CHE 402 Kinetics & Reactor Design

Oct. 13, 2008

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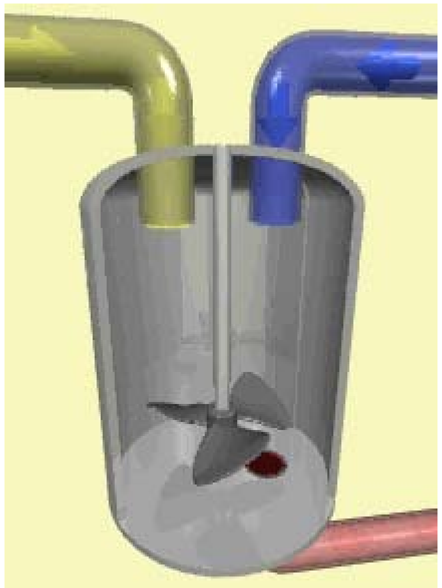
Exams Times

- 1st Exam: Nov. 16, 2008
- 2nd Exam: Dec. 23, 2008

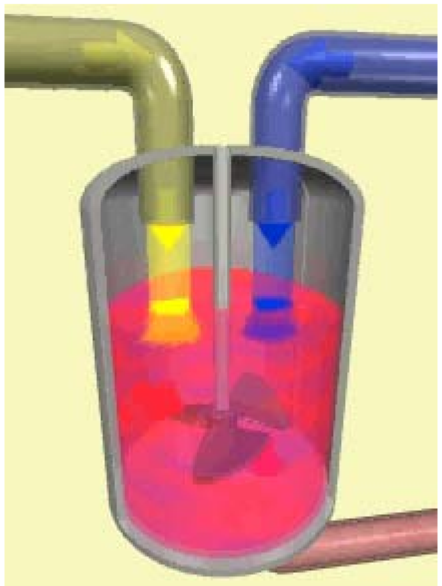
Batch Reactors

- Batch reactors are the simplest reactors used in chemical processes.
- Reactants are first placed inside the reactor and then allowed to react over time.
- Applications: typically used for liquid phase reactions.
  - When only a small amount of product is desired (process in testing phase OR product is expensive)



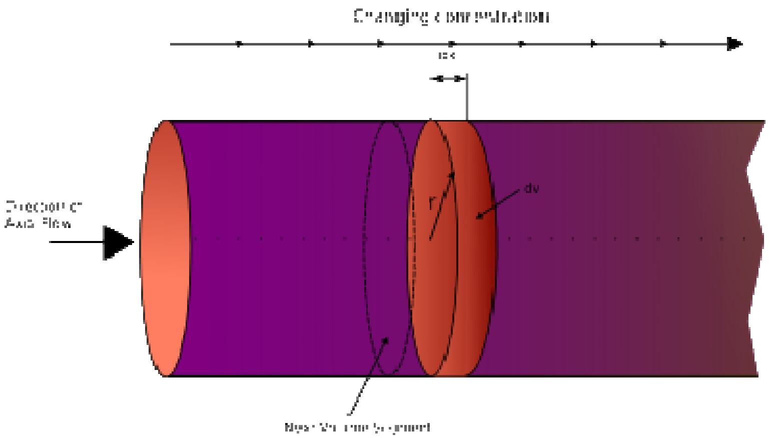
CSTR

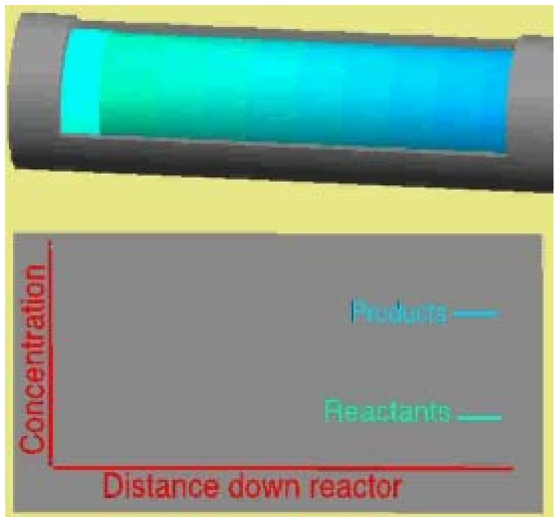
- CSTRs are very well mixed ►contents have uniform properties (temperature, density, etc)
- Reactants are continuously introduced into the reactor, while products are continuously removed.



