Foodborne Bacteria Modeling

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September 17, 2019

1 Introduction

Foodborne illnesses, such as Salmonella and E. Coli, are common and affect millions of Americans each year. The Center for Disease and Control states that roughly 48 million people are reported sick, 128,000 are hospitalized, and 3,000 die from foodborne illnesses and diseases annually [1].

Freezing and refrigerating foods is known to slow bacterial growth. One way people thaw foods is by leaving them out at room temperature. Mesophiles, the category of bacteria that includes Salmonella and E. Coli, grow rapidly at room temperature. For this reason, the USDA does not recommend thawing foods this way [2].

In this project, we seek to model bacterial growth on food thawing at room temperature. We will first discuss the quantitative background, giving an overview of how heat spreads through food, along with the bacterial growth rate's dependence on temperature. We will then give an overview of the past models used to describe bacterial growth. Next, we will survey some common numerical methods to solve partial differential equations (PDEs). We will conclude by stating our problem quantitatively, and giving the assumptions that define the scope of our model.

2 Background and Motivation

We intend to describe the bacteria colony size on a piece of food thawing at room temperature (296 K). Bacteria have a wide array of factors that affect their growth rate, such as sample temperature, availability of resources, and competing bacteria [3]. In this section we will describe the diffusion constant as a function of its medium. We then discuss bacterial growth rate's direct dependence on the change in temperature.

2.1 The Diffusion Constant

Due to the complexity of making accurate predictions of these factors, we make the assumption that bacterial growth is only related to the diffusion of heat through the thawing food. This is justified by the fact that bacteria in the mesophile family, such as E. Coli and Salmonella, thrive at room temperature and experience higher growth rates as they approach their optimal temperature. The task is now to model the rate that the temperature increases through the sample, which can be considered using Fick's model of diffusion:

$$\frac{\partial T}{\partial t} = D\nabla^2 T, \tag{1}$$

where T is the temperature, t is time, D is the diffusion constant, and $\nabla^2 = \nabla \cdot \nabla$ is the Laplacian operator. The diffusion constant D is measured in units of (m^2/s).

The diffusion constant for a given food substance is based on the content of protein, carbs and fat within the sample. Each macro-nutrient has its own expression for the diffusion constant. The nutrients we will consider and their expressions are detailed in Table 1 (copied from [4]). The diffusion constant for the total food sample will be a linear combination of each expression multiplied by their respective weight fractions, written as

$$D_{tot} = X_p D_p + X_c D_c + X_f D_f + X_{fb} D_{fb} + X_a D_a, \tag{2}$$

where X_m represents the weight fraction of each macro-nutrient and D_m represents the diffusion coefficient of each macro-nutrient. P, c, f, fb, and a represent protein, carbohydrate, fat, fiber and ash respectively. Protein, carbohydrates, fats and fiber are all organic molecules, i.e are assembled through carbon chains. Ash refers to non organic molecules that exist within the food (vitamins, minerals, mercury, etc). Since the temperature will vary over time and we desire a single constant, we will be finding the average temperature within the sample from the start to the end of our experiment. The temperature of the sample will vary from frozen solid (273 K) to room temperature (296 K).

Macro-nutrient	**Diffusion Constant Model** (m^2/s)
Protein	$D = 6.88714 \times 10^{-8} + 4.7578 \times 10^{-10}t - 1.4646 \times 10^{-12}t^2$
Carbohydrate	$D = 8.80842 \times 10^{-8} + 5.3052 \times 10^{-10}t - 2.3218 \times 10^{-12}t^2$
Fat	$D = 9.8777 \times 10^{-8} - 1.2569 \times 10^{-10}t - 3.8286 \times 10^{-14}t^2$
Fiber	$D = 7.3976 \times 10^{-8} + 5.1902 \times 10^{-10}t - 2.2202 \times 10^{-12}t^2$
Ash	$D = 1.2461 \times 10^{-7} + 3.7321 \times 10^{-10}t - 1.2244 \times 10^{-12}t^2$

Table 1: Each macro-nutrient and its temperature dependent diffusion constant are listed, where t is the temperature and may vary from 233 K to 423 K

2.2 The Effect of Temperature on Bacterial Growth Rate

The growth rate of bacteria is closely related to the temperature. The Arrhenius Equation is a model that describes the reaction rate's dependence on temperature. The model is provided by [5] and based on the research of [6]

$$k = Ae^{-\frac{E_a}{RT}}, \tag{3}$$

where k represents the rate constant, T represents the absolute temperature in Kelvin, E_a is the activation energy, A is he pre-exponential factor which is a constant for each chemical reaction and R is the universal gas constant.

