

# Chapter 1

## Derivation of Reaction-Diffusion Equations

### 1.1 Fick's Law

Diffusion mechanism models the movement of many individuals in an environment or media. The individuals can be very small such as basic particles in physics, bacteria, molecules, or cells, or very large objects such as animals, plants, or certain kind of events like epidemics, or rumors. The particles reside in a region, which we call  $\Omega$ , and we assume that  $\Omega$  is open subset of  $\mathbf{R}^n$  (the  $n$ -th dimensional space with Cartesian coordinate system) with  $n \geq 1$ . In particular, we are interested in the cases of  $n = 1, 2$  and  $3$ , but most material here are true regardless of the dimensions of the space (sometimes  $n = 1$  and  $n \geq 2$  may be different as we will see.)

The main mathematical variable we consider here is the density function of the particles:  $P(t, x)$ , where  $t$  is the time, and  $x \in \Omega$  is the location. The dimension of the population density usually is number of particles or organisms per unit area (if  $n = 2$ ) or unit volume (if  $n = 3$ ). For example, the human population density is often expressed in number of people per square kilometer. A list of world population and population density can be found at

[http://en2.wikipedia.org/wiki/List\\_of\\_countries\\_by\\_population\\_density](http://en2.wikipedia.org/wiki/List_of_countries_by_population_density).

However in such data table, we can only find the population density for countries, and a country is not a “point” on our map. In reality, population density is always associated with a scale, like country, city, county, town, and street. But as in many other mathematical models, we will assume that the function  $P(t, x)$  has nicer properties, like continuity and differentiability, which is in fact reasonable, when a population with a large number of organisms is considered. Technically, we define the population density function  $P(t, x)$  as follows: let  $x$  be a point in the habitat  $\Omega$ , and let  $\{O_n\}_{n=1}^{\infty}$  be a sequence of spatial regions (which have the same dimension as  $\Omega$ ) surrounding  $x$ ; here  $O_n$  is chosen in a way that the spatial measurement  $|O_n|$  of  $O_n$  (length, area, volume, or

mathematically, the Lebesgue measure) tends to zero as  $n \rightarrow \infty$ , and  $O_n \supset O_{n+1}$ ; then

$$P(t, x) = \lim_{n \rightarrow \infty} \frac{\text{Number of organisms in } O_n \text{ at time } t}{|O_n|}, \quad (1.1)$$

if the limit exists. Realistically, as long as the scale of data collecting is small enough, the population density function is usually very well defined. Clearly the total population in any sub-region  $O$  of  $\Omega$  at time  $t$  is

$$\int_O P(t, x) dx. \quad (1.2)$$

The question we are interested now is how the function  $P(t, x)$  changes as time  $t$  evolves, and as the location  $x$  varies. Population can change in two ways: one is that the individual particles can move around, and the second is they may produce new individuals or kill existing individuals due to physical, chemical, or biological reasons. We shall model these two different phenomena separately.

How do the particles move? In general that is a highly complicated process which can be attributed to a lot of reasons. For example, the reasons of the emigration of human can be looking for a better life, looking for a better job, political reason, or religious reason, etc. Let's review a few historical emigration trends: since the sixteenth century, European emigrated westward to America; in the last two centuries, Asian emigrated eastward to America; inside United States, people move to west from east, and people move to Rocky mountain area from eastern or western coasts. Although economical reason can be quoted as motivation to move, we can see clearly, in all these cases, people move from areas where population density is high to areas where it is lower. This is similar to many physical phenomena, like the heat transfer (from warmer place to colder place), or the dilution of chemical in water.

A Chinese proverb is "People goes to high place, water flows to low place". It is a natural phenomenon that a substance goes from high density regions to low density regions. The movement of  $P(t, x)$  is called the **flux** of the population density, which is a vector. The "high to low" principle now means that, the flux always points to the most rapid decreasing direction of  $P(t, x)$ , which is the negative **gradient** of  $P(t, x)$ . This principle is called **Fick's law**, and it can be represented as

$$\mathbf{J}(t, x) = -d(x) \nabla_x P(t, x), \quad (1.3)$$

where  $\mathbf{J}$  is the flux of  $P$ ,  $d(x)$  is called **diffusion coefficient** at  $x$ , and  $\nabla_x$  is the gradient operator  $\nabla_x f(x) = (\partial f / \partial x_1, \partial f / \partial x_2, \dots, \partial f / \partial x_n)$ .

On the other hand, the number of particles at any point may change because of other reasons like birth, death, hunting, or chemical reactions. We assume that the rate of change of the density function due to these reasons is  $f(t, x, P)$ , which we usually call the **reaction rate**. Now we derive a differential equation using the balanced law. We choose any region  $O$ , then the total population in  $O$  is  $\int_O P(t, x) dx$ , and the rate of change of the total population is

$$\frac{d}{dt} \int_O P(t, x) dx. \quad (1.4)$$

The net growth of the population inside the region  $O$  is

$$\int_O f(t, x, P(t, x)) dx, \quad (1.5)$$

and the total out flux is

$$\int_{\partial O} \mathbf{J}(t, x) \cdot \mathbf{n}(x) dS, \quad (1.6)$$

where  $\partial O$  is the boundary of  $O$ , and  $\mathbf{n}(x)$  is the outer normal direction at  $x$ . Then the balance law implies

$$\frac{d}{dt} \int_O P(t, x) dx = - \int_{\partial O} \mathbf{J}(t, x) \cdot \mathbf{n}(x) dS + \int_O f(t, x, P(t, x)) dx \quad (1.7)$$

From the Divergence Theorem in multi-variable calculus, we have

$$\int_{\partial O} \mathbf{J}(t, x) \cdot \mathbf{n}(x) dS = \int_O \text{div}(\mathbf{J}(t, x)) dx. \quad (1.8)$$

Combining (1.3), (1.7) and (1.8), and interchanging the order of differentiation and integration, we obtain

$$\int_O \frac{\partial P(t, x)}{\partial t} dx = \int_O [\text{div}(d(x) \nabla_x P(t, x)) + f(t, x, P(t, x))] dx. \quad (1.9)$$

Since the choice of the region  $O$  is arbitrary, then the differential equation

$$\frac{\partial P(t, x)}{\partial t} = \text{div}(d(x) \nabla_x P(t, x)) + f(t, x, P(t, x)) \quad (1.10)$$

holds for any  $(t, x)$ . The equation (1.10) is called a **reaction diffusion equation**. Here  $\text{div}(d(x) \nabla_x P(t, x))$  is the diffusion term which describes the movement of the individuals, and  $f(t, x, P(t, x))$  is the reaction term which describes the birth-death or reaction occurring inside the habitat or reactor.