PFR (Tubular)

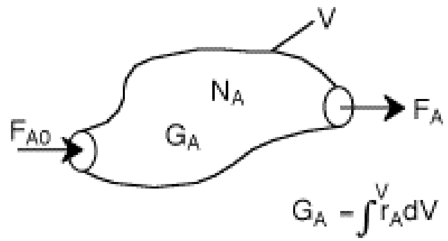
Plug flow or tubular reactors consist of a hollow pipe or tube through which reactants and products to flow through.
Applications: wide variety of operations (gas or liquid phases)
Gasoline production
Oil cracking





General Mole Balance Equation

IN - OUT + GENERATION = ACCUMULATION



IN - OUT + GENERATION = ACCUMULATION

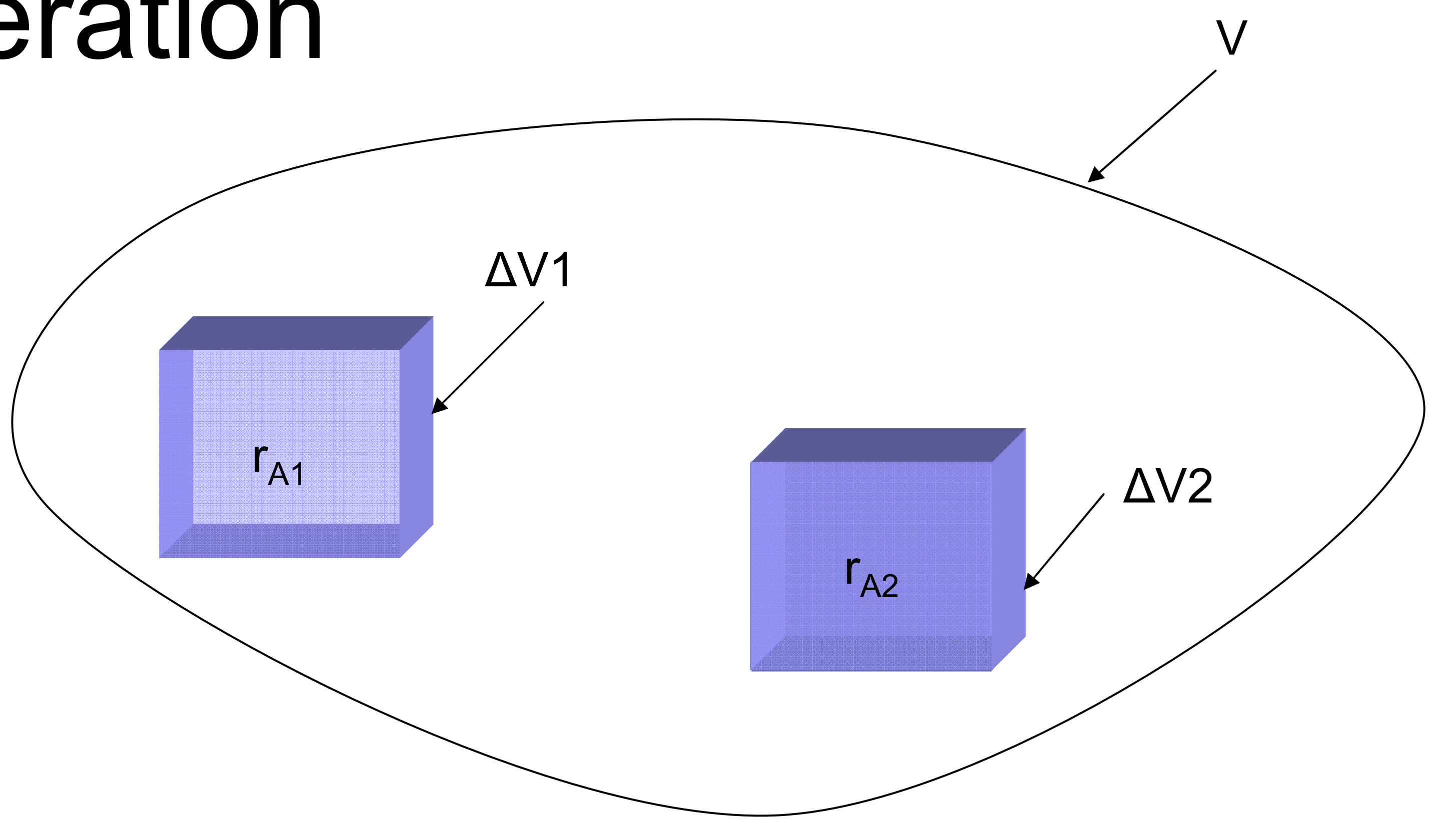
{Rate of flow of A into the system (mole/time)} - {Rate of flow of A out of the system (mole/time)} + {Rate of Generation of A by chemical reaction within the system (mole/time)}

