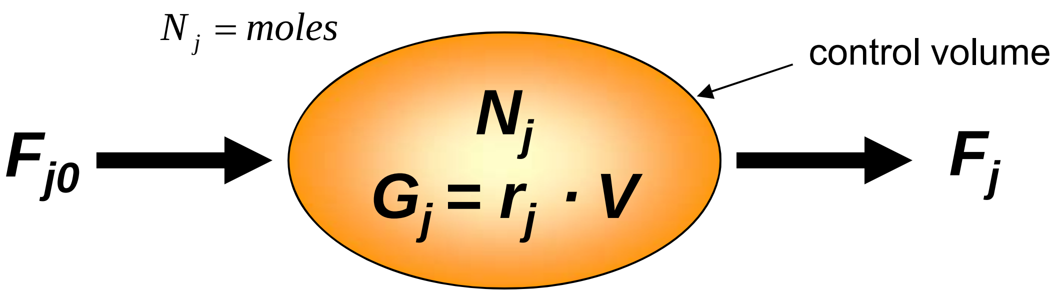
Characteristics	**Tubular reactor that is packed with solid catalyst**
Phases	**Gas/Solid catalyst, Gas/Solid**
Application	**Heterogeneous gas phase reaction with a catalyst**
Advantages	**High conversion per unit mass of catalyst** **Low operating (labor) cost** **Continuous operation**
Disadvantages	**Undesired thermal gradients** **Poor temperature control (hot spot)** **Channeling** **Shutdown and cleaning may be expensive**

Fluidized-Bed Reactor (PBR)

Characteristics	**Heterogeneous reaction** **Like a CSTR in that the reactants are well mixed**
Phases	**Gas/Solid catalyst, Gas/Solid**
Application	**Heterogeneous gas phase reaction with a catalyst**
Advantages	**Good mixing** **Good uniformity of temperature** **Catalyst can be continuously regenerated** **with the use of an auxiliary loop**
Disadvantages	**Bed-fluid mechanics are not well known** **Severe agitation can result in catalyst destruction** **and dust formation** **Uncertain scale-up**

General Mole Balance on control volume

Balance on control volume



$$G_j = \frac{moles}{time} = \frac{moles}{time \cdot volume} \cdot volume$$

A mole balance on species *j*, at any time, t, yields

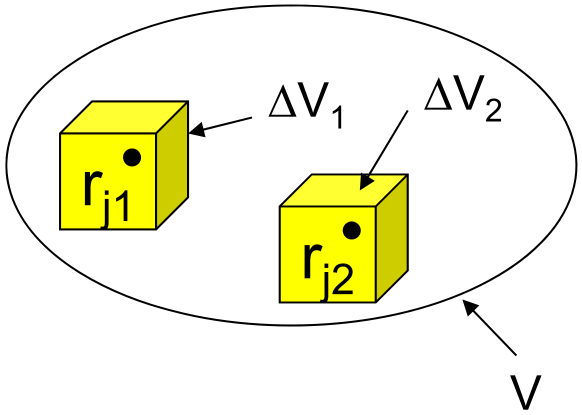
Rate of flow of j ***into*** the system (mole/time)	-	Rate of flow of j ***out of*** the system (mole/time)	+	Rate of ***generation*** of j by chem. rxn within the system (mole/time)	=	Rate of ***accumulation*** of j within the system (mole/time)
in	-	out	+	generation	=	accumulation

$$F_{j0} - F_j + G_j = \frac{dN_j}{dt}$$

Rate of formation of species *j* by chem. rxn

Suppose that the rate of formation of species *j* for the reaction varies with the position in the *control volume*. The rate of generation, ΔG_{j1}, in terms of r_{j1} and sub-volume ΔV_1 is

$$\Delta G_{j1} = r_{j1} \cdot \Delta V_1$$



If the total control volume is divided into M sub-volume, the total rate of generation is

$$G_j = \sum_{i=1}^{M} \Delta G_{ji} = \sum_{i=1}^{M} r_{ji} \Delta V_i$$

By taking the limits (i.e., let $M \to \infty$ and $\Delta V \to 0$) and making use of the definition of integral, we can rewrite the foregoing equation in the form

$$\boxed{G_j = \int^{V} r_j \, dV}$$

r_j can have different values at difference locations in the reactor since the properties of the reacting materials (e.g., conc., temp.)

