

Asynchronous Learning of Chemical Reaction Engineering

Revitalization of Chemical Engineering
Workshop III
June 12, 2003

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University of Michigan
Department of Chemical Engineering
Ann Arbor, Michigan

Introduction

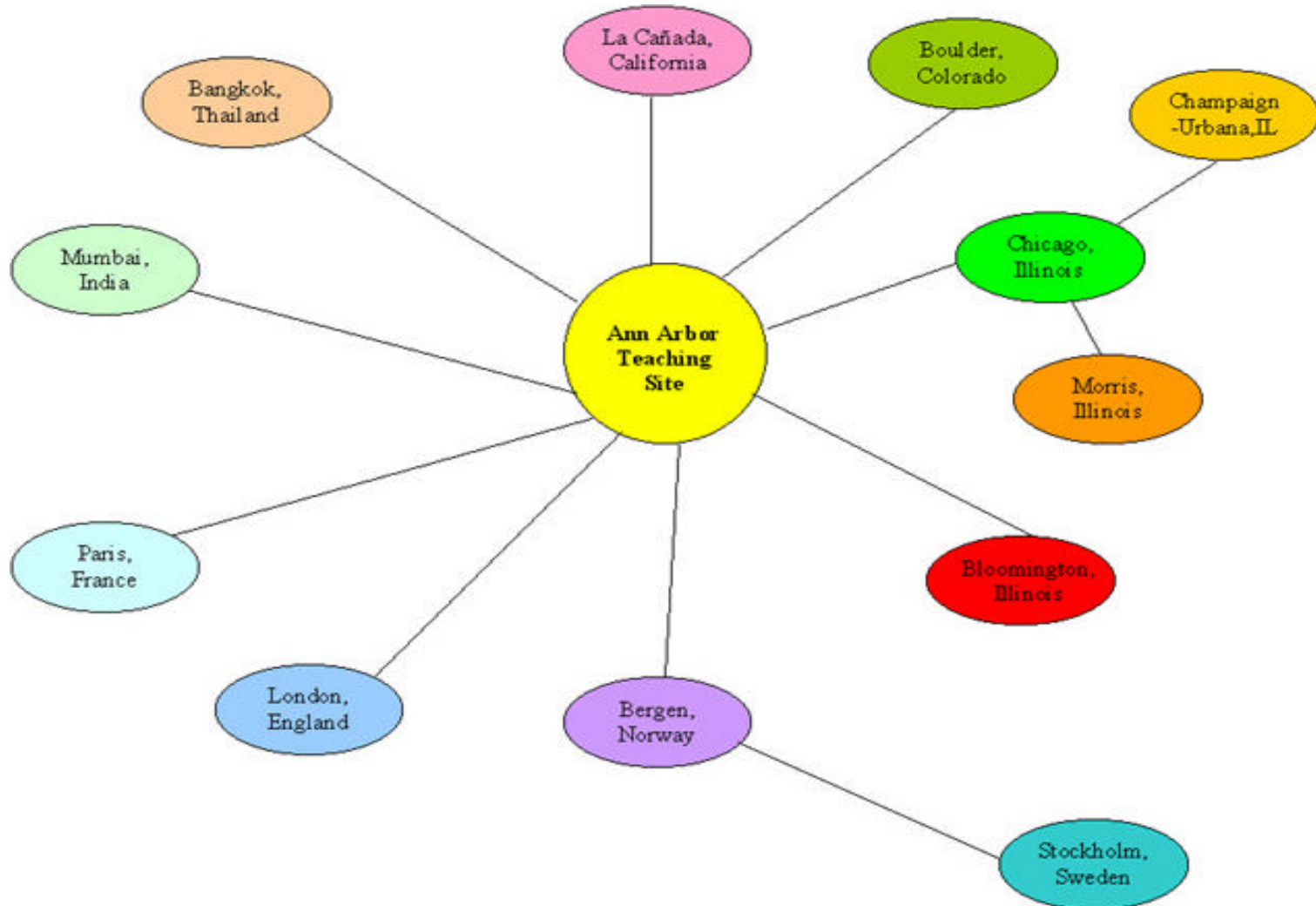
Asynchronous Learning (AL) means that students learn at different times and locations. Asynchronous Learning is a part of Problem Based Learning because students are given a homework problem set to work on and they must then find and use the necessary learning resources to solve the problem.





Asynchronous Learning

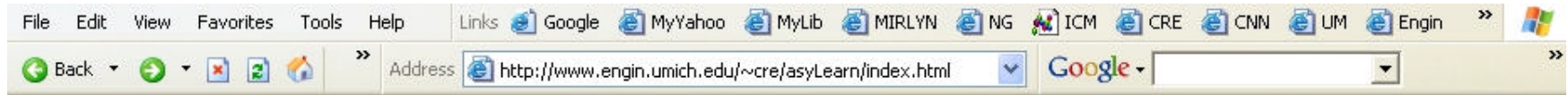
Students can be located both with and outside the United States



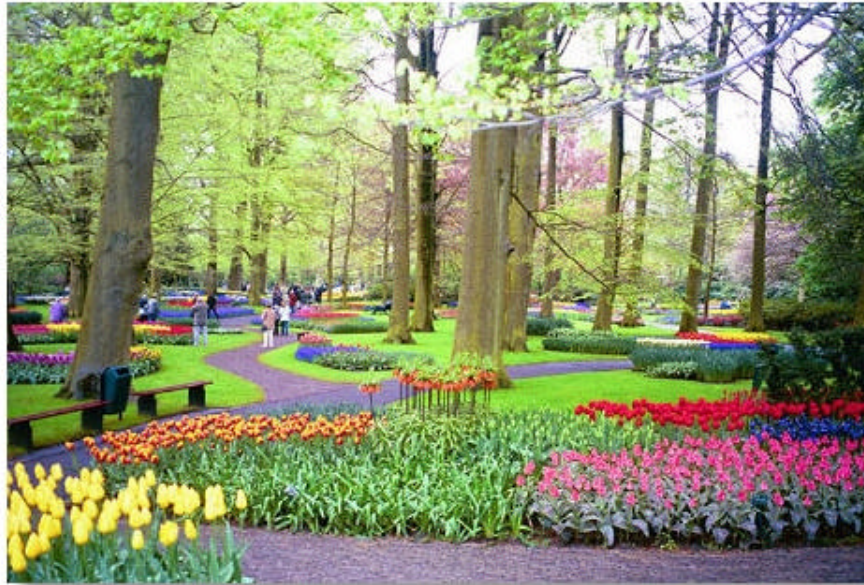
Asynchronous Learning

- With increased focus on technology, AL is rapidly becoming an alternative to traditional lecture-based classes (synchronous learning).
- AL also has the advantage of accommodating students who are on a co-op assignment or who can not make it on a regular basis to lecture.
- Some feel that a better description of AL is Location Independent Learning (LIL)
- ChE 344, Chemical Reaction Engineering (CRE), is the first class offered asynchronously in the chemical engineering department at the University of Michigan.

Asynchronous Learning Main Web Page



Asynchronous Learning



Tulips and Asynchronous Learning, two beautiful ideas
(Keukenhof, Holland)

Do you have "The Knack"?

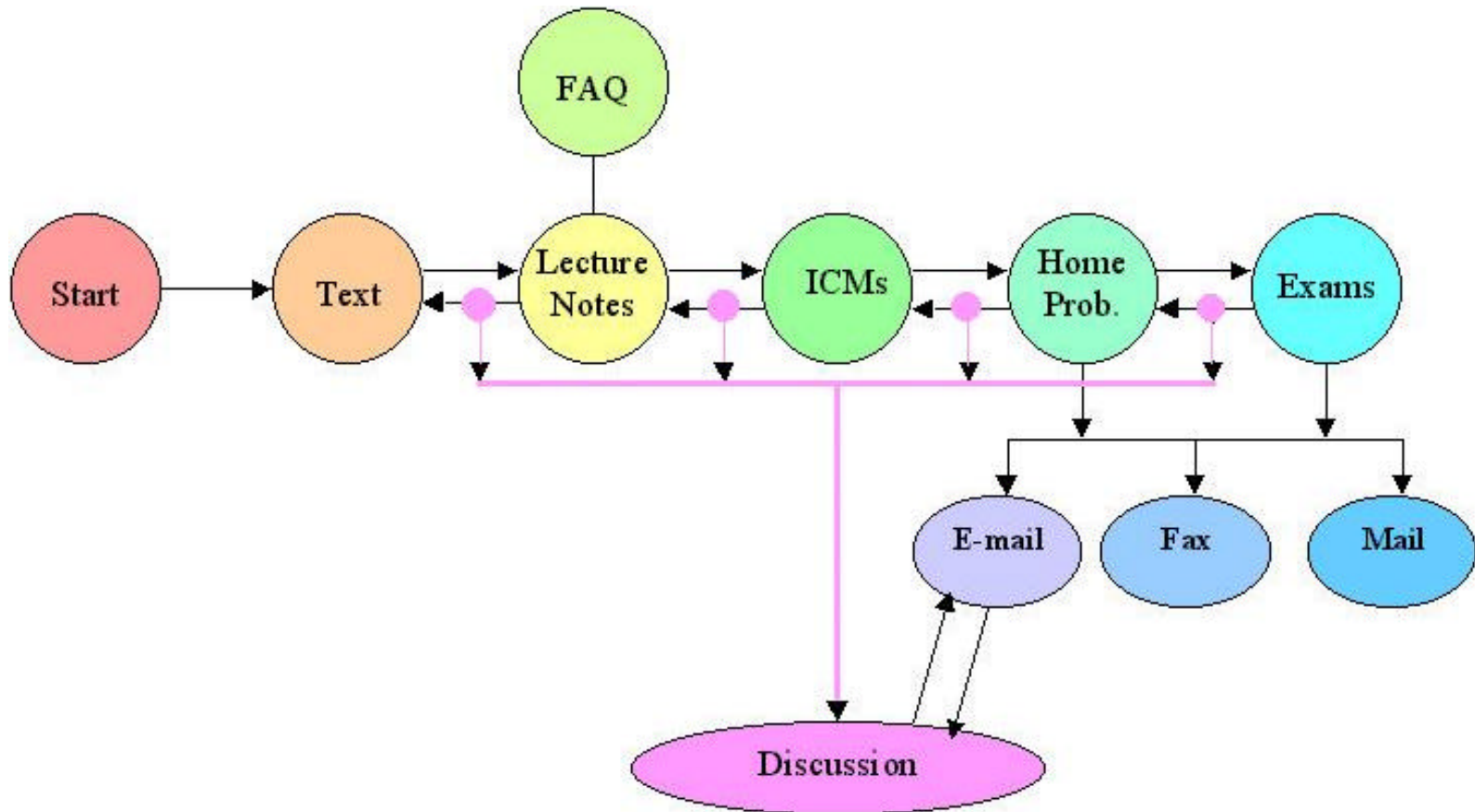
You are visitor number 17282 since 5/16/2000

CDROM/WEB Resources

- Chapter outlines
- Web modules
- Summer notes with audio notes
- Equation derivations
- Self tests
- Video Clips
- Living example problems
- FAQ's
- Interactive computer modules

Asynchronous Learning

The student progression for the asynchronous CRE course at the University of Michigan is shown below:



- [Preface](#)
- [Unit 0](#)
- [Unit 1](#)
- [Unit 2](#)
- [Unit 3](#)
- [Unit 4](#)
- [Unit 5](#)
- [Unit 6](#)
- [Unit 7](#)
- [Unit 8](#)
- [Unit 9](#)
- [Unit 10](#)
- [Unit 11](#)
- [Unit 12](#)
- [Unit 13](#)
- [Unit 14](#)
- [Unit 15](#)
- [Unit 16](#)
- [Unit 17](#)
- [Unit 18](#)

CRE - Asynchronous Learning

Unit 11

Energy Balance and It's Application to the CSTR

Objectives	<p>After completing Unit 11 of the text and associated CD-ROM material, the reader will be able to</p> <ul style="list-style-type: none"> • Discuss each term in the energy balance • Describe the algorithm for CSTRs that are not operated isothermally • Size adiabatic and nonadiabatic CSTRs
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Reading Assignment	<p>Text: Chapter 8, pages 426-450</p> <p>CD-ROM: Lecture Notes 13 and 14</p>
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Time Estimate: 2 1/2 hours

Problem Assignment	<p>CDROM ICMs: Review Section Only</p> <p>Heat Effects 1</p> <p>Heat Effects 2</p> <p>P8-6</p> <p>Review all the audio clips and self tests in lectures 1-13. Pick three in each category that need to be improved. Explain why and how they need to be improved. Pick the two best in each category and explain why they are the best. Where would you suggest adding in audio clips? Finally, write a sentence stating the most confusing part in the text, on the lecture notes or add an FAQ. Email your answers to sfogler@umich.edu with a cc to byrnecc@umich.edu.</p>
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Time Estimate: 3 1/2 hours

Study Problems	<p>P8-3</p> <p>P8-4</p>
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Unit 11 Total Time Estimate: 6 hours

Critical and Creative Thinking

- **Thinking critically** is the process we use to reflect on, assess, and judge the assumptions underlying own and others' ideas and actions.