F_{A0} F_{A0} G_A

= {Rate of accumulation of A within the system (mol/time)}

dN_A/dT

Generation



$\Delta G_{A1} = r_{A1}\,\Delta V_1$

$G_A = \sum \Delta G_{Ai} = \sum r_{Ai}\,\Delta V_i$

$$G_A = \int^{V} r_A\,dV$$

IN - OUT + GENERATION = ACCUMULATION

$$F_{A0} \quad - \quad F_A \quad + \quad G_A \quad = \quad dN_A/dT$$

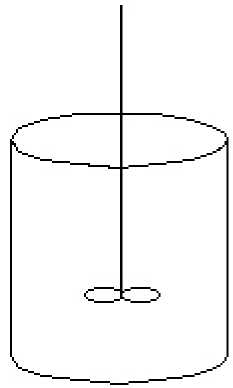
$$F_{A0} - F_A + \int_0^V r_A \, dV = \frac{dN_A}{dt}$$

Batch Reactor Mole Balance

- General Mole Balance on System Volume V

$$\text{In} - \text{Out} + \text{Generation} = \text{Accumulation}$$

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$



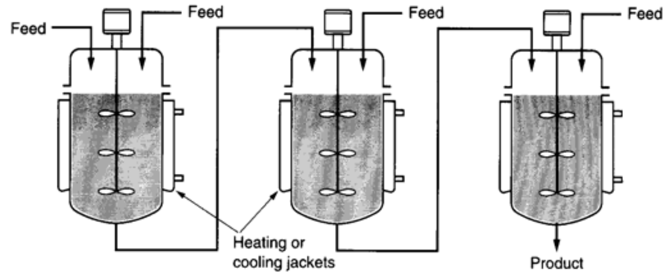
-No inflow or outflow $F_{A0} = F_A = 0$

Assumptions

Well mixed $\int r_A dV = r_A V$

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

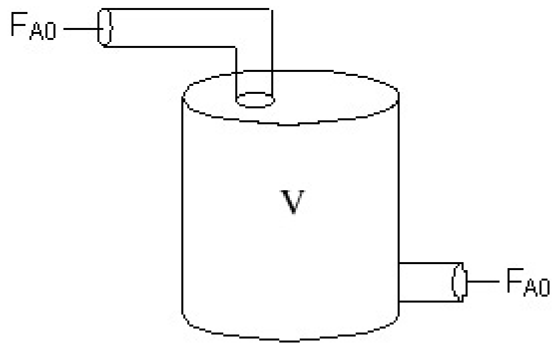
CSTR Mole Balance



- General Mole Balance on System Volume V

In − Out + Generation = Accumulation

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$



Assumptions

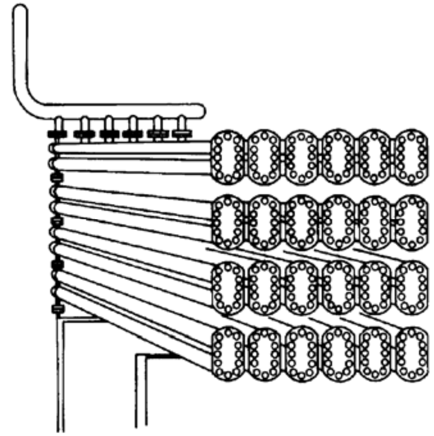
Steady State $\frac{dN_A}{dt} = 0$

Well mixed $\int r_A dV = r_A V$ $F_{A0} - F_A + r_A V = 0$

NO spatial variations in r_A

$$V = \frac{F_{A0} - F_A}{-r_A}$$

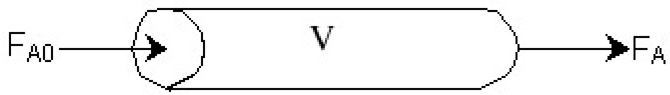
PFR Mole Balance



General Mole Balance on System Volume V

$$\text{In} - \text{Out} + \text{Generation} = \text{Accumulation}$$

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$



Steady State $\frac{dN_A}{dt} = 0$ $\quad F_{A0} - F_A + \int r_A dV = 0$

Differentiate with respect to V

$$0 - \frac{dF_A}{dV} = -r_A$$

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

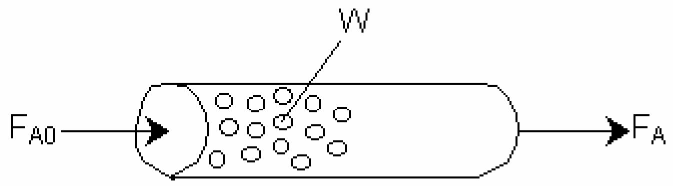
The integral form is:

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

This is the volume necessary to reduce the entering molar flow rate (mol/s) from F_{A0} to the exit molar flow rate of F_A.

