Model

1 Abstract

The model in the paper is divided into two parts: the reaction rate problem in electrochemical system and the yield problem of Roxella.The Assumption of Arrhenius relation and the Butler Volmer Equation were used to obtain the relationship between the reaction rate and the current.Meanwhile, We used logistics differential equation to solve and fit the yield of Roche, and the fitting results were close to the experimental data. More explanation about the yield of product can be seen in wiki.

2 Assumption:

[1]The constant of rate has the form of Arrhenius, which is k = A e^{E}

Where E = - $\frac{Ea}{RT}$

[2]We also make assumptions that we the amount of bacteria in the system is directly proportion to the amount of product

3 Reason:

In this section, we will explain why it is reasonable to use the formula of Arrhenius. The simple collision model is used in the discussion.And at last it can be seen that the result from collision is consistent with the formula of Arrhenius.The collision model conceive that when two particles collide with each other, the reaction could happen if their energy surpassed the activate energy. First and the foremost, we consider the amount of particles a electron will encounter in the time interval of $\triangle$ t.
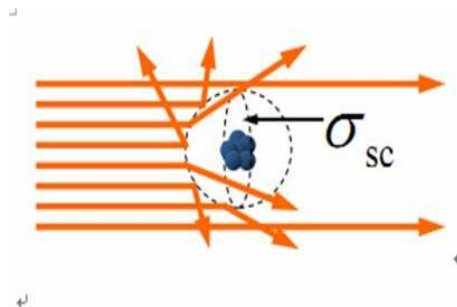

Figure 1: Scattering Section

As the collision of particles could only take place in space of cylinder with the volume of $\sigma\mathbf{L}$. We consider the collision takes place in a really small interval which implies $\triangle$ t goes zero. The velocity of the particle could be estimated as the average velocity. Thus the length the particle travels in $\triangle$ t. is $\nu \triangle$ t where ν represents average velocity. So far, we can get the number of collision happens in a short interval is nearly ρ_A V. As the volume V we consider equals $\sigma \nu \triangle$t , the result of number of collision equals $\rho_A \sigma \nu \triangle$t.

$$
\begin{aligned}
\nu &= -\frac{\mathrm{d}[A]}{\mathrm{d}t} = -\frac{\mathrm{d}[N_\mathrm{A}/(\mathcal{N}_\mathrm{A}V)]}{\mathrm{d}t} \\
&= -\frac{1}{\mathcal{N}_\mathrm{A}V}\frac{\mathrm{d}N_\mathrm{A}}{\mathrm{d}t} = \frac{1}{\mathcal{N}_\mathrm{A}V}\frac{N_\mathrm{coll}\mathcal{P}_\mathrm{rxn}}{\mathrm{d}t}
\end{aligned}
$$

Figure 2:

$$
\nu = \frac{1}{\mathcal{N}_\mathrm{A}}\rho_\mathrm{A}\rho_\mathrm{B}\sigma_\mathrm{AB}\langle v_\mathrm{AB}\rangle p\mathcal{P}(E_\mathrm{AB} > E_a)
$$

Figure 3: The result chemical reaction rate

The condition of a reaction to happen is not only particles hit each other but they also need to have certain energy level that's higher than activate energy $\mathbf{E}_a$. We can use the partition function of the canonical ensemble to find out the possibility that the encountered particle has a energy level that's higher than certain amount $\mathbf{E}_a$. In the canonical ensemble, the possibility of a particle in the state of $\mathbf{E}$ equals to $\frac{e^E}{\sum e^{E_i}}$. In this case, p is the possibility of a reaction to take place if they reach the activate energy.

Then, the possibility of the reaction to take place equals $\frac{e^{-E_a}}{\sum e^{E_i}}$. β constant is set to one in this case where it should be at power term.

$$
\nu = \frac{1}{\mathcal{N}_\mathrm{A}}\rho_\mathrm{A}\rho_\mathrm{B}\sigma_\mathrm{AB}\langle v_\mathrm{AB}\rangle pe^{-E_a/kT}
$$

Figure 4: The result chemical reaction rate

It exactly conforms to the formula obtained by Arrhenius according to experimental data fitting: k = A $e^{\frac{Ea}{RT}}$ Thus, it is reasonable to consider the reaction rate has the form it takes in the assumption part.

4   Butler Volmer Equation

In this model, Butler-Volmer Equation is used to connect the chemical reaction rate we derived from

B-V equation can be used in this scenario because electrolysis of water is a simple REDOX reaction.

And we have assumed that the Arrhenius formula is correct.

