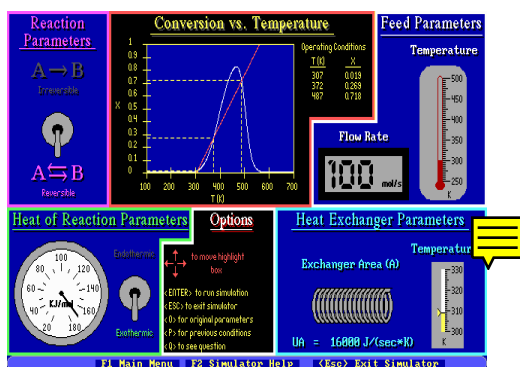
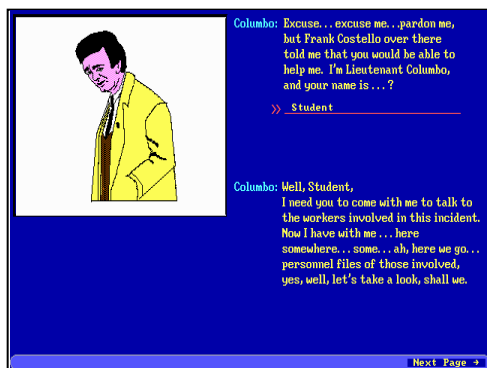


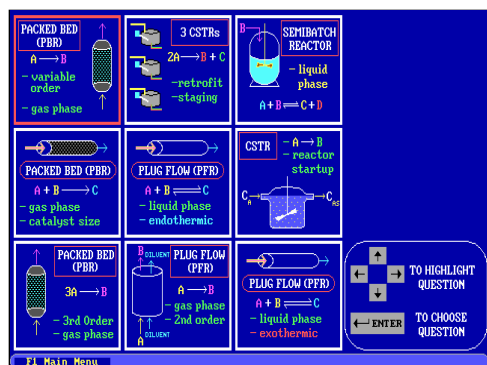
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NSF Project - "A Focus on Developing Innovative Engineers"  
Interactive Computer Modules Project

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## **Introduction**

---

## Package Contents

This package includes the "Kinetics" computer modules developed under an NSF grant "A Focus on Developing Innovative Engineers." This booklet describes how to install and run the modules, and contains a brief description of the modules, including the material covered, and references to the appropriate chapters in Fogler, The Elements of Chemical Reaction Engineering, Prentice-Hall, 2nd ed., 1992, for easy integration into a reaction kinetics course. An insert describes how to decipher the performance numbers generated by the module to obtain the student's score.

The modules included in the diskette are:

KINCHAL1	Kinetics Challenge 1 - Introduction to kinetics
STAGING	Reactor staging and optimization
KINCHAL2	Kinetics Challenge 2 - Stoichiometry and rate laws
COLUMBO	CSTR-Volume Algorithm - A murder mystery.
TICTAC	Ergun, Arrhenius, and Van't Hoff equations in isothermal reactor design.
ECOLOGY	Collection and analysis of rate data - Ecological engineering
HETCAT	Heterogeneous catalysis.
HEATFX-1	Simulation - Mole and energy balances in a CSTR.
HEATFX-2	Simulation - Mole and energy balances in a PFR.

Additional module sets are available for chemical engineering courses in material and energy balances, fluids and transport, and separations.

---

## Project History

Interactive computer instruction has been in use at the University of Michigan's Chemical Engineering department since the mid 1970's. At that time interactive computer modules that ran on our mainframe computer were created for the kinetics course by Prof. H. Scott Fogler. These activities have become more sophisticated over the years, always taking advantage of the current state of computer technology.

---

## Educational Benefits

It is becoming well established that students learn best when they experiment with subject matter themselves, and are actively involved in the subject matter (Felder, R.M. *Engineering Education*, April 1988, pp. 674-681). The current generation of interactive computer modules, developed over a 5 year period, take advantage of three of the unique features of computers – computation, interactivity, and graphical animations – to address a variety of learning modes.

---

## Module Components

Interactive computer modules typically include:

- Menu
- Review of pertinent fundamentals
- Interactive testing of fundamentals
- Demonstration
- Interactive exercise
- A solution to the exercise
- Evaluation

---

## Module Features

Using interactive computer modules allows students to “review and demonstrate mastery of the material at his/her own pace, provides them with immediate feedback to their responses, and allows them to explore the effects of parameter variations on a system, perform simulations to optimize its performance, and carry out simulated experiments from which they can obtain the data needed to model the system.” (Fogler, Montgomery and Zipp, *Comp. Appl. in Eng. Educ.*, Vol 1(1) 11-12, September/October 1992).

During the 5-year development process, we have incorporated the pedagogical expertise we have gained during extensive testing both at the University of Michigan and many other universities. This testing has allowed us to ensure that the modules best address the issues that ensure success in interactive computer learning:

- Ease of use
- Maintaining focus on the concepts
- Minimal tediousness
- Promoting learning
- Individual guidance.

Additional features included in some modules include introduction to new technologies using graphical animations, and entertaining motivators, which have been shown to increase the students’ interest and motivation for the module content (R. Snow and M. Farr, *Aptitude, Learning, and Instruction. Vol 3: Conative and Affective Process Analysis.* Hillsdale, NJ, Erlbaum, 1987).

# Installation and Information

---

**Computer Requirements** These modules run on IBM-PCs and compatibles with EGA or better graphics. The recommended system includes DOS 5.0, 25Mh 80386 processor and math co-processor. 500 kB executable program size should be sufficient to run most of the modules. Hetcat requires approx. 570 kB of memory to perform correctly.

---

**Installing the Modules** The modules cannot be executed from the floppy disk, since it contains compressed files. You should install the files in a directory on your hard disk, and run them from that directory. Run the installation routine provided from the drive that the diskette is in. For example, if you place the diskette in drive A:, type:

```
C:> A:  
A:> INSTALL
```

This installation routine will place some required files in the directory you specify, and the files needed to run each individual module in corresponding subdirectories.

Should you have any problems installing or running the modules, please contact Prof. Susan Montgomery at (313) 936-1890, or e-mail [smontgom@engin.umich.edu](mailto:smontgom@engin.umich.edu).