The diffusion coefficient  $d(x)$  is not a constant in general since the environment is usually heterogeneous. But when the region of the diffusion is approximately homogeneous, we can assume that  $d(x) \equiv d$ , then (1.10) can be simplified to

$$\frac{\partial P}{\partial t} = d\Delta P + f(t, x, P), \quad (1.11)$$

where  $\Delta P = \text{div}(\nabla P) = \sum_{i=1}^n \frac{\partial^2 P}{\partial x_i^2}$  is the Laplacian operator. When there is no reaction occurs, the equation is **diffusion equation**:

$$\frac{\partial P}{\partial t} = d\Delta P, \quad (1.12)$$

In classical mathematical physics, the equation  $T_t = \Delta T$  is called **heat equation**, where  $T$  is the temperature function. So sometimes (1.11) is also called a nonlinear heat equation. Conduction of heat can be considered as a form of diffusion of heat.

## 1.2 Random Walk

A random walk considers a “walker” (a particle, or a rabbit) which starts at a point, and takes steps in a random direction. Sometimes the steps can also be of random length as well. The random walk can take place in a plane, along a line, or in higher dimensions.

The simplest random walk considers a walker that takes steps of length  $\Delta x$  to the left or right along a line, and after each  $\Delta t$  time units, the walker will take one step. If the walker is at location  $x_0$  at the time  $t_0$ , then at time  $t = t_0 + \Delta t$ , the walker will either be at  $x_0 - \Delta x$  or  $x_0 + \Delta x$ . Normally the chances of going left or right should be equal, thus the probability of the walker going left or right is  $1/2$ . Now we assume that many walkers are walking with the same time frame simultaneously, with the same step size and on the same lattice on the line. We define  $P(t, x)$  as the number of walkers at time  $t$  and location  $x$ . Then after one time step  $\Delta t$ , everyone who is at  $x_0$  is gone now (go to  $x_0 - \Delta x$  or  $x_0 + \Delta x$ ), and half of those who are at  $x_0 - \Delta x$  and half of those who are at  $x_0 + \Delta x$  move to  $x = x_0$  now. So we have

$$P(t_0 + \Delta t, x_0) = \frac{1}{2}P(t_0, x_0 - \Delta x) + \frac{1}{2}P(t_0, x_0 + \Delta x). \quad (1.13)$$

We use the Taylor expansion of the function  $P(t, x)$ :

$$P(t_0 + \Delta t, x_0) = P(t_0, x_0) + \frac{\partial P}{\partial t}(t_0, x_0)\Delta t + \frac{1}{2}\frac{\partial^2 P}{\partial t^2}(t_0, x_0)(\Delta t)^2 + \dots, \quad (1.14)$$

$$\frac{1}{2}P(t_0, x_0 - \Delta x) = \frac{1}{2}P(t_0, x_0) + \frac{1}{2}\frac{\partial P}{\partial x}(t_0, x_0)(-\Delta x) + \frac{1}{4}\frac{\partial^2 P}{\partial x^2}(t_0, x_0)(-\Delta x)^2 + \dots, \quad (1.15)$$

$$\frac{1}{2}P(t_0, x_0 + \Delta x) = \frac{1}{2}P(t_0, x_0) + \frac{1}{2}\frac{\partial P}{\partial x}(t_0, x_0)(\Delta x) + \frac{1}{4}\frac{\partial^2 P}{\partial x^2}(t_0, x_0)(\Delta x)^2 + \dots. \quad (1.16)$$

By substituting (1.15), (1.16) and (1.14) into (1.13), we obtain

$$\frac{\partial P}{\partial t}(t_0, x_0)\Delta t + \dots = \frac{1}{2}\frac{\partial^2 P}{\partial x^2}(t_0, x_0)(\Delta x)^2 + \dots. \quad (1.17)$$

Here we assume that both  $\Delta t$  and  $\Delta x$  are small quantities, thus the higher order terms in the Taylor expansions (the  $\dots$  parts) are smaller terms compared to the two remaining terms in (1.17). By dividing  $\Delta t$ , we now have

$$\frac{\partial P}{\partial t}(t_0, x_0) = \frac{(\Delta x)^2}{2\Delta t}\frac{\partial^2 P}{\partial x^2}(t_0, x_0) + \dots. \quad (1.18)$$

Now we assume that

$$\Delta t \rightarrow 0, \quad \Delta x \rightarrow 0, \quad \text{and} \quad \frac{(\Delta x)^2}{2\Delta t} \rightarrow D > 0. \quad (1.19)$$

The last assumption can be satisfied by designing the scale of the random walk, and when the limits in (1.19) are taken, we arrive at

$$\frac{\partial P}{\partial t}(t_0, x_0) = D\frac{\partial^2 P}{\partial x^2}(t_0, x_0), \quad (1.20)$$

the one-dimensional diffusion equation.

