CBE 255 — Course Review and Study Guide

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1 Introduction

This document provides a compact summary of the concepts covered in this course. It may be helpful as a study guide for the final exam in CBE 255 and as a refresher for using MATLAB to solve problems in later courses. Also feel free to download the latest version of the course MATLAB m-files at the top of this webpage `http://cbe255.che.wisc.edu`.

If you discover bugs or errors in this document or the course m-files, please report them by email to the author.

2 Chemical and Biological Engineering Concepts

3 Computational Concepts

4 Programming Concepts

5 Summary of MATLAB commands

We have used the following MATLAB functions and commands in this course. You should recall the general purpose of each of these commands. You can always find the details of the syntax by typing `help command` at the MATLAB command line.

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CBE Course	Title	Coverage in CBE 255	
		Module	Level
250	Process Synthesis	4	✓✓
211			
311			
320	Transport Phenomena	3	✓✓
324		6	
326			
424			
426			
440/450	Materials/Polymers	5	✓
430	Chemical kinetics and reactor design	2, 5	✓✓✓
450	Process design	4	✓✓
470	Process dynamics and feedback control	2, 5, 6	✓✓

Table 1: CBE 255 support of subsequent chemical and biological engineering courses. Number of ✓ indicate amount of support.

Module	Title	Concepts
1	Programming and programming languages	
2	Stoichiometry of chemical reactions	
3	Diffusion and heat transfer	
4	Process systems steady-state modeling and design	
5	Chemical kinetics in well-mixed reactors	
6	Staged separations	
7	Estimating parameters from data	

Table 2: CBE 255 module summary as of 2014. See also website `http://cbe255.che.wisc.edu`.

6 Exercises

The following exercises are a selected list taken from the CBE 255 modules Exercises, Examples and Exams. All of the modules are represented in this selection. These exercises provide students and instructors with an overview of the problem difficulty level that CBE students are prepared to solve after taking this course.

Module 2: Stoichiometry of Chemical Reactions

Examples and Exercises	Title	Programming
Module 1	**Programming and programming languages**	
Module 2	**Stoichiometry of chemical reactions**	
Exercise 1	Stoichiometric matrix for a single reaction	
Exercise 2	Finding independent sets of reactions	`rank`
Exercise 3	The stoichiometric matrix	`[ ] , ;`
Exercise 4	Finding reaction rates from production rates	`inv`
Exercise 5	Independent reactions for bromine hydrogenation	`rank`
Exercise 6	Independent reactions for methane oxidation	`:`
Exercise 7	Production rates from reaction rates	`*`
Exercise 8	Eliminating reaction intermediates	
Exercise 9	Stoichiometry short questions	
Exercise 10	Reaction rates from production rates	`inv`
Exercise 11	Least squares estimate for multiple measurements	`inv`
Exercise 12	Don't retype data!	`load`
Exercise 13	Writing functions in MATLAB and Octave	`function`
Exercise 14	Functions with multiple return arguments	`function`
Module 3	**Diffusion and heat transfer**	
Example 1	Dimensionless variables	
Example 2	Heating of a finite slab	`colloc` `ode15s`
Example 3	Heating of a semi-infinite slab	`colloc` `ode15s`
Example 4	Single-pellet profile	`colloc` `ode15i`
Example 5	Quasi-steady state assumption gives rise to DAEs	`ode15i`
Exercise 1	Checking the derivative formulas. Oscillating function	`colloc`
Exercise 2	Checking the derivative formulas. Exponential function	`colloc`
Exercise 3	Stopping conditions for radioactive decay reactions	`ode15s` `Event`
Exercise 4	Heat equation with an insulated end	`colloc` `ode15i`
Exercise 5	Cooking the turkey	`colloc` `ode15i` `Event`
Exercise 6	Turkey with increased heat transfer resistance	`colloc` `ode15i` `Event`
Exercise 7	Using a heat transfer coefficient	`colloc` `ode15i` `Event`