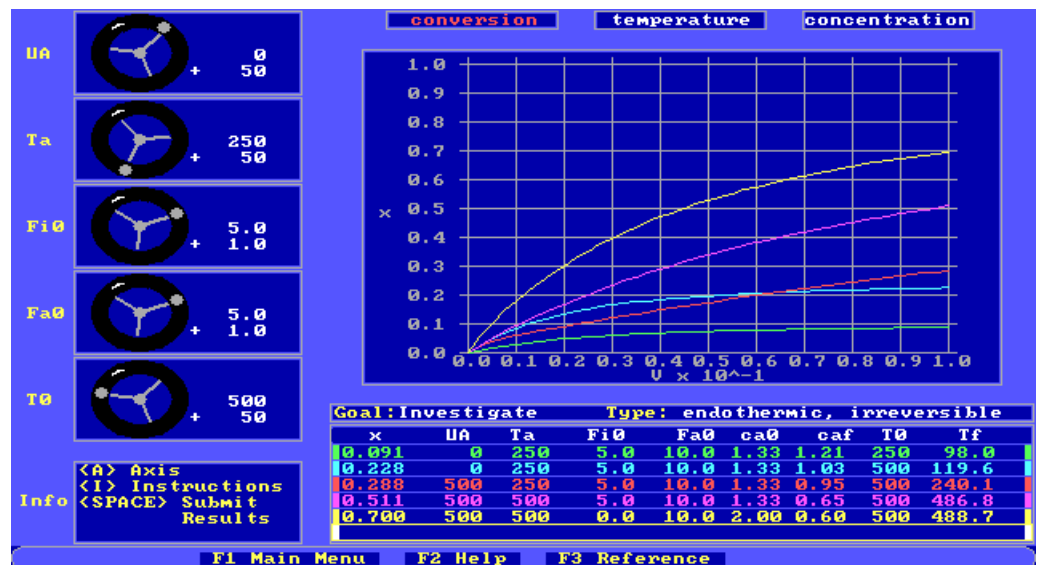
---

**Running the Modules** Be sure the modules have been installed first, and that you are in the newly created directory. Then type the batch file name corresponding to the module. For example, if you installed the modules in the C:\MODULES directory, and want to run the module HEATFX1, the steps would be:

```
C:> CD MODULES  
C:\MODULES> HEATFX1
```

---

**Hot Keys** Most screens contain a bright blue command bar at the bottom of the screen. This command bar lists the F-keys that are currently active:



By pressing one of the F-keys listed in the command bar, the corresponding option is executed:

- F1: Main Menu - This option allows the user to exit to the module's main menu.
- F2: Hints - If a hint is available, this option activates a pop-up hint.
- F3: Reference - This option activates a pop-up screen containing information relevant to the problem. For example, it may contain conversion factors, measured results, or necessary equations.
- F4: Tools - This allows access to a pop-up calculator.

In addition to active F-keys, a few other instructions are included. For example, pressing the right arrow will typically lead to the next screen. Note: The arrow keys on the numeric key pad may only be used if "Num Lock" is turned off.

---

## Authoring System

The modules were written using the Quest Authoring System, versions 3.0, 4.0 and 4.1. Quest is a product of Allen Communication, 140 Lakeside Plaza II, 5225 Wiley Post Way, Salt Lake City, Utah, 84116 (801) 537-7800.

# KinChal1: Kinetic Challenge 1 - Introduction To Kinetics

## Concepts

Definitions of rates of reaction.  
Types of reactors  
General mole balances for batch reactors, CSTR's and PFR's.

$$\int^V r_j dV_{\text{Batch}} = \frac{dN_j}{dt}, \quad V_{\text{CSTR}} = \frac{F_{j0} - F_j}{-r_j}, \quad \frac{dF_j}{dV_{\text{PFR}}} = r_j$$

## Time

29 minutes  $\pm$  10 minutes

## Reference

Fogler: Chapter 1

## Description

This module allows the students to test their knowledge of the general mole balance equation, reaction rate laws, as well as types of reactions and reactors. The interaction occurs in the form of an interactive game with timed responses and computer competitors. Twenty questions are selected from a pool of approximately 100 multiple choice questions. Students can choose questions from any of four categories (mole balance, reactions, rate law, and reactor types) and five difficulty levels (100 - 500 points):



The student has one minute to choose the correct answer. The module responds to the student's choice, either reinforcing the reasoning for a correct answer, or immediately clarifying a misunderstanding if an incorrect answer is entered. If

no response is entered within the time limit, or if an incorrect response is entered, the points are lost, and one of the computer competitors tries to answer the question:

What are the units of k in the equation  $-R_a = k C_a^2 C_b$  ?

1. moles/time
2. moles \* time/volume<sup>2</sup>
3. moles/volume
4. volume<sup>2</sup>/moles<sup>2</sup>/time

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

Host: 1 is incorrect. Ra has units of mol/time/volume.  
Columbo: This reminds me of a class I had in high school. My chemistry teacher was showing the class an experiment, and ...  
Arrhenius: The answer is 4.  
Host: Correct. The units work out fine this way.

F1 Main Menu      Return to Board →

The competitor who last answered a question correctly gets to pick the following category and degree of difficulty. (Note that this will not necessarily always be the student). In addition to regular questions, one question is randomly assigned as the "Double Challenge" in which the student has the option of betting points. After all twenty questions have been answered, the contestants with positive scores go on to the "Final Challenge" question, in which they are also allowed to bet points.

---

## Grade Base

The game score is the number of accumulated points, including gains or losses from Double Challenge and Final Challenge. For the performance scores, the student is given 3 points for every correct answer in the 100-300 point range, and 7 points for the 400-500 point questions. The Final Challenge question is worth 8 points. 75 points are needed to achieve mastery.

---

## Comments

Students have used this module as review material before an exam, to ensure that they had a solid grasp of the basics of reaction kinetics. Some professors have also made use of it in recitation sections, inviting student volunteers to enter responses, then discussing any conceptual misunderstandings that might be discovered.

# Staging: Reactor Staging Optimization

## Concepts

Concentration as a function of conversion  
CSTR vs. PFR volume-conversion relationships  
Effect of changing order of reactor placement on final conversion.

