

# UTILIZATION OF TOTAL MASS AS A CONTROL IN DIFFUSION PROCESSES

MOHAMED SALMAN  
B.S. Suez Canal University, 1990  
M.S. Kuwait University, 1997  
M.S. University of Central Florida, 2002

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Major Professor:  
John R. Cannon

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## ABSTRACT

As motivation for the mathematical problems considered in this work, consider a chamber in the form of a long linear transparent tube. We allow for the introduction or removal of material in a gaseous state at the ends of the tube. The material diffuses throughout the tube with or without reaction with other materials. By illuminating the tube on one side with a light source with a frequency range spanning the absorption range for the material and collecting the residual light that passes through the tube with photo-reception equipment, we can obtain a measurement of the total mass of material contained in the tube as a function of time. Using the total mass as switch points for changing the boundary conditions for introduction or removal of material. The objective is to keep the total mass of material in the tube oscillating between two set values such as  $m < M$ . The physical application for such a system is the control of reaction diffusion systems such as production of a chemical material in a reaction chamber via the introduction of reactants at the boundary of chamber.

In Chapter 1, we study the diffusion problem  $u_t = u_{xx}$ ,  $0 < x < 1$ ,  $t > 0$ ;  $u(x, 0) = 0$ , and  $u(0, t) = u(1, t) = \psi(t)$ , where  $\psi(t) = u_0$  for  $t_{2k} < t < t_{2k+1}$  and  $\psi(t) = 0$  for  $t_{2k+1} < t < t_{2k+2}$ ,  $k = 0, 1, 2, \dots$  with  $t_0 = 0$  and the sequence  $t_k$  is determined by the equations  $\int_0^1 u(x, t_k) dx = M$ , for  $k = 1, 3, 5, \dots$ , and  $\int_0^1 u(x, t_k) dx = m$ , for  $k = 2, 4, 6, \dots$  and where  $0 < m < M < u_0$ . Note that the switching points  $t_k$ ,  $k = 1, 2, 3, \dots$  are unknown.

Existence and uniqueness are demonstrated. Theoretical estimates of the  $t_k$  and  $t_{k+1} - t_k$  are obtained and numerical verifications of the estimates are presented.

In Chapter 2, we consider the problem  $u_t = u_{xx} - u$ ,  $0 < x < 1$ ,  $t > 0$ ;  $u(x, 0) = 0$ , and  $u(0, t) = u(1, t) = \psi(t)$ , where  $\psi(t) = u_0$  for  $t_{2k} < t < t_{2k+1}$  and  $\psi(t) = 0$  for  $t_{2k+1} < t < t_{2k+2}$ ,  $k = 0, 1, 2, \dots$  with  $t_0 = 0$  and the sequence  $t_k$  is determined by the equations  $\int_0^1 u(x, t_k) dx = M$ , for  $k = 1, 3, 5, \dots$ , and  $\int_0^1 u(x, t_k) dx = m$ , for  $k = 2, 4, 6, \dots$  and where  $0 < m < M$ . Note that the switching points  $t_k$ ,  $k = 1, 2, 3, \dots$  are unknown. Existence and uniqueness are demonstrated. Theoretical estimates of the  $t_k$  and  $t_{k+1} - t_k$  are obtained and numerical verifications of the estimates are presented. The case of  $u_x(0, t) = u_x(1, t) = \psi(t)$  is also considered and analyzed.

In Chapter 3, study the problem  $u_t = u_{xx}$ ,  $0 < x < 1$ ,  $t > 0$ ;  $u(x, 0) = 0$ , and  $-u_x(0, t) = u_x(1, t) = \psi(t)$ , where  $\psi(t) = 1$  for  $t_{2k} < t < t_{2k+1}$  and  $\psi(t) = -1$  for  $t_{2k+1} < t < t_{2k+2}$ ,  $k = 0, 1, 2, \dots$  with  $t_0 = 0$  and the sequence  $t_k$  is determined by the equations  $\int_0^1 u(x, t_k) dx = M$ , for  $k = 1, 3, 5, \dots$ , and  $\int_0^1 u(x, t_k) dx = m$ , for  $k = 2, 4, 6, \dots$  and where  $0 < m < M$ . The sequence  $t_k$  is analytically determined. A finite difference method is used to compute this sequence. Under certain restrictions on the mesh size, the answer coincides with the one found analytically. Numerical estimates are presented.