Examples and Exercises	Title	Programming
Module 4	**Process systems steady-state modeling and design**	
Exercise 1	Solve $f(x) = x^3 2x^2 + 3x6 = 0$	Newton's method
Exercise 2	Solve $f(x) = x^3 - 3x - 2 = 0$	`while input`
Exercise 3	Solve $f(x) = x^3 - 2x^2 - x + 2 = 0$	`isempty if fprint`
Exercise 4	Solve $f_1(x_1, x_2) = 2x_1^2 + x_2^2 5 = 0$	Newton's method
	$f_2(x_1, x_2) = x_1 + 2x_2 3 = 0$	`fsolve`
Exercise 5	Process flowsheet	`fsolve`
Exercise 6	Process flowsheet over a range of recycle	`fsolve`
Exercise 7	Process flowsheet with nonsharp separation	`fsolve`
Module 5	**Chemical kinetics in well-mixed reactors**	
Example 1	Radioactive Decay	`ode15s`
Example 2	Passing arguments to a function with the `global` statement	`global`
Exercise 1	Solving ordinary differential equations (ODEs) in MATLAB	`ode15s`
Exercise 2	Second-order, irreversible reaction	
Exercise 3	More ODE solving in MATLAB	`ode15s`
Exercise 4	Radioactive decay with fast intermediate species	
Exercise 5	Writing your own simple ODE solver: Euler's method	Euler's method
Exercise 6	Complex dynamic behavior with nonlinear ODEs	`ode15s`
Exercise 7	More oscillations. Coupled mass and energy balance in a continuous well-stirred reactor	`ode15s`
Exercise 8	Estimating rate constant and activation energy from rate constant measurements at different temperatures	least squares `inv`
Exercise 9	Multiple steady states. Coupled mass and energy balance in a continuous well-stirred reactor	`ode15s`

Table 3: Programming concepts by Example and Exercise.

Exercise 1: Finding independent sets of reactions

Consider the following set of chemical reactions,

$$2N_2O_5 \rightleftharpoons 2N_2O_4 + O_2 \quad (1)$$

$$N_2O_5 \rightleftharpoons NO_2 + NO_3 \quad (2)$$

$$NO_2 + NO_3 \rightleftharpoons N_2O_5 \quad (3)$$

$$NO_2 + NO_3 \rightleftharpoons NO_2 + O_2 + NO \quad (4)$$

$$NO + N_2O_5 \rightleftharpoons 3NO_2 \quad (5)$$

$$NO_2 + NO_2 \rightleftharpoons N_2O_4 \quad (6)$$

(a) Determine the stoichiometric matrix, $\boldsymbol{\nu}$, and the species list, $\boldsymbol{A}$, for this reaction system

Looping
- `for`
- `while`
- `break`
- `end`

Conditionals
- `if`
- `elseif`
- `else`

Screen/file input/output
- `input`
- `who`
- `fprint`
- `disp`
- `print`
- `save load`
- `format short/long e`
- `%g %e %i`

Math Operations
- `+ - * / ^`
- `.+ .- .* ./ .^`
- `exp log`
- `abs min max`
- `fix ceil floor`

Comparison and Boolean Operators
- `== <= >= !=`
- `~ || &&`

Matrix/submatrix operations
- `[ ] ( )`
- `, ;` (comma, semi-colon)
- `'` (apostrophe)
- `:`
- `size length`
- `inv`
- `repmat`
- `reshape`

Generate indices and intervals
- `linspace`
- `logspace`
- `nchoosek`

Functions
- `function`
- `return`
- `global`
- `@`

Continuation and comment lines
- `\ ... %`

ODE/algebraic/PDE equation solvers
- `fsolve`
- `ode15s`
- `ode15i`
- `colloc`

Plotting
- `figure`
- `plot`
- `semilog loglog`
- `hold on hold off`

Table 4: Summary of MATLAB commands used in CBE 255.

so the reaction network is summarized by

$$\boldsymbol{\nu A} = \mathbf{0}$$

(b) Use Octave, MATLAB, or your favorite software package to determine the rank of the stoichiometric matrix. How many of the reactions are linearly independent?

(c) Now that you have found the number of independent reactions, n_i, which n_i of the original set of 6 reactions can be chosen as an independent set? Try guessing some set of n_i reactions and determine the rank of the new stoichiometric matrix. Stop when you have determined successfully one or more sets of n_i independent reactions.