## Time

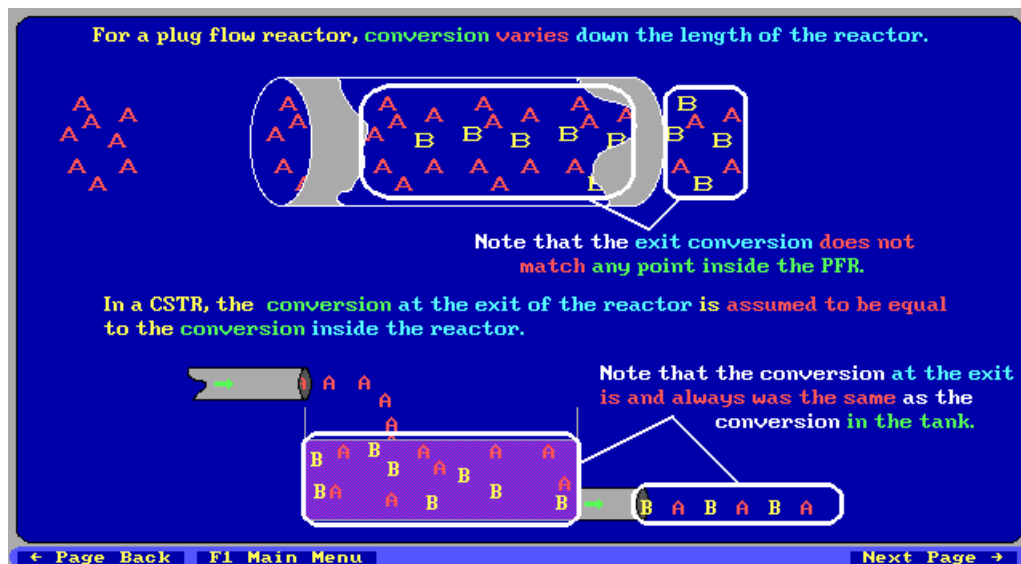
35 minutes  $\pm$  10 minutes

## Reference

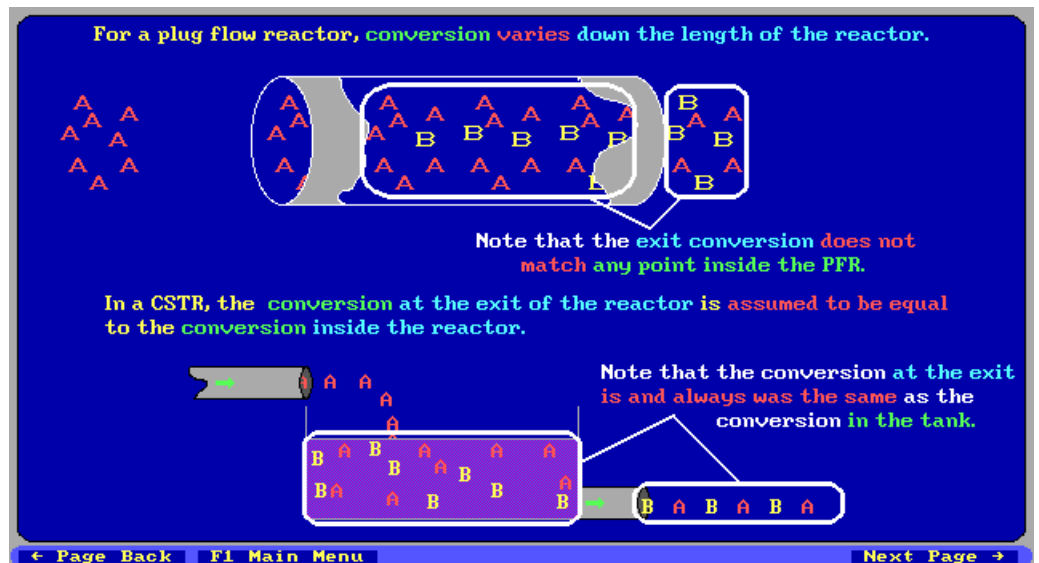
Fogler: Chapter 2

## Description

In the interaction portion of this module the student must arrange a group of five reactors – CSTRs and PFRs – in the order that will result in at least 75% conversion, while maximizing the product flow rate for the reaction  $A \rightarrow B$ . Both the  $-F_{A0}/r_A$  vs.  $X$  graph and the reactor volumes are specified, and many arrangements of reactor order and inlet flow rate can be tested using an interactive simulation:



The student may at any time access a reference section that reviews the derivation of the design equations for PFRs and CSTRs, clarifying the change in conversion down a PFR, and the well-mixedness of the CSTR:



The reactor optimization simulator can also be run independently of the scenario. This allows the professor to present the student with a variety of open-ended problems to be investigated using the simulator.

---

## Grade Base

The student's score is based on the conversion achieved, as well as the total flow rate of material produced.

---

## Comments

This module makes use of a scenario to increase the level of interest of the student. In the scenario, the student must generate a sufficient amount of an antidote of high enough purity to help Mr. Hyde get back to his Dr. Jeckyll persona.

# KinChal2: Kinetic Challenge 2 - Stoichiometry And Rate Laws

Concepts Arrhenius equation  
Stoichiometry tables  
Rate laws.

Time 36 minutes ± 16 minutes

Reference Fogler: Chapter 3

Description This module focuses on rate laws and stoichiometry, allowing the students to master the elements of the stoichiometric table:

**EXPRESSING CONCENTRATIONS IN TERMS OF CONVERSION – cont.**

If the reaction is in the **gas** phase, we have to keep track of possible changes in volume with reaction. For the two **gas** phase reactions

$$A + 2B \rightarrow C \qquad A + 2B \rightleftharpoons C$$

we can adapt the **stoichiometric table** to account for volume changes:

Species	Feed rate	Change	Effluent rate	Concentration
A	$F_{Ao}$	$- F_{Ao} X$	$F_A = F_{Ao} (1 - X)$	$C_A = \frac{F_{Ao}}{v} (1 - X)$
B	$F_{Bo}$	$- 2 F_{Ao} X$	$F_B = F_{Ao} (\theta_B - 2X)$	$C_B = \frac{F_{Ao}}{v} (\theta_B - 2X)$
C	$F_{Co}$	$+ F_{Ao} X$	$F_C = F_{Ao} (\theta_C + X)$	$C_C = \frac{F_{Ao}}{v} (\theta_C + X)$
volume :	$F_{To}$	$- 2 F_{Ao} X$	$F_T = F_{To} - 2 F_{Ao} X$	$C_T = \left( \frac{F_{Ao}}{v} - 2 \frac{F_{Ao}}{v} X \right)$

$$v = v_o \frac{F_T}{F_{To}} \frac{P_o}{P} \frac{T}{T_o} = v_o \frac{F_{To} - 2 F_{Ao} X}{F_{To}} \frac{P_o}{P} \frac{T}{T_o} = v_o (1 - 2y_{Ao} X) \frac{P_o}{P} \frac{T}{T_o}$$

[Continue →](#)

The interaction portion of the module is similar to that in Kinetic Challenge 1. Students can choose from four categories (reactants, products, rate law, potpourri) and four levels of difficulty (200-1,000 points).

The key focus in this module is to provide the students with practice so they will avoid the more prevalent mistakes: Expressing the reaction rate law for an irreversible reaction as if it were reversible, and using the ideal gas law for liquid-phase reactions:

Which of the following is the concentration of D for the nonisothermal elementary, irreversible, gas phase reaction  $A + 2B \rightarrow 2C + 3D$ ? The feed is equimolar in A and B.