In Chapter 4, we study the problem  $u_t = u_{xx} - au$ ,  $0 < x < 1$ ,  $t > 0$ ;  $u(x, 0) = 0$ , and  $-u_x(0, t) = u_x(1, t) = \phi(t)$ , where  $a = a(x, t, u)$ , and  $\phi(t) = 1$  for  $t_{2k} < t < t_{2k+1}$  and  $\phi(t) = 0$  for  $t_{2k+1} < t < t_{2k+2}$ ,  $k = 0, 1, 2, \dots$  with  $t_0 = 0$  and the sequence  $t_k$  is determined by the equations  $\int_0^1 u(x, t_k) dx = M$ , for  $k = 1, 3, 5, \dots$ , and  $\int_0^1 u(x, t_k) dx = m$ , for  $k = 2, 4, 6, \dots$

and where  $0 < m < M$ . Note that the switching points  $t_k$ ,  $k = 1, 2, 3, \dots$  are unknown. A maximum principal argument has been used to prove that the solution is positive under certain conditions. Existence and uniqueness are demonstrated. Theoretical estimates of the  $t_k$  and  $t_{k+1} - t_k$  are obtained and numerical verifications of the estimates are presented.

In conclusion, the analytical and computational results of chapters 1 through 4 show that such control mechanisms are feasible.

*This Work is Dedicated to my Parents and my Professors.*

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# CHAPTER 1

## DIFFUSION PROBLEM WITH DIRICHLET BOUNDARY CONTROL

### 1.1 Introduction

In this chapter we study the diffusion equation

$$u_t = u_{xx}, \quad 0 < x < 1, \quad t > 0, \quad (1.1.1)$$

subject to the initial concentration

$$u(x, 0) = 0, \quad 0 < x < 1,$$

and boundary conditions controlled by the total mass  $\mu(t) = \int_0^1 u(x, t) dx$ . We are going to begin by setting the concentration to be  $u = u_0$  at both boundary points  $x = 0$  and  $x = 1$ , where  $u_0$  is a positive constant. We shall watch the total mass  $\int_0^1 u(x, t) dx$  until it reaches a certain specified level  $M$  at time  $t = t_1$ , where  $0 < M < u_0$ . At this moment,  $t = t_1$  we switch the concentration to

$$u(0, t) = u(1, t) = 0 \quad t_1 < t.$$

We keep watching the total mass until it drops down to a prespecified level  $m$  at time  $t = t_2$ , where  $0 < m < M < u_0$ . We keep switching the concentration according to the level of the total mass so that we always have

$$m \leq \int_0^1 u(x, t) dx \leq M.$$

In other words, the boundary conditions will be

$$u(0, t) = u(1, t) =: \phi(t) = \begin{cases} u_0, & t_{2n} \leq t \leq t_{2n+1}, \\ 0, & t_{2n+1} \leq t \leq t_{2n+2} \end{cases} \quad (1.1.2)$$

where  $n = 0, 1, 2, \dots$ ; and the sequence  $\{t_n\}$  will be strictly increasing, i.e.

$$0 = t_0 < t_1 < t_2 < \dots$$

and its terms are defined by the equations

$$\begin{aligned} \int_0^1 u(x, t_n) dx &= M, & n = 1, 3, 5, \dots, \\ \int_0^1 u(x, t_n) dx &= m, & n = 2, 4, 6, \dots \end{aligned}$$

## 1.2 Existence of the Time Switching Points

For the sake of simplicity, we will take  $u_0 = 1$ . Consider the problem

$$\begin{aligned} u_t &= u_{xx}, & 0 < x < 1, & \quad t > 0, \\ u(0, t) &= u(1, t) = \phi(t), & t > 0, \\ u(x, 0) &= 0. \end{aligned} \quad (1.2.1)$$



Then the solution will be (see [16])

$$u(x, t) = \int_0^t \left[ \frac{\partial \theta}{\partial x}(x-1, t-\tau) - \frac{\partial \theta}{\partial x}(x, t-\tau) \right] \phi(\tau) d\tau, \quad (1.2.2)$$

where [46]

$$\theta(x, t) = \frac{1}{2} + \sum_{n=1}^{\infty} e^{-n^2 \pi^2 t} \cos n\pi x. \quad (1.2.3)$$

Upon integrating (1.2.2) with respect to  $x$  from 0 to 1 we get

$$\mu(t) := \int_0^1 u(x, t) dx = 4 \int_0^t [\theta(0, t-\tau) - \theta(1, t-\tau)] \phi(\tau) d\tau. \quad (1.2.4)$$

Substituting (1.2.3) in (1.2.4), we obtain

$$\mu(t) = 8 \int_0^t \phi(\tau) \left( \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2 (t-\tau)} \right) d\tau, \quad (1.2.5)$$

where  $\lambda_k = k\pi$ .

