A model on the process of Cu^{2+} elimination by "Copper Terminator"

Abstract The process which this equipment "Copper Terminator" uptaking Cu2+ is modeled by ordinary differential equations. Parameters in this models are both inferred from our experiments or obtained from literature. Second order Runge-Kutta method is utilized in simulation and the result shows that Cu2+ is almost entirely eliminated within 300 minutes from 1mg/L. Finally, Morris sensitivity analysis is carried out and shows that four controllable parameters are most important to the effect of elimination and this demonstrate the possibility of its application.

1. Introduction

In our "Copper Terminator" (figure 2.2.1), E.coli reproduce in a relatively environment in which the temperature is set constant by a temperature sensor , a heater and a microcontroller. Polymers are covered on a framework to keep E.coli form spreading into outside space but let Cu^{2+} pass through. Cu^{2+} which have entered this equipment is uptaken by E.coli.

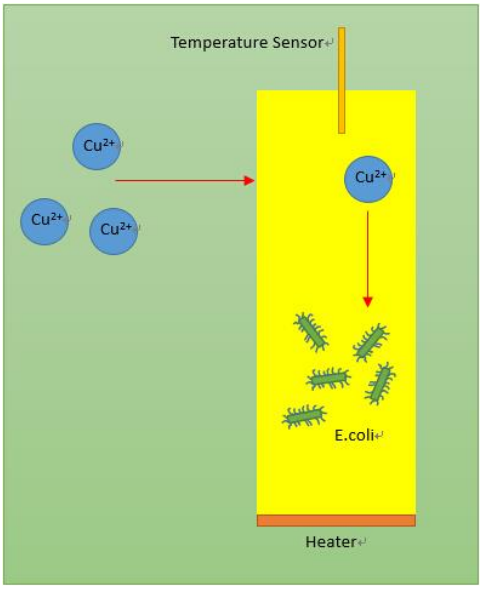

Figure 2.2.1 "Copper Terminator" Device

2. Assumptions

Due to our experiment, Cu^{2+} concentration have little influence on the growth of E.coli. The critical values of tolerance of Cu^{2+} for DH5α and BL21 is 165mg/L and 160mg/L which are all beyond the normal concentration in water. We assume that the growth of E.coli is not influenced by Cu^{2+} concentration.

Since we have polymers covering the surface of this equipment, the environment inside is relatively independent from the environment outside. The growth of E.coli can hardly be disturbed by environment outside. The assumption is that the growth of E.coli is subject to logistic model, in other words, the environmental resistance only comes from the competition on nutrition within the population.

How Cu^{2+} is transported into E.coli is still undiscovered. So that it is difficult to come up with an exact description by mathematical equations for this process. To simplify this model, we assume that the rate of Cu^{2+} uptaken is not related to the physiological status of E.coli. They are equal under different stage of a single E.coli.

For this model here, we assume uniformity of Cu^{2+} and E.coli in the solution.

3. Model

a) Variables and Parameters

i. Variables

Variables	Description	Unit
C_1	Cu^{2+}	mg L^{-1}

	concentration outside “Copper Terminator”	
C_2	Cu^{2+} concentration inside “Copper Terminator”	mg L^{-1}
C_3	E.coli concentration inside “Copper Terminator”	CFU L^{-1}
t	Time	min

ii. Parameters

Parameters	Description	Unit
D	Density of “Copper Terminator” in water body	L^{-1}
h	Height of each “Copper Terminator”	m
R	Bottom radius of each “Copper Terminator”	m
k	Diffusion rate coefficient for Cu2+	m min^{-1}
λ	Cu2+ uptaken coefficient by E.coli	CFU^{-1} min^{-1} L
r	intrinsic rate of increase	min^{-1}
K	Environmental capacity	CFU L^{-1}

b) Model Development

The simple model which describes forward diffusion from compartment i to j :

$$\left(\frac{dQ_i}{dt}\right)_f = -\frac{kQ_i}{V_i} \qquad (3.1)$$

Similarly, a back diffusion from j to i is described as:

$$\left(\frac{dQ_j}{dt}\right)_b = \frac{kQ_j}{V_j} \qquad (3.2)$$

The change in the substance of each compartment can be derivated as :

$$\frac{dQ_i}{dt} = k\left(\frac{Q_j}{V_j} - \frac{Q_i}{V_i}\right) \qquad (3.3)$$

$$\frac{dQ_j}{dt} = k\left(\frac{Q_i}{V_i} - \frac{Q_j}{V_j}\right) \qquad (3.4)$$

In our model, taking the effective surface area of each “Copper Terminator” into consideration, we derivate the change of Cu^{2+} concentration outside the equipment as:

$$\frac{dC_1}{dt} = 2\pi kRh(C_1 - C_2)D \qquad (3.4)$$

Parameter k here has a different unit from previous ones.