1.  $C_D = C_{A0}^{3X}$

2.  $C_D = C_{A0} \frac{3X}{(1-X)} \frac{P}{P_0} \frac{T_0}{T}$

3.  $C_D = C_{A0} \frac{3X}{(1+X)} \frac{P}{P_0} \frac{T_0}{T}$

4.  $C_D = C_{A0}^X$

Select an answer (1-4) or  
<ESC> to forfeit (no gain or loss): 3

Host: Correct.



F1 Main Menu

Return to Board →



---

## Grade Base

The game score is the number of accumulated points, including gains or losses from Double Challenge and Final Challenge. For the performance scores, the student is given 3 points for every correct answer in the 200-600 point range, and 7 points for the 800-1,000 point questions. The Final Challenge question is worth 8 points.

---

## Comments

Students report that they find this module very useful as a review before the first examination. In some instances, some of the text strings in the last few questions and the Final Challenge question will become garbled, and the computer will lock up at the end of the module. We have been unable to determine the circumstances that give rise to this effort.

Some students comment that the one minute time limit does not allow them enough time to derive the required expressions. It is helpful to suggest to students that they examine the four options available and choose the correct answer by process of elimination, based on the information provided in the problem statement, rather than trying to derive the expressions.

# Columbo : CSTR - Volume Algorithm - A Murder Mystery

---

Concepts                      Isothermal CSTR reactor design  
                                    Problem solving and analysis

---

Time                            32 minutes  $\pm$  10 minutes

---

Reference                    Fogler: Chapter 4

---

Description                    The principal purpose of this module is to allow students to practice the algorithm for CSTR design:

**The General Algorithm to Follow is. . .**

1. Mole Balance
2. Rate Law
3. Stoichiometry
4. Combine
5. Evaluate Parameters

Next Page →

In the interaction portion of the module the student must solve a murder mystery, with the aid of Lieutenant Columbo. It seems that overnight there was a slight irregularity in the conversion in the reactor at the Nutmeg company:

**Columbo:** I also have the facts on the CSTR as well as the readings off of the conversion vs. time graph found at the scene...

Normal conv.=0.900  
conv. 2  
conv. 1

```

cstr vol: 150 gal
flow of A: 1 mole/min
flow of B: 8 mole/min
Total Flow: 20 gal/min
initial conv.= 90%
conversion 1=0.8592
conversion 2=0.8800
A + B → C
  
```

**Columbo:** Oh, by the way, student, should you ever want to take a look at any of the information that we have gathered, just get my attention by pressing the F3 key.

F3 Reference      Next Page →

It is feared that one of the employees may have been murdered by a fellow employee, and the dead body left within the reactor. By analyzing the conversion data, and using personnel information and knowledge of CSTR reactor design, the student must determine the identity of the murderer and the victim. Help may be obtained by questioning the suspects:

Suspects Available for Questioning

<p>QUESTIONED</p>  <p>Lizzy Borden</p> <p>Reactor Volume Changed</p>	<p>QUESTIONED</p>  <p>Clyde Barrow</p> $U = \frac{F_{Ao} X}{-r_a}$	 <p>Scarface</p>
---	--	---

**Note:** clues obtained from suspects are given in white

use ← or → to move highlight box  
<Enter> to select a suspect

Grade Base

Successful solution of the murder mystery with a minimum of assistance.

Comments

Students have always enjoyed the murder mystery scenario in this module.

# Tictac: Isothermal Reactor Design - Ergun, Arrhenius And Van't Hoff Equations

Concepts

Interaction of the Ergun, Arrhenius, and Van't Hoff equations and other considerations in isothermal reactor design.

Time

33 minutes  $\pm$  9 minutes

Reference

Fogler: Chapter 4

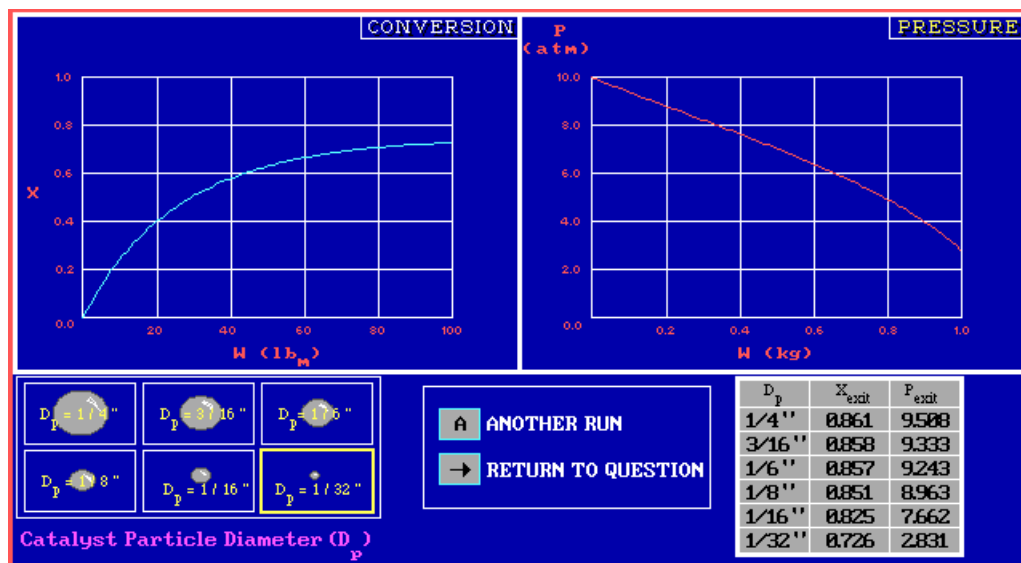
Description

This module allows the student to examine nine reactor design problems, and investigate the effect of varying reactor parameters on process performance. The problems are organized as in a tic-tac-toe board. The reactors covered by these problems include PFRs, CSTRs, packed bed reactors and semi-batch reactors:

<b>PACKED BED (PBR)</b> $A \rightarrow B$ - variable order - gas phase	<b>3 CSTRs</b> $2A \rightarrow B + C$ - retrofit - staging	<b>SEMI-BATCH REACTOR</b> - liquid phase $A + B \rightleftharpoons C + D$
<b>PACKED BED (PBR)</b> $A + B \rightarrow C$ - gas phase - catalyst size	<b>PLUG FLOW (PFR)</b> $A + B \rightleftharpoons C$ - liquid phase - endothermic	<b>CSTR</b> - $A \rightarrow B$ - reactor startup $C_A \rightarrow C_{ns}$
<b>PACKED BED (PBR)</b> $3A \rightarrow B$ - 3rd Order - gas phase	<b>PLUG FLOW (PFR)</b> $A \rightarrow B$ - gas phase - 2nd order	<b>PLUG FLOW (PFR)</b> $A + B \rightleftharpoons C$ - liquid phase - exothermic

TO HIGHLIGHT QUESTION  
 TO CHOOSE QUESTION

The student must master the concepts in enough squares to successfully win the tic-tac-toe game (Three adjacent squares horizontally, vertically, or diagonally). Each problem allows the student the opportunity to examine the effect of a specified operational parameter on reactor performance, using simulators:



After performing the “experiments” the student proceeds to answer three questions that examine the effects observed. These effects can be explained through the Ergun, Arrhenius, and Van’t Hoff equations. In many cases, competing effects are highlighted. The square is "won" by answering two out of the three questions correctly.