1.2 The General Mole Balance Equation

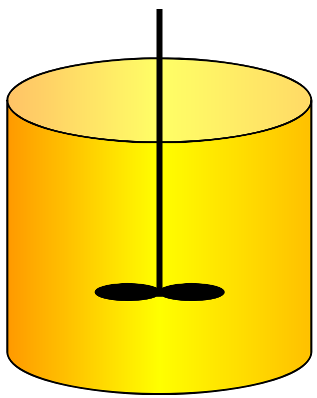
(GMBE)

$$F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt} \qquad (1\text{-}4)$$

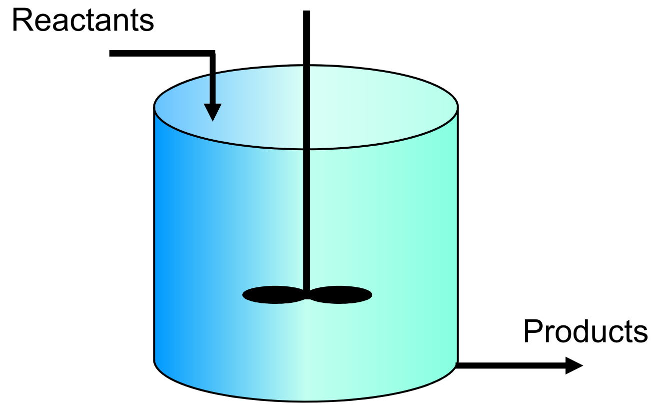
With this GMBE, we can develop the design equations for the various types of industrial reactors: *batch*, *semi-batch*, *and continuous-flow*. Upon evaluation of these equations we can determine the time (batch) or reactor volume (continuous-flow) necessary to convert a specified amount of reactants to products.

The most common industrial reactors

batch reactor

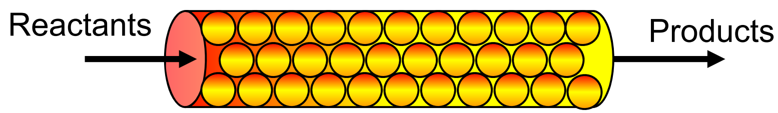


CSTR
(backmix reactor)



PFR
(tubular reactor)

PBR
(packed-bed reactor)



Ideal Reactor Type

Batch Reactor

- uniform composition everywhere in the reactor
- the composition changes with time

Continuous-Stirred Tank Reactor (CSTR)

- uniform composition everywhere in the reactor (well mixed)
- same composition at the reactor exit

Tubular Reactor (PFR)

- fluid passes through the reactor with no mixing of earlier

  and later entering fluid, and with no overtaking.
- It is as if the fluid moved in single file through the reactor
- There is no radial variation in concentration (plug-flow reactor)

1.3 Batch Reactors

GMBE

$$\cancelto{0}{F_{j0}} - \cancelto{0}{F_j} + \int^V r_j dV = \frac{dN_j}{dt}$$

$$\int^V r_j dV = V r_j$$

If the reaction mixture is perfectly mixed so that there is no variation in the rate of reaction throughout the reactor volume, we can take r_j out of the integral and write the GMBE in the form

Design Equation for Batch reactor

$$\frac{dN_A}{dt} = r_A V \quad \textbf{(1-5)}$$

$$dt = \frac{dN_A}{r_A V}$$

Integrating with limits that
at $t = 0$, $N_A = N_{A0}$
at $t = t_1$, $N_A = N_{A1}$