According to [7], the Arrhenius Equation fits the data of bacterial growth poorly. Instead the following linear model was constructed based on the experimental results:

$$\sqrt{r} = b(T - T_{min}), \tag{4}$$

where r is bacterial the growth rate, T is temperature and T_{min} is a constant which is a property of the organism. However, this model only describes the change in the growth rate of bacteria up to its maximum growth rate. A more complete model is shown by [8]

$$\sqrt{r} = b(T - T_{min})\{1 - \exp\left[c(T - T_{max})\right]\}, \tag{5}$$

where b is a regression coefficient in equation (4) and c is the parameter to fit for the growth rate after it reaches its maximum. A plot of equation (5) is shown in Fig. 1.

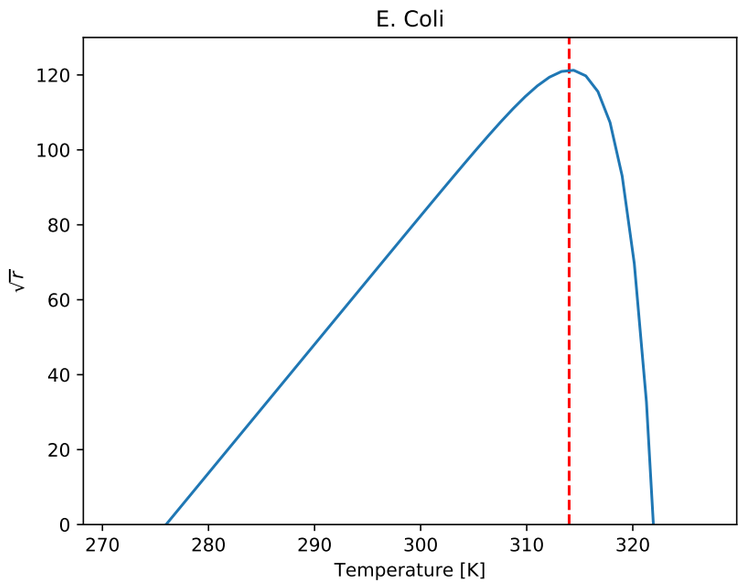

Figure 1: Plot of the *sqrtr* versus temperature curve for E. Coli. The blue curve is growth rate relation from (5), and the red dashed line is T_{opt}.

The T_{min} is the minimum temperature at which $r = 0$. Similarly, $r(T_{max}) = 0$. They define T_{opt} as the temperature at which the growth rate of bacteria reaches its maximum. In this model, as the temperature increases, the growth rate of bacteria would increase until the temperature reaches T_{opt}, and decline significantly to zero when temperature is higher than T_{opt}. This new model is an extension of equation (4), and shows how the growth rate of bacteria is nonlinear from T_{min} to T_{max}.

3 Quantitative Methods Overview

This section will first cover analytic models of population growth, then give an overview of numerical methods to solve PDEs.

3.1 Model Review

In this section we review three well-know ODE models which describe the grow of population.

3.1.1 Exponential Growth Model

Exponential growth is one of the simplest model of population growth, and has the form of

$$\frac{dN}{dt} = rN, \tag{6}$$

with initial value N_0, where N is the number of population with respect to time t, r is the growth rate. In reality, the population is always limited by available resources. Thus, the exponential growth model often works in some particular region.

3.1.2 Gompertz's Model

The Gompertz function is a sigmoid function which is widely used to model populations. It was first employed by Benjamin Gompertz to describe the law

of human mortality [9]. Later, the Gompertz function was applied to model tumor growth, bacterial populations, among other fields.

According to [10], the definition of the Gompertz model of growth is based on the assumption that the specific growth rate $\mu(t)$ is related to the amount of population $x(t)$ at time t, by

$$\mu(t) = c \cdot \ln \frac{x_{max}}{x(t)} \tag{7}$$

where x_{max} is the maximum value of $x(t)$ and c is a constant. The specific rate is defined as

$$\mu(t) = \frac{dx(t)/dt}{x(t)}, \tag{8}$$

which can be written as

$$\mu(t) = \frac{d(\ln x(t))}{dt} \tag{9}$$

when $x(t)$ is positive. According to equation (7) and (9), the solution of $x(t)$ is

$$x(t) = \exp\left[\ln x_{max} - a\exp(-ct)\right] \tag{10}$$

where a and c are constants.

