

MATH 319, Fall 2013, Assignment 4

Due date: Friday, October 11

Name (printed): _____

UW Student ID Number: _____

Discussion Section: (circle)

Liu Liu:	301	302	303	304
Huanyu Wen:	305	306	323	324
Dongfei Pei:	325	326	329	
Kai Hsu:	327	328		

Instructions

- Fill out this cover page **completely** and affix it to the front of your submitted assignment.

Correctness

/20

- Staple** your assignment together and answer the questions in the order they appear on the assignment sheet.

Completeness

/5

- You are encouraged to collaborate on assignment problems but you must write up your assignment independently. **Copying is strictly forbidden!**

Total:	/25
--------	-----

Bonus:	/3
--------	----

Applications, Numerical Methods

Suggested problems:

Section 2.3: 1-5, 13-19

Section 2.7: 1-4, 11-19

Section 8.3: 1-15

Problems for submission:

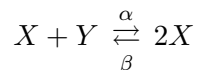
Section 2.3: 3, 5(a)

Section 2.7: 3(a,b)

Section 8.3: 3(a) (compare with *exact* solution as well)

(*Justify your answers for full marks!*)

1. Consider the reversible chemical reaction



where X and Y are chemical species (i.e. molecules). Assuming the solution is well-stirred, it is reasonable to model the reaction rate by the *law of mass action*, which says the rate of a reaction is proportional to the product of the reactant concentrations. For example, the reaction rate of the forward reaction $X + Y \xrightarrow{\alpha} 2X$ would be $\alpha[X][Y] = \alpha xy$ where α is a proportionality constant. The differential equation governing the concentration of X can then be given by

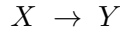
$$\frac{dx}{dt} = \alpha xy - \beta x^2, \quad x(0) = x_0. \quad (1)$$

(*Note:* This equation cannot be solved directly because it depends on a second variable, y , which depends on t .)

- (a) Note that the variables x and y are related by the *conservation* relationship $x + y = C$ (that is to say, the total amount of X and Y remains constant over time). Use this relationship to rewrite the RHS of (1) so that it only depends on x (i.e. eliminate y from the equation).
- (b) Solve the initial value problem found in part (a) for $x(t)$ with the values $\alpha = \beta = C = x_0 = 1$.
- (c) Use the conservation relationship to solve for $y(t)$.

- (d) Describe the long-term behavior of $x(t)$ and $y(t)$. How does this depend on the initial conditions? Does this make sense in the context of the physical problem? (*Hint:* Note that the initial conditions are related by $x_0 + y_0 = C$.)

2. Consider the irreversible chemical reaction



subject to continuous inflow and outflow of X and Y (constant inflow can be modeled by a constant, while outflow is typically assumed to be proportional to the current concentration, x or y , respectively). This can be modeled by the *system* of first-order differential equations

$$\begin{aligned} \frac{dx}{dt} &= \alpha - \beta x, & x(0) &= x_0 \\ \frac{dy}{dt} &= \gamma + \delta x - \eta y, & y(0) &= y_0 \end{aligned}$$

where $\alpha, \beta, \gamma, \delta, \eta > 0$ are constants. (*Note:* Positive signs corresponds to terms of inflow, while negative signs correspond to terms of outflow.)

- (a) Solve this differential equation for the parameter values $\alpha = \beta = \gamma = \delta = 1$, $\eta = 2$, $x_0 = 0$ and $y_0 = 1$. [**Hint:** Solve the equation for x first, and then substitute it into the equation for y .]
 (b) What are the limiting values (i.e. $t \rightarrow \infty$) of the concentrations?

Bonus! Adapt the MATLAB code given online to perform the forward Euler method for the system in Question #2(a) with $\Delta t = 0.1$ and $\Delta t = 0.01$ over the range $t = 0$ to $t = 5$. Print off the results of the numerical simulations of both the x and y variables. Also include plots of the real solutions found in Question # 2(a), for comparison. *Note:* You will need to modify the code to keep track of *two* independent variables, x and y , which both depend on t . In general, for a system of two variables

$$\begin{aligned} \frac{dx}{dt} &= f_1(x, y, t) \\ \frac{dy}{dt} &= f_2(x, y, t) \end{aligned}$$

the forward Euler method is given by

$$\begin{aligned} x_{n+1} &= x_n + f_1(x_n, y_n, t_n)\Delta t \\ y_{n+1} &= y_n + f_2(x_n, y_n, t_n)\Delta t \\ t_{n+1} &= t_n + \Delta t. \end{aligned}$$