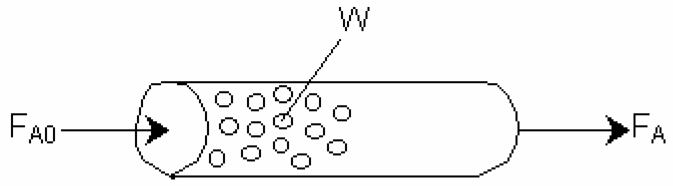
Packed Bed Reactor Mole Balance

PBR



Packed Bed Reactor Mole Balance

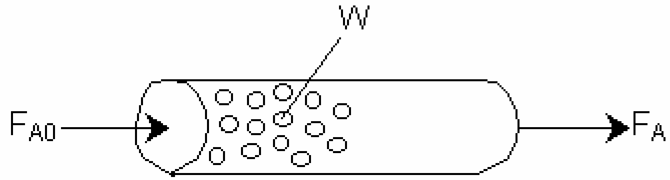
PBR



$$F_{A0} - F_A + \int r'_A dW = \frac{dN_A}{dt}$$

Packed Bed Reactor Mole Balance

PBR



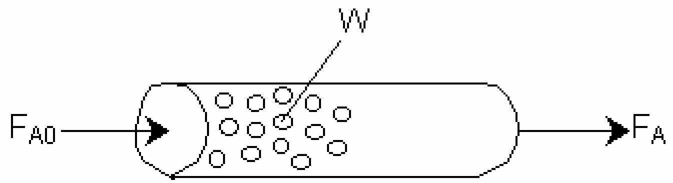
$$F_{A0} - F_A + \int r_A' dW = \frac{dN_A}{dt}$$

Steady State $\frac{dN_A}{dt} = 0$

$$F_{A0} - F_A + \int r_A' dW = 0$$

Packed Bed Reactor Mole Balance

PBR



$$F_{A0} - F_A + \int r_A' dW = \frac{dN_A}{dt}$$

Steady State $\quad \frac{dN_A}{dt} = 0$

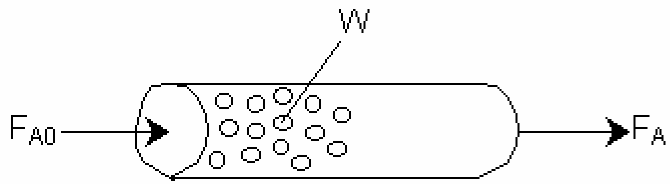
$$F_{A0} - F_A + \int r_A' dW = 0$$

Differentiate with respect to W and rearrange

$$\boxed{\frac{dF_A}{dW} = r_A'}$$

Packed Bed Reactor Mole Balance

PBR



$$F_{A0} - F_A + \int r'_A dW = \frac{dN_A}{dt}$$

Steady State $\quad \frac{dN_A}{dt} = 0$

$$F_{A0} - F_A + \int r'_A dW = 0$$

Differentiate with respect to W and rearrange

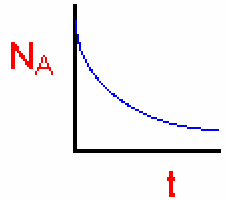
$$\boxed{\frac{dF_A}{dW} = r'_A}$$

The integral form to find the catalyst weight is: $\quad W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$

Reactor Mole Balance Summary

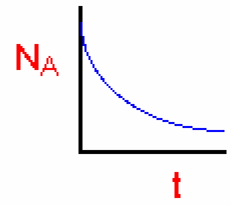
Reactor	Differential	Algebraic	Integral

Reactor Mole Balance Summary

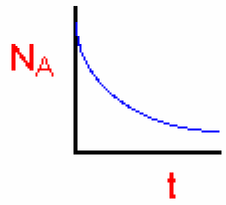
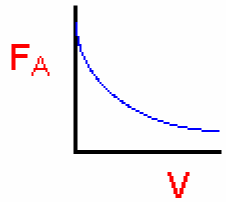
Reactor	Differential	Algebraic	Integral	
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$	

Reactor Mole Balance Summary

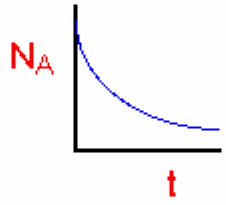
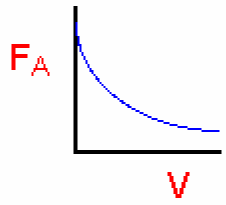
Reactor	Differential	Algebraic	Integral
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$	



Reactor Mole Balance Summary

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	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$	

Reactor Mole Balance Summary

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	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$