---

### Grade Base

Grade based on mastery of concepts within each square, and successful completion of the tic-tac-toe game.

---

### Comments

Some students have found the questions in this module to be slightly above their current level of understanding. They have mentioned, however, that the process was helpful in exploring these concepts.

# Ecology: Collection And Analysis Of Rate Data - Ecological Engineering

---

Concepts                      Collection and analysis of rate data  
Ecological engineering concepts

---

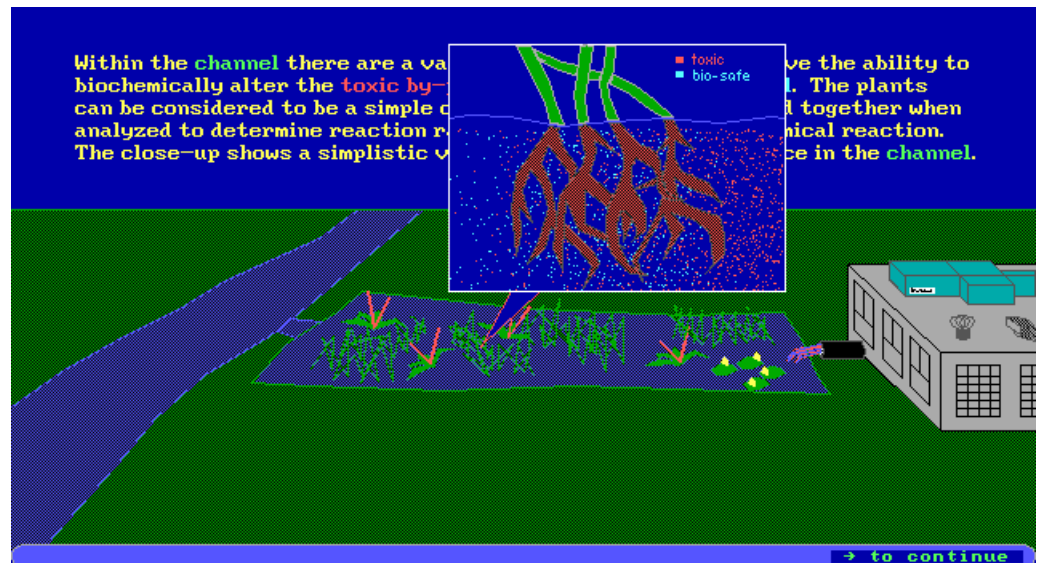
Time                              49 minutes  $\pm$  21 minutes

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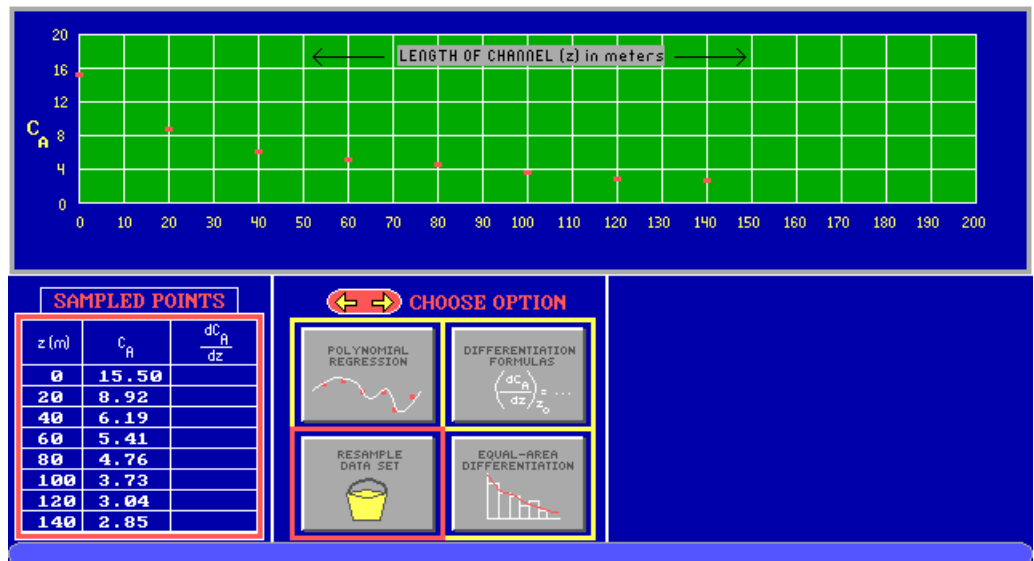
Reference                      Fogler: Chapter 5

---

Description                      The student, as an employee of a company trying to meet environmental regulatory agency standards, must sample concentration data for a toxic material found in a wetlands channel between a chemical plant upstream and a protected waterway to analyze the rate of decay of the toxic material.



The wetlands are modeled as a PFR. The student must first develop the necessary reactor design equation for a PFR, then start collecting data. This concentration data (which includes experimental error) is then analyzed in various ways (polynomial fit of the data followed by differentiation of the resulting equation, difference equations, etc.) to determine the rate law, as well as the rate constants and reaction order. Students must determine which points are to be excluded from the analysis (if any) and which points may be resampled:



The student then analyzes this information and submits a memo with the requested parameters:

The figure shows a software interface for data analysis. On the left is a graph of  $\ln(-\frac{dC_A}{dz})$  vs.  $\ln C_A$  with a linear regression line. The equation is  $y = 1.89x + -5.88$ ,  $R = 0.995$ . Below the graph is text: 'Here's a hard copy of the graph you produced...' and 'The form of the equation you used to produce the graph above was:'. Below that is a boxed equation:  $\ln \frac{-dC_A}{dz} = \alpha \ln C_A + \ln \frac{whk}{v}$ . On the right is a memo template with a 'To: Mr. Supervisor' header, a 'WORK TO DATE:' section, and three numbered options for the rate constant k. Option 1 is  $k = \frac{wh}{v} \text{EXP} \left[ \frac{\text{intercept}}{\text{slope}} \right]$ . Option 2 is  $k = \frac{v}{wh} \text{EXP} \left[ \frac{\text{intercept}}{\text{slope}} \right]$ . Option 3 is  $k = \frac{v}{wh} \text{EXP} \left[ \text{intercept} \right]$ . A red box highlights option 3. At the bottom is a red instruction: '<TOGGLE TO THE DESIRED EXPRESSION AND PRESS ENTER>'. The memo text states: 'Rate law analysis has been completed and the reaction order for the channel was determined to be 1.89. The reaction rate constant was also evaluated to be of the form:'.