The first stage we set  $\phi(t) = 1$ . This will give

$$\mu(t) = 8 \sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2} \left[ 1 - e^{-\lambda_{2k+1}^2 t} \right]$$

which is a strictly increasing function of  $t$ , and it ranges between 0 and 1 as  $t$  ranges from 0 to  $\infty$ . Therefore, there exists a positive  $t_1$  such that

$$\mu(t_1) = M, \quad 0 < M < 1.$$

For  $t > t_1$ , we set  $\phi(t) = 0$ . Then equation (1.2.5) implies

$$\begin{aligned} \mu(t) &= 8 \int_0^{t_1} \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2 (t-\tau)} d\tau, \quad t > t_1 \\ &= 8 \sum_{k=0}^{\infty} \frac{e^{-\lambda_{2k+1}^2 t}}{\lambda_{2k+1}^2} \left[ e^{\lambda_{2k+1}^2 t_1} - 1 \right], \end{aligned}$$

which is a strictly decreasing function that falls from  $M$  to 0 as  $t$  goes from  $t_1$  to  $\infty$ . Hence, there exists a  $t_2$  such that

$$\mu(t_2) = m, \quad 0 < m < M < 1.$$

In an inductive fashion, we obtain as  $t > t_{2n}$  and  $\phi(t) = 1$ ,

$$\begin{aligned} \mu(t) &= 8 \sum_{j=0}^{n-1} \int_{t_{2j}}^{t_{2j+1}} \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2(t-\tau)} d\tau \\ &\quad + 8 \int_{t_{2n}}^t \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2(t-\tau)} d\tau \\ &= 8 \sum_{k=0}^{\infty} \frac{e^{-\lambda_{2k+1}^2 t}}{\lambda_{2k+1}^2} \sum_{j=0}^{n-1} \left[ e^{\lambda_{2k+1}^2 t_{2j+1}} - e^{\lambda_{2k+1}^2 t_{2j}} \right] \\ &\quad + 8 \sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2} \left[ 1 - e^{-\lambda_{2k+1}^2(t-t_{2n})} \right] \\ &= 8 \sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2} \left\{ 1 - e^{-\lambda_{2k+1}^2 t} \left[ \sum_{j=0}^{2n} (-1)^j e^{\lambda_{2k+1}^2 t_j} \right] \right\}, \quad t > t_{2n}, \end{aligned}$$

which increases from  $m$  to 1 as  $t$  goes from  $t_{2n}$  to infinity. Thus, there exists a  $t_{2n+1}$  such that

$$\mu(t_{2n+1}) = M.$$

When  $t > t_{2n+1}$ ,  $\phi(t) = 0$ , we have

$$\begin{aligned} \mu(t) &= 8 \int_0^{t_{2n+1}} \phi(\tau) \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2(t-\tau)} d\tau \\ &= 8 \sum_{j=0}^n \int_{t_{2j}}^{t_{2j+1}} \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2(t-\tau)} d\tau \\ &= 8 \sum_{k=0}^{\infty} \frac{e^{-\lambda_{2k+1}^2 t}}{\lambda_{2k+1}^2} \left\{ \sum_{j=0}^{2n+1} (-1)^{j+1} e^{\lambda_{2k+1}^2 t_j} \right\}, \quad t > t_{2n+1}. \end{aligned}$$

Hence,  $\mu(t)$  will continuously decrease down from  $M$  to 0 as  $t$  goes from  $t_{2n+1}$  to infinity.

This ensures the existence of  $t_{2n+2}$  such that

$$\mu(t_{2n+2}) = m.$$

From the argument above, we have constructed the sequence  $\{t_n\}$ , where

$$0 = t_0 < t_1 < t_2 < \dots .$$

Given the switching sequence  $\{t_n\}$ , the existence and uniqueness of the solution follows immediately.