Hint: you want to examine the rank of sub-matrices obtained by deleting rows (i.e., reactions) from the original stoichiometric matrix. In Octave, if you assign the original stoichiometric matrix to a name, `stoi`, then you can obtain the rank of the stoichiometric matrix associated with deleting the fifth reaction, for example, by

```
stoi2 = [stoi(1:4,:);stoi(6,:)]
rank(stoi2)
```

Do you see how the indices in forming `stoi2` work out? Notice we do not have to enter any more matrices after we build the original stoichiometric matrix to test the ranks of various reaction networks.

(d) What do you think of a colleague's answer that contains Reactions 2 and 3 in the final set. Can this be correct? Why or why not?

Exercise 2: Least squares estimate for multiple measurements

Consider again the water gas shift reaction.Consider the first two reactions as a linearly independent set.

$$\begin{aligned} H_2O + CO &\rightleftharpoons CO_2 + H_2 \\ H_2O + H &\rightleftharpoons H_2 + OH \end{aligned}$$

We are provided with the following six replicate experimental measurements of the species production rates, all of which are subject to small measurement errors.

$$\boldsymbol{R}_{\text{meas}} = \begin{bmatrix} R_{\text{H}} \\ R_{\text{H}_2} \\ R_{\text{OH}} \\ R_{\text{H}_2\text{O}} \\ R_{\text{CO}} \\ R_{\text{CO}_2} \end{bmatrix} = \begin{bmatrix} -2.05 & -2.06 & -1.93 & -1.97 & -2.04 & -1.92 \\ 2.94 & 3.02 & 3.04 & 2.93 & 3.06 & 3.04 \\ 2.01 & 1.94 & 2.01 & 1.92 & 2.01 & 2.04 \\ -2.98 & -2.98 & -2.98 & -2.99 & -2.96 & -2.96 \\ -1.03 & -1.03 & -0.98 & -1.07 & -0.95 & -1.08 \\ 0.97 & 1.05 & 1.06 & 1.09 & 1.00 & 1.07 \end{bmatrix}$$

(a) Consider each column of $\boldsymbol{R}_{\text{meas}}$, that is each production rate measurement, and compute a least-squares estimate of $\boldsymbol{r}$ for that measurement. Confirm that your six least-squares estimates are:

$$\boldsymbol{r}_{\text{est}} = \begin{bmatrix} 0.97 & 1.03 & 1.03 & 1.06 & 0.98 & 1.05 \\ 2.01 & 1.99 & 1.98 & 1.92 & 2.03 & 1.96 \end{bmatrix}$$

(b) Next consider all six measurements simultaneously. Find one estimate of $\boldsymbol{r}$ that simultaneously minimizes the squared errors of all six of the measured production rates. Confirm that your estimate is

$$\boldsymbol{r}_{\text{est}} = \begin{bmatrix} 1.02 \\ 1.98 \end{bmatrix} \qquad \text{all six measurements considered}$$

Hint: Consider the least squares problem $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$. To create the $\boldsymbol{b}$ vector for this problem, you can manually insert the six $\boldsymbol{R}_{\text{meas}}$ vectors into one column vector, or you may want to try the MATLAB command: `reshape`. To create the $\boldsymbol{A}$ matrix, you can manually insert the stoichiometric matrix six times, or you may want to use the MATLAB command: `repmat` or `kron`. The functions `reshape`, `repmat`, and `kron` are powerful and convenient tools for reorganizing matrices and vectors. See the MATLAB help for their use.

(c) Plot the six single-measurement estimates and the one multiple-measurement estimate with r_1, r_2 as the x-y axes. Where does the multiple-measurement estimate lie with respect to the six single-measurement estimates? Which of the seven estimates available do you think is the most reliable estimate of the two reaction rates and why?

Exercise 3: Don't retype data!

Next consider Exercise 2 with 500 measurements. The measurements are in the file

`lots_of_data.dat`

with the first few measurements shown below

```
-2.05   -2.06   -1.93   -1.97   -2.04   -1.92   -1.99   -2.00   -2.05
 2.94    3.02    3.04    2.93    3.06    3.04    3.00    2.94    3.01
 2.01    1.94    2.01    1.92    2.01    2.04    2.06    1.90    1.98
-2.98   -2.98   -2.98   -2.99   -2.96   -2.96   -2.99   -2.96   -2.96
-1.03   -1.03   -0.98   -1.07   -0.95   -1.08   -1.04   -1.01   -1.00
 0.97    1.05    1.06    1.09    1.00    1.07    0.98    1.02    1.01
```

Download the 500 measurements with your browser, save them to a file, and load the data into MATLAB using the `load` command.