From the above argument, the diffusion constant  $d$  have the dimension as  $(\Delta x)^2/\Delta t$ , or

$$\frac{(\text{distance})^2}{\text{time}}. \quad (1.21)$$

The diffusion constant can often be estimated through experiment, since (1.21) implies the time that the substance diffuses is proportional to the square of the distance that the substance diffuses, *i.e.*

$$T \sim D^2, \quad (1.22)$$

where  $T$  is the time that the substance diffuses, and  $D$  is the distance that the substance diffuses. We will get a more precise conclusion later with calculations, but we can see from the following chart of the diffusion constant of oxygen that  $D$  depends on the nature of the substance, the media where it is diffusing and the temperature:

Temperature ( $^{\circ}C$ )	Media	$D$ ( $cm^2/sec$ )
0	air	$1.78 \times 10^{-1}$
20	air	$2.01 \times 10^{-1}$
18	water	$2.41 \times 10^{-5}$
25	water	$4.58 \times 10^{-5}$

The assumption that the random walk is unbiased may not be true for certain cases, and when one direction in the random walk is favored, an equation with a first order derivative is the result (see homework problem):

$$\frac{\partial P}{\partial t} + V \frac{\partial P}{\partial x} = D \frac{\partial^2 P}{\partial x^2}. \quad (1.23)$$

The first order derivative term is called a **convection term**, and (1.23) is a **diffusion equation with convection**. In higher dimensional space, the random walk can be biased on any direction, and the general reaction-diffusion equation with convection is

$$\frac{\partial u}{\partial t} + V \nabla u \cdot \gamma = D \frac{\partial^2 u}{\partial t^2} + f(t, x, u), \quad (1.24)$$

where  $\gamma \in \mathbf{R}^n$  is a vector indicating the direction of the biased motion (see homework problem). Such equation is more realistic when the media of the diffusion moves to a direction—for example, the wind or the water flow.

## 1.3 Reaction

In the reaction-diffusion equation:

$$\frac{\partial P}{\partial t} = d\Delta P + f(t, x, P), \quad (1.25)$$

the  $f(t, x, P)$  represents the birth/death, or reaction process. as will see in the following chapters, reaction and diffusion both contribute to the interesting dynamical behavior of the solutions of the equation, and sometimes, it is intriguing to compare the dynamics of (1.25) with its more familiar and less sophisticated cousin:

$$\frac{\partial P}{\partial t} = f(t, P), \quad (1.26)$$

where  $P = P(t)$  is usually not the density function but the function of total number of the particles at time  $t$ . Generic population model usually assume that

$$f(P) = kP, \text{ (Malthus linear growth)}, \quad f(P) = kP \left(1 - \frac{P}{N}\right), \text{ (Logistic growth)}. \quad (1.27)$$

The analytic methods for (1.26) with these growth rate functions are well-known in the undergraduate differential equation textbooks. Reaction diffusion equations corresponding to these reaction rates are

$$\frac{\partial P}{\partial t} = D\Delta P + kP, \quad \text{Diffusive Malthus equation}, \quad (1.28)$$

$$\frac{\partial P}{\partial t} = D\Delta P + kP \left(1 - \frac{P}{N}\right), \quad \text{Diffusive logistic equation}. \quad (1.29)$$

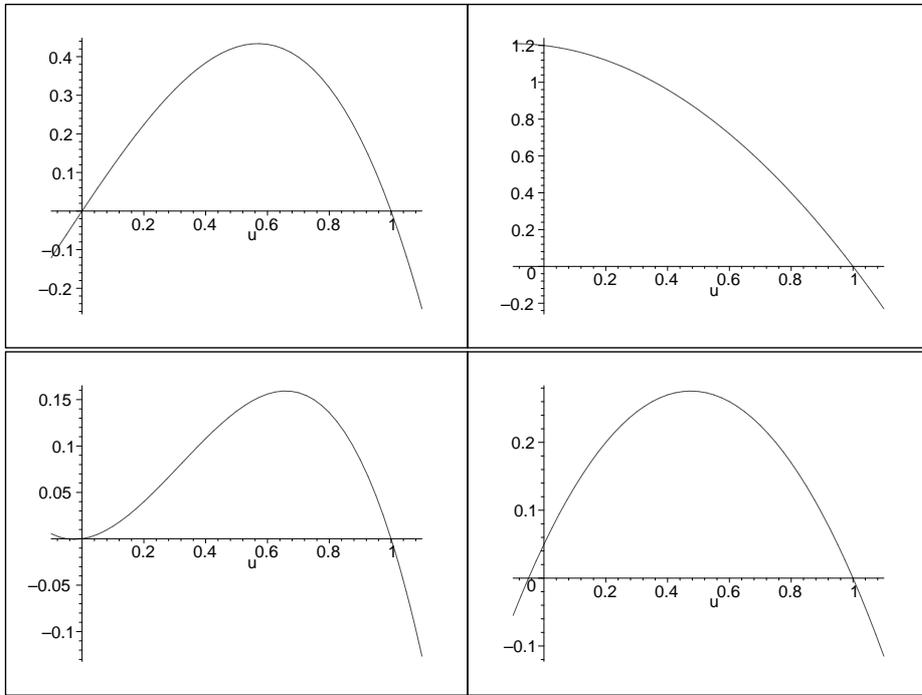


Figure 1.1: **(a)** Logistic (upper); **(b)** Weak Allee effect (middle): growth rate (left), growth rate per capita (right).

Similar to the non-spatial versions, (1.28) and (1.29) are equations describing the evolution of a spatially distributed population which satisfies generical growth patterns. In these two examples, if we rewrite the equation as

$$\frac{\partial P}{\partial t} = D\Delta P + Pg(P), \quad (1.30)$$

then the growth rate per capita  $g(P)$  are constant  $g_1(P) = k$  for Malthus equation and decreasing linear function  $g_1(P) = k(1 - P/N)$  for logistic equation.

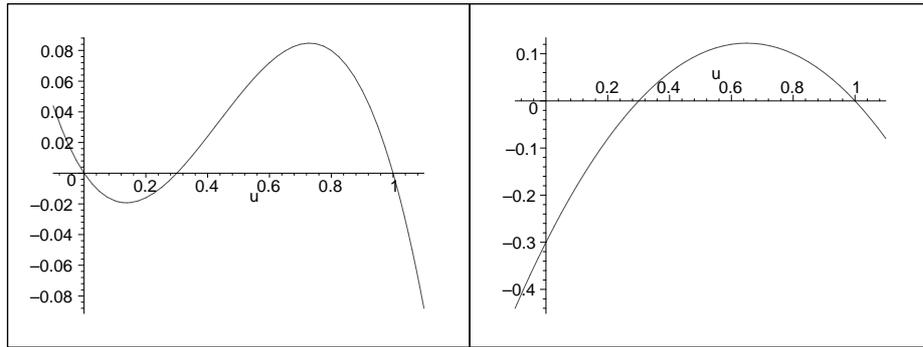


Figure 1.2: Strong Allee effect: growth rate (left), growth rate per capita (right).