### 1.3 A First Term Approximation

In this section we study equation (1.2.5) by using the first term of the infinite series, that is

$$\tilde{\mu}(t) := 8 \int_0^t \phi(\tau) e^{-\lambda_1^2(t-\tau)} d\tau \simeq \mu(t) \tag{1.3.1}$$

where  $\lambda_1 = \pi$ .

We will find an approximation to the sequence  $\{t_n\}$  in an explicit form. For the sake of simplicity, the upper and lower bound on total mass are taken to be

$$M = \frac{8}{\pi^2}(1 - \alpha) \tag{1.3.2}$$

$$m = \frac{8}{\pi^2}\alpha \tag{1.3.3}$$

where the restriction  $0 < \alpha < \frac{1}{2}$  has been set in order to  $0 < m < M$ . The first time step  $t_1$  can be calculated through the equation

$$\tilde{\mu}(t_1) = M,$$

which gives,

$$\frac{8}{\lambda_1^2} \left[ 1 - e^{-\lambda_1^2 t_1} \right] = \frac{8}{\lambda_1^2} (1 - \alpha),$$

i.e.

$$e^{-\lambda_1^2 t_1} = \alpha. \tag{1.3.4}$$

The second time step can be found by

$$\tilde{\mu}(t_2) = m.$$

This gives

$$\frac{8e^{-\lambda_1^2 t_2}}{\lambda_1^2} \left[ e^{\lambda_1^2 t_1} - 1 \right] = \frac{8}{\pi^2} \alpha. \tag{1.3.5}$$

By using (1.3.4), the above equation implies

$$e^{-\lambda_1^2 t_2} = \frac{\alpha^2}{1 - \alpha}. \tag{1.3.6}$$

Using a similar argument, we can inductively obtain

$$e^{-\lambda_1^2 t_3} = \frac{\alpha^3}{(1 - \alpha)^2},$$

$$e^{-\lambda_1^2 t_4} = \frac{\alpha^4}{(1 - \alpha)^3},$$

⋮

$$e^{-\lambda_1^2 t_n} = \frac{\alpha^n}{(1-\alpha)^{n-1}}, \quad n \geq 1. \quad (1.3.7)$$

Next we use mathematical induction to prove (1.3.7). The point  $t_{2n}$  can be obtained by

$$\begin{aligned} \tilde{\mu}(t_{2n}) &= 8 \int_0^{t_{2n-1}} \phi(\tau) e^{-\lambda_1^2(t_{2n}-\tau)} d\tau \\ &= \left[ \int_0^{t_1} e^{-\lambda_1^2(t_{2n}-\tau)} d\tau + \dots + \int_{t_{2n-2}}^{t_{2n-1}} e^{-\lambda_1^2(t_{2n}-\tau)} d\tau \right] \\ &= \frac{8e^{-\lambda_1^2 t_{2n}}}{\lambda_1^2} [e^{\lambda_1 t_{2n-1}} - e^{\lambda_1 t_{2n-2}} + \dots + e^{\lambda_1 t_1} - 1] = m. \end{aligned}$$

Assuming formula (1.3.7) is valid for all  $k < 2n$ , then the last equation is equivalent to

$$e^{-\lambda_1^2 t_{2n}} \left[ \frac{(1-\alpha)^{2n-2}}{\alpha^{2n-1}} - \frac{(1-\alpha)^{2n-3}}{\alpha^{2n-2}} + \dots + \frac{1}{\alpha} - 1 \right] = \alpha.$$

Upon adding all the terms inside the brackets as a finite geometric sum, we will obtain

$$e^{-\lambda_1^2 t_{2n}} = \frac{\alpha^{2n}}{(1-\alpha)^{2n-1}}. \quad (1.3.8)$$

