PHYC30170 Physics with Astronomy and Space Science Lab 1; The Brusselator - A Computational Example of Chemical Oscillations

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This is the abstract...

I. INTRODUCTION

What are chemical oscillations and what are their modern applications.

A chemical oscillator is a nonlinear system of reacting chemicals in which exhibits

Nonlinear systems have many applications in modern areas of science and engineering [1] particularly in .

The Brusselator is one such system.

A. Oscillations in a Chemical System

Talk about the origins of chemical oscillations. Boris Belousov. The beliefs of the scientific community at the time that oscillations in a chemical system couldn't exist due to the laws of thermodynamics.

B. Chemical Equations

Discuss how chemical equations work and how you can get rate equations from these. Describe how this can be broken down into differential equations.

C. The Brusselator

Discribe the specific brussellator system and the rate equations involved. Describe the break down into two first order ODEs. Define the species of interest and discuss how they are autocatylitic.

The chemical equations of the Brusselator are described in the lab manual as follows [2]:

$$\begin{aligned} A &\rightarrow X && (a) \\ B + X &\rightarrow Y + D && (b) \\ 2X + Y &\rightarrow 3X && (c) \\ X &\rightarrow C && (d) \end{aligned} \tag{1}$$

With ODEs given by:

$$\begin{aligned} \frac{dX}{dt} &= A - (B+1)X + X^2Y && (a) \\ \frac{dY}{dt} &= BX - X^2Y && (b) \end{aligned} \tag{2}$$

The steady state solution of this system is one which stays stationary over time, sometimes refered to as a stable point. At any stable point, the rate of change of X and Y is zero.

$$\frac{dX}{dt} = 0 \;;\; \frac{dY}{dt} = 0 \tag{3}$$

Hence we can find the stable point by solving for X and Y. A full derivation is inlcuded in appendix 1, however a single point at $(X,Y) = \left(A, \frac{B}{A}\right)$ is calculated to be the only stable point in the system.

In this report we will investigate the evolution of the Brusselator system over time, and discuss the oscillatory nature of the reaction using phase space diagrams and concentration diagrams. This will be carried out over a range of initial conditions for X and Y, but also varying ratios of A and B.

II. COMPUTATIONAL METHODS

A. The Euler Method

The Euler Method was chosen to numerically integrate the rate equations to evolve the system over time. The Euler Method is used to solve the first-order initial value problem [3]:

$$\frac{dy}{dx} = f\left(x, y\right), \; y(x_0) = y_0 \tag{4}$$

Here we have first-order ordinary differential equation with a known initial condition. Euler's Method makes use of a relativly simple process where it takes the slope of the function at an initial point and assumes a linear path between that point and the next some arbitrary step away. The formula is given as follows [4]:

$$y(x+h) = y(x) + hf(x,y) \tag{5}$$

where h is the step size. This will construct the tangent at coordinate x, and find the value of $y(x+h)$ to determine the next point.

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1. *The Application of the Euler method to the System*

B. Error Analysis of the Euler Method

Note how the error scales with h.