This information is reviewed by the boss, who evaluates the parameter values and makes recommendation.

Grade Base

Based on correct determination of rate law parameters.

---

## Comments

This module is useful in exposing the student to experimental error and the dangers of using curve-fitting tools without discretion. It also exposes the student to “real world” applications of reaction kinetics. To introduce an element of levity, the student performs the analysis in a "Mr. Potatohead" persona. Students have reported enjoying this.

# Hetcat: Heterogeneous Catalysis

---

Concepts	Derivation of catalytic rate equations based on experimental data Selection of reaction mechanism and rate-limiting step that support the rate equation.
----------	---

---

Time	33 minutes $\pm$ 13 minutes
------	-----------------------------

---

Reference	Fogler: Chapter 6
-----------	-------------------

---

Description	The review section of this module reviews the essential elements of heterogeneous catalysis:
-------------	--

This module focuses on the steps that take place at sites on the pore surface:

- Reactant adsorption
- Surface reaction
- Product desorption

Let's take a closer look at the surface of the pore and each of these steps!

**Bulk Fluid** (containing a pink circle labeled 'B')

**Catalyst Pellet**

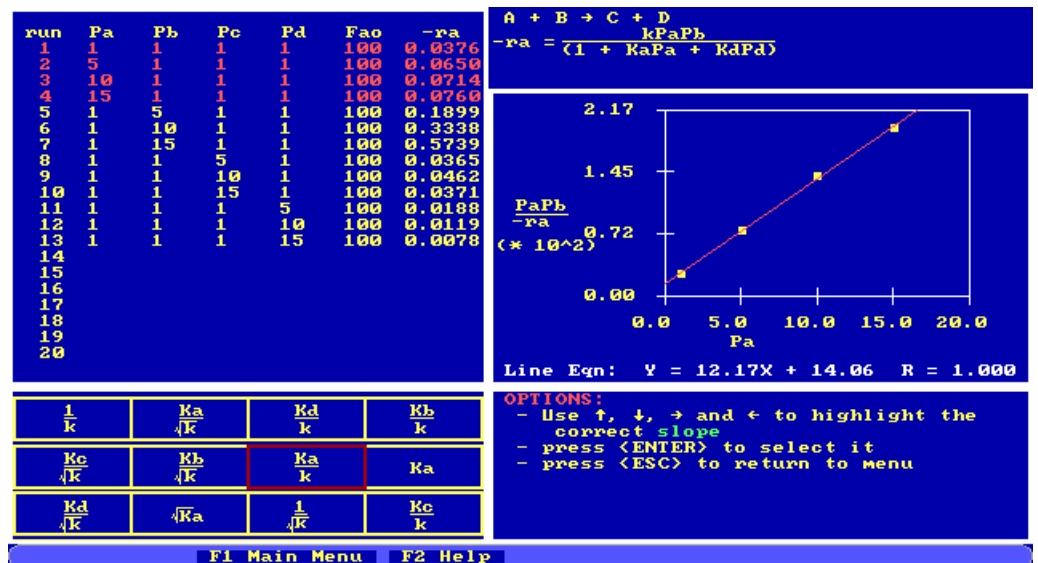
**Pore Mouth**

**Pore**

1. Mass transfer—reactant
2. Diffusion into pore
3. Reactant adsorption
4. Surface reaction
5. Product desorption
6. Diffusion out of pore
7. Mass transfer – product

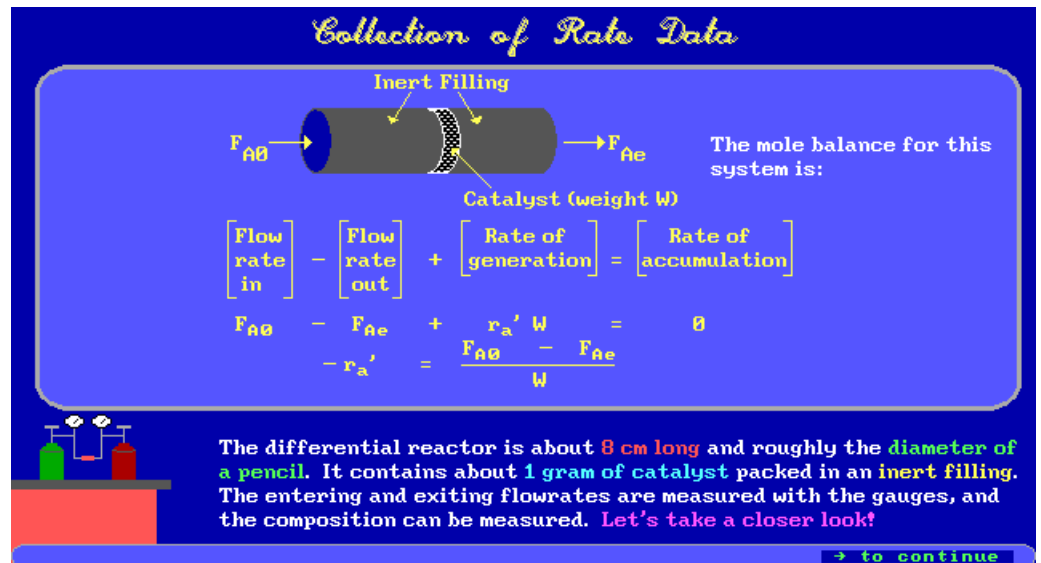
Navigation: [← Page Back](#) | [F1 Main Menu](#) | [Next Page →](#)

The student must derive the rate equation for a given reactive system by analyzing the rate data obtained in a differential reactor. The student must choose which experiments to run, that is, the entering pressures of each species and total flow rate. In order to obtain the dependence of the rate equation on the pressure of a given species, the student must select which of the points are to be included in a plot of reaction rate vs. species partial pressure. Given the requested plot, the student must determine the form of the dependence of the rate law on the pressure of the given species:



Once all dependencies have been established, the student must decide which rate law parameters can be determined, through judicious plotting of the experimental data.