- **Creative thinking** is the process we use to develop the ideas that are unique, useful, and worthy of further elaboration.

Felder/Soloman's Learning Style Inventory

- Active learners/Reflective learners
- Global learners/Sequential learners
- Visual learners/Verbal learners
- Sensing learners/Intuitive learners

Learning Styles Explained

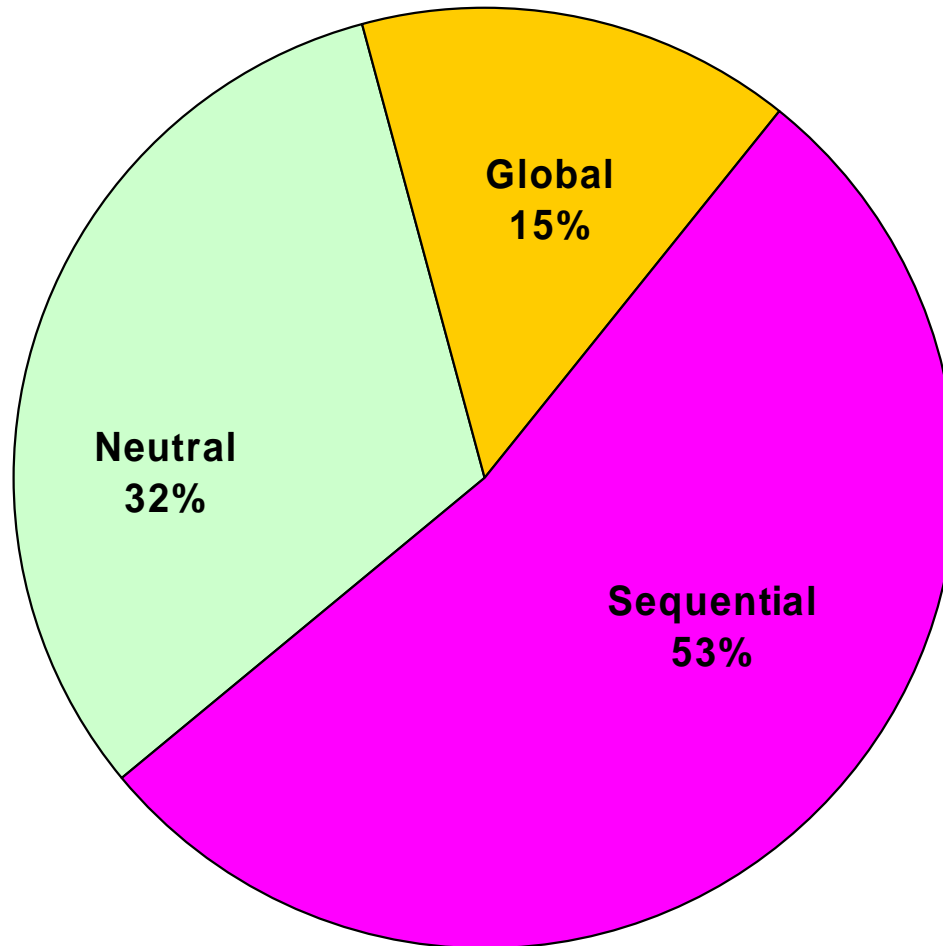
Global vs. Sequential learners

- **Global learners** tend to learn in large jumps, absorbing material almost randomly without seeing connections, and then suddenly “getting it”.
- **Sequential learners** tend to gain understanding in linear steps, with each step following logically from the previous one.

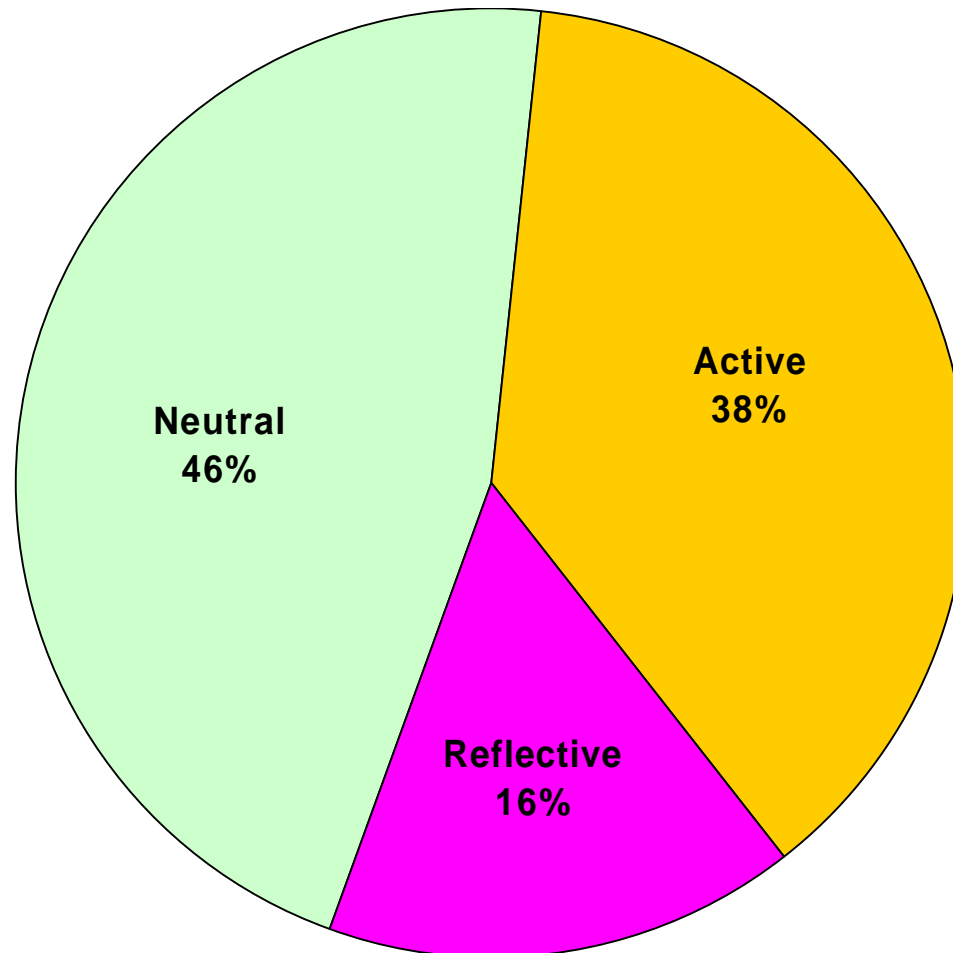
Active vs. Reflective learners

- **Active learners** like to learn by doing or trying things out in order to understand them.
- **Reflective learners** like to learn by reflecting, trying to understand things before experimenting with them.

Global vs. Sequential Learners



Active vs. Reflective



How the CD ROM and Web Can Help Your Learning Style

● Active

- Use all the hot buttons to interact with the material
- Use self tests as a good source of practice problems
- Use living example problems to change settings/parameters and see the results
- Review for exams using the ICM's

● Reflective

- Self tests allow you to consider the answer before seeing it
- Use web modules to think about topics independently

How the CD ROM and Web Can Help Your Learning Style

● Global

- Use the summary lecture notes to get an overview of each chapter on the CD and see the big picture
- Review real world examples and pictures on the CD
- Look at concepts outlined in the Interactive Computer Modules (ICMs)

● Sequential

- Use the *derive* hot button to go through the derivations in lecture notes on the web
- Follow all derivations in the ICMs step by step
- Do all self-tests, audios, and examples as you progress through the CD ROM lecture notes step by step.

Chapter Four - Microsoft Internet Explorer

File Edit View Favorites Tools Help Links Google MyYahoo MyLib MIRLYN NG ICM CRE CNN UM Engin UMRes

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CHAPTER 4

- Chapter Outline
- Software Toolbox
ASPEN
MATLAB
POLYMATH
- Computer Modules
- Thoughts on Problem Solving
- Updates & FAQs
- Representative Syllabi and Exams
- Help

Chapter Outline

4

- **Learning Resources**
 1. *Summary Notes for Lectures 3 and 4*
Summary Notes for Lectures 5 and 6
Summary Notes for Lectures 7 and 8
Summary Notes for Lectures 9 and 10
 2. *Web Modules*
 - A. Wetlands
 - B. Membrane Reactors
 - C. Reactive Distillation
 - D. Aerosol Reactors
 3. *Interactive Computer Modules*
 - A. Murder Mystery
 - B. Tic Tac -- A Game of Reaction Engineering Tic-Tac-Toe
 4. *Solved Problems*
 - A. CD P4-A_B A Sinister Gentleman Messing with a Batch Reactor
 - B. Solution to a California Registration Exam Problem
 - C. Ten Types of Home Problems: 20 Solved Problems
 5. *Analogy of CRE Algorithms to a Menu in a Fine French Restaurant*
 6. *Algorithm for Gas Phase Reaction*

HOME 1 2 3 4 5 6 7 8 9 10 11 12 13 14

APPENDICES

My Computer

Chapter Four - Microsoft Internet Explorer

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CHAPTER 4

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Updates & FAQs

Frequently Asked Questions (FAQs)

Chapter 4

- In solving problems for this class, is there ever a case where you need more steps than the mole balance, rate law, stoichiometry, and combining? (When do you deviate from this algorithm?)**

We will always use this basic algorithm and then just add to these steps to it, e.g. the energy balance. We will not deviate from these first four steps.
- What specifically causes a CSTR in series to have a higher conversion than a CSTR in parallel?**

The CSTR is always operating at the lowest concentration, the exit concentration. When say two CSTRs are in series, the first operates at a higher concentration, therefore the rate is greater, therefore the conversion is greater. The second reactor in series builds on the conversion in the first reactor. The conversion in the parallel scheme is the same as the conversion to the first reactor to the series scheme. See Figure p.50 and Example 4-2.
- When are reactors in parallel used since it seems as though reactors in series would always achieve higher conversion?**

The PBRs in parallel are used when there would otherwise be a large pressure drop in one long reactor or identically several PBRs connected in series.
- Is it possible to have a pressure drop for a liquid phase reaction, as is possible for a gas phase reaction?**