To find out the relationship between the reaction rate and the current of the electrode, the equation is

used

$$ i = FAk^0 \left[c_O(0,t) \exp \frac{-\beta F(E - E^{0\prime})}{RT} - c_R(0,t) \exp \frac{(1-\beta)F(E - E^{0\prime})}{RT} \right] $$

Figure 5: Butler Volmer Equation

C0(0,t): concentration of substance O on the electrode surface;

CR(0,t): the concentration of substance R on the electrode surface;

In particular, we want to know how changes in potential affect the rate of reaction at the electrode, that

is, the relationship between potential and current – in electrochemical systems we think of current and

rate of reaction as equivalent.

$$ v = \frac{i}{nFA} $$

Figure 6: Relation between the current and reaction rate

Further, with this relation, we will be able find out how will the system affect the reaction rate of water

electrolysis from the above formula we derive. It can be seen that this model works in a variety of

different environments, it can be at different temperatures, in different elementary reactions, and in a

certain range of electrode voltage to draw relatively reliable conclusions, with universal applicability.

5   The Model Results

This is the graph we draw of the growth model of germs comparison to the result of experiment in the

lab.

The curve we derived from the differential equation in the growth of bacteria.
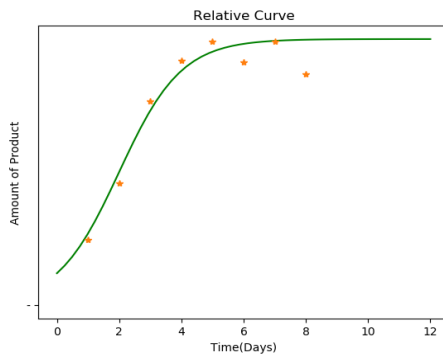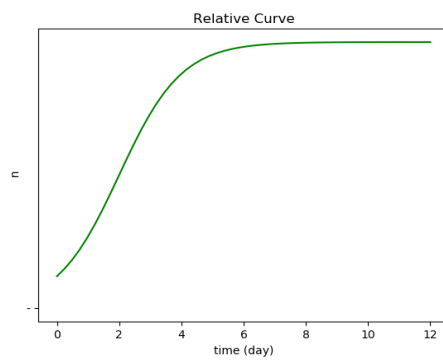
Figure 7: The fit curve of products

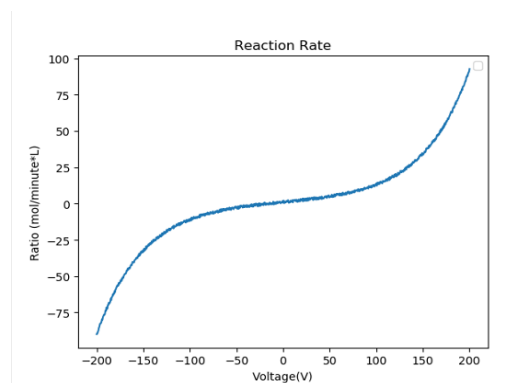Figure 8: The fit curve derived of products derived from Model

Figure 9: The Reaction rate curve derived from the model

6 Strengths and weaknesses

6.1 Strengths

- **Simple calculations**

  It can be seen that Boltzmann statistical method is very applicable because its energy level is very narrow for collision.

- **Multiple factors concerned**

  The electrochemical system of this experiment is relatively simple, and electrolysis of water as a simple elemental reaction can well meet the application conditions of Butler Volmer Equation.This allows the model to work in a variety of different environments, it can be at different temperatures, in different elementary reactions, and in a certain range of electrode voltage to draw relatively reliable conclusions, with universal applicability.

- **Reliable sources** We incorporate data from reliable sources to reduce subjectivity. We also show our results through visual graphs, making the results easier to interpret.

6.2 Weakness

- **Subjective assumption**

  Due to missing data, we make assumptions, making calculations simpler. We also make assumptions that we the amount of bacteria in the system is directly proportion to the amount of product.

- **Distribution in the solution**

  If we care about reactions in solution, we actually need to think more carefully about distribution and environment.

7 References

[1] Arnold Sommerfeld Thermodynamics and Statistical Mechanics Chapter 5.

[2] M. Brouard and C. Vallance Ed. Tutorials in Molecular Reaction Dynamics.

[3] G. C. Schatz, Mark Ratner, Quantum Mechanics in Chemistry

8 Appendix

```python
import numpy as np;

import torch

import matplotlib.pyplot as plt

a = 2

z = 0.01

F= 1

RT = 1

E_eq = 0

J0 = 10

n =1

A =6

E = np.linspace(0,12, 50)

'''


 lab result


'''

Sx = [1,2,3,4,5,7,6,8]

Sy = [0.4,0.75,1.25,1.5,1.62,1.62,1.49,1.42]


def BV(E):

    return (J0 *( np.exp(a*z*F*(1/RT)*(E-E_eq)) - np.exp(-a*z*F*(1/RT)*(E-E_eq)) ))/ (n
                                                        * F *A)


def sig(z):

    return 1.4/(1+np.exp(-z+2))




#plt.scatter(E,BV(E))


A  = 13

plt.plot(E,BV(35)*sig(E),'g','-')

plt.plot(Sx,Sy,'*')

plt.show()
```

```
plt.show()
```