(a) Repeat Exercise 2 (a)–(c) on these data.

(b) Describe the pattern of points for the 500 estimates? Do you see any structure to these estimates?

Exercise 4: Functions with multiple return arguments

Let's write a function to do Exercise 1. Use the `nchoosek` function inside your function to make your code as general as possible.

Write a function

```
[indreac, r] = ind_sets(V)
```

in which `V` is a stoichiometric matrix, `r` is its rank r, and `indreac` is a matrix containing the set of all linearly independent reactions, with each row containing a set of r integers corresponding to a set of reactions that are linearly independent. A function can return more than one argument, by placing the list of return arguments inside square brackets as above.

(a) Pass in the stoichiometric matrix from Exercise 1 to check your function. Print out the returned matrix `indreac` for this problem.

(b) Find your own favorite chemical reaction set with 7 or more reactions and species whose rank is at least 2 less than the number of reactions. Apply your function to this stoichiometric matrix and print out the list of all linearly independent reactions.

Notice that when you have a calculation that you need to repeat many times on different data, it's convenient to write and store a function to perform the calculation.

Module 3: Diffusion and Heat Transfer

Exercise 5: Stopping conditions for radioactive decay reactions

Consider again the two radioactive decay reactions of Example 1 of the "Chemical kinetics in well-mixed reactors" module.

$$\begin{aligned} \mathrm{Ra} &\longrightarrow \mathrm{Rn} + \mathrm{He} \\ \mathrm{Rn} &\longrightarrow \mathrm{Po} + \mathrm{He} \end{aligned}$$

(a) Use an ODE solver to find the time at which the Ra mass reaches half of its initial value. Plot Ra, Rn, He, Po versus time up to this time.

(b) Compare the value reported by the ODE solver to the half life given in the problem. What is the relative error in the ODE solver's value? If you wanted more accuracy in the ODE solver's reported time, how would you obtain it?

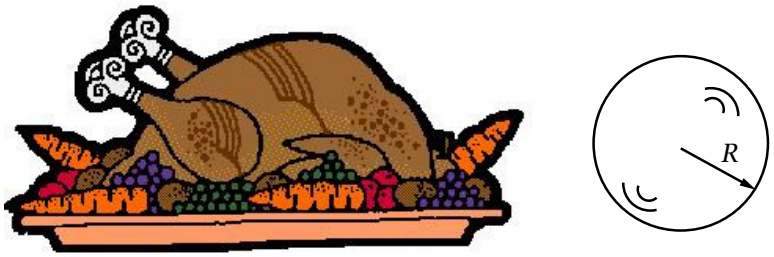

Figure 1: Model the stuffed turkey as a sphere filled with water.

Exercise 6: Cooking the turkey [1]

For heat transfer and cooking purposes, consider modeling a stuffed turkey as a sphere filled with water as depicted in Figure 1. The oven is set at 325°F. Assume the turkey's outer temperature is 50°F lower than the oven temperature. The turkey is finished cooking when the center temperature reaches 180°F.

(a) Write out the dimensionless heat equation in spherical coordinates starting with the dimensional heat equation in spherical coordinates

$$\rho \hat{C}_P \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 k \frac{\partial T}{\partial r} \right) \tag{7}$$

Convenient dimensionless variables are

$$\Theta = \frac{T - T_0}{T_1 - T_0} \qquad \xi = \frac{r}{R} \qquad \tau = \frac{kt}{\rho \hat{C}_P R^2}$$

in which T_0 is room temperature, T_1 is the turkey's outer temperature during cooking, and R is the sphere radius.

What is the dimensionless center temperature when the turkey is finished cooking?

(b) Solve the dimensionless heat equation with a stopping condition to find the time when the center temperature reaches the value found in the previous part. Note you will require a DAE solver for this problem.

What is the dimensionless stopping time when the turkey is finished cooking?

Plot the temperature profile in the sphere at this dimensionless stopping time?

(c) Prepare a cooking time versus turkey weight chart over the turkey weight range 10 to 25 pounds. How many times must you solve the heat equation to prepare this plot?