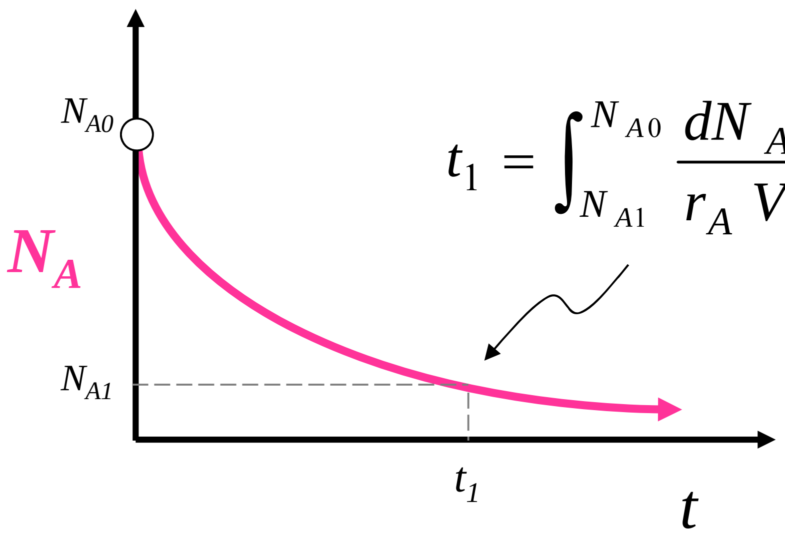
What time is necessary to reduce the initial number of moles from N_{A0} to a final desired number N_{A1}?

$$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V} \quad \textbf{(1-6)}$$

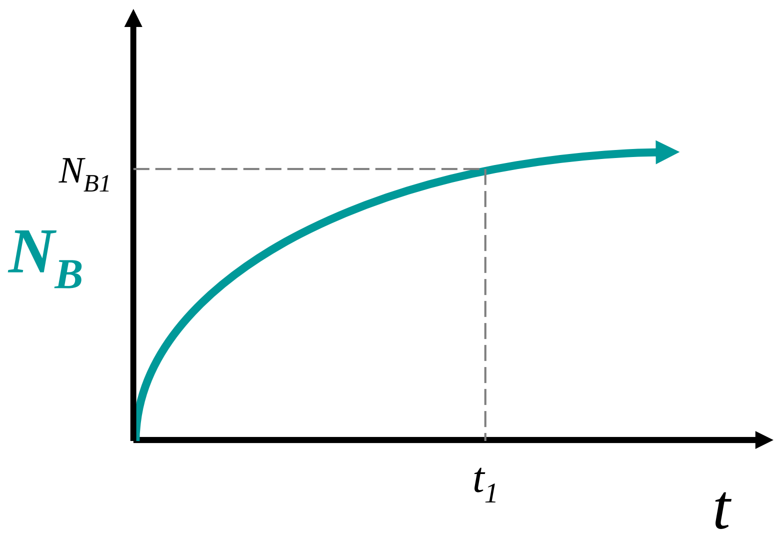
1.3 Batch Reactors

$$A \longrightarrow B$$

$$\frac{dN_A}{dt} = r_A V$$



Moles of A change with time



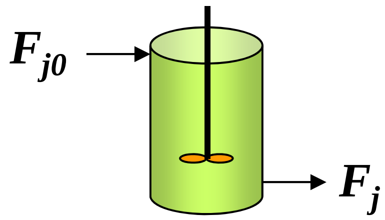
Moles of B increase with time

1.4.1 Continuous-Stirred Tank Reactor (CSTR)

GMBE

$$F_{j0} - F_j + \int^V r_j dV = \cancelto{0}{\frac{dN_j}{dt}}$$

$$\int^V r_j dV = V r_j$$



Design Equation for CSTR

$$V = \frac{F_{j0} - F_j}{-r_j} \qquad \textbf{(1-7)}$$

The CSTR is normally run **at steady state** and is assumed to be **perfect mixed**.

- No temporal, spatial variations in conc., temp., or rxn rate throughout the vessel
- Conc. and temp at exit are the same as they are elsewhere in the tank
- Non-ideal mixing, residence-time distribution model is needed

$$F_j = C_j \cdot v$$

$$\frac{moles}{time} = \frac{moles}{volume} \cdot \frac{volume}{time}$$

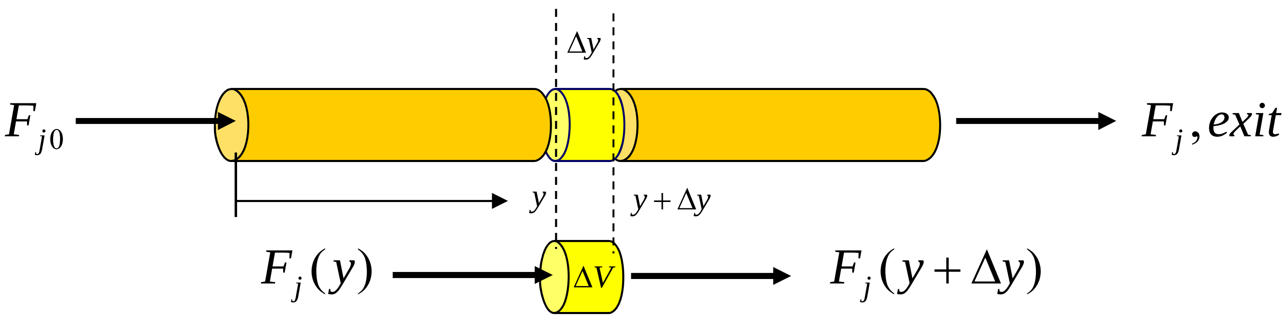
$$F_j = C_j \cdot v \qquad \textbf{(1-8)}$$

The reactor volume, ***V***, necessary to reduce the entering flow rate from F_{j0} to the exit flow rate F_j at reaction rate of r_j.

$$V = \frac{v_0 C_{A0} - v C_A}{-r_A} \qquad \textbf{(1-9)}$$

1.4.2 Tubular Reactor (PFR)

- The reactants are continually consumed as they flow down the length of the reactor
- The concentration varies continuously in the axial direction through the reactor.
- Consequently, the reaction rate will also vary axially.
- To develop the PFR design equation, we shall divide (conceptually) the reactor into a number of sub-volumes so that within each sub-volume ΔV, the reaction rate may be considered spatially uniform.



Let $F_j(y)$ represent the molar flow rate of species j into volume ΔV at y

$F_j(y+\Delta y)$ represent the molar flow rate of species j out of volume ΔV at $(y+\Delta y)$

In a spatially uniform sub-volume ΔV,

$$\int^{\Delta V} r_j dV = r_j \Delta V$$

1.4.2 Tubular Reactor (PFR)

GMBE in ΔV

$$F_j\big|_V - F_j\big|_{V+\Delta V} + \int^V r_j dV = \cancel{\frac{dN_j}{dt}}^{\,0}$$

$$\int^{\Delta V} r_j dV = r_j \Delta V$$

$$\lim_{\Delta V \to 0}\left[\frac{F_j\big|_{V+\Delta V} - F_j\big|_V}{\Delta V}\right] = r_j \qquad \textbf{(1-10)}$$

Design Equation for PFR

$$\frac{dF_j}{dV} = r_j \qquad \textbf{(1-11)}$$

Integrating with limits that
at $V = 0$, $F_A = F_{A0}$
at $V = V_1$, $F_A = F_{A1}$

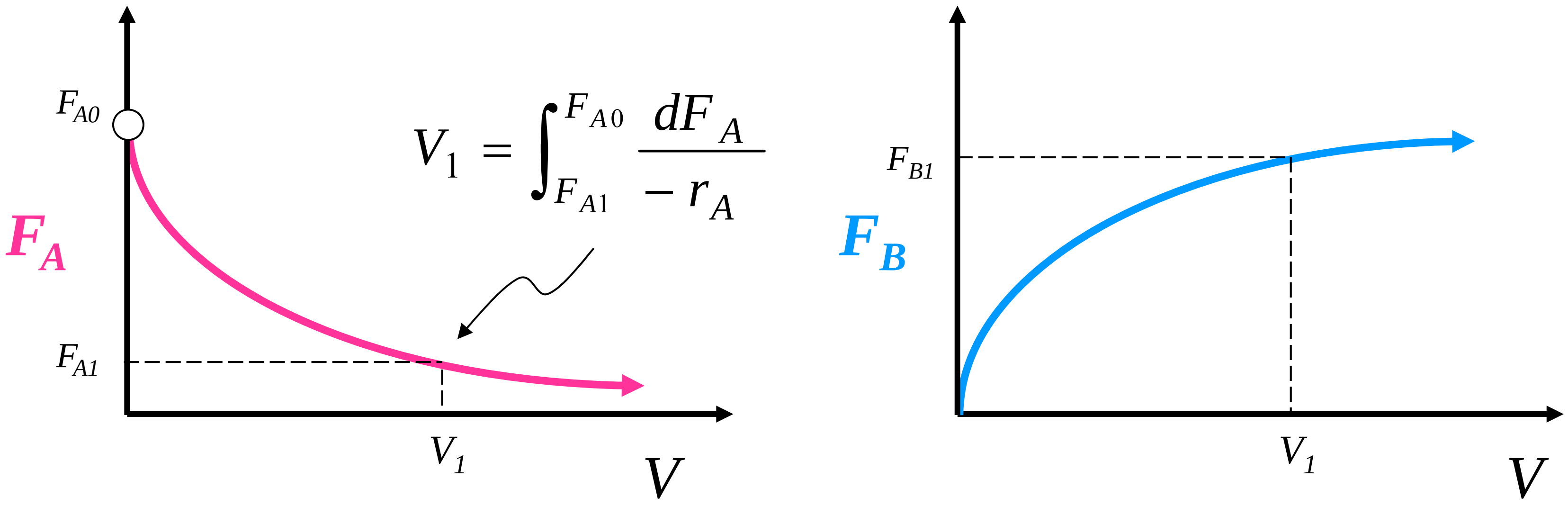
$$V_1 = \int_{F_{A0}}^{F_{A1}} \frac{dF_A}{r_A} \qquad \textbf{(1-13)}$$

The reactor volume, $\boldsymbol{V_1}$, necessary to reduce the entering molar flow rate F_{A0} to some specified value F_{A1} at reaction rate of r_A.

1.4.2 Tubular Reactor (PFR)

$$A \longrightarrow B$$

$$\frac{dF_A}{dV} = r_A$$



$$V_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r_A}$$

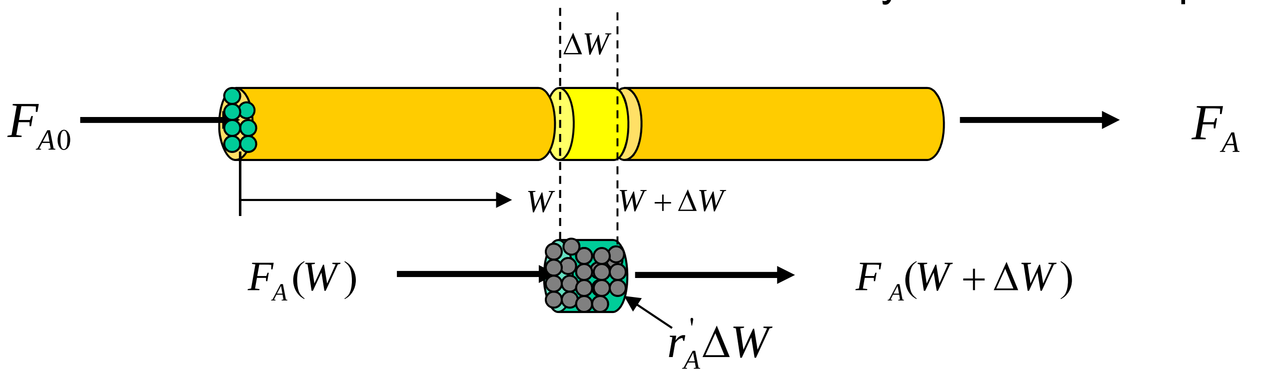
Figure 1-12 profiles of molar flow rates in a PFR

1.4.3 Packed-Bed Reactor (PBR)

For a fluid-solid heterogeneous system, the rate of reaction of a substance A is defined as

$$-r_A' = \frac{gmol\ A\ reacted}{\sec \cdot g\ catalyst}$$

The mass of solid is used because the amount of the catalyst is what is important to the $-r'_A$



$$F_A(W) \quad - \quad F_A(W + \Delta W) \quad + \quad r_A' \Delta W \quad = \quad 0$$

In - out + generation = accumulation

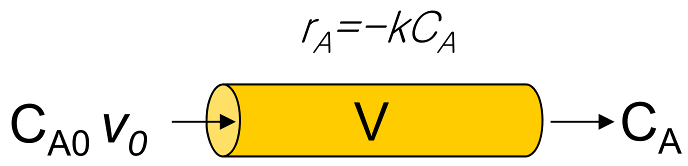
Design Equation for PBR

$$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A'}$$

No pressure drop
No catalyst decay

Example 1-1 How large is it? (PFR)

The first-order reaction (liquid phase rxn)



$A \rightarrow B$

is carried out in a tubular reactor in which the volumetric flow rate, v_0, is constant.