In population biology, for some species, a small or sparse population may not be favorable, since for example, mating may be difficult. This is called **Allee effect**. Mathematically the growth rate per capita function  $g(P)$  will not have the maximum value at  $P = 0$ . If  $g(P)$  is negative when  $P$  is small, we call such a growth pattern has a **strong Allee effect**. A typical example is

$$\frac{dP}{dt} = kP \left(1 - \frac{P}{N}\right) \left(\frac{P}{M} - 1\right) = P \cdot g(P), \quad (1.31)$$

where  $0 < M < N$ ,  $M$  is the sparsity constant and  $N$  is the carrying capacity. If the growth rate per capita  $g(P)$  is smaller than the maximum but still positive for small  $P$ , we call such a growth pattern has a **weak Allee effect**. A typical example is

$$\frac{dP}{dt} = kP \left(1 - \frac{P}{N}\right) \left(\frac{P}{M} - 1\right) = P \cdot g(P), \quad (1.32)$$

where  $M < 0 < N$ . The corresponding reaction-diffusion equation with Allee effect is

$$\frac{\partial P}{\partial t} = D\Delta P + aP \left(1 - \frac{P}{N}\right) \left(\frac{P}{M} - 1\right), \quad (1.33)$$

where  $a > 0$ ,  $N > 0$  and  $N > M$ .

Chemical mixing and reaction can also be modeled by reaction-diffusion equations. We first consider a typical “mixing problem” in ordinary differential equation course:

*A tank currently holds 100 gallons of pure water. A solution containing 2 lb of salt per gallon enters the tank at a rate of 3 gallon/minute. Assume that the solution is well-stirred so the salt is evenly resolved in the solution. A drain is opened at the bottom of the tank so that the volume of the solution in the tank remains constant. How much salt is in the tank after 60 minutes? How about after a long long time?*

Let  $A(t)$  be the concentration of the salt the tank. Then by the balance law,  $A(t)$  satisfies an ordinary differential equation:

$$\frac{dA}{dt} = 0.06 - 0.03A, \quad A(0) = 0. \quad (1.34)$$

The solution of the equation is  $A(t) = 2(1 - e^{-3t/100})$ , and as  $t \rightarrow \infty$ ,  $A(t) \rightarrow 2\text{lb/gallon}$ . While the model (1.34) correctly describes the mixing as an exponential approach to an equilibrium state, it is a simplification of the real chemical process—especially the spatial distribution of the chemical is ignored, and the chemical is assumed to be evenly resolved in the solution immediately, which is also not true.

We use the reaction-diffusion equation to model the problem again. The tank which holds 100 gallon is the spatial domain  $\Omega$  in  $\mathbf{R}^3$ , which can be a cylinder or cube shaped; the concentration of the salt in the water is  $A(t, x)$ , where  $t \geq 0$ ,  $x \in \Omega$ ; we assume that the salt molecules moves randomly in the media (water). Since there is no reaction involved here, the evolution of the density function  $A$  can be described by a diffusion equation with an initial condition:

$$\frac{\partial A}{\partial t} = D\Delta A, \quad A(0, x) = 0. \quad (1.35)$$

Note that (1.35) does not include the addition from the inflowing solution (which contains 2 lb per gallon of salt) and the subtraction from the drain. In fact, these additions or subtractions occur not in the domain, but on the boundary of the domain. For example, the inflowing solution comes into the tank from the solution surface, and the drain is on the bottom of the tank. We shall discuss such boundary conditions of the problem in the next section.

In the above problem, if salt is replaced by a chemical which will react, say the name of chemical is  $A$ , and the chemical reaction is



where  $C$  and  $D$  are two other kinds of molecules, and  $k$  is the reaction rate (the percentage of  $B$  molecules which will react in a unit time and a unit volume.) Then the reaction-diffusion equation is

$$\frac{\partial A}{\partial t} = D\Delta A - kA, \quad (1.37)$$

where  $A(t, x)$  is the concentration function of  $A$ . Of course most chemical reactions involve more than one chemicals, thus a system of reaction-diffusion equation is required to describe such reactions. For example, we consider a chemical reaction:



This is called an autocatalytic reaction, as one  $A$  molecule acting as catalyst. Let  $A(t, x)$  and  $B(t, x)$  be the concentration of  $A$  and  $B$  respectively. Since over all one  $B$  molecule is consumed and one  $A$  molecule is generated in the reaction, the equations are:

$$\frac{\partial A}{\partial t} = D_A\Delta A + kAB, \quad \frac{\partial B}{\partial t} = D_B\Delta B - kAB. \quad (1.39)$$

Here we assume the possibility of  $A$  and  $B$  molecules colliding in a unit volume of media is  $AB$ , and reaction rate  $k$  is defined as the percentage of reaction when a collision occurs. The possibility of a multiple molecule reaction occurring is proportional to the multiplication of concentration of each reactant. For example, consider



where  $p > 1$  is an integer. Then similar to (1.39), we have

$$\frac{\partial A}{\partial t} = D_A \Delta A + kA^p B, \quad \frac{\partial B}{\partial t} = D_B \Delta B - kA^p B. \quad (1.41)$$

A simple reaction which has been studied extensively is Gray-Scott model. Consider reactions:



and we assume that  $A$  is continuously and evenly feeded into the reactor, and  $A$ ,  $B$  and  $C$  are continuously and evenly removed from the reactor, all with the same rate  $k_3$ . Then the reaction-diffusion model is:

$$\frac{\partial A}{\partial t} = D_A \frac{\partial^2 A}{\partial t^2} - k_1 AB^2 + k_3 - k_3 A, \quad \frac{\partial B}{\partial t} = D_B \frac{\partial^2 B}{\partial t^2} + k_1 AB^2 - k_2 B - k_3 B. \quad (1.43)$$

We will come back to (1.43) in Chapter 4 to discuss the behavior of the solutions.