III. RESULTS AND DISCUSSION

A. Varying the initial conditions

IV. CONCLUSION

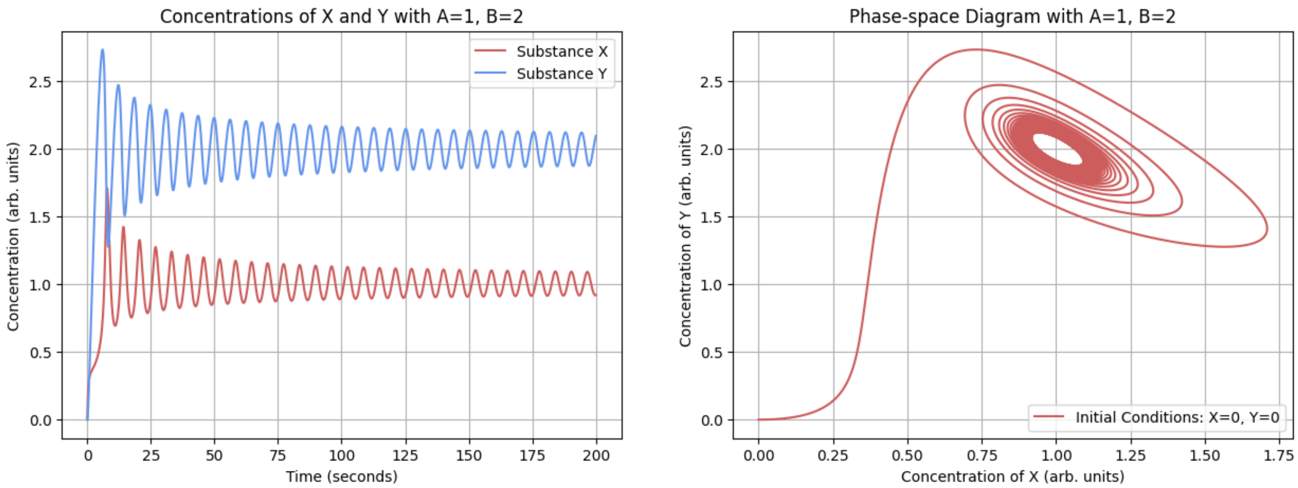

Figure 1: Example caption

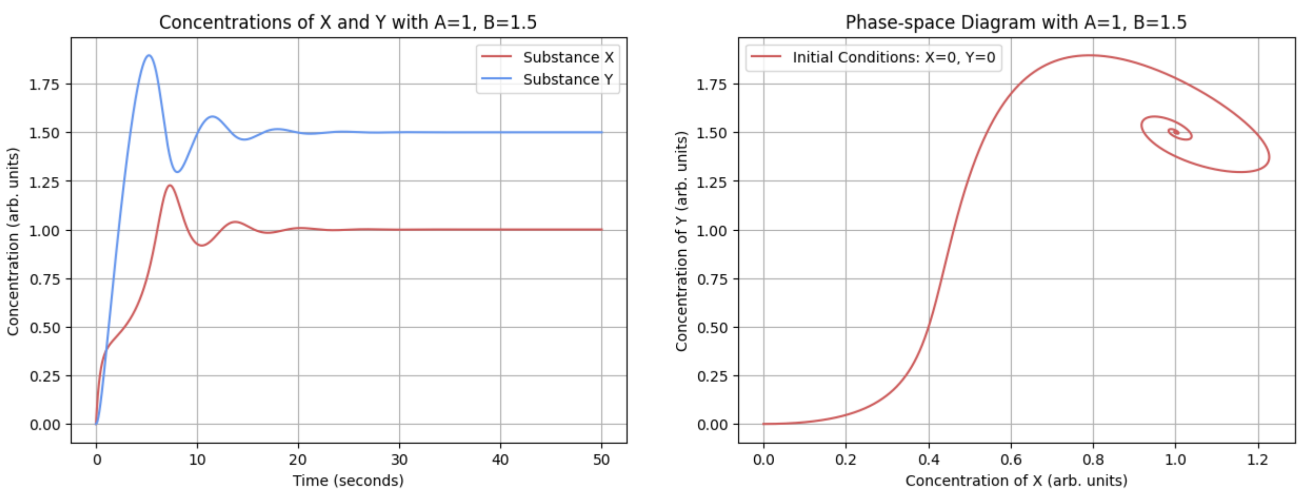

Figure 2: Falls to stable point

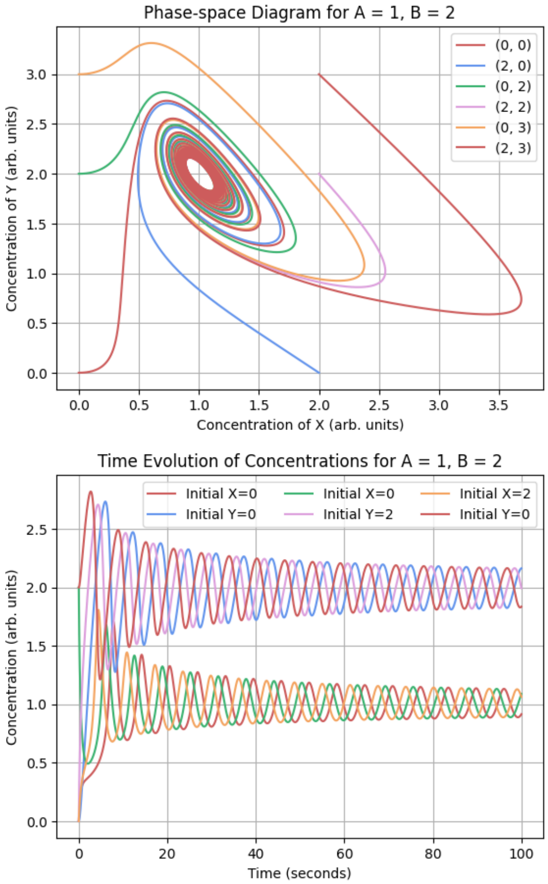

Figure 3: Variation of initial conditions

[1] J. H. Lozano-Parada, H. Burnham, and F. Machuca Martinez, Pedagogical approach to the modeling and simulation of oscillating chemical systems with modern software: The brusselator model, Journal of chemical education **95**, 758 (2018).

[2] *Chemical Oscillations*, University College Dublin.

[3] R. B. Israel, Error analysis of the euler method, `https://personal.math.ubc.ca/~israel/m215/euler2/euler2.html`, visited on 01/02/23.

[4] P. Dawkins, Euler's method, `https://tutorial.math.lamar.edu/classes/de/eulersmethod.aspx`, visited on 01/02/23, last modified on 16/11/22.

APPENDIX 1 - DERRIVATION OF THE STABLE POINT

$$A - (B+1)X + X^2Y = 0$$
$$BX - X^2Y = 0$$

$$\therefore \qquad X^2Y = BX$$

$$\implies A - (B+1)X + BX = 0$$
$$X = A$$

$$A^2Y = BA$$
$$\implies Y = \frac{B}{A}$$

$$(X, Y) = \left(A, \frac{B}{A}\right)$$