HOME 1 2 3 4 5 6 7 8 9 10 11 12 13 14

APPENDICES

My Computer

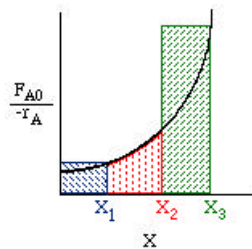
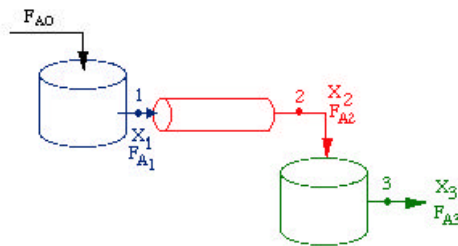
Lecture Outlines

Reactors in Series

Given $-r_A$ as a function of conversion, one can also design any sequence of reactors:

$$X_i = \frac{\text{moles of A reacted up to point } i}{\text{moles of A fed to first reactor}} \quad \text{Only valid if there are no side streams}$$

Consider a PFR between two CSTRs



$$V_1 = \frac{F_{A0} X_1}{-r_{A1}}$$

$$V_2 = \int_{X_1}^{X_2} \frac{F_{A0}}{-r_{A2}} dX$$

$$V_3 = \frac{F_{A0}(X_3 - X_2)}{-r_{A3}}$$

Example

Reactors in Series

Index - Microsoft Internet Explorer


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Address <http://www.engin.umich.edu/~cre/course/lectures/one/mast> Google

You can tell the overall reaction order by the units of k

C_A	$-r_A$	Reaction Order	Rate Law	k
(mol/dm^3)	$(\text{mol}/\text{dm}^3 \cdot \text{s})$	zero	$-r_A = k$	$(\text{mol}/\text{dm}^3 \cdot \text{s})$
		1st	$-r_A = kC_A$	s^{-1}
		2nd	$-r_A = kC_A^2$	$(\text{dm}^3/\text{mol} \cdot \text{s})$

Example Activation Energy

Self Test Crickets 

Rate Laws (p. 73)

Example: If the rate law for the non-elementary reaction

$$A + B \rightarrow C + D$$

is found to be

$$-r_A = kC_A^2 C_B$$

then the reaction is said to be 2nd order in A, 1st order in B, and 3rd order overall.

Elementary Reactions (p. 75)

A reaction follows an *elementary rate law* **if and only if the (iff)** stoichiometric coefficients are the same as the individual reaction order of each species. For the reaction in the previous example ($A + B \rightarrow C + D$), the rate law would be:

$$-r_A = kC_A C_B$$

if $2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$ then $-r_{\text{NO}} = k_{\text{NO}} C_{\text{NO}}^2 C_{\text{O}_2}$ if elementary!

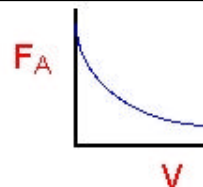
Lecture Notes

Include colored notes with audio clips, examples, and self-tests.

PFR

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

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

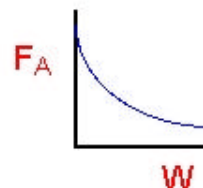


Derive

PBR

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

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



Derive



Self Test

Multiple Choice Questions

Self Test

Batch Reactor Times

Self Test

What's wrong with this solution? Chapter 1

Self Assessment of Chapter Objectives

Chapter 1

Thoughts on Problem Solving: Sample Registration Exam Problem - Microsoft Internet Explorer

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Address http://www.engin.umich.edu/~cre/probsolv/closed/Alg/CRE-t Google Search Web

[HOME](#) > [CLOSED](#) > [ALGORITHM](#) > [CRE EXAMPLES](#)
SREP - Part II :CSTR & PFR

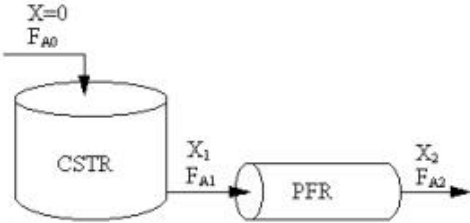
4. Identify and Name:

A. Relative Theories and Equations

Algebraic Form of CSTR equation:

$$V_{CSTR} = \frac{F_{A0}X_1}{-r_{A1}}$$

[derive CSTR volume](#)



For reactors in series, such as a PFR after a CSTR, the integral form of a PFR equation becomes:

$$V_{PFR} = F_{A0} \int_{X_1}^{X_2} \frac{dX_2}{-r_{A2}}$$

[derive PFR volume](#)

B. Systems

Volume of PFR

Volume of CSTR

C. Dependent and Independent Variables

Independent: $V_{CSTR}, V_{PFR}, F_{A0}, F_{B0}, T$

Dependent: k, X_1, X_2

Thoughts on Problem Solving: Sample Registration Exam Problem - Microsoft Internet Explorer

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HOME > CLOSE

problem solving

SREP - Part II : C

4. Identify and Name:

A. Relative Theories and Equations

Algebraic Form of CSTR equation:

$$V_{CSTR} = \frac{F_{A0}X_1}{-r_{A1}}$$

[derive CSTR volume](#)

For reactors in series, such as

$$V_{PFR} = F_{A0} \int_{X_1}^{X_2} \frac{dX_2}{-r_{A2}}$$

[derive PFR volume](#)

B. Systems

Volume of PFR

Volume of CSTR

C. Dependent and Independent Variables

Independent: V_{CSTR}, V_{PFR}

Dependent: k, X_1, X_2

http://www.engin.umich.edu/~cre/probsolv/closed/Alg/CRE-Exam/SRP/Clicks/click12.htm - Microsoft Internet Explorer

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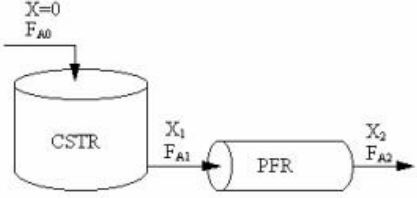


Figure 1. Schematic of a CSTR and a PFR in series

When reactors are connected in series, the effluent stream of the first reactor becomes the feed stream for the second reactor. Let's start with the definition for conversion:

$$X_1 = \frac{\text{amount of A reacted up to point i}}{\text{amount of A fed initially}}$$

We see that our two conversions, which correspond to the points marked in Figure 1 (above), are:

$$X_1 = \frac{F_{A0} - F_{A1}}{F_{A0}}$$

$$X_2 = \frac{F_{A0} - F_{A2}}{F_{A0}}$$

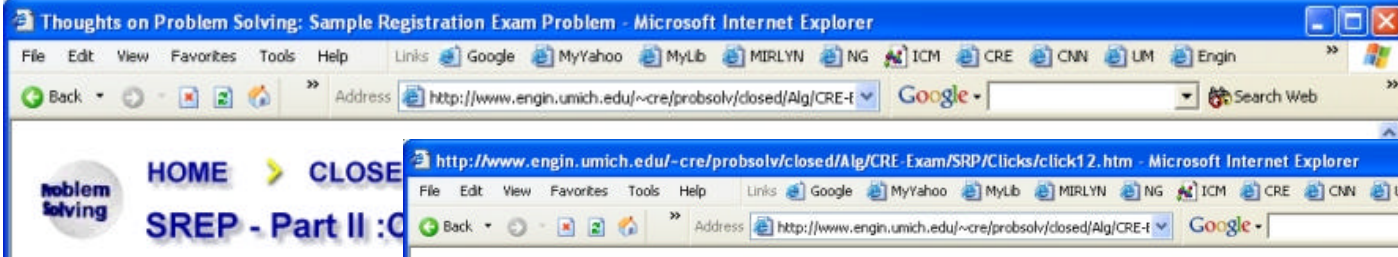
We can rearrange the equations to get our flow rates:

$$F_{A1} = F_{A0} - F_{A0}X_1$$

$$F_{A2} = F_{A0} - F_{A0}X_2$$

As we saw for the [CSTR derivation](#):

$$V_1 = \frac{F_{A0}X_1}{-r_{A1}}$$



The general mole balance for a CSTR is:

$$\left[\begin{array}{l} \text{rate of flow of} \\ \text{A into the} \\ \text{system} \\ \text{(moles/time)} \end{array} \right] + \left[\begin{array}{l} \text{rate of generation} \\ \text{of A by chemical} \\ \text{reaction within} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right] - \left[\begin{array}{l} \text{rate of flow} \\ \text{of A out of} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right] = \left[\begin{array}{l} \text{rate of accumulation} \\ \text{of A within the} \\ \text{system (moles/time)} \end{array} \right]$$

$$F_{A0} + r_{A1} V_1 - F_{A1} = \frac{dN_A}{dt}$$

We assume there are no spatial variations in the rate of reaction. At steady state:

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

After some rearranging:

$$V_1 = \frac{F_{A0} - F_{A1}}{-r_{A1}}$$

Working in terms of conversion: $F_{A1} = F_{A0}(1 - X_1)$

Substituting into the equation:

$$V_1 = \frac{F_{A0} - F_{A0}(1 - X_1)}{-r_{A1}}$$

$$V_1 = \frac{F_{A0} - F_{A0} + F_{A0}X_1}{-r_{A1}}$$

$$V_1 = \frac{F_{A0}X_1}{-r_{A1}}$$

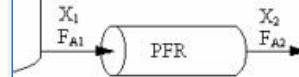


Diagram of a CSTR and a PFR in series

The outlet stream of the first reactor becomes the feed stream for the second reactor.

The amount of A reacted up to point i
is the amount of A fed initially

Therefore, the points marked in Figure 1 (above), are:

$$X_1 = \frac{F_{A0} - F_{A1}}{F_{A0}}$$

$$X_2 = \frac{F_{A0} - F_{A2}}{F_{A0}}$$

$$F_{A1} = F_{A0} - F_{A0}X_1$$

$$F_{A2} = F_{A0} - F_{A0}X_2$$

$$V_1 = \frac{F_{A0}X_1}{-r_{A1}}$$



Self Tests

Allow for practice and understanding of lecture material

Elementary Reactions (p. 75)

A reaction follows an *elementary rate law* **if and only if the (iff)** stoichiometric coefficients are the same as the individual reaction order of each species. For the reaction in the previous example ($A + B \rightarrow C + D$), the rate law would be:

$$-r_A = kC_A C_B$$

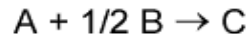
if $2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$ then $-r_{\text{NO}} = k_{\text{NO}} C_{\text{NO}}^2 C_{\text{O}_2}$ if elementary!

Example More examples of Rate Laws

Self Test Rate Laws

Self Test - Rate Laws

What is the reaction rate law for the reaction



if the reaction is elementary? What is r_B ? What is r_C ? Calculate the rates of A, B, and C in a CSTR where the concentrations are $C_A = 1.5 \text{ mol/dm}^3$, $C_B = 9 \text{ mol/dm}^3$ and $k_A = 2 \text{ (dm}^3/\text{mol)}^{(1/2)}(1/\text{s})$.

Hint 1: What is $-r_A$?

Hint 2: What is r_B ?

Chapter Three - Microsoft Internet Explorer

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SELF TEST

What Four Things are Wrong with This Solution? - Chapter 3

Problem

The elementary gas phase reaction

$$3A + 2B \longrightarrow 3C + 5D$$

is carried out in a flow reactor operated isothermally at 427°C and 28.7 atmospheres. Pressure drop can be neglected. Express the rate law and the concentration of each species as a function of conversion and as a function of the total molar flow rates. The entering volumetric flow rate is 10 dm³/s and the specific reaction rate is 200 dm¹²/mol⁴*s. The feed is equal molar in A and B.

Solution

$$3A + 2B \longrightarrow 3C + 5D$$

A is the limiting reactant

$$A + \frac{2}{3}B \longrightarrow C + \frac{5}{3}D$$

$$-r_A = kC_A C_B^{2/3}$$

$$C_A = \frac{C_{A0}(1-X)}{(1+\epsilon X)}$$

$$\epsilon = 3 + 5 - 2 - 3 = 3$$

$$C_A = C_{A0} \frac{(1-X)}{1+3X}$$

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APPENDICES

CHAPTER 3

- Chapter Outline
- Software Toolbox
ASPEN
MATLAB
POLYMATH
- Computer Modules
- Thoughts on Problem Solving
- Updates & FAQs
- Representative Syllabi and Exams
- Help

Main Menu

1. Introduction (Rules)
2. Review (Commercial Break)
3. Interaction (Introduce Contestants and Start the Game)
4. Exit Module

Please enter a number from 1-4 :

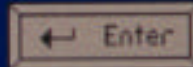
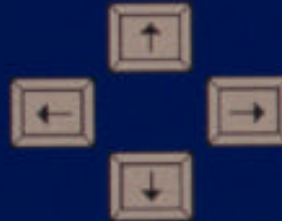
Review Menu

1) Energy Balance

2) Heat Effects

3) Simulator

4) Main Menu



Hit enter to continue

The Energy Balance



The energy balance for this single component system will be,

$$\frac{dE}{dt}\bigg|_{\text{sys}} = \dot{Q} - \dot{W} + F_{\text{in}}E_{\text{in}} - F_{\text{out}}E_{\text{out}}$$

[rate of energy leaving system by mass flow out of the system]

$$\left. \frac{dE}{dt} \right|_{sys} = \dot{Q} - \dot{W} + \sum_{i=1}^n E_i F_i|_{in} - \sum_{i=1}^n E_i F_i|_{out}$$

We will now define the work term (\dot{W}).

$$\dot{W} = \underbrace{- \sum_{i=1}^n F_i P U_i|_{in} + \sum_{i=1}^n F_i P U_i|_{out}}_{\text{flow work}} + \dot{W}_s$$

+ to Continue

$$\dot{Q} - \dot{W}_s + F_{R0} \sum_{i=1}^n \phi_i (H_{i0} - H_i) - F_{R0} \sum_{i=1}^n z_i H_i = 0$$

Now we can integrate this expression.

$$\int_{H(T_R)}^H dH_i = \int_{T_R}^T C_{P_i} dT$$

To obtain,

$$H_i - H_i(T_R) = \int_{T_R}^T C_{P_i} dT \quad \Delta H_{vi}$$

Who are you?

→ to Continue

$$\dot{Q} - \dot{W}_s + F_{R0} \sum_{i=1}^n \phi_i (H_{i0} - H_i) - F_{R0} \sum_{i=1}^n \nu_i H_i = 0$$

Now we can integrate this expression.

$$\int_{H(T_R)}^H dH_i = \int_{T_R}^T C_{Pi} dT$$

To obtain,

$$H_i - H_i(T_R) = \int_{T_R}^T C_{Pi} dT$$

ΔH_{vi}

I'm the phase change term.

→ to Continue

$$\dot{Q} - \dot{W}_s + F_{A0} \sum_{i=1}^n \Theta_i (H_{i0} - H_i) - F_{A0} \sum_{i=1}^n \nu_i H_i = 0$$

Now we can integrate this expression.

$$\int_{H(T_R)}^H dH_i = \int_{T_R}^T C_{P_i} dT$$

To obtain,

$$H_i - H_i(T_R) = \int_{T_R}^T C_{P_i} dT$$

We're neglecting
you this time.

ΔH_{H_i}

→ to Continue

$$\dot{Q} - \dot{W}_s + F_{A0} \sum_{i=1}^n \phi_i (H_{i0} - H_i) - F_{A0} \sum_{i=1}^n \nu_i H_i = 0$$

Now we can integrate this expression.

$$\int_{H(T_R)}^H dH_i = \int_{T_R}^T C_{P_i} dT$$

To obtain,

$$H_i - H_i(T_R) = \int_{T_R}^T C_{P_i} dT$$

ΔH_{iH}

I feel so unwanted.

→ to Continue

Reaction Parameters

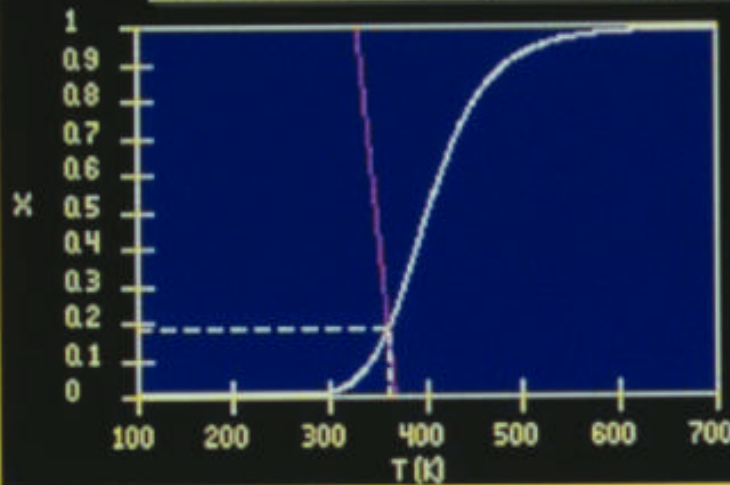


Irreversible



Reversible

Conversion vs. Temperature



Operating Conditions

T (K)	X
359	0.182

Feed Parameters

Temperature



Flow Rate



Heat of Reaction Parameters




Endothermic



Exothermic

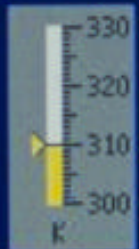
Options

 to move highlight box
<ENTER> to enter parameter box
<ESC> to exit simulator

Heat Exchanger Parameters

Temperature

Exchanger Area (A)



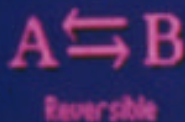
UA = 4000 J/(sec*K)

F1 Main Menu

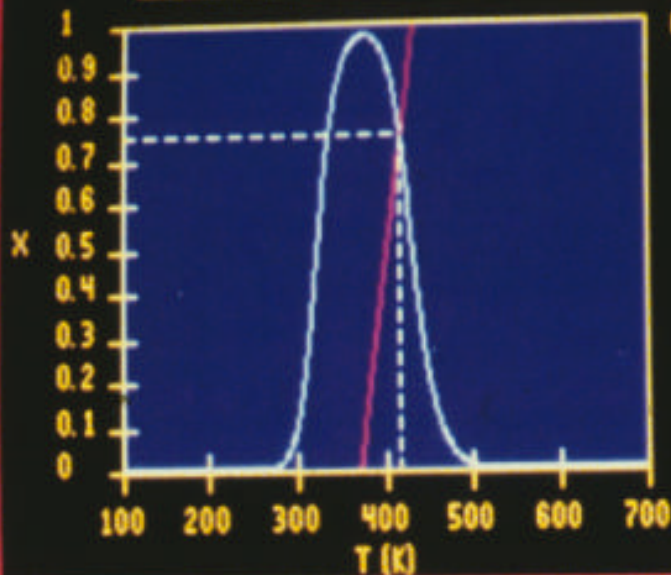
F2 Simulator Help

<Esc> Exit Simulator

Reaction Parameters



Conversion vs. Temperature



Operating Conditions

T (K)	X
415	0.75

Feed Parameters

Temperature



Flow Rate

100 mol/s

Heat of Reaction Parameters



Endothermic



Exothermic

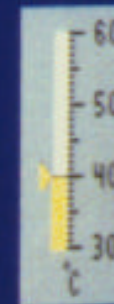
Heat Exchanger Parameters

Temperature

Exchanger Area (A)



UA = 10000 J/(sec*K)



F1 Main Menu F2 Simulator Help

Kinetics Challenge I

mole balance	reactions	rate laws	reactor types	Module score: 0
100	100	100	100	 Score: 0 Dieter
200	200	200	200	 Score: 0 Arrhenius
300	300	300	300	
400	400	400	400	
500	500	500	500	 Score: 0 Nigel

F1 Main Menu Select a box with the arrow keys and <ENTER>

Which of the following is a characteristic of an ideal CSTR ?

- 1. Intense mixing.**
- 2. Minimal side reactions.**
- 3. Hot spots.**
- 4. A good personality.**

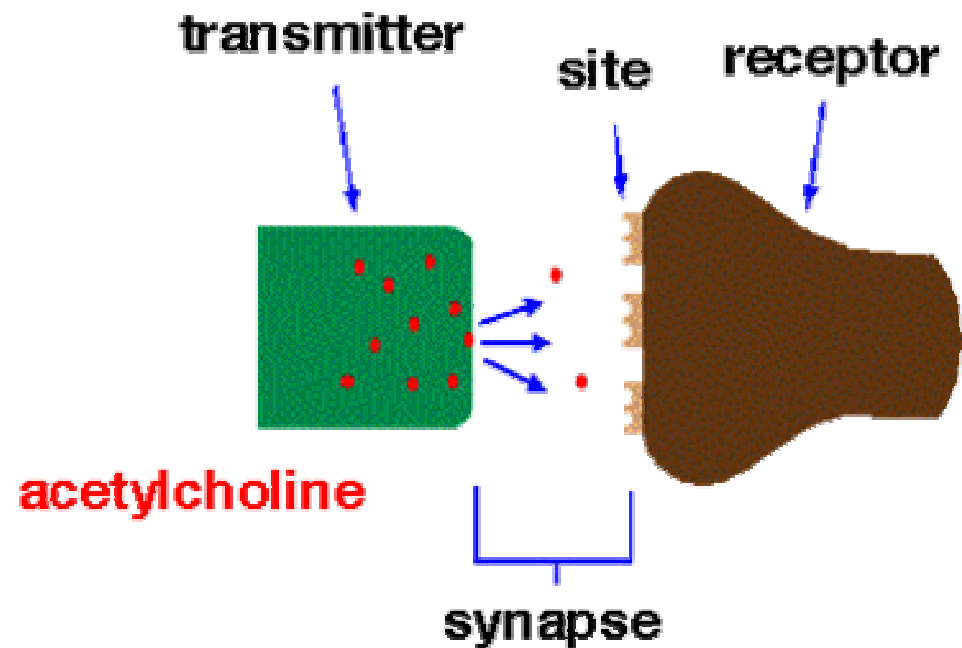
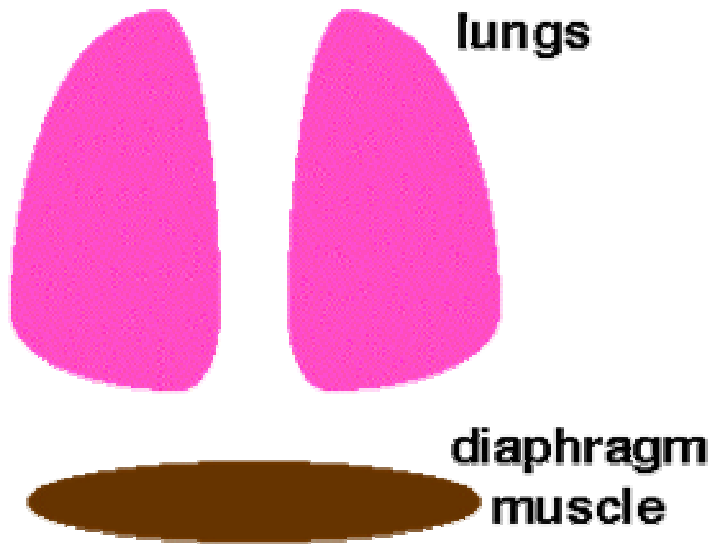
**Select an answer (1-4) or
<ESC> to forfeit (no gain or loss) :**