## 1.4 Boundary Conditions

As we can see from the example of chemical mixing model, the boundary conditions are as important as the differential equations in the model. In the situation of a chemical reaction, additions and subtractions of chemicals can be included in the equation, but often they are imbedded in the boundary conditions. The simplest boundary condition is when there is no additions and subtractions of any chemicals through the boundary, and all chemicals are generated inside the reactor and they remain there. for example the chemical reactions occurring in a Petri dish with an impermeable wall. Such system is called a **closed** one. For each chemical involved, if  $\mathbf{J}(t, x)$  is the flux of the chemical, then the flux across on a boundary point  $x$  is  $\mathbf{J}(t, x) \cdot \mathbf{n}(x)$ , and if we assume the Fick's law (1.3), then for a close system, at each boundary point  $x$ :

$$\nabla u(t, x) \cdot \mathbf{n}(x) = 0, \quad (1.44)$$

where  $u(t, x)$  is the concentration function of the chemical. Therefore a well-posed (which means solution is uniquely determined under reasonable assumptions) closed reaction-diffusion equation is an initial value boundary value problem

$$\begin{cases} \frac{\partial u}{\partial t} = d\Delta u + f(t, x, u), & t > 0, x \in \Omega, \\ u(0, x) = u_0(x), & x \in \Omega, \\ \nabla u(t, x) \cdot \mathbf{n}(x) = 0, & t > 0, x \in \partial\Omega. \end{cases} \quad (1.45)$$

Here  $\partial\Omega$  is the common notation used for the boundary of  $\Omega$ . Closed reaction-diffusion systems are similar. In mathematical physics or fluid dynamics, (1.44) is called **no-flux** or homogeneous **Neumann** boundary condition. The second one is named after Germany mathematician and physicist Franz Ernst Neumann (1798-1895). The closed system is also relevant in many population ecological models. For example, an isolated island can be considered as the spatial domain of the system; if all living species on the island do not attempt to emigrate from the island, then the

ecosystem of the island can be considered as a closed one. For the classical heat conduction equation  $T_t = d\Delta T$ , the no-flux boundary condition means the boundary is heat-insulated. The no-flux boundary condition can also be called as **reflecting** since particles diffusing to the boundary can be considered as reflected back. In the case of spatial dimension  $n = 1$ , the domain  $\Omega$  is an interval  $(a, b)$ , then the no-flux boundary condition becomes

$$\frac{\partial u}{\partial x}(t, a) = \frac{\partial u}{\partial x}(t, b) = 0. \quad (1.46)$$

Now we can come back to the chemical mixing model considered in Section 1.3. The system there is not closed. We assume that the inflow comes in from a portion  $\Gamma_1$  of the boundary  $\partial\Omega$ , and the outflow comes out from another portion  $\Gamma_2$ . Then the total flux across  $\Gamma_1$  in a unit time is

$$\int_{\Gamma_1} \mathbf{J}(t, x) \cdot \mathbf{n}(x) ds = 6, \quad (1.47)$$

and we assume that the inflow is evenly distributed on  $\Gamma_1$ , then for each  $x \in \Gamma_1$ ,

$$\mathbf{J}(t, x) \cdot \mathbf{n}(x) = -D\nabla u(t, x) \cdot \mathbf{n}(x) = \frac{6}{|\Gamma_1|}, \quad (1.48)$$

where  $D > 0$  is the diffusion constant, and  $|\Gamma_1|$  is the surface area of  $\Gamma_1$ . Thus

$$\nabla A(t, x) \cdot \mathbf{n}(x) = -\frac{6}{D|\Gamma_1|}, \quad t > 0, \quad x \in \Gamma_1. \quad (1.49)$$

Similarly,

$$\nabla A(t, x) \cdot \mathbf{n}(x) = \frac{3A(t, x)}{D|\Gamma_2|}, \quad t > 0, \quad x \in \Gamma_2. \quad (1.50)$$

For the other parts of the boundary, the no-flux boundary condition is appropriate. Therefore the full initial value boundary value problem is

$$\begin{cases} \frac{\partial A}{\partial t} = D\frac{\partial^2 A}{\partial t^2}, & t > 0, \quad x \in \Omega, \\ u(0, x) = 0, & x \in \Omega, \\ \nabla A(t, x) \cdot \mathbf{n}(x) = -\frac{6}{D|\Gamma_1|}, & t > 0, \quad x \in \Gamma_1, \\ \nabla A(t, x) \cdot \mathbf{n}(x) - \frac{3}{D|\Gamma_2|}A(t, x) = 0, & t > 0, \quad x \in \Gamma_2, \\ \nabla A(t, x) \cdot \mathbf{n}(x) = 0, & t > 0, \quad x \in \partial\Omega/(\Gamma_1 \cup \Gamma_2). \end{cases} \quad (1.51)$$

The boundary condition on  $\Gamma_2$  is a special case of homogeneous **Robin** boundary condition.

In general there are three commonly used boundary conditions:

$$\text{(Neumann)} \nabla u(t, x) \cdot \mathbf{n}(x) = \phi(x), \quad t > 0, \quad x \in \partial\Omega; \quad (1.52)$$

$$\text{(Robin)} \nabla u(t, x) \cdot \mathbf{n}(x) + a(x)u(t, x) = \phi(x), \quad t > 0, \quad x \in \partial\Omega; \quad (1.53)$$

$$\text{and (Dirichlet)} \quad u(t, x) = \phi(x), \quad t > 0, \quad x \in \partial\Omega. \quad (1.54)$$

In the Robin boundary condition,  $a(x) \geq 0$ , and  $\phi(x)$  is a function defined on the boundary  $\partial\Omega$ . As we can see from the previous example,  $\phi(x)$  may not be a continuous function, so we assume that  $\phi$  is an integrable function. The precise and optimal setting for such problems requires much more mathematical knowledge, thus we will not go deeper in that direction. Often we consider the case when  $\phi(x) \equiv 0$ , the **homogeneous** boundary condition. When  $\phi(x)$  is not zero, then the boundary condition is **non-homogeneous**. Again as we can learn from the previous example, it is unrealistic that the boundary condition is uniformly one type on the whole domain  $\partial\Omega$ . In fact, the boundary conditions in (1.51) is a **mixed** boundary condition, which is one of the three boundary conditions on each of several components of  $\partial\Omega$ .

Dirichlet boundary condition assumes that the solution presumes the value  $\phi(x)$  for each point on the boundary. For many cases, the homogeneous Dirichlet boundary condition makes the mathematical analysis easier, so in many examples of this book, we will consider that case. For most chemical reaction, no-flux is more appropriate than Dirichlet boundary condition. When the problem assumes Dirichlet boundary condition  $u(t, x) \equiv c$ , a constant, we can think  $u(t, x)$  takes the value  $c$  for all the points outside of  $\Omega$ . For example, for the heat equation  $T_t = D\Delta T$ , constant Dirichlet condition means the outside environment has a constant temperature  $T_0$ . For ecological applications, sometimes we can assume homogeneous Dirichlet boundary condition  $u(t, x) \equiv 0$  on  $\partial\Omega$ , which implies that any individual of the species cannot survive outside of  $\Omega$  on even on the boundary of  $\Omega$ . Thus in this case, the boundary is lethal (sometimes called **absorbing**), and any individual who wanders outside (due to diffusion) is killed by the sterile exterior environment or the deadly boundary. A good example perhaps is the high-voltage electric fence around the Jurassic Park.

When studying the periodic patterns generated by the reaction-diffusion mechanism, we will encounter **periodic boundary condition**. First of all, for such problem, the domain and the media of diffusion both should have a periodic structure. For example, the one-dimensional diffusion equation with periodic boundary condition is

$$\begin{cases} \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, & t > 0, \quad x \in (a, b), \\ u(0, x) = u_0(x), & x \in (a, b), \\ u(t, a) = u(t, b), & t > 0, \quad x \in (a, b), \\ \frac{\partial u}{\partial x}(t, a) = \frac{\partial u}{\partial x}(t, b), & t > 0, \quad x \in (a, b). \end{cases} \quad (1.55)$$

When the function  $u$  satisfies (1.55), we can extend  $u$  spatially to  $x \in (-\infty, \infty)$  periodically. The extended function satisfies the differential equation for all  $x \in (-\infty, \infty)$ , since the function values and the derivative values at the boundary match, and the second derivative values will also match because of the equation.

Finally in some models of physics and biology, we may consider the reaction-diffusion equation on the whole space  $\mathbf{R}^n$ . The “boundary” of the whole space is  $x = \infty$ , or more precisely, the boundary condition is the limiting behavior of the solution when  $|x| \rightarrow \infty$ , where  $|x|$  is the the distance from  $x$  to the origin. In that situation, a natural condition is that

$$\lim_{|x| \rightarrow \infty} u(t, x) = 0, \quad \lim_{|x| \rightarrow \infty} \nabla u(t, x) = 0. \quad (1.56)$$

It means that the chance of the dispersal of the articles to infinity is zero.

## 1.5 Nondimensionalization

In both qualitative and numerical methods, the dependence of solutions on the parameters plays an important role, and there are always more difficulties when there are more parameters. We describe a technique that changes variables so that the new variables are “dimensionless”. This technique will lead to a simple form of the equation with fewer parameters. It makes clear that the parameters can interact in the equation and a simpler combined parameter can suffice for more than one parameter. We illustrate this technique which is called Nondimensionalization, with an example of an ordinary differential equation.

**Example.** Consider the following model of an outbreak of the spruce budworm:

$$\frac{dP}{dt} = kP \left(1 - \frac{P}{N}\right) - \frac{BP^2}{A^2 + P^2}, \quad P(0) = P_0. \quad (1.57)$$

We give a step by step approach to nondimensionalize this initial value problem.

**Step 1.** List all of the variables, parameters, and their dimensions. For the dimensions we use  $\tau$  for time, and  $\rho$  for population in number of worms.

Variable	Dimension	Parameter	Dimension
$t$	$\tau$	$k$	$1/\tau$
$P$	$\rho$	$N$	$\rho$
		$A$	$\rho$
		$B$	$\rho/\tau$
		$P_0$	$\rho$

**Step 2.** Take each variable and create a new variable by dividing by the combination of parameters that has the same dimension in order to create a dimensionless variable. Note that there is not always a unique way to do that, so some experimentation may be necessary. Here we create

$$u = \frac{P}{A}, \quad s = \frac{Bt}{A}.$$

We can use our table of dimensions above to check that these new variables are now dimensionless.

**Step 3.** Now use the chain rule to derive a new differential equation.

$$\frac{dP}{dt} = \frac{dP}{du} \cdot \frac{du}{ds} \cdot \frac{ds}{dt} = A \frac{du}{ds} \cdot \frac{B}{A} = B \frac{du}{ds}$$

The term  $kP \left(1 - \frac{P}{N}\right)$  becomes  $kAu \left(1 - \frac{Au}{N}\right)$  and the term  $\frac{BP^2}{A^2 + P^2}$  simplifies to  $\frac{Bu^2}{1 + u^2}$ . Thus the equation simplifies to

$$B \frac{du}{ds} = kAu \left(1 - \frac{Au}{N}\right) - \frac{Bu^2}{1 + u^2}$$

Dividing by  $B$  gives

$$\frac{du}{ds} = \frac{kA}{B} u \left(1 - \frac{u}{N/A}\right) - \frac{u^2}{1 + u^2}$$

Noting that the combinations of the parameters that occur above leads us to introduce two new dimensionless parameters

$$\alpha = \frac{kA}{B}, \quad \beta = \frac{N}{A}$$

The equation then becomes

$$\frac{du}{ds} = \alpha u \left(1 - \frac{u}{\beta}\right) - \frac{u^2}{1 + u^2}$$

At the meantime, the initial condition  $P(0) = P_0$  becomes  $u(0) = P_0/A$  through the change of variable  $u = P/A$ . Thus if we introduce another new parameter  $\gamma = P_0/A$ , then the initial condition becomes

$$u(0) = \gamma$$

Note that the equation has two dimensionless variables  $s, u$  and three dimensionless parameters  $\alpha, \beta, \gamma$  which are combinations of the original parameters. This simplified form of the equation has reduced the number of parameters from 5 to 3, which makes the analysis of the equation simpler.