In the literature, the Gompertz function has various forms for different systems. One common reparameterization of the Gompertz model provided by [11] is

$$W(t) = A\exp\left\{-\exp\left[-k_G(t - T_i)\right\}\right], \tag{11}$$

where t represents time, $W(t)$ is the expected value of the population at time t, A is an asymptote, k_G is the growth rate coefficient, and T_i is a constant. Also shown in [11], two other common reparameterizations of Gompertz model which are more difficult to interpret are

$$W(t) = A\exp\left[-\exp\left(-k_G t + b\right)\right], \tag{12}$$

and

$$W(t) = A\exp\left\{-c[\exp\left(-k_G t\right)]\right\}. \tag{13}$$

3.1.3 Logistic Model

The logistic model studies the population growth within a constrained environment. The growth rate is related to the size of both the population and total capacity of the environment. It was adjusted from exponential growth model (6) by Pierre-François Verhulst with the form of

$$\frac{dN}{dt} = rN\left(1 - \frac{N}{N_{max}}\right). \tag{14}$$

In bacteriology, this represents the growth rate in number of bacteria in a medium at time t, so the solution $N = N(t)$ gives the number of bacteria at any given time. N_{max} is the maximum amount of bacteria, which forms where the solution asymptotes [12]. N_0 is the initial amount of bacteria. The solution of the logistic function is

$$N(t) = \frac{N_{max}}{1 + Ae^{-rt}}, \qquad A = \frac{K - N_0}{N_0}. \tag{15}$$

One property of the logistic model is

$$\lim_{t\to\infty} N(t) = N_{max},$$

which implies the population is limited by the availability of resources.

The logistic equation (14) contains qualitative features that are appropriate for modeling population growth, but it is unsuitable for bacteria since it does not form a sigmoid in $\log N$ [12]. A modified form presented by [12] is

$$\frac{dN}{dt} = rN\left(1 - \frac{N}{N_{max}}\right)\left(1 - \frac{N_{min}}{N}\right)^c. \tag{16}$$

Where the extra $1 - N_{min}/N$ term describes the lag time of the bacteria, $c \geq 0$ is a fitting parameter, and $N_{min} = (1 - \delta)N(0)$, where $\delta > 0$ is small.

3.2 Comparison of Numerical Methods

In this section we will give an overview of finite element analysis (FEM), the method of lines and the finite difference method. All of these methods rely on discretizing the PDE in order to make approximations of the solution, which can be difficult to find analytically.

3.2.1 Finite Element Analysis

Finite element analysis, also called the finite element method, posits the solution to a PDE can be approximated by a linear combination of n functions. That is, if u is the solution then to a PDE then $\tilde{u}$ approximates u and is given by

$$\tilde{u} = \sum_{i=1}^{n} c_i \phi_i \tag{17}$$

where ϕ_i is the previously chosen function, and c_i is the coefficient.

Functions are chosen beforehand and are solved to be 1 at a point and 0 everywhere else. This construction is convenient because if a function $\phi_i(x_i) = 1$, then $\tilde{u}(x_i) = c_i$. The domain is discretized via triangulation, a method that breaks up the domain into triangles. The vertices of these triangles are used to determine the functions ϕ_i in equation (17) such that at the ith vertex, $\phi_i = 1$ and 0 everywhere else [13, p. 222-223].

Finite element analysis is incredibly important for engineering design analysis. For instance, the automotive industry uses FEM to simulate car collisions [14, p. 10].

3.2.2 The Method of Lines

The method of lines involves discretizing a PDE in all but one variable, then solving a system of ODEs in that one variable. Another way to think about this is in two dimensions, discritizing in one variable gives us planes to solve the ODE on.

More formally, say we have an equation in two variables x and y, and $u = u(x, y)$ is a solution of this equation. We discretize one variable, say x, to x_i with some step size. We can then form a vector $\tilde{\boldsymbol{u}}(y)$ with elements $\tilde{u}(y) \approx u(x_i, y)$. From this we form a system of ODEs which approximate our PDE [15, p. 456-457].

The system of ODEs can be solved either analytically or with an ODE solver. This makes the method of lines a semi-analytic method, which is one of its advantages. Another advantage is the ease of implementation. One can discretize a PDE using techniques similar to the finite difference method (see below), then use software packages such as python's scipy module to solve the ODEs numerically.