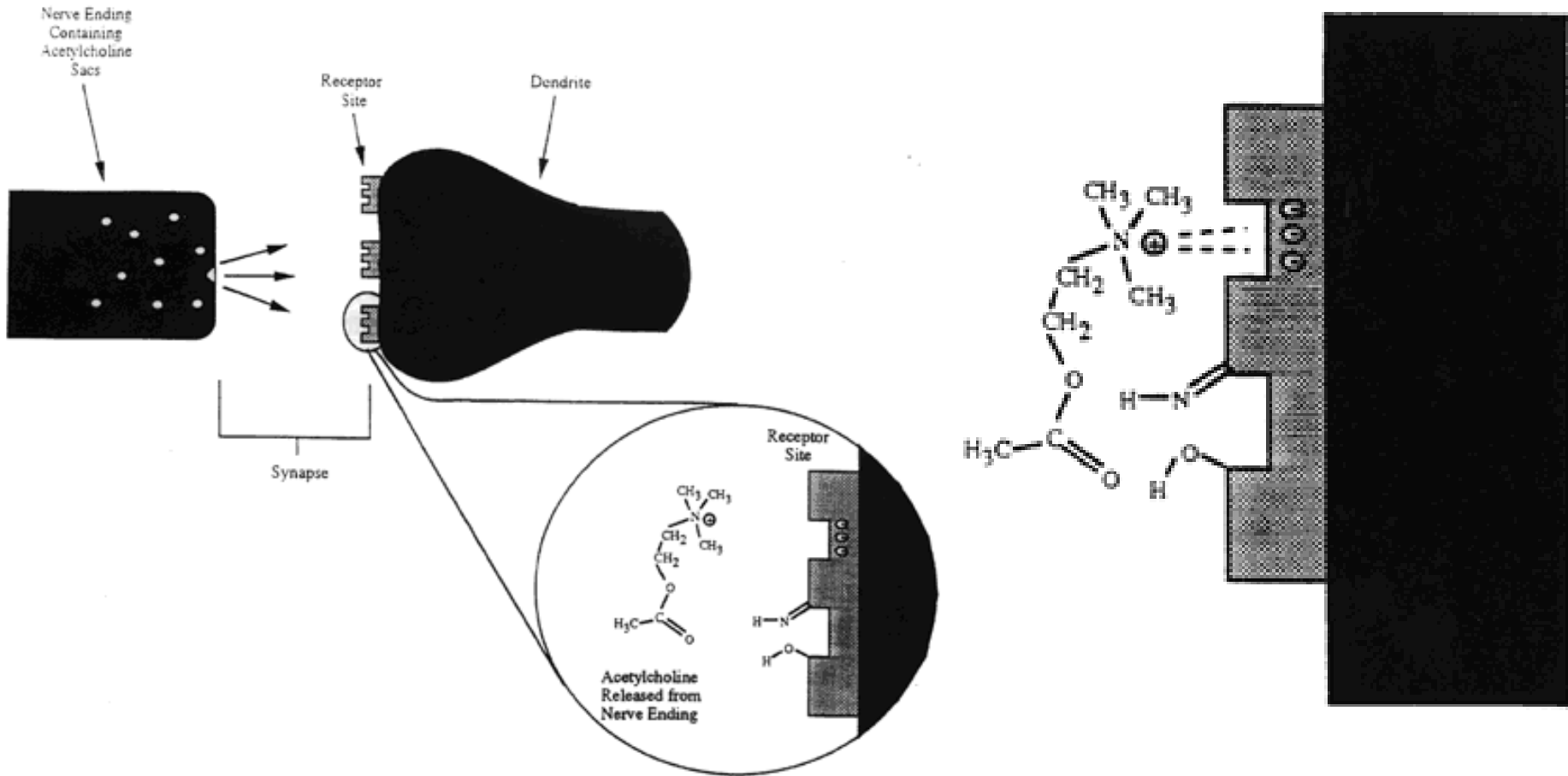


Venom kills within 30 minutes
Antivenom is only known treatment

Effects of Cobra Venom

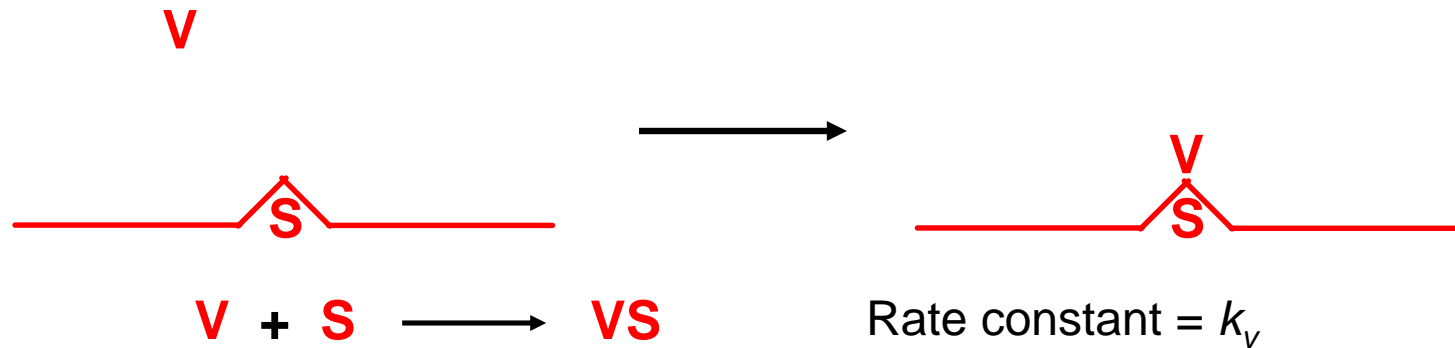


Effects of Cobra Venom

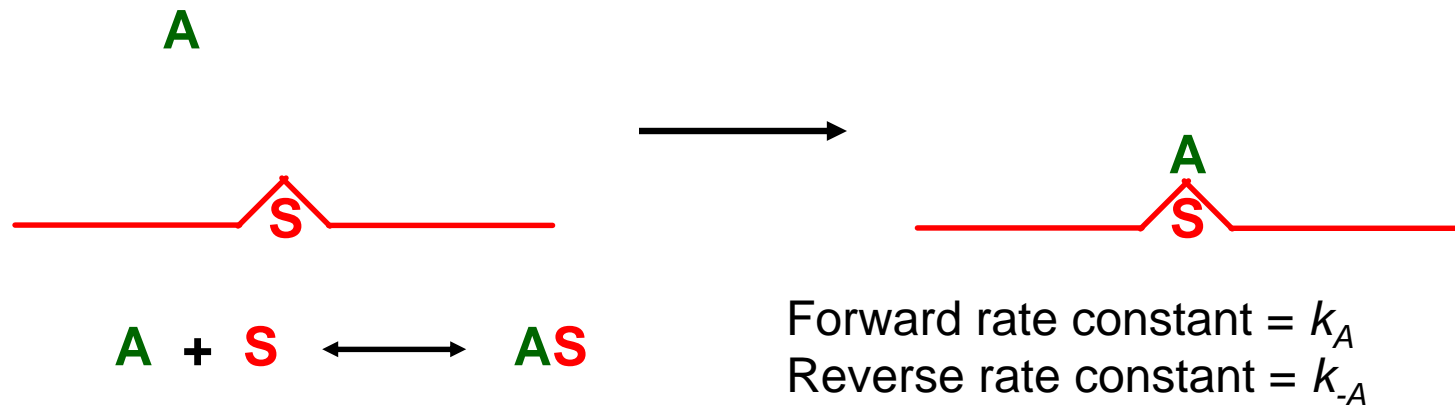


Cobra Venom Reactions

Adsorption of venom onto site:

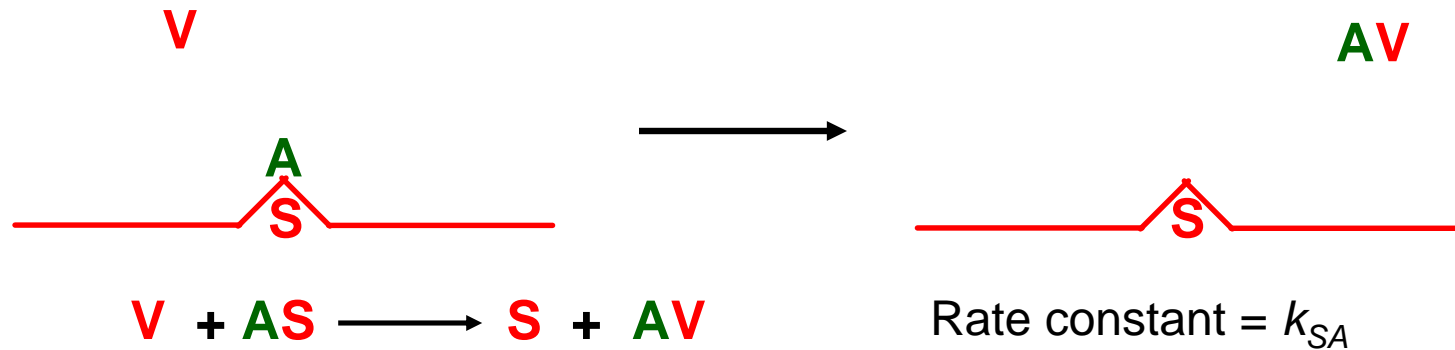


Adsorption of antivenom onto site:

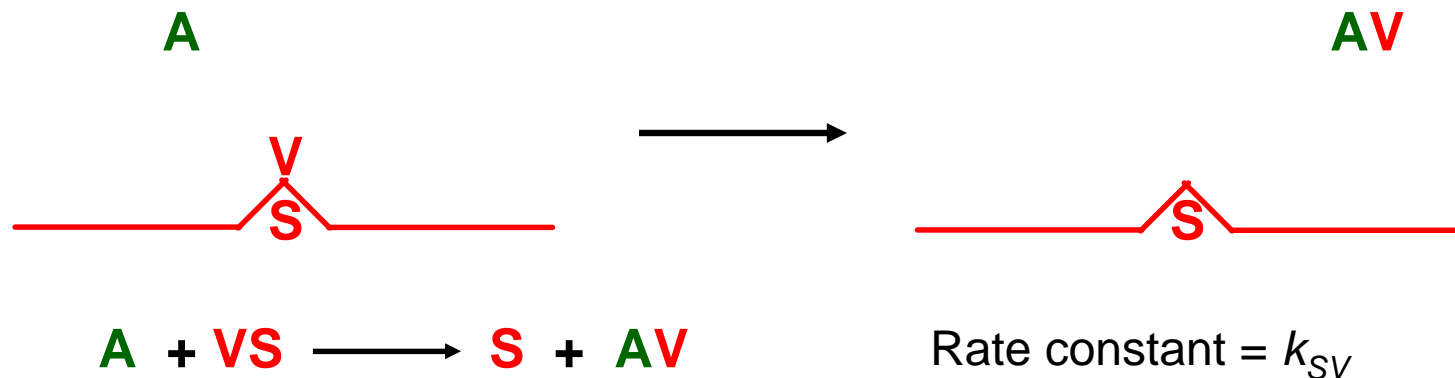


Cobra Venom Reactions

Reaction of venom with antivenom on site:

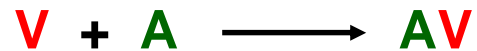


Reaction of antivenom with venom on site:



Cobra Venom Reactions

Reaction of venom and antivenom in blood:



Rate constant = k_p

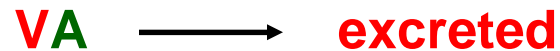
Removal of products and reactants from system:



Rate constant = k_{0V}



Rate constant = k_{0A}



Rate constant = k_{0P}

Concentration of venom in the blood

$$\frac{d(C_V)}{dt} = \left[\begin{array}{l} \text{initial concentration} \\ \text{of free sites} \end{array} \right] \left(- \left[\begin{array}{l} \text{fraction of sites being} \\ \text{uncovered by venom} \end{array} \right] + \left[\begin{array}{l} \text{fraction of sites already} \\ \text{covered by antivenom that} \\ \text{are reacting with venom} \end{array} \right] \right) \\ - \left[\begin{array}{l} \text{concentration of sites being occupied} \\ \text{by venom - antivenom reaction} \end{array} \right] - \left[\begin{array}{l} \text{concentration of venom} \\ \text{leaving the body} \end{array} \right]$$

$$\frac{d(C_V)}{dt} = C_{S0} (-k_V f_S C_V - k_{SA} f_{SA} C_V) - k_P C_V C_A - k_{OV} C_V$$

Rate Law and Material Balances contd.