Next we consider a reaction-diffusion equation with logistic growth:

$$\begin{cases} u_t = Du_{xx} + au \left(1 - \frac{u}{N}\right), & t > 0, \quad x \in (0, L), \\ u(t, 0) = u(t, L) = 0, \\ u(0, x) = f(x), & x \in (0, L). \end{cases} \quad (1.58)$$

We list the dimension of all variables and parameters

Variables	Dimension	Parameters	Dimension
$t$	$\tau$	$D$	$\tau^{-1}\theta^2$
$x$	$\theta$	$a$	$\tau^{-1}$
$u$	$\mu$	$N$	$\mu$
		$L$	$\theta$

To reduce the number of parameters, we introduce dimensionless variables:

$$s = \frac{Dt}{L^2}, \quad y = \frac{x}{L}, \quad v = \frac{u}{N}. \quad (1.59)$$

Then from the chain rule, we have

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial v} \cdot \frac{\partial v}{\partial s} \cdot \frac{\partial s}{\partial t} = \frac{DN}{L^2} \frac{\partial v}{\partial s}, \quad \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial v} \cdot \frac{\partial^2 v}{\partial y^2} \cdot \left(\frac{\partial y}{\partial x}\right)^2 = \frac{N}{L^2} \frac{\partial^2 v}{\partial y^2},$$

and the equation becomes

$$\begin{cases} \frac{\partial v}{\partial s} = \frac{\partial^2 v}{\partial y^2} + \lambda v(1 - v), & s > 0, \quad y \in (0, 1), \\ v(t, 0) = v(t, 1) = 0, \\ v(0, y) = f_1(y), \end{cases} \quad (1.60)$$

where

$$\lambda = \frac{aL^2}{D}, \quad f_1(y) = \frac{f(Ly)}{N}. \quad (1.61)$$

In the following sections, we will use (1.60) in the analysis, but since we normally use variables  $(t, x, u)$  instead of  $(s, y, v)$ . Thus we rewrite (1.60) in the old variables:

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \lambda u(1 - u), & t > 0, x \in (0, 1), \\ u(t, 0) = u(t, 1) = 0, \\ u(0, x) = f(x), x \in (0, 1). \end{cases} \quad (1.62)$$

The way of reducing parameters is not unique. The new equation (1.62) is sometimes called a *nonlinear eigenvalue problem* with  $\lambda$  as a bifurcation parameter. Another nondimensionalization will result in an equation with the length of interval as the parameter (see the exercises.)

## Chapter 1 Exercises

- Let (a)  $f(x, y) = \sin x \cos y$ , and (b)  $f(x, y) = 3x^2 + 5y^2$ .
  - Calculate  $\nabla f$ ;
  - Calculate  $\Delta f$ ;
  - Use `Maple` to draw the graphs of  $f(x, y)$ , and the level curves of  $f(x, y)$  (contour graphs.)
- Let  $f(x, y, z) = \cos(xy)e^{2z}$ .
  - Calculate  $\nabla f$ ;
  - Calculate  $\Delta f$ ;
  - Show that  $\Delta(f^2) = 2\nabla f \cdot \nabla f + 2f\Delta f$ , and use that to calculate  $\Delta(f^2)$ .
- From satellite pictures, the forest service find that a new species of wild grass is spreading fast. A data matching turns out that the density function  $P(t, x, y)$  is approximately

$$P(t, x, y) = \frac{1}{4\pi t} e^{2t} e^{-\frac{x^2 + y^2}{4t}}. \quad (1.63)$$

- Verify that  $P(t, x, y)$  satisfies a reaction-diffusion equation:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + 2P. \quad (1.64)$$

- Use the simulation function in `Maple` to simulate the spread of the this wild grass.

4. The two-dimensional diffusion equation is

$$\frac{\partial P}{\partial t} = D \left( \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} \right) \quad (1.65)$$

where  $D > 0$ . Show that via a change of variables:

$$x = r \cos \theta, \quad y = r \sin \theta, \quad (1.66)$$

(1.65) becomes

$$\frac{\partial P}{\partial t} = D \left( \frac{\partial^2 P}{\partial r^2} + \frac{1}{r} \frac{\partial P}{\partial r} + \frac{1}{r^2} \frac{\partial^2 P}{\partial \theta^2} \right). \quad (1.67)$$

5. Let  $P(t, x)$  be the population density of species  $A$  at the location  $x$  and time  $t$ . We assume that species  $A$  lives on a line, and the movement of the individuals follows a random walk. Suppose that in the random walk, there is a bias to the right, that is the probability of moving right is  $a > 0.5$ , and the probability of moving left is  $b < 0.5$ , but  $a - b$  is a small number. Show that  $P(t, x)$  satisfies a diffusion equation (here we assume that there is no reaction) with a convection term:

$$\frac{\partial P}{\partial t} + V \frac{\partial P}{\partial x} = D \frac{\partial^2 P}{\partial x^2} \quad (1.68)$$

where  $V$  and  $D$  are constants which you should define.

6. (a) Let  $P(t, x, y)$  be the population density of species  $A$  at the location  $(x, y)$  and time  $t$ . We assume that species  $A$  lives on a two-dimensional space, and the movement of the individuals follows a random walk. Suppose that in the random walk, there is no bias to any direction. Set up a rectangular grid on  $\mathbf{R}^2$  to model the random walk, and show that  $P(t, x, y)$  satisfies a diffusion equation

$$\frac{\partial P}{\partial t} = D \left( \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} \right) \quad (1.69)$$

where  $D$  is a constant which you should define.

(b) Suppose that  $(X, Y)$  is another coordinate system in  $R^2$  which is a rotation of  $(x, y)$ :  $X = ax + by$ ,  $Y = -bx + ay$ , where  $a^2 + b^2 = 1$ . Show that  $\Delta_{XY} u = \Delta_{xy} u$ . (This shows that the derivation of (1.69) is independent of the choice of the the coordinate system.)

