Exercise Sheet 10

Belousov Zhabotinsky Reaction

The Belousov-Zhabotinsky reaction is a special chemical reaction. It oscillates. Several chemical reactions take place simultaneously in an aqueous solution with different substances. As a result of the chemical reactions, the concentrations of the substances involved change continuously. Three of the substances involved are subject to periodic fluctuations in their concentrations.

Table 1 lists the chemical substances involved. The variables *A*, *B*, *X*, *Y*, *Z* and *P* are to be used to describe the concentrations of these substances in *mol/l*. At the beginning of the experiment, the six substances are added to the water and stirred. At this point in time, the concentrations of substances shall have the values in the right-hand column of the table.

Substance	*Concentration*	*Initial Value*
BrO_3^-	A	$0{,}03\,\frac{mol}{l}$
$CH_2(COOH)_2$	B	$0{,}02\,\frac{mol}{l}$
$HBrO_2$	X	$4{,}2\cdot 10^{-4}\,\frac{mol}{l}$
Br^-	Y	$8{,}4\cdot 10^{-7}\,\frac{mol}{l}$
Ce(IV)	Z	$0{,}08467\,\frac{mol}{l}$
HOBr	P	$0{,}001\,\frac{mol}{l}$

Table 1

After the start of the experiment, different chemical reactions occur in the solution. Table 2 describes these chemical reactions by stoichiometric reaction equations. The stoichiometric reaction equations show the quantity ratio in which the reactants are involved and the quantity ratio of the products produced by this chemical reaction. The last stoichiometric equation in table 2 contains a stoichiometric factor *f*. It is assumed that *f* has the value 1.

Reaction Equations	*Reaction Rate*	
A + Y → X + P	$k_1 A Y$	$k_1 = 2 \frac{l^3}{mol^3 s}$
X + Y → 2P	$k_2 X Y$	$k_2 = 3 \cdot 10^6 \frac{l^3}{mol^3 s}$
A + X → 2X + 2Z	$k_3 A X$	$k_3 = 42 \frac{l^3}{mol^3 s}$
X + X → A + P	$k_4 X^2$	$k_4 = 3 \cdot 10^3 \frac{l^3}{mol^3 s}$
B + Z → 1/2 f Y	$k_5 B Z$	$k_5 = 1 \frac{l^3}{mol^3 s}$ $f = 1$

Table 2

Each chemical reaction contributes to a reduction in the concentration of the reactants involved and to an increase in the concentration of the products involved. The concentration of a substance is influenced by all the reactions in which the substance occurs as a reactant or as a product. The reaction rate describes the concentration changes per unit of time caused by the chemical reaction. The reaction rate shall be applied to all substances involved in the reaction. With this speed, the reaction reduces the concentrations of the reactants and increases the concentrations of the products.

The reaction speed of all reactions is proportional to each reactant involved in the reaction. The specific proportionality factors for each chemical reaction are indicated by k_1, k_2, k_3, k_4 and k_5. These proportionality factors were determined experimentally.

Due to the chemical reactions, the substances BrO_3^- and $CH_2(COOH)_2$ are consumed and more and more HOBr is produced. This would lead to the chemical reactions becoming weaker over time. Simplifyingly, it is assumed that the variables *A*, *B* and *P* have a constant value during the entire experiment, namely their initial value. For this purpose, the concentration of these three substances must be kept constant during the chemical reaction: BrO_3^- and $CH_2(COOH)_2$ must be continuously fed and HOBr must be continuously discharged.

Exercise 1

Use the approach from exercise sheet 1 to describe this physical system. Determine the constants, state variables, and dependent variables that are involved in this physical system. Specify the units for all physical variables. Specify the values for all constants. Specify the initial values and the first derivations for all state variables. Specify formulas for all dependent variables, which you can use to calculate their values from the state values and constants.

Exercise 2

Program the physical system and simulate it in the Physolator!

The physical system is to be simulated for about half an hour. For this reason, the simulation shall run in fast motion with a factor of 100. To run simulate your physical system in fast motion, insert the following program code into your physical system.

```
public void initSimulationParameters(SimulationParameters s) {
    s.fastMotionFactor = 100;
    s.framesPerSecond = 20;
    s.recordFramesFactor = 10;
    s.iterationsPerFrame = 1000;
    s.allowAdaptive = true;
}
```

A few explanations of this program code: The assignment

s.fastMotionFactor=100;

causes the simulation to run in fast motion. In order to obtain a sufficiently accurate result in numerical simulation, the step size must be selected sufficiently small. This is ensured by the following assignments. The status of the system shall be displayed on the screen 20 times per second. Between these steps, 10 sub-steps are to be calculated and recorded. Between these steps, approximately 1000 iterations of the numerical method (standard procedure: Dormand-Prince) are to be carried out. The value 1000 is only a default value. The step size of the iterations shall be adjusted automatically (adaptive) in such a way that the highest possible accuracy is achieved.

Display concentrations X, Y and Z in the plotter! These three variables have very different value ranges. It is therefore advisable to display the variables in different graphs, each with scales for the y-axis that are adapted to the scales. Proposal:

```
public void initPlotterDescriptors(PlotterParameters r) {
    r.add("X", 3000, 0, 0.5e-3);
    r.add("Z", 3000, 0, 0.1);
    r.add("Y", 3000, 0, 5e-3);
}
```

Note: By default, only the first function graph is displayed in the plotter window of the Physolator. In the plotter window there is a settings dialogue. Use this dialog to define which of the function graphs shall be displayed and thus switch to other function graphs. By default, only one plotter window is displayed in the Physolator. If several plotter windows are to be displayed at the same time, additional plotter windows can be added. To add a plotter window to Physolator's menu and press *Window - add Plotter.*

Exercise 3

After a settling phase, the physical system shows a periodically recurring behavior. How long does such a cycle last? What is the maximum value of the concentration X? Vary the concentration A and carry out the experiment with the changed values of A. What influence does A have on the cycle time? What influence does A have on the maximum value of X?

Reference: R. J. Field „Oreganator“, http://www.scholarpedia.org/article/Oregonator