(1) Derive an equation relating the reactor volume (V) to the entering concentration of A (C_{A0}), the rate constant k, and the volumetric flow rate v_0.

(2) Determine the reactor volume necessary to reduce the exiting concentration (C_A) to 10% of the entering concentration (C_{A0}) when the volumetric flow rate (v_0) is 10 ℓ/min and the specific reaction rate, k, is 0.23 min^{-1}.

Example 1-1 How large is it? (PFR)

GMBE for PFR

$$\boxed{\frac{dF_A}{dV} = r_A}$$

$$\frac{dF_A}{dV} = r_A$$

$$-r_A = kC_A$$

(1st-order reaction)

$$\frac{dF_A}{dV} = \frac{d(C_A v_0)}{dV} = v_0 \frac{dC_A}{dV}$$

Combine both side

$$v_0 \frac{dC_A}{dV} = -kC_A$$

$$-\frac{v_0}{k}\left(\frac{dC_A}{C_A}\right) = dV$$

$$-\frac{v_0}{k}\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^V dV$$

$$\boxed{V = \frac{v_0}{k}\ln\frac{C_{A0}}{C_A}}$$

Tubular, 1st order rxn

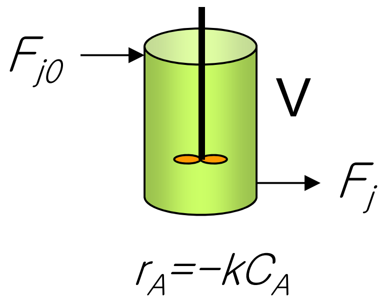
$$V = \frac{10 l/\min}{0.23 \min^{-1}} \ln \frac{C_{A0}}{0.1 C_{A0}}$$

$$= \frac{10 l}{0.23}\ln 10$$

$$= 100 l$$

A reactor volume of 100L is necessary to convert 90% of species A entering into product B for the parameter given.

P1-6$_B$ How large is it? (CSTR)



The first-order reaction (liquid phase rxn)

$$A \rightarrow B$$

is carried out in a CSTR in which the volumetric flow rate, v_0, is constant.

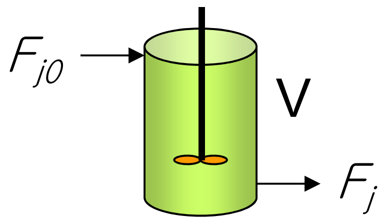
(1) Derive an equation relating the reactor volume (V) to the entering concentration of A (C_{A0}), the rate constant k, and the volumetric flow rate v_0.

(2) Determine the reactor volume necessary to reduce the exiting concentration (C_A) to 10% of the entering concentration (C_{A0}) when the volumetric flow rate (v_0) is 10 ℓ/min and the specific reaction rate, k, is 0.23 min^{-1}.

P1-6$_B$ How large is it? (CSTR)

For CSTR,

the mole balance on species A was shown to be



$$\boxed{V = \frac{F_{A0} - F_A}{-r_A} = \frac{C_{A0}v_0 - C_A v_0}{kC_A}}$$

$$C_A = 0.1C_{A0}, \quad v_0 = 10\ell/\min, \quad and \quad k = 0.23\min^{-1}$$

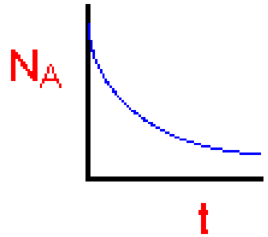
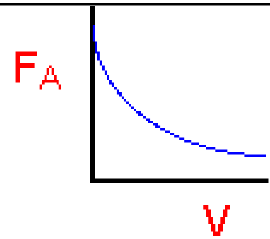
$$V = \frac{C_{A0}v_0 - C_A v_0}{0.1kC_{A0}} = \frac{0.9v_0}{0.1k}$$

$$= (9)(10\ell/\min)/(0.23\min^{-1})$$

$$= 391.3\ell$$

The CSTR is almost 4 times larger than the PFR for getting 90% conversion

Mole Balance on Different Reactor

Reactor	Differential	Algebraic	Integral	
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$	
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$		
PFR	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$	
PBR	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$