The review section also outlines the derivation of the governing equations of heterogeneous catalysis:



Grade Base

Based merely on completion of the module, i.e. derivation of the reaction rate expression.

Comments

Students reported that this module was very helpful to them in preparing to do the homework problems from the textbook. This module requires a large amount of memory to run.

# Heatfx1: Simulation - Mole and Energy Balances in a CSTR

---

Concepts Effect of parameter variations on operation of a nonisothermal CSTR

---

Time 36 minutes ± 14 minutes

---

Reference Fogler: Chapter 8

---

Description This module allows students to investigate the effect of parameter variations on the operation of a nonisothermal CSTR. An extensive review section derives the energy balance for the CSTR, and also describes the terms in the mole balance that are temperature dependent:

$$X_{EB} = \frac{C_{P0}(1 + \kappa)}{-\Delta H_R(T_R)} (T - T_c) \quad \text{where } \kappa = \frac{U\bar{a}}{F_{R0}C_{P0}} \quad \text{and} \quad T_c = \frac{\kappa T_a + T_0}{1 + \kappa}$$

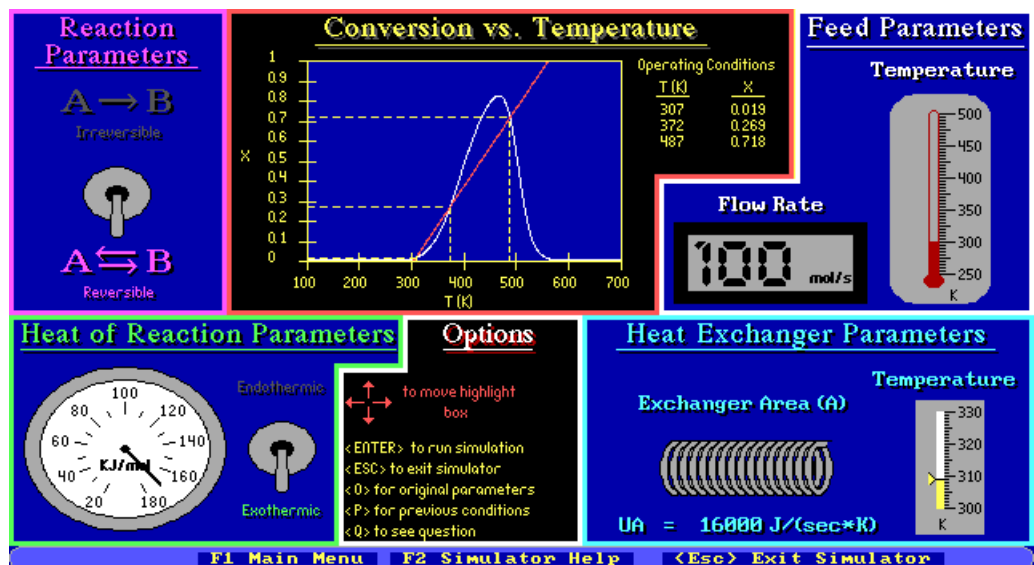
The energy balance is satisfied for every point on this line. However, to find the operating point of the reactor, both the energy balance and the mole balance must be satisfied.

Alright. Who is temperature dependent?

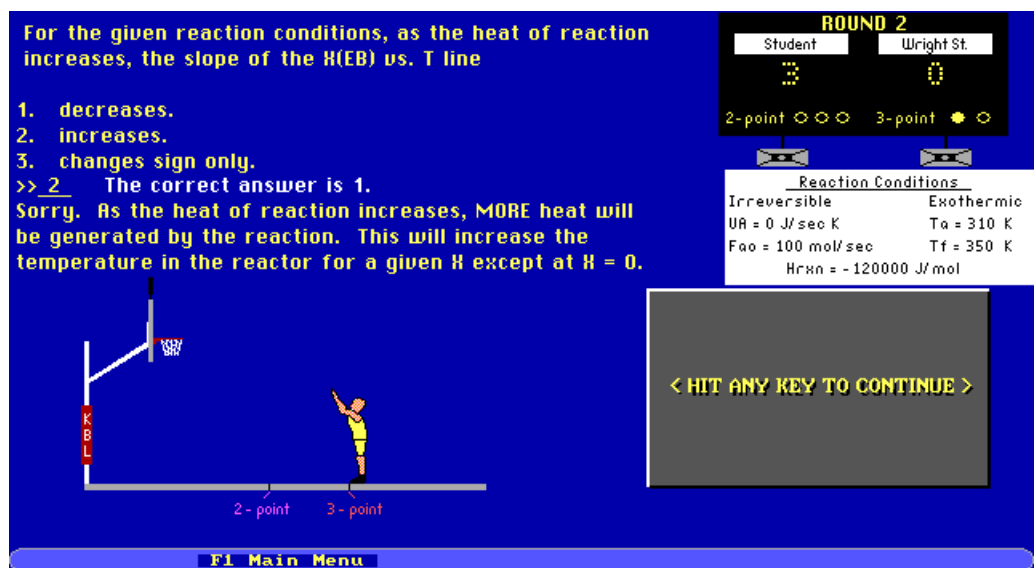
$$U = \frac{F_{R0} X}{-r_R}$$

→ to Continue

A simulator is also included in the review section. This allows the student to vary parameters and observe the effects on the conversion-temperature relationships as described by both the mole balance and the energy balance. The parameters that may be varied include: feed flow rate and temperature, the reversibility/irreversibility of the reaction, heat of reaction, heat exchanger area and heat transfer fluid temperature. The operating conditions can be determined from the intersections of the mole balance and energy balance:



The module can also be run in the interactive mode, in which the scenario takes the student to a basketball tournament. They have the choice of two-point and three-point questions:



The simulator is available to help the student in answering the three point questions.

## Grade Base

A grade is only assigned in the interactive mode. The student is given a "shooting percentage" for the two point and three point questions, as well as an overall shooting percentage. A shooting percentage greater than 85% demonstrates mastery.

## Comment

This module requires a lot of memory to run.