3.2.3 Finite Difference Method

The finite difference method uses the idea of the partial derivative as a difference between two closely-spaced points. Say x_1 and $x_2 = x_1 + \Delta x$ are two x-values close together, and let $f(x, y)$ be some continuous function. Then if $\Delta x = x_2 - x_1$ is some small change in x, we can write

$$\frac{\partial f}{\partial x} \approx \frac{f(x_1 + \Delta x, y) - f(x_1, y)}{\Delta x}. \tag{18}$$

We can also apply this reasoning to higher-order derivatives [16, p. 3-4].

This method is straightforward both to understand and to implement. One caveat is, depending on the equation, stability conditions must be met which determine the maximum size of the discretized steps. This affects computation time. If the steps must be small, then the PDEs will take longer to compute. The major drawback of this method is that it works well on rectangular domains, but is harder to implement for other geometries [13, p. 205-206].

4 Problem Statement

We seek to model the number of bacteria on a piece of thawing food at specified point and time. We first state the assumptions we are making in our model. Then we will state what we expect our model to look like qualitatively.

4.1 Assumptions

- The room temperature is constant. If we want to use the heat equation, this will determine our boundary conditions.
- The initial distribution of bacteria is uniform over our domain.
- The bacteria spread in a thin film on the food, so we confine our analysis to two spatial dimensions.
- The diffusion coefficient in the heat equation is constant over our range of temperatures.
- The bacteria are mesophiles, and different species of mesophiles will be assumed to grow identically
- There are no competing bacteria present on the food.
- The food nutrient distribution is uniform at any point. This means given the mass fractions of protein, carbohydrates and fat content we can assume that any given point on the food substance follows said distribution.
- The growth rate of the bacteria is only a function of temperature.

4.2 Problem Proposition

We expect the solution $N = N(x, t)$, the number number of bacteria at the point x and time t, to be a sigmoid in $\log N$. An example of a sigmoid curve in $\log N$ is presented in Fig. 2. We use logarithms since the the number of bacteria will be very large.

We expect the equation for N to be in the form

$$\frac{\partial N}{\partial t} = rN(1 - N/N_{max})(1 - N_{min}/N)^c, \tag{19}$$

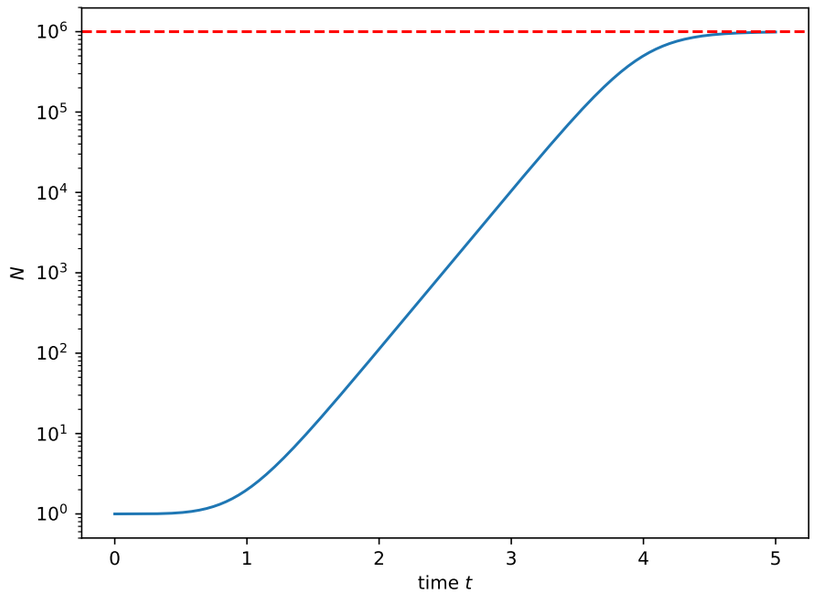

Figure 2: Example of a sigmoid curve in $\log N$. The solid blue curve is the solution to the modified logistic equation (16), and the red dashed line represents N_{max}, the maximum population the system can hold.

which is the modified logistic equation (16) with $d \to \partial$. The parameters are defined the same as in (16). Note that r depends on T. Our model for the temperature of the food T will be the heat equation

$$\frac{\partial T}{\partial t} = D\nabla^2 T \tag{20}$$

Note this is equivalent to equation (1), and the parameters are defined the same. This implies $T = T(x, t)$, that is, temperature depends on position and time. Since the growth rate r in equation (16) depends on T, it also depends on position and time. Hence these differential equations are coupled, and we will have to solve equation (20) first in order to solve (19).

This procedure should give us the number of bacteria N, and from here we can make predictions such as when the food will become dangerous to eat, and if putting ice packs on food really does slow bacterial growth.

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