Concentration of antivenom in the blood

$$\begin{aligned} \frac{d(C_A)}{dt} = & \left[\begin{array}{l} \text{initial concentration} \\ \text{of free sites} \end{array} \right] \left(- \left[\begin{array}{l} \text{fraction of sites being} \\ \text{covered by antivenom} \end{array} \right] + \left[\begin{array}{l} \text{fraction of sites being} \\ \text{uncovered by antivenom} \end{array} \right] \right) \\ & + \left[\begin{array}{l} \text{initial concentration} \\ \text{of free sites} \end{array} \right] \left(- \left[\begin{array}{l} \text{fraction of sites already} \\ \text{covered by venom that are} \\ \text{reacting with antivenom} \end{array} \right] \right) \\ & - \left[\begin{array}{l} \text{concentration of sites being occupied} \\ \text{by venom - antivenom reaction} \end{array} \right] - \left[\begin{array}{l} \text{concentration of venom} \\ \text{leaving the body} \end{array} \right] \end{aligned}$$

$$\frac{d(C_A)}{dt} = C_{S0} (-k_A f_S C_A + k_{-A} f_{SA} - k_{SV} f_{SV} C_A) - k_P C_V C_A - k_{OA} C_A$$

Base Case: Polymath Input

Indep Var Initial Value
 Solve with Final Value

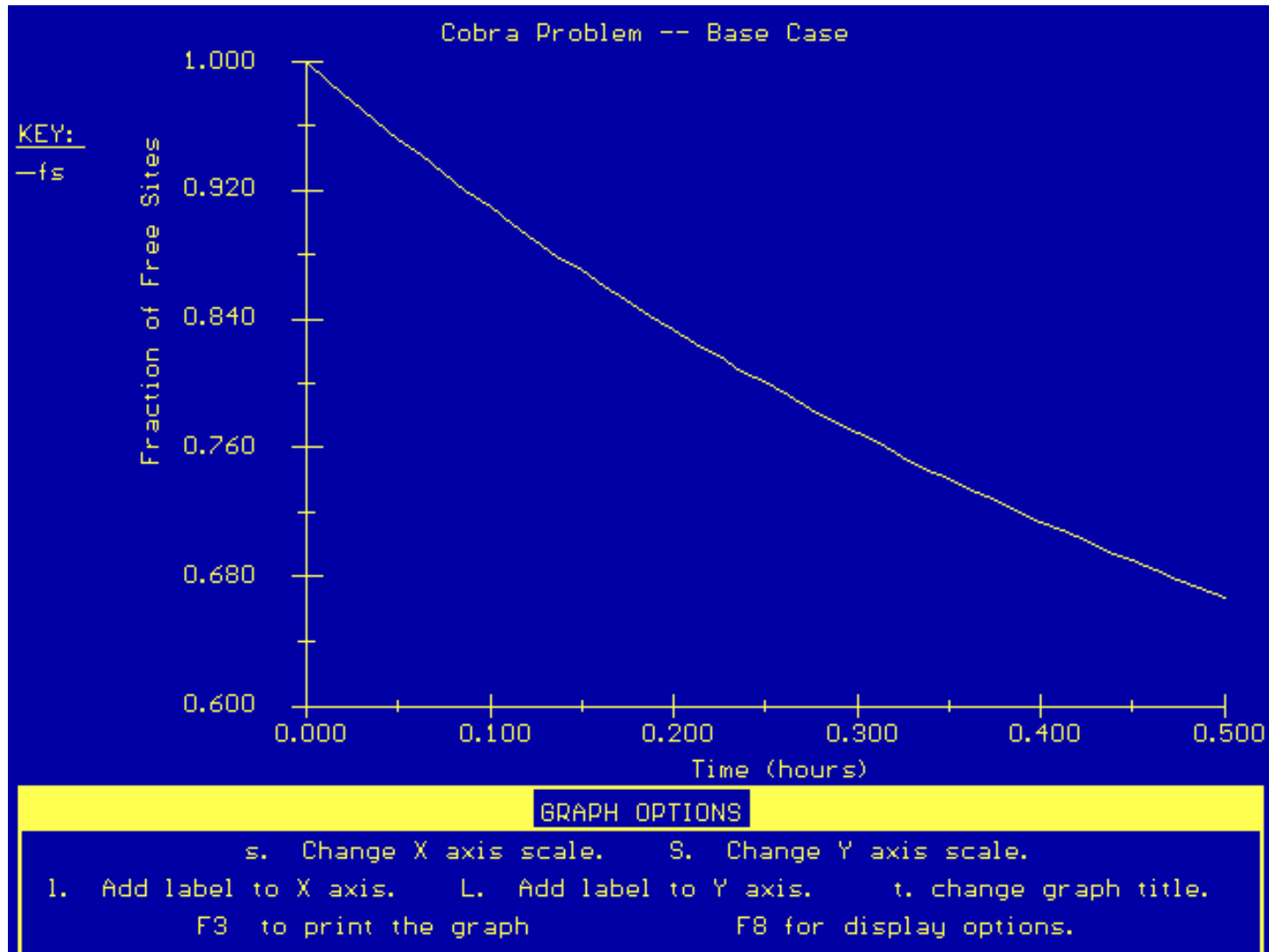
Comments

	Differential equations / explicit equations	Initial value
1	$d(fsv)/d(t) = kv*fs*Cv - ksv*fsv*Ca$	0
2	$d(fs)/d(t) = -kv*fs*Cv - ka*fs*Ca + kia*fsa + g$	1
3	$d(Cv)/d(t) = Cso*(-kv*fs*Cv - ksa*fsa*Cv) + h$	5e-09
4	$d(Ca)/d(t) = Cso*(-ka*fs*Ca + kia*fsa) + j$	0
5	$d(fsa)/d(t) = ka*fs*Ca - kia*fsa - ksa*fsa*Cv$	0
6	$d(Cp)/d(t) = Cso*(ksv*fsv*Ca + ksa*fsa*Cv) + m$	0
7	$kv = 2e8$	n.a.
8	$ksv = 6e8$	n.a.
9	$ka = 2e8$	n.a.
10	$kia = 1$	n.a.
11	$Cso = 5e-9$	n.a.
12	$ksa = 6e8$	n.a.
13	$kp = 1.2e9$	n.a.
14	$kov = 0$	n.a.
15	$koa = 0.3$	n.a.
16	$kop = 0.3$	n.a.
17	$g = ksa*fsa*Cv + ksv*fsv*Ca$	n.a.
18	$h = -kp*Cv*Ca - kov*Cv$	n.a.
19	$m = kp*Cv*Ca - kop*Cp$	n.a.
20	$j = -Cso*ksv*fsv*Ca - kp*Cv*Ca - koa*Ca$	n.a.

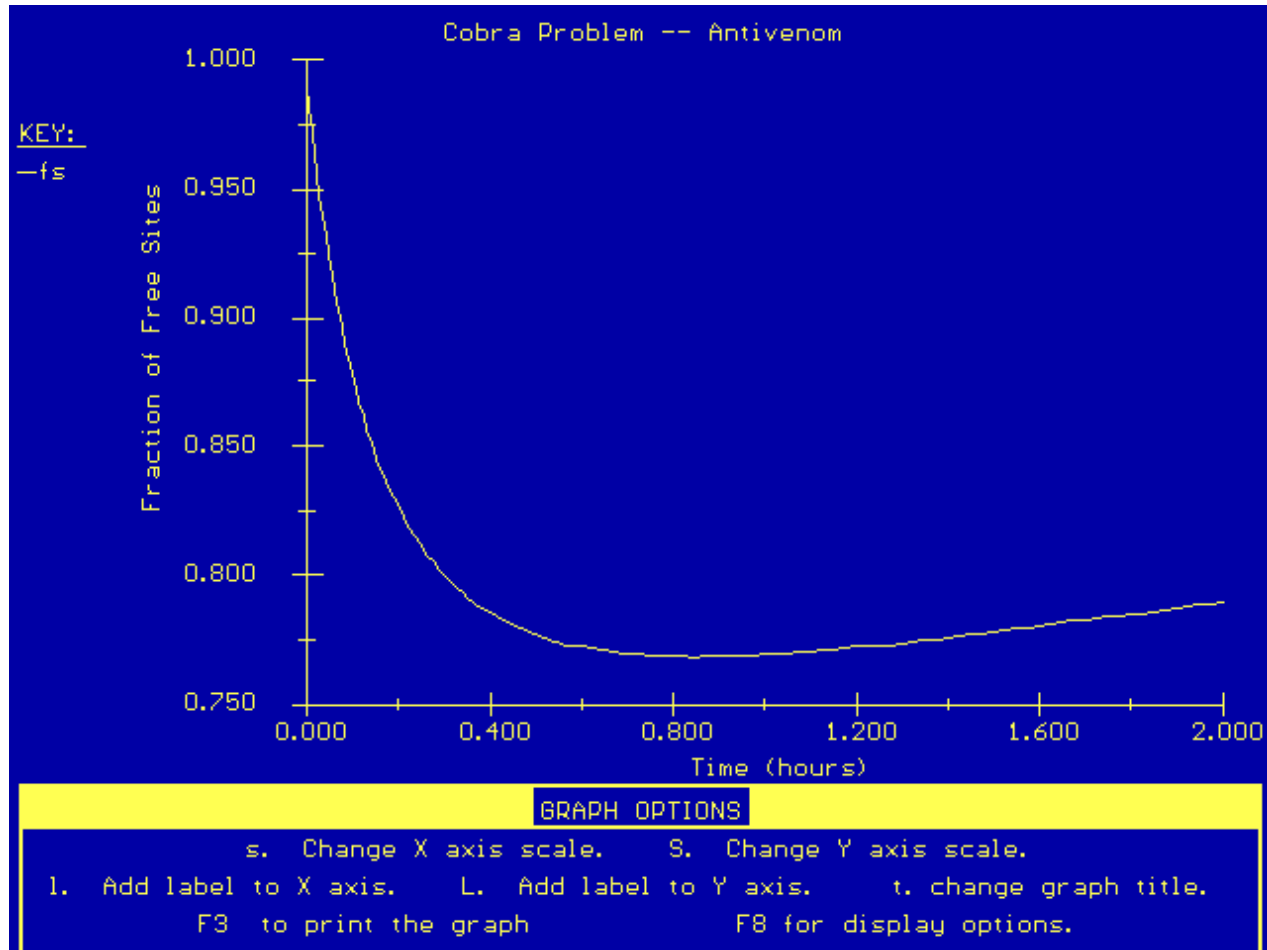
Assumptions:

1. Body is a batch reactor
2. Body is well-mixed

Polymath Solution for the Base Case



Polymath Solution for the Antivenom Case



Hippo

Modeling the Digestive System of a Hippopotamus^{*}

Matthew Robertson, Fredrik Persson, Professor H. Scott Fogler



"Even hippo's like Chemical Reaction Engineering."