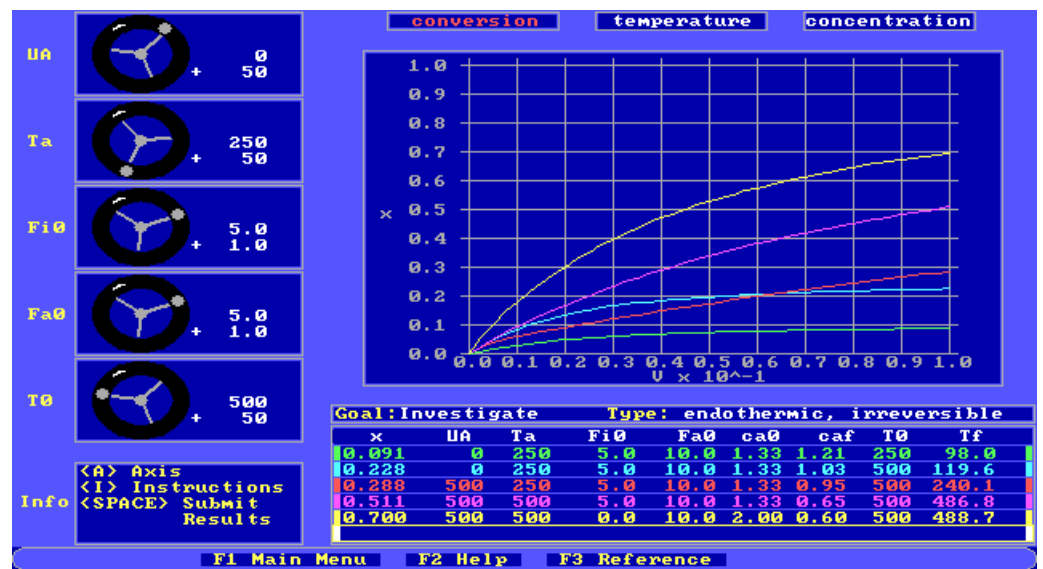
# Heatfx2: Simulation - Mole and Energy Balances in a PFR

Concepts Effect of parameter variations on operation of a nonisothermal plug flow reactor

Time 61 minutes ± 36 minutes

Reference Fogler: Chapter 8

Description This simulation allows the student to explore the effect of various parameters on the performance of a non-isothermal plug flow reactor. The student may choose from eight simulations, that span all combinations of exothermic/ endothermic, reversible/irreversible conditions, as well as one simulation that includes the effect of pressure drop. The parameters that may be varied include heat transfer coefficient, inlet reactant and diluent flow rate, inlet temperature, and ambient temperature:



The results of the simulator may be analyzed in the form of plots of concentration, conversion or temperature as a function of reactor volume. The module may also be run in the interaction mode, in which the student must achieve specific goals (e.g. achieve a given conversion without exceeding a given temperature within the reactor), in order to get to the center of the reactor complex.

The review section includes a derivation of the energy balance equation for a PFR:

**The Energy Balance**  
First Law of Thermodynamics

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

rate of accumulation of energy within the system

Continuous-flow reactors are considered to be open systems in which mass crosses the system boundary. The energy balance for the system is composed of the following parts.

+ to continue

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## Grade Base

In the interactive mode, mastery is based on the correct solution of two consecutive problems, i.e., arriving at the center of the reactor complex.

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## Comments

We have used the simulator portion of this module as a tool in a group problem solving exercise. Students had to vary various parameters and explain their observations, then use the newly gained insight to optimize a system. A sample assignment, for System 2 in the “individual problems” menu, follows. Since the assignment was to be completed within a one hour class period, explicit instructions and suggestions for parameter values were given.

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## Sample assignment

*You are to investigate the effect of some important reactor parameters on the conversion and temperature profiles down a tubular reactor. You will be told which parameter to vary, then asked to explain the results you observe.*

*In each case, in addition to a general statement (“increase UA”), you will be given a set of optional reactor conditions to use, in the order they appear in the left-hand side of the simulation screen: (UA, T<sub>a</sub>, F<sub>io</sub>, F<sub>ao</sub>, T<sub>o</sub>). You may use these conditions if you wish, or pick your own for your investigation.*

## GETTING STARTED

Choose "5. individual problems" from the main menu , then choose problem 2. "Endothermic irreversible." Once the F-key bar at the bottom shows up, you may want to hit "F2" for a short description of each of the components of the simulator.

Things to keep in mind, once you are running the simulator:

- To change the step size in varying the parameters: 1(smallest step size) 10 (largest one)
- To delete a run so its curve doesn't show up on the graph-select it and hit backspace.
- Not sure what keys to hit?-**Press I for Information.**

## EFFECT OF HEAT EXCHANGER

To analyze the effect of the heat exchanger on the reaction, compare the conversion and temperature profiles with and without heat exchange:

Set the y-axis to temperature - Choose temperature with the arrow keys.  
Select your first run - Hit <Enter> until the yellow selector box is around the UA box

Perform a run with UA equal to 0  
(e.g.,  $UA=0$ ,  $T_a=300$ ,  $F_{iO}=10$ ,  $F_{aO}=10$ ,  $T_O=300$ )

*How does the temperature change with volume down the reactor with no heat exchange for an endothermic irreversible reaction?*

Select a second run - Use the arrows to select the blue run.

Perform a new run with a higher UA  
(e.g.  $UA=250$ ,  $T_a=300$ ,  $F_{iO}=10$ ,  $F_{aO}=10$ ,  $T_O=300$ )

*How does the temperature change down the reactor with heat exchange for an endothermic irreversible reaction?*

Set the y-axis to conversion - Press "A" for axes

*How do the conversion profiles for the cases with and without heat exchange compare?*

## EFFECT OF FLOW PARAMETERS

Perform a new run with no inerts.  
(e.g.  $UA=250$ ,  $T_a=300$ ,  $F_{iO}=0$ ,  $F_{aO}=10$ ,  $T_O=300$ )  
Now perform a run with a higher reactant rate.  
(e.g.  $UA=250$ ,  $T_a=300$ ,  $F_{iO}=0$ ,  $F_{aO}=20$ ,  $T_O=300$ )

*How does the presence of inerts affect the results from the previous question?*

*Perform a run with inerts  
(e.g.  $UA=250$ ,  $T_a=300$ ,  $F_{i0}=10$ ,  $F_{a0}=20$ ,  $T_0=300$ ).*

*Compare the temperature profiles for the above three cases.*

### **APPLICATION**

*Given your new-found intuition, try to get the highest conversion given the limitation that the reactor temperature (at ALL positions within the reactor), must be between 250-300 K. An easily achieved value is 0.50. The highest conversion found so far is 0.711. Turn in the conditions you used ( $UA, T_a, F_{i0}, F_{a0}, T_0$ ) as well as the conversion obtained, and a few sentences explaining what you learned.*

### **SUMMARY**

*Write a paragraph (1/2 to 1 page) describing the effect of heat exchange, the reactant flowrate and the inert flowrate on conversion and temperature profiles for the tubular reactor. Include sketches illustrating the trends and the equations necessary to predict the results. Based on these results can you predict what would happen in an exothermic, irreversible reaction? How about reversible reactions?*

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