[1] See also Bird, Stewart, and Lightfoot (2002, Problem 12B.7)

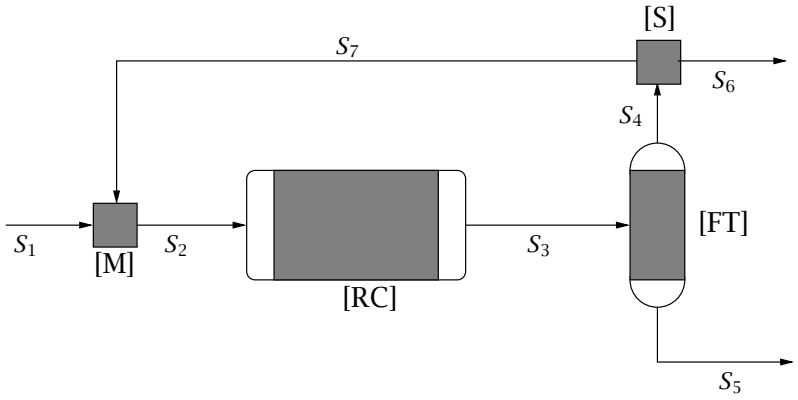

Figure 2: Process flow diagram for the production of C from A and B.

Exercise 7: Using a heat transfer coefficient

Consider using the heat transfer coefficient to model the outer boundary of the sphere in Exercise 6.

(a) Solve the dimensionless version of Equation 7 with the boundary condition given in Equation 8.

$$\boxed{\left.\frac{\partial \Theta}{\partial \xi}\right|_{\xi=1} = \left(\frac{hR}{k}\right)(1-\Theta(1,t)) \qquad \text{heat transfer boundary condition}} \tag{8}$$

Prepare the cooking chart for the following dimensionless heat transfer coefficient

$$\frac{hR}{k} = 3$$

Does the cooking time increase or decrease compared to the chart in Exercise 6?

(b) Plot the sphere's outer temperature versus time.

(c) Repeat the calculations for

$$\frac{hR}{k} = 5$$

Module 4: Process Systems Steady-State Modeling and Design

Exercise 8: Process Flowsheet Over a Range of Recycle. Optimal Operation.

Write the model for the process flowsheet shown above.

(a) Vary the recycle ratio, R, and plot the production rate of C and Q^{S3} versus R for $0 \leq R < 1$. What production rate is achieved without recycle? What is the largest production rate that can be achieved with this process?

(b) Examine the Q^{S3} versus R plot. Discuss the competing factors in selecting R for the best economics of this process. What R do you expect to be near the economic optimum for this process?

Exercise 9: Process flowsheet with nonsharp separation

Repeat Exercise 5 of Module 4 with the separation factors changed to

$$\phi_A = 0.8 \qquad \phi_B = 0.9 \qquad \phi_C = 0.2$$

(a) Assume the production rate of C is the molar flow in $S5$ only and you cannot recover the C in $S6$. Does production rate go up or down compared to the sharp separation case considered in Exercise 2.3? How much C is lost in $S6$?

(b) How has the economic situation changed with respect to choosing the recycle ratio for this case compared to the sharp separation case considered in Exercise 5? What value of R do you expect to be near the economic optimum for this process?

Module 5: Material Balance for the well-mixed, batch reactor

Exercise 10: Complex dynamic behavior with nonlinear ODEs. Belousov-Zhabotinsky reaction.

Belousov and Zhabotinsky discovered chemical reactions that can remain far from equilibrium for long periods of time. The following mechanism due to Field and Noyes (1974) while working at the University of Oregon, known as the Oregonator, is the simplest model that explains some of the observed behavior

$$\mathrm{A} + \mathrm{Y} \longrightarrow \mathrm{X} + \mathrm{P} \qquad r_1 = k_1 AY \tag{9}$$

$$\mathrm{X} + \mathrm{Y} \longrightarrow 2\mathrm{P} \qquad r_2 = k_2 XY \tag{10}$$

$$\mathrm{A} + \mathrm{X} \longrightarrow 2\mathrm{X} + 2\mathrm{Z} \qquad r_3 = k_3 AX \tag{11}$$

$$2\mathrm{X} \longrightarrow \mathrm{A} + \mathrm{P} \qquad r_4 = k_4 X^2 \tag{12}$$

$$\mathrm{B} + \mathrm{Z} \longrightarrow \frac{1}{2}\mathrm{fY} \qquad r_5 = k_5 BZ \tag{13}$$

in which A=$HBrO_3^-$, B is the sum of all oxidizable organic species, P=HOBr, X=$HBRO_2$, Y=Br, and Z=metal oxides. We may assume the A and B concentrations are much higher than the intermediates X, Y, and Z and can be assumed constant at A=0.06M and B=0.02M.

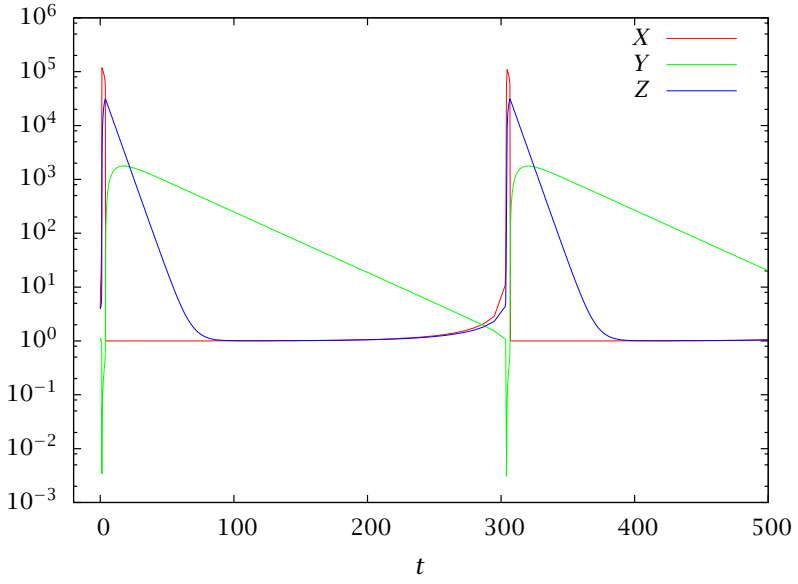

Figure 3: Complex dynamic behavior of the Oregonator model of the Belousov-Zhabotinsky reaction.

We wish to solve this model for the intermediates using the following values of rate constants and initial conditions

$$\frac{dX}{dt} = \alpha(Y - XY + X - \beta X^2)$$
$$\frac{dY}{dt} = (Z - XY - Y)/\alpha$$
$$\frac{dZ}{dt} = \gamma(X - Z)$$

in which

$$\alpha = 77.27 \qquad \beta = 8.375 \times 10^{-6} \qquad \gamma = 0.161$$
$$X_0 = 4 \qquad Y_0 = 1.1 \qquad Z_0 = 4$$

Be prepared, your solution is going to look something like Figure 3. In order to capture the sudden transient occurring at about $t = 303$, try using the following times for reporting the ODE solution in your call to `ode15s`

```
time = [0, ...
     (logspace (-1, log10 (303), 300)), ...
     (logspace (log10 (303.01), log10 (500), 300))]';
```

echo `time` back to the command line so you can see where these time points are placed. The command `logspace` is handy for dividing an interval evenly on a log scale. Contrast its behavior to the command `linspace`.

Exercise 11: More oscillations. Coupled mass and energy balance in a continuous well-stirred reactor. Default error tolerances in MATLAB's `ode15s` unreliable

Consider again the irreversible reaction

$$\mathrm{A} \xrightarrow{k} \mathrm{B} \qquad r = kc_A$$

The mass and energy balances for a continuous-stirred-tank reactor (CSTR) are given by (Rawlings and Ekerdt, 2012, p. 298)

$$\frac{dc_A}{dt} = \frac{c_{Af} - c_A}{\tau} - kc_A \tag{14}$$

$$\frac{dT}{dt} = \frac{U^o A}{V_R \rho \hat{C}_P}(T_a - T) + \frac{T_f - T}{\tau} - \frac{\Delta H_R}{\rho \hat{C}_P} kc_A \tag{15}$$

$$k(T) = k_m e^{-E(1/T - 1/T_m)} \tag{16}$$

in which c_A is the reactor A concentration and T is the reactor temperature. Notice the rate constant k also depends on the reactor temperature. Including the energy balance to describe the reactor temperature allows the reactor to exhibit complex behavior. We wish to solve the model for the following parameter values