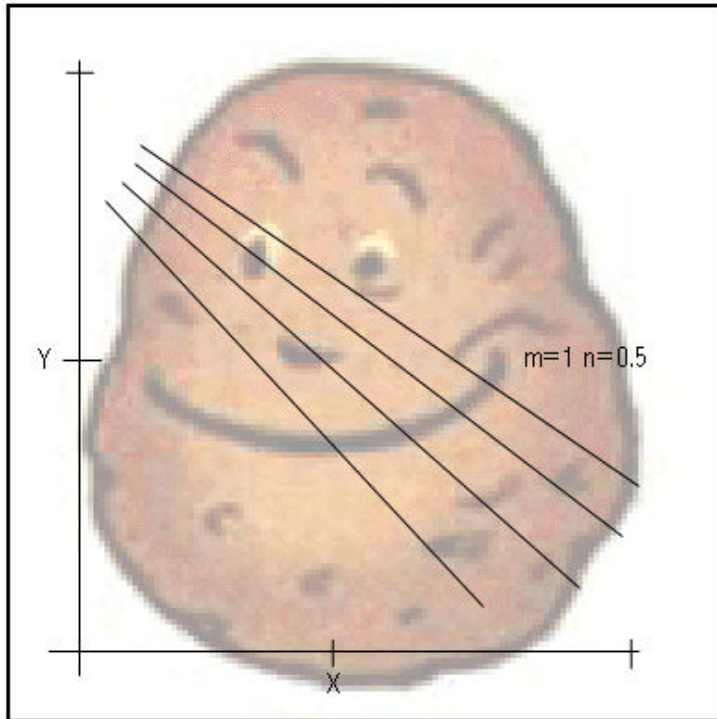


^{*}From a problem suggested by **Professor Alice P. Gast**
["Animal Guts as Ideal Reactors", Chemical Engineering Education, Winter 1998, pp 24-29]

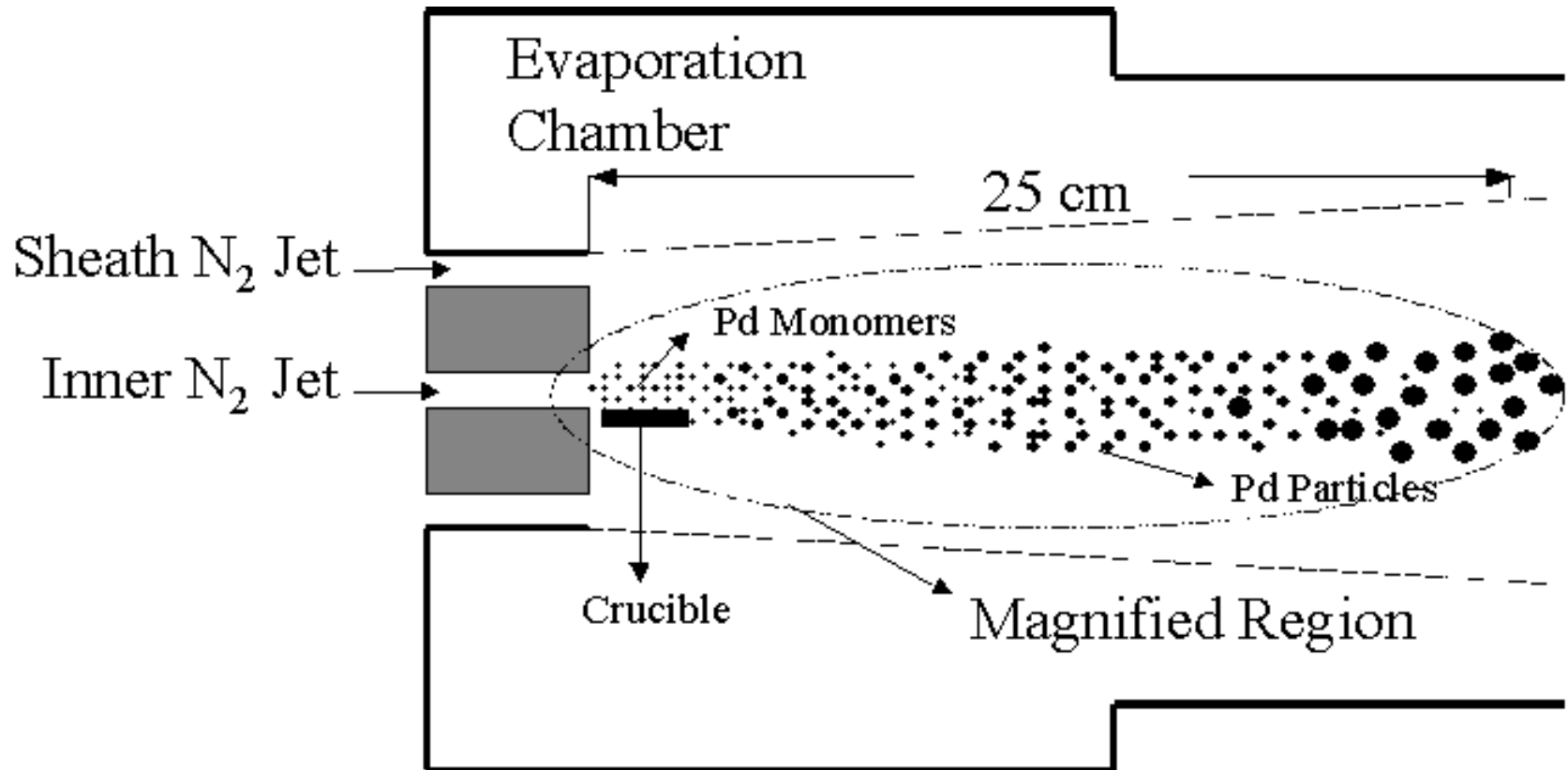
Potato

Baking a Potato!

*A basic chemical engineering experiment by:
Matthew Robertson, Fredrik Persson, Lander Coronado-Garcia,
Professor H Scott Fogler and Professor Levi Thompson*

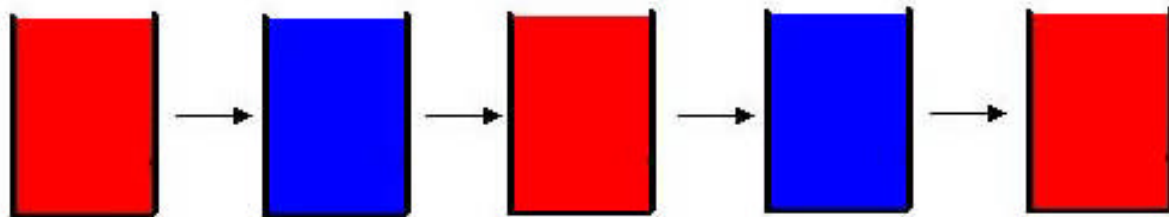
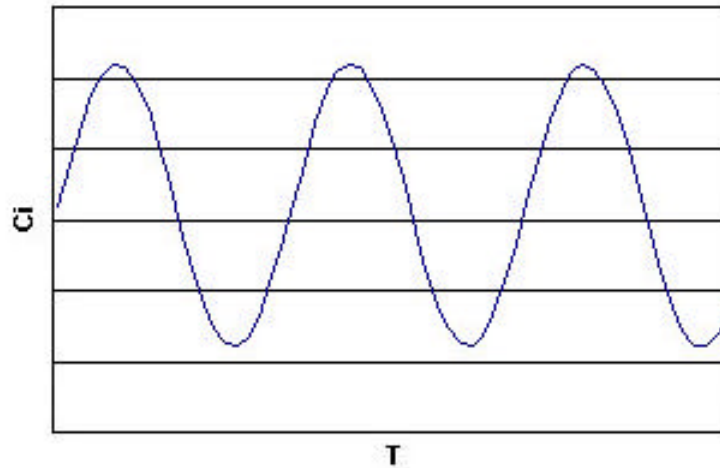


Aerosol Reactors



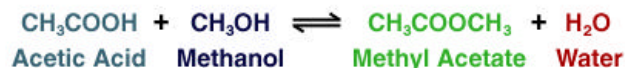
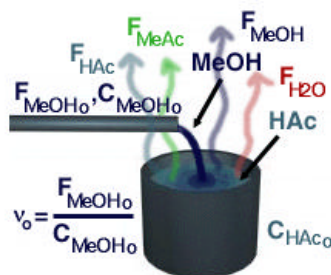
Oscillating Reactions

Oscillating Reactions Web Module



Reactive Distillation

Introduction



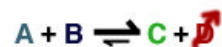
Reactive distillation is used with **reversible, liquid phase** reactions. Suppose a reversible reaction had the following chemical equation :



For many reversible reactions the equilibrium point lies far to the left and little product is formed :



However, if one or more of the products are removed more of the product will be formed because of Le Chatlier's Principle :

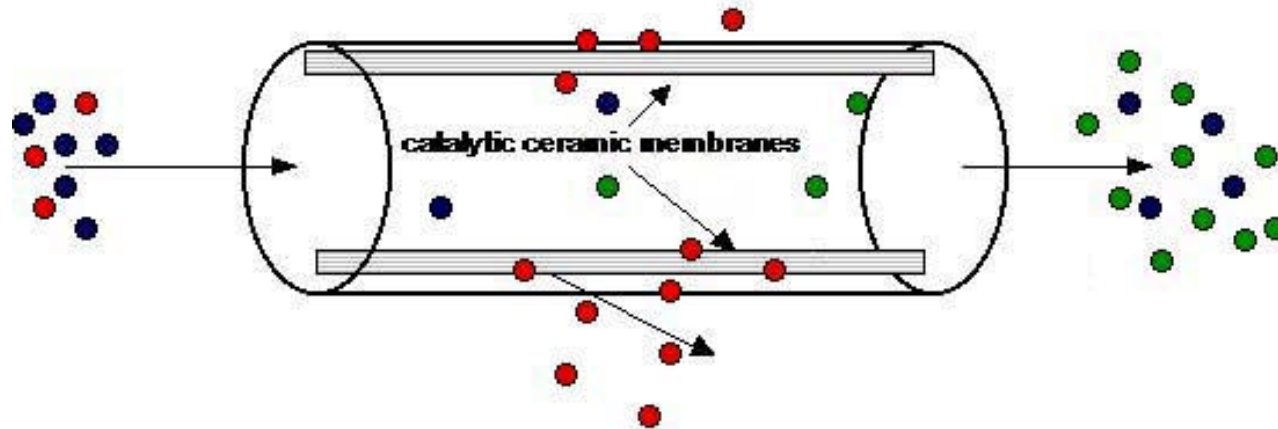
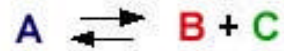


Removing one or more of the products is one of the principles behind reactive distillation. The reaction mixture is heated and the product(s) are boiled off. However, caution must be taken that the reactants won't boil off before the products.

For example, Reactive Distillation can be used in removing acetic acid from water. Acetic acid is the byproduct of several reactions and is very useful in its own right. Derivatives of acetic acid are used in foods, pharmaceuticals, explosives, medicinals and solvents. It is also found in many homes in the form of vinegar. However, it is considered a pollutant in waste water from a reaction and must be removed.



Membrane Reactors



A mixed feed of **A** and **B** enters the membrane reactor. **C** is produced in the reactor, and **B** diffuses out through the membrane pores. There are multiple ceramic membranes, but only two are shown for simplicity.