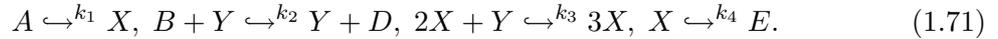
(c) A more general diffusion equation is the **anisotropic diffusion equation**:

$$\frac{\partial P}{\partial t} = D_1 \frac{\partial^2 P}{\partial x^2} + D_2 \frac{\partial^2 P}{\partial y^2}. \quad (1.70)$$

How do you change the assumptions in (a) to derive (1.70)? (Note that (1.69) is called isotropic diffusion equation in comparison with (1.70).)

7. Use the approach in Section 1.1 to derive the (1.24).

8. The first chemical “respectable” model is proposed by Prigogine and Lefever in 1968, which is later called Brusselator since Prigogine’s lab was located in Brussels at that time. The reactions are:



Suppose that  $A$  and  $B$  are feeded so that they keep constant concentrations in the reactions. Write a system of reaction-diffusion equations for  $X$  and  $Y$ .

9. A tube with length  $L$  connects two reservoirs which contain salt waters. The cross-section ( $yz$ -direction) of the tube is so small so we can assume that the concentration of the salt water is same for any point on a cross-section. Let the concentration of the salt water in the tube be  $c(t, x)$ ,  $0 < x < L$ . We assume that the diffusion of the salt is one-dimensional in the tube:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}. \quad (1.72)$$

Determine the boundary and initial conditions according to the following setups:

- (a) Initially the tube contains pure water, the concentration of the salt water in the reservoir at  $x = 0$  is kept at constant  $C_1$ , and the concentration of the salt water in the reservoir at  $x = L$  is kept at constant  $C_2$ ;
- (b) Initially the concentration of the salt water in the tube is a linear function which decreases from  $C_3$  at  $x = 0$  to 0 at  $x = L$ , the tube is sealed at  $x = 0$ , and the concentration of the salt water in the reservoir at  $x = L$  is kept at constant 0.
10. Consider the equation:

$$\frac{dP}{dt} = kP \left( 1 - \frac{P}{N} \right) - \frac{BP^2}{A^2 + P^2}.$$

Use the following change of variables:

$$(a) Q = \frac{P}{N}, s = kt, \quad (b) Q = \frac{kP}{B}, s = kt,$$

to get nondimensionalized equations.

11. Consider a population model:

$$\frac{dx}{dt} = kx \left( 1 - \frac{x}{N} \right) - M, \quad x(0) = x_0,$$

where  $k, M, N, x_0$  are positive parameters.

- (a) In the following table, fill in the dimensions of all parameters in terms of the dimensions of variables.

Variable	Dimension	Parameter	Dimension
$t$	$\tau$	$k$	
$x$	$\lambda$	$M$	
		$N$	
		$x_0$	

(b) Use the change of variable:

$$y = \frac{x}{N}, \quad s = kt.$$

Derive the new equation (including the initial condition) in the new variables  $y$  and  $s$ .

12. Consider a population model:

$$\frac{dx}{dt} = kx \left(1 - \frac{x}{N}\right) - \frac{\beta x^2}{m+x}, \quad (1.73)$$

where  $k, N, \beta, m > 0$  are parameters. Use the change of variable:

$$y = \frac{x}{m}, \quad s = \beta t.$$

Derive the equation in the new variables.

13. Use the substitution

$$s = at, \quad y = \sqrt{\frac{a}{D}}x, \quad v = \frac{u}{N} \quad (1.74)$$

to deduce a new equation from

$$\begin{cases} u_t = Du_{xx} + au \left(1 - \frac{u}{N}\right), & t > 0, \quad x \in (0, L), \\ u(t, 0) = u(t, L) = 0, \\ u(0, x) = f(x), & x \in (0, L). \end{cases} \quad (1.75)$$

Express the new parameters and initial values in terms of old ones.

14. Find a substitution different from (1.59) and (1.74) to deduce a nondimensionalized equation from (1.75).

15. Consider diffusive population model with Allee effect

$$\begin{cases} u_t = Du_{xx} + au \left(1 - \frac{u}{N}\right) \left(\frac{u}{M} - 1\right), & t > 0, \quad x \in (0, L), \\ u(t, 0) = u(t, L) = 0, \\ u(0, x) = f(x), & x \in (0, L). \end{cases} \quad (1.76)$$

Use a table to list the dimensions of all quantities and parameters, and convert the equation to a dimensionless equation.

16. Consider the diffusive predator-prey model

$$\begin{cases} \frac{\partial U}{\partial t} = D_U \frac{\partial^2 U}{\partial y^2} + AU - BUV, & s > 0, \quad y \in (0, L), \\ \frac{\partial V}{\partial t} = D_V \frac{\partial^2 V}{\partial y^2} - CV + DUV, & s > 0, \quad y \in (0, L), \\ \frac{\partial U}{\partial y}(t, 0) = \frac{\partial U}{\partial y}(t, L) = \frac{\partial V}{\partial y}(t, 0) = \frac{\partial V}{\partial y}(t, L) = 0, \\ U(0, y) = U_0(y), \quad V(0, y) = V_0(y). \end{cases} \quad (1.77)$$

Use the substitution

$$t = \frac{D_U}{L^2}s, \quad x = \frac{y}{L}, \quad u = \frac{B}{A}U, \quad v = \frac{D}{C}V,$$

to show the nondimensionalized equation has the form

$$\begin{cases} u_t = u_{xx} + \lambda[Au - (C/D)uv], & t > 0, \quad x \in (0, 1), \\ v_t = dv_{xx} + \lambda[-Cv + (A/B)uv], & t > 0, \quad x \in (0, 1), \\ u_x(t, 0) = u_x(t, 1) = v_x(t, 0) = v_x(t, 1) = 0, \\ u(0, x) = u_0(x), \quad v(0, x) = v_0(x). \end{cases} \quad (1.78)$$

Express the new parameters  $d$  and  $\lambda$  in terms of old parameters.