Param.	Value	Units
T_f	298	K
T_a	298	K
T_m	298	K
$\hat{C}_P$	4.0	kJ/(kg K)
c_{Af}	2.0	kmol/m^3
$k_m(T_m)$	0.004	min^{-1}
E	1.5×10^4	K
ρ	10^3	kg/m^3
ΔH_R	-2.2×10^5	kJ/kmol
$U^o A/V_R$	340	kJ/(m^3 min K)
τ	73.1	min

(a) Solve the two differential equations describing the reactor from the following initial condition using MATLAB's default parameters

$$c_{A0} = 0.36 \text{ mol/L} \qquad T_0 = 315 \text{ K}$$

Plot c_A, T versus t for this solution out to $t = 20\tau$.

Next plot c_A versus T for this solution. This type of plot is called a phase plot or phase portrait. Notice it gives you a clear indication when a system is approaching a persistent oscillation known as a limit cycle.

(b) Next we tighten the absolute and relative error tolerance for `ode15s` using the `odeset` function. Learn more about this function by typing at the command line

```
help odeset
```

The machine precision is stored in the variable `eps`. Try setting both the absolute and relative error tolerances to the square root of the machine precision. The `odeset` command is

```
opts = odeset ('AbsTol', sqrt (eps), 'RelTol', sqrt (eps));
```

After setting `opts`, you pass this extra argument to the ODE solver to use the tighter tolerances with

```
[tout, x] = ode15s (@oderhs, tout, x0, opts);
```

Resolve the ODEs with the same initial conditions and the tighter tolerances. Plot the solution with both loose and tight tolerances on the same graph. What do you conclude about MATLAB's default error tolerances?

(c) Try your function `euler` on this problem. Can you obtain an accurate solution? If so, what step size h do you recommend? Note: I have not tried this part myself so I am not sure what happens here.

(d) Resolve the Oregonator with tighter tolerances and compare to your solution in Exercise 10. Do you notice a difference in the two solutions?

Exercise 12: Estimating rate constant and activation energy from rate constant measurements at different temperatures

Assume a reaction rate has been measured at several different temperatures in the range $300\ \text{K} \leq T \leq 500\ \text{K}$. Model the rate (rate constant) as

$$k = k_0 \exp(-E/T) \tag{17}$$

in which k_0 (min^{-1}) is the pre-exponential factor and E (K) is the activation energy scaled by the gas constant. To make the estimation problem linear, transform the data by taking the logarithm of Equation 17

$$\ln k = \ln k_0 - E/T$$

(a) Estimate the parameters $\ln k_0$ and E using least squares given the following single experiment consisting of nine rate constant measurements at the following temperatures

T	k
300	0.01658
325	0.06151
350	0.09822
375	0.2751
400	0.9982
425	2.113
450	4.401
475	4.505
500	13.42

What are the least squares estimates of $\ln k_0$ and E for this experiment?

(b) Plot the data and least squares fit on two plots: one plot of k versus T and a separate plot of $\ln k$ versus $1/T$. How well does Equation 17 represent these data?

(c) Next we wish to analyze the following 50 replicate experiments in which each experiment consists of nine measurements of k at different T. The first four of these experiments are shown here

T1	k1	T2	k2	T3	k3	T4	k4
303	0.01145	302	0.0175	302	0.01208	301	0.00955
323	0.0483	321	0.04742	326	0.06483	329	0.05799
351	0.167	345	0.1456	354	0.2289	354	0.1729
376	0.3197	379	0.5643	375	0.436	376	0.2612
402	1.221	396	0.9718	401	0.877	404	0.8787
429	1.278	425	2.166	427	2.152	422	1.052
453	3.844	447	2.853	452	2.354	448	3.882
479	4.519	476	5.098	477	4.685	475	5.931
501	13.8	504	12.05	496	8.29	496	6.235

Download these data from the file

`kt_lotsmeas.dat`

Calculate a least squares estimates for each experiment. Plot the 50 estimates using the estimate of $\ln k_0$ as the abscissa and the estimate of E as the ordinate.

(d) Next combine all 50 experiments into one dataset of k, T values and estimate $\ln k_0$ and E using all 450 measurements. What are the values of the estimates?

(e) Plot all 450 measurement and the least squares fit on two plots: one plot of k versus T and a separate plot of $\ln k$ versus $1/T$. How well does Equation 17 represent all of the measurements.

References

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