Creative Thinking

Elementary Principles of Chemical Processes, 3/e

- Felder and Rousseau

CREATIVITY EXERCISE

The costs of petroleum and natural gas have increased dramatically since the early 1970's, and there is some question about their continued long-term availability. List as many alternative energy sources as you can think of, being as creative as you can, and then go back and suggest possible drawbacks to each one.

Vehicles to Develop Creative Thinking Skills

“Thinking creatively is an active, purposeful, cognitive process we use to develop ideas that are unique, useful, and worthy of further elaboration.”

- Techniques to develop creative ideas
- Solving Open-Ended Problems (OEPs)
- Solving OEP enhanced home problems
- Learning how to choose open ended problems

Untitled - Microsoft Internet Explorer

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The Des Plaines River Wetlands Project

The Des Plaines River is located in southern Wisconsin and northeast Illinois (See image below). It runs along the city of Chicago and finally empties into the Illinois and Kankakee rivers.

The map displays the geographical context of the Des Plaines River. Wisconsin is shown in green at the top, Illinois in yellow in the center, and Indiana in red at the bottom right. Lake Michigan is a blue body of water on the right side. The Des Plaines River is a blue line flowing from the top right towards the bottom center. A small blue square on the river in Illinois is labeled 'Des Plaines Wetlands' with an arrow. The city of Chicago is marked with a black dot and labeled. At the bottom of the map, the Illinois and Kankakee rivers are labeled. The browser interface includes a status bar at the bottom with 'Done' and 'Internet' indicators.

Des Plaines River Wetlands

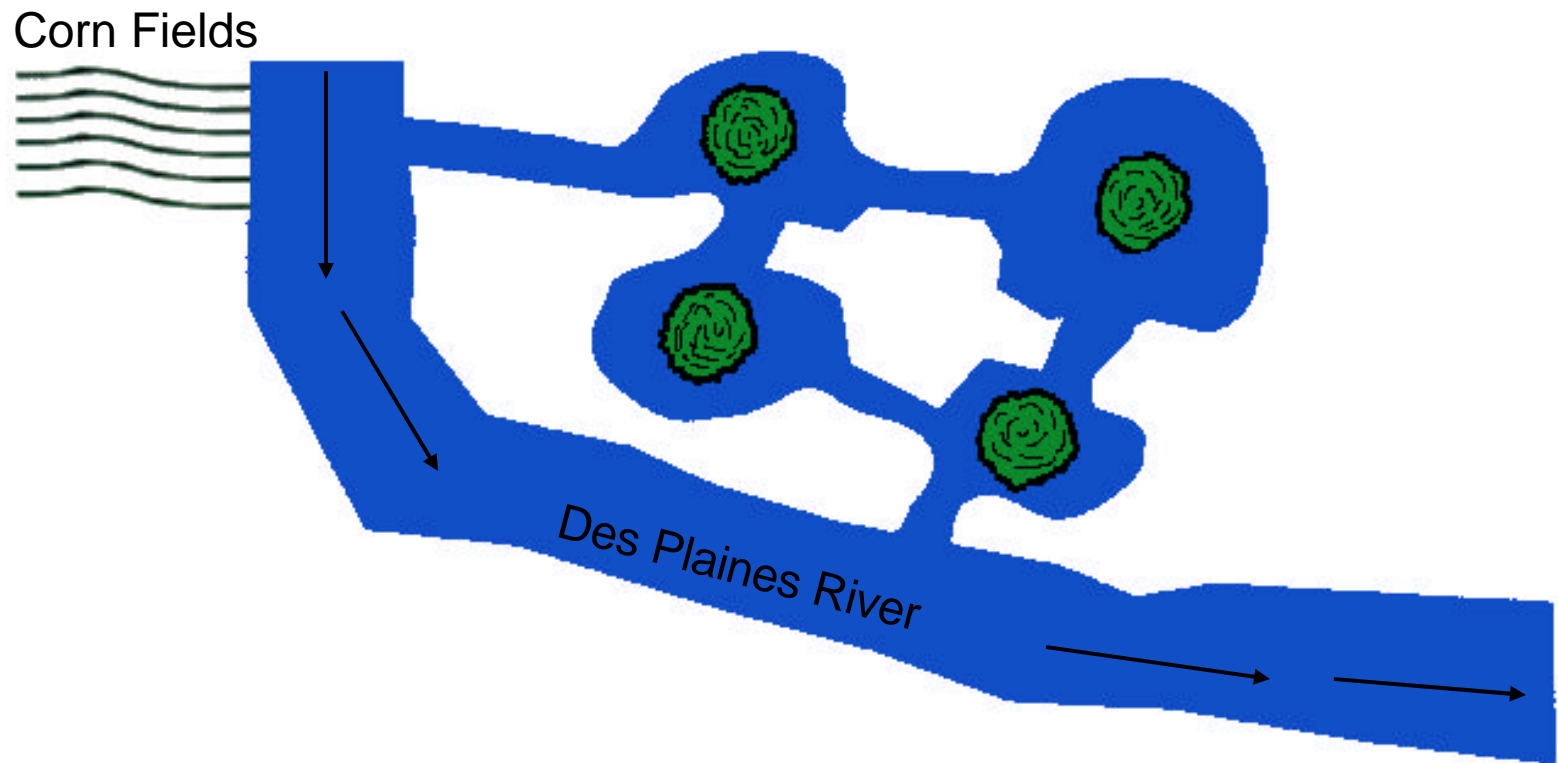


Des Plaines River Wetlands



Des Plaines River Wetlands

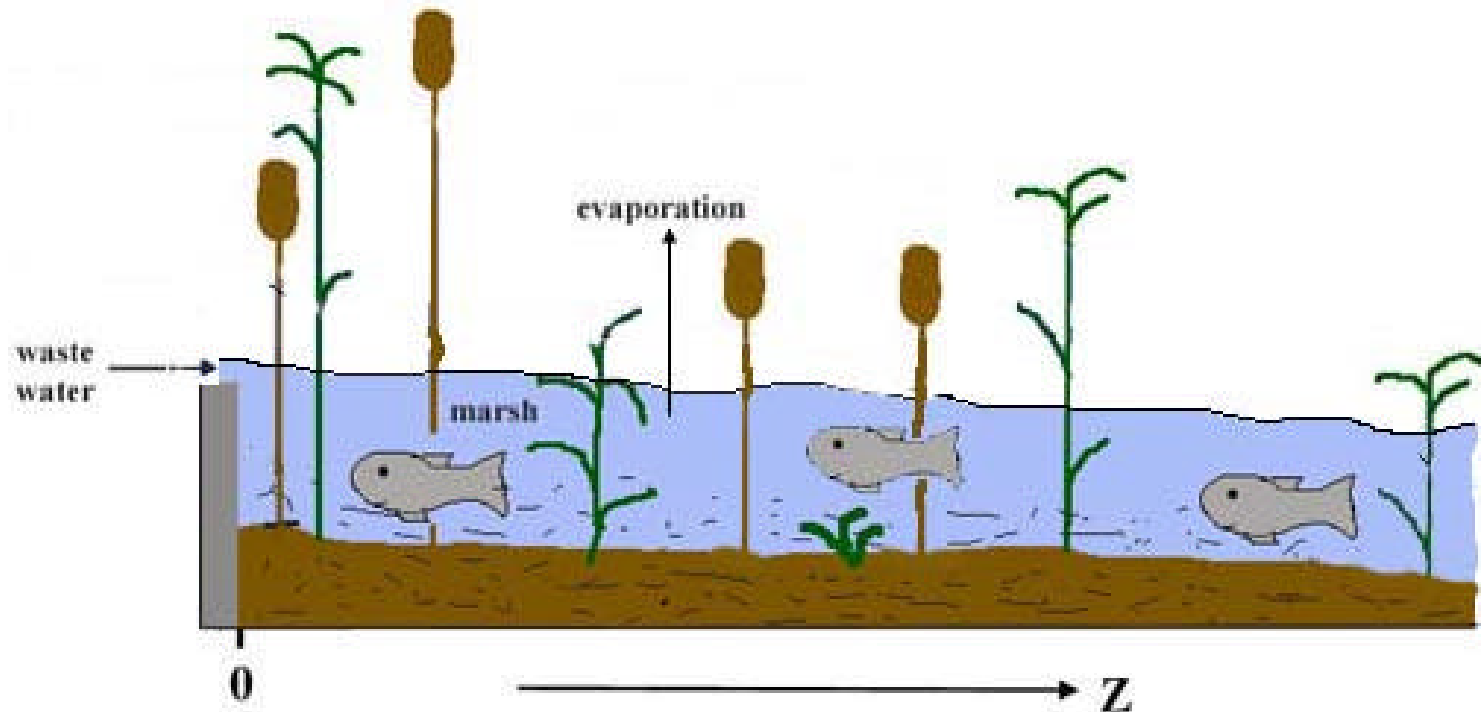
Wetlands to degrade Atrazine



Des Plaines River Wetlands



Modeling a Treatment Wetland as a simple PFR



The Equations

Wetlands

Mole Balance $F_{A0} \frac{dX}{dV} = -r_A$ (1)

Rate Law $-r_A = k_1 C_A$ (2)

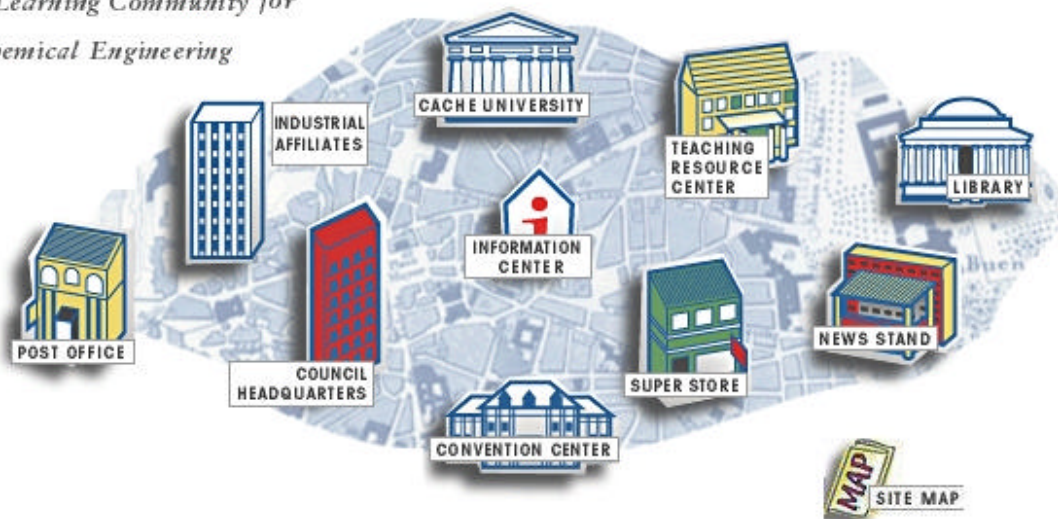
Stoichiometry $\mathbf{u} = \mathbf{u}_o + \frac{Q^* W^* z}{\mathbf{r}_m}$ (3)

$$C_A = \frac{F_{A0}}{\mathbf{u}} \quad (4)$$

Combine
$$C_{A0} = \frac{C_{A0}(1-X)}{1 - \frac{Q^* W^* z}{\mathbf{r}_m^* \mathbf{u}_o}} \quad (5)$$

Solve
$$X(z) = 1 - \left(1 - \frac{Q^* W^* z}{\mathbf{r}_m^* \mathbf{u}_o} \right)^{\left(\frac{1}{\frac{Q^* W^*}{\mathbf{r}_m^* \mathbf{u}_o} k_1^* W^* \frac{D}{\mathbf{u}_o}} \right)} \quad (6)$$

*A Learning Community for
Chemical Engineering*



Map key

									
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