The time step  $t_{2n+1}$  can be found as a solution of

$$\begin{aligned} \tilde{\mu}(t_{2n+1}) &= 8 \int_0^{t_{2n+1}} \phi(\tau) e^{-\lambda_1^2(t_{2n+1}-\tau)} d\tau \\ &= 8 \left[ \int_0^{t_1} + \int_{t_2}^{t_3} + \dots + \int_{t_{2n}}^{t_{2n+1}} e^{-\lambda_1^2(t_{2n+1}-\tau)} d\tau \right] \\ &= \frac{8e^{-\lambda_1^2 t_{2n+1}}}{\lambda_1^2} [e^{\lambda_1^2 t_{2n+1}} - e^{\lambda_1^2 t_{2n}} + e^{\lambda_1^2 t_{2n-1}} - e^{-\lambda_1 t_{2n-2}} + \dots + e^{\lambda_1^2 t_1} - 1] \\ &= M. \end{aligned}$$

Assuming the validity of (1.3.7) for all  $k \leq 2n$ , and using (1.3.8), the above equation implies

$$e^{-\lambda_1^2 t_{2n+1}} \left[ \frac{(1-\alpha)^{2n-1}}{\alpha^{2n}} - \frac{(1-\alpha)^{2n-2}}{\alpha^{2n-1}} + \dots - \frac{1}{\alpha} + 1 \right] = \alpha.$$

If we add these terms which constitute finite geometric series, we can obtain

$$e^{-\lambda_1^2 t_{2n+1}} = \frac{\alpha^{2n+1}}{(\alpha-1)^{2n}}. \quad (1.3.9)$$

Hence, formula (1.3.7) is valid.

Formula (1.3.7) implies that

$$t_n = \frac{1}{\pi^2} \ln \frac{(1-\alpha)^{n-1}}{\alpha^n}, \quad n \geq 1.$$

Therefore,

$$t_{n+1} - t_n = \frac{1}{\pi^2} \ln \frac{1-\alpha}{\alpha}, \quad n \geq 1,$$

which is obviously independent of  $n$ .

## 1.4 A Higher Order Approximation

In this section we will study a higher order approximation of the sequence  $\{t_n\}$ . This approximation is based on dropping all the terms that have  $e^{-\lambda_{2k+1}^2 t_n}$  from the expression of the mass, except for a few dominating terms. The upper and lower bounds on the mass are not necessarily symmetric. For simplicity of computation, the bounds are chosen to be

$$M = 8 \left[ \sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2} - \frac{\alpha}{\lambda_1^2} \right],$$

and

$$m = \frac{8}{\lambda_1^2} \beta,$$

where  $\lambda_{2k+1}^2 = (2k+1)^2 \pi^2, k = 0, 1, \dots$ ;  $\alpha$  and  $\beta$  are positive numbers that are chosen so that the inequality  $0 < m < M$  holds. Since  $\sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2} = \frac{1}{\pi^2} \sum_{k=0}^{\infty} \frac{1}{(2k+1)^2} = \frac{1}{8}$ , then we have  $M = 1 - \frac{8}{\pi^2} \alpha$ .

To find  $t_1$ , we need to solve the equation

$$\mu(t_1) = M,$$

which is

$$8 \left[ \frac{1 - e^{-\lambda_1^2 t_1}}{\lambda_1^2} + \sum_{k=1}^{\infty} \frac{1 - e^{-\lambda_{2k+1}^2 t_1}}{\lambda_{2k+1}^2} \right] = M.$$

Upon dropping all the terms that have  $e^{-\lambda_{2k+1}^2 t_1}$  for all  $k \geq 1$ , we get

$$8 \left[ \sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2} - \frac{e^{-\lambda_1^2 t_1}}{\lambda_1^2} \right] = 1 - \frac{8}{\pi^2} \alpha,$$

which implies

$$e^{-\lambda_1^2 t_1} = \alpha. \tag{1.4.1}$$

In a similar fashion, we compute  $t_2$  by solving

$$\mu(t_2) = 8 \int_0^{t_1} \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2 (t_2 - \tau)} d\tau = m,$$

i.e.,

$$8 \sum_{k=0}^{\infty} \frac{e^{-\lambda_{2k+1}^2 t_2}}{\lambda_{2k+1}^2} \left[ e^{\lambda_{2k+1}^2 t_1} - 1 \right] = m.$$

By dropping all the terms that have  $e^{\lambda_{2k+1}^2 t_2}$  for all  $k \geq 1$ , we get

$$e^{-\lambda_1^2 t_2} \left( e^{\lambda_1^2 t_1} - 1 \right) = \beta.$$

Using (1.4.1) we obtain

$$e^{-\lