CHE 402
Kinetics & Reactor Design

Oct. 18, 2008

Dr. Eid Al-Mutairi

Announcements

- 1st Exam: Nov. 16, 2008 - Evening
- 2nd Exam: Dec. 23, 2008 – Evening
- HW1

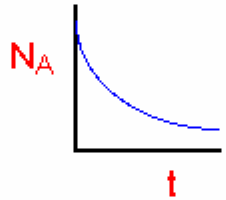
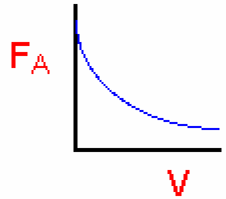
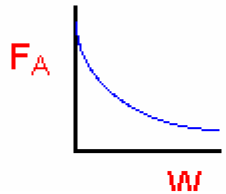
Chapter 2: Conversion and Reactor Sizing

Dr. Eid Al-Mutairi

Objectives

- Define conversion and space time.
- Write the mole balances in terms of conversion for a batch reactor, CSTR, PFR, and PBR.
- Size reactors either alone or in series once given the molar flow rate of A, and the rate of reaction, $-r_A$, as a function of conversion, X.

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

Conversion

Consider the general equation

$$aA + bB \longrightarrow cC + dD$$

We will choose A as our basis of calculation.

$$A + \frac{a}{b}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D$$

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The basis of calculation is most always the limiting reactant. The conversion of species A in a reaction is equal to the number of moles of A reacted per mole of A fed.

$$X = \frac{\text{moles reacted}}{\text{moles fed}}$$

Batch

$$X = \frac{(N_{A0} - N_A)}{N_{A0}}$$

Flow

$$X = \frac{(F_{A0} - F_A)}{F_{A0}}$$

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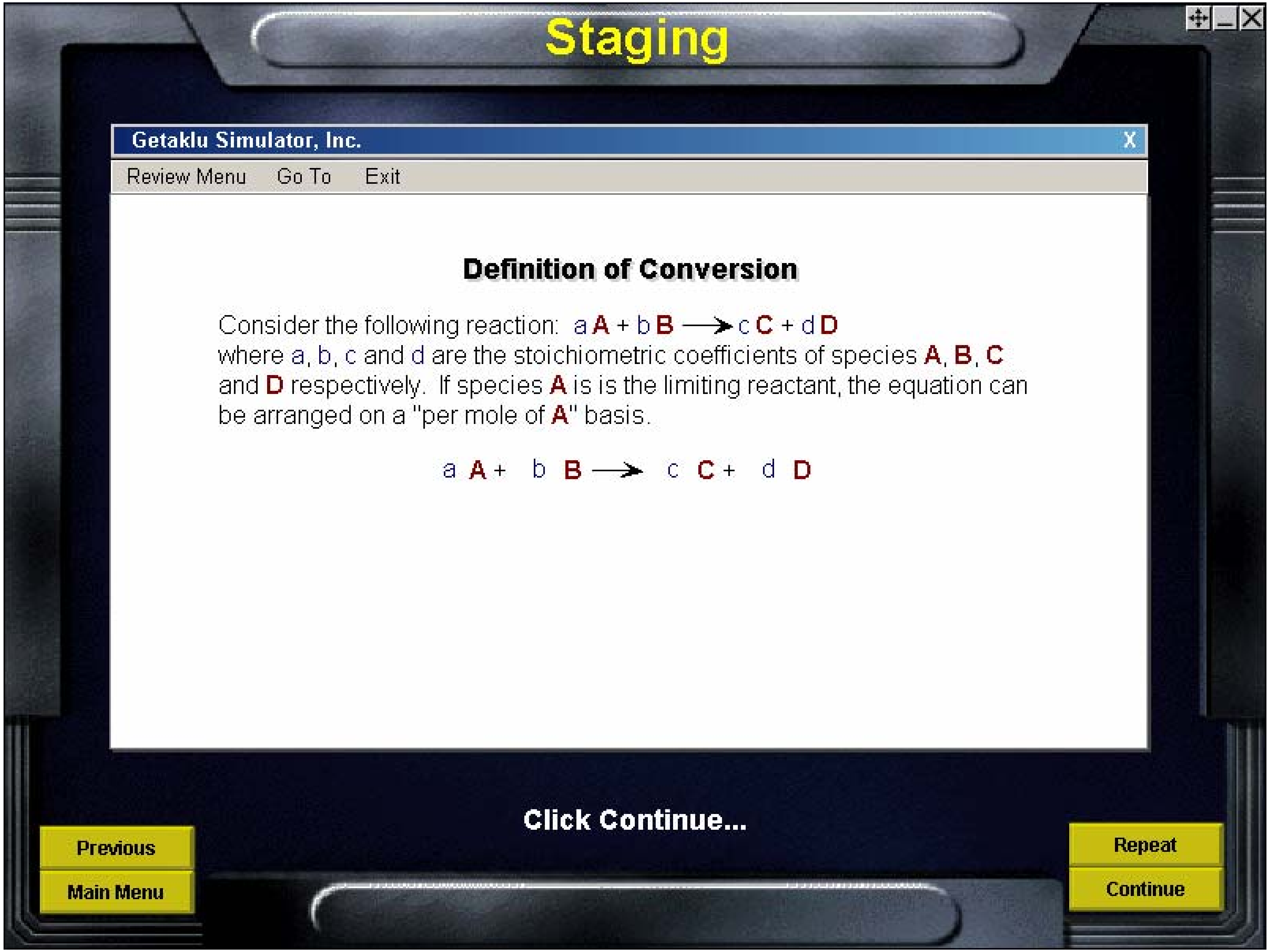
Batch

$$X = \frac{(N_{A0} - N_A)}{N_{A0}}$$

For irreversible reaction, the maximum value of X is that for complete conversion, i.e. X=1.0

For reversible reactions, the maximum value of X is the equilibrium conversion, i.e. X=Xe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X
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Definition of Conversion
Consider the following reaction: a A + b B ⟶ c C + d D
where a, b, c and d are the stoichiometric coefficients of species A, B, C
and D respectively. If species A is is the limiting reactant, the equation can
be arranged on a "per mole of A" basis.
a A + b B ⟶ c C + d D
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Definition of Conversion

Consider the following reaction: $aA + bB \longrightarrow cC + dD$
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$$\frac{a}{a}A + \frac{b}{a}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D$$

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Definition of Conversion

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$$A + \frac{b}{a}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D$$

With this relationship, species **A** can now be used to define **CONVERSION** of the system. Conversion for a flow system can be stated as:

$$X = \frac{\text{Moles of A reacted}}{\text{Moles of A fed}}$$

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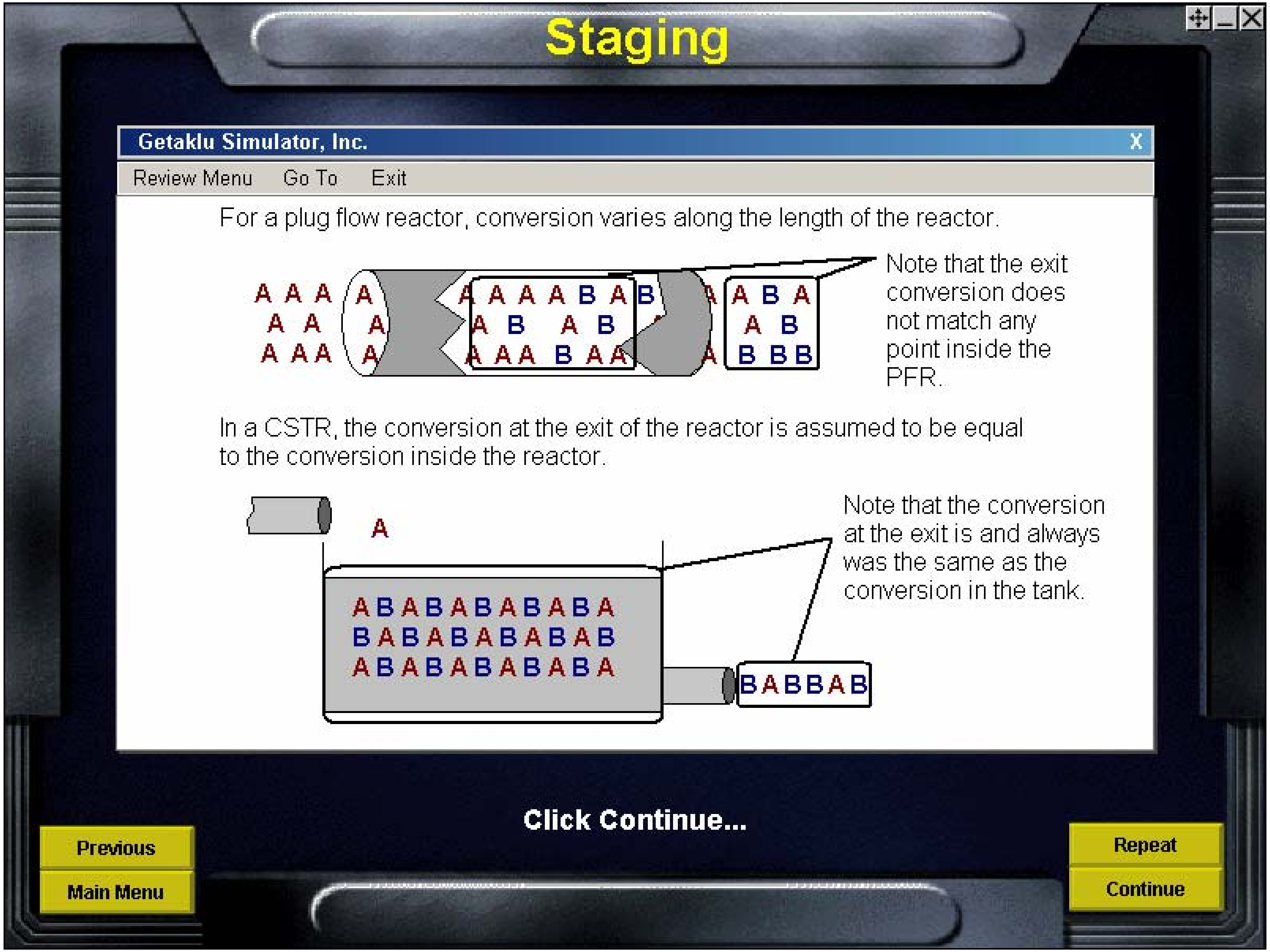
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For a plug flow reactor, conversion varies along the length of the reactor.
Note that the exit conversion does not match any point inside the PFR.
In a CSTR, the conversion at the exit of the reactor is assumed to be equal to the conversion inside the reactor.
Note that the conversion at the exit is and always was the same as the conversion in the tank.
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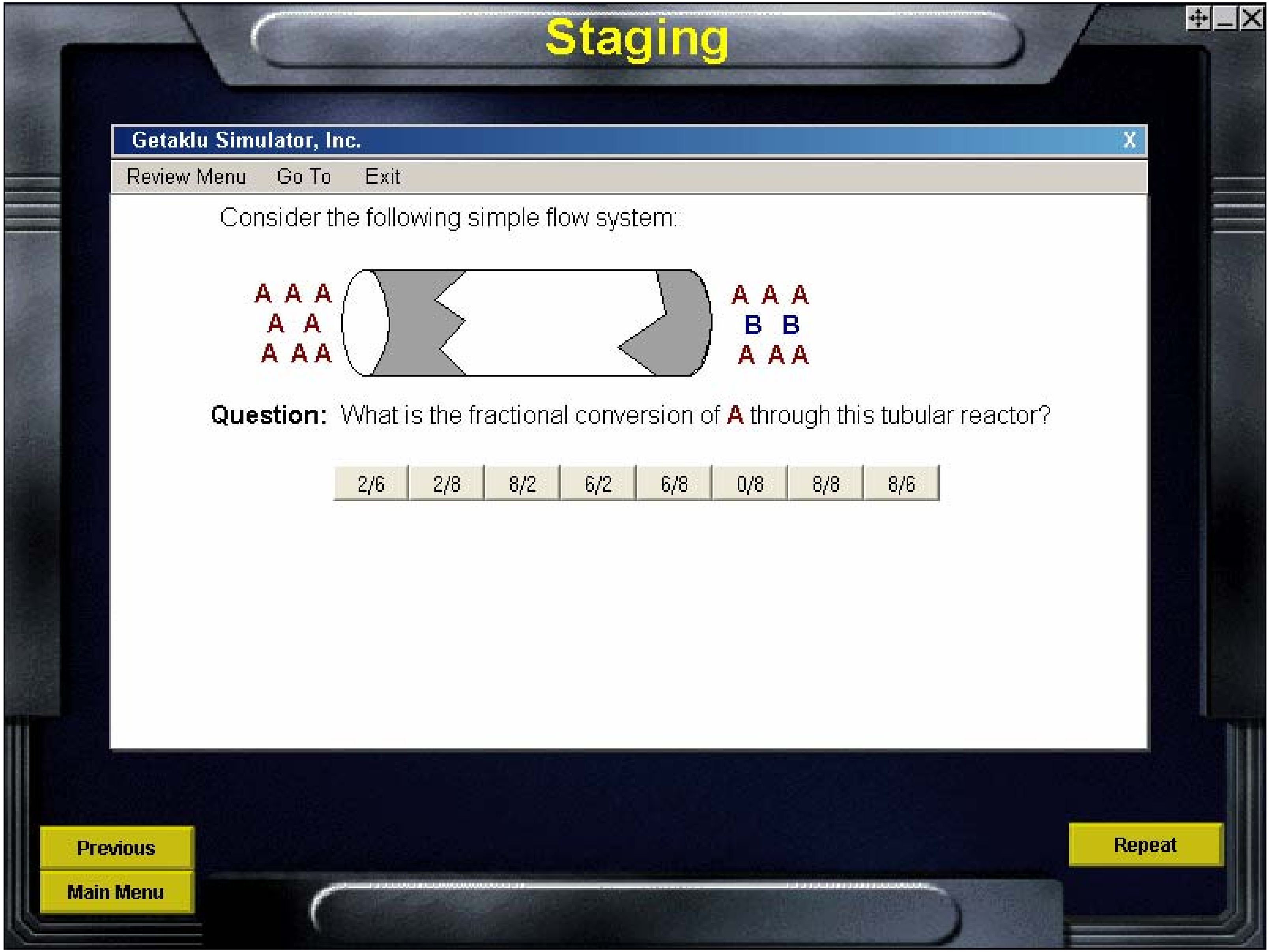
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Consider the following simple flow system:
A A A
A A
A A A
A A A
B B
A A A
Question: What is the fractional conversion of A through this tubular reactor?
2/6
2/8
8/2
6/2
6/8
0/8
8/8
8/6
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Consider the following simple flow system:

Question: What is the fractional conversion of **A** through this tubular reactor?

Correct!! Great Job! There were 8 moles of **A** fed into the reactor and two of those moles reacted to form **B**.

$$X = \frac{\text{Moles of A reacted}}{\text{Moles of A fed}} = \frac{2}{8} = 0.25 \text{ (25\% conversion)}$$

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Batch Reactor Conversion

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$$N_A = N_{A0} - N_{A0}X$$

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Differential Form:

$$N_{A0}\frac{dX}{dt} = -r_A V$$

Integral Form:

$$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$$

CSTR Conversion

CSTR

$$F_A = F_{A0} - F_{A0}X$$

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

Algebraic Form: $$\boxed{V = \frac{F_{A0}X}{-r_A}}$$

There is no differential or integral form for a CSTR.

PFR Conversion

PFR

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

$$F_A = F_{A0}(1 - X)$$

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Differential Form:

$$\boxed{F_{A0}\frac{dX}{dV} = -r_A}$$

Rearranging

Integral Form:

$$\boxed{V = F_{A0}\int_0^X \frac{dX}{-r_A} = \int_0^X \frac{F_{A0}\,dX}{-r_A}}$$

Design Equations

The following design equations are for single reactions only. Design equations for multiple reactions will be discussed later.

Reactor Mole Balances in Terms of Conversion

Reactor	**Differential**	**Algebraic**	**Integral**

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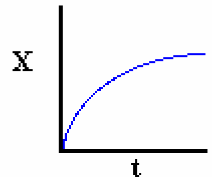

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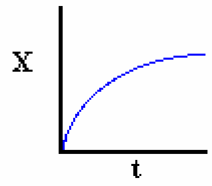

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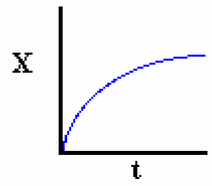
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$	
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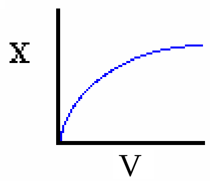
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V = F_{A0}\int_0^X \frac{dX}{-r_A}$	

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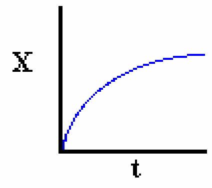
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$	
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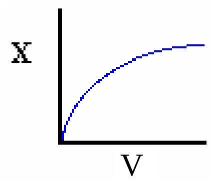
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V = F_{A0}\int_0^X \frac{dX}{-r_A}$	
PBR	$F_{A0}\frac{dX}{dW} = -r'_A$		$W = F_{A0}\int_0^X \frac{dX}{-r'_A}$