The concentration of Cu^{2+} inside is increased by diffusion while decreased by E.coli uptaking. So that the change of Cu^{2+} concentration inside can be described as :

$$\frac{dC_2}{dt} = \frac{2k(C_1 - C_2)}{R} - \lambda C_1 C_2 \qquad (3.5)$$

The growth of E.coli follow logistic equation :

$$\frac{dC_3}{dt} = rC_3\left(1 - \frac{C_3}{K}\right) \qquad (3.6)$$

c) Model Simulation

Simulation is carried out by second order Runge-Kutta method with a step of 0.1 min and 3000 times iteration. The parameters are both from our experiment and some

literatures. Figure 2.2.2 shows the Cu^{2+} concentration change with time both inside and outside. Figure 2.2.3 shows the growth curve of E.coli.

d) Global Sensitivity Analysis

Global sensitivity analysis is a method to analyse all the parameters at one time to find out the influence on the result for each parameter and the interaction between those parameters.

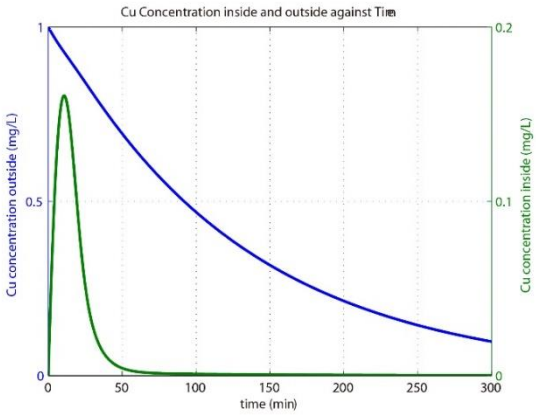

Figure 2.2.2 Simulation of the ^{2}Cuptaken Process with R = 0.5, h = 1, k = 0.075, λ = 0.0005, r = 0.1, K = 30000, D = 1/3000. Initial Cu^{2+} outside is 1mg/L and inside is 0.

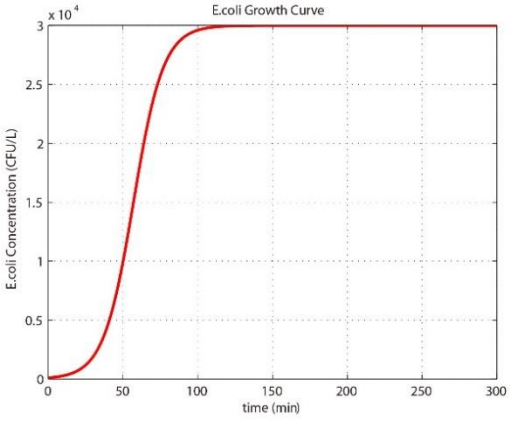

Figure 2.2.3 Growth curve of E.coli, with a initial concentration of 100CFU/L.

Morris (1991) proposed conducting individually randomized experiments that evaluate the effect of changing one parameter at a time. Each input may assume a discrete number of values, called levels, that are selected from within an allocated range of variation for the parameter.

For each parameter, two sensitivity measures are proposed by Morris (1991): (1) the mean, μ, which estimates the overall effect of the parameter on a given output; and (2) the standard deviation of the effect, σ, which estimates the higher-order characteristics of the parameter (such as curvatures and interactions).

We define $t_{0.5}$ as the time when Cu^{2+} concentration outside reaches 0.5mg/L, which is the maximum value allowed in city water. Monte Carlo method is applied to generate 80 groups of 7 parameters randomly with certain distributions. $t_{0.5}$ of each sample can be calculated and then they are undergoing Morris sensitivity analysis. According to figure 2.2.4, the most significant parameters which have most effect on the result in this model are R, h, D, and k. Those parameters are all controllable parameters.

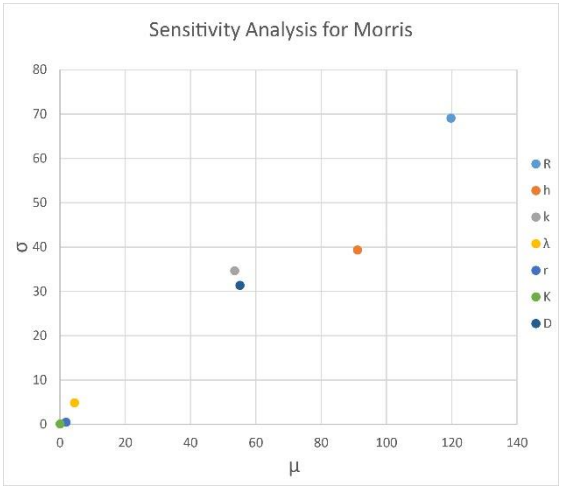

Figure 2.2.4. Morris SA. μ represents the overall effect of the parameter on a given out put while σ means the higher-order characteristics of the parameter.

The result of Morris analysis gives us a direction on design and application of these “Copper Terminator” equipment.: As long as we set proper R, h, D, and k, we will make an outstanding improvement on the performance.

Reference

[1] Keen, Robert E., and James D. Spain. *Computer simulation in biology: a BASIC introduction*. John Wiley & Sons, Inc., 1994.

[2] Morris, Max D. "Factorial sampling plans for preliminary computational experiments." *Technometrics* 33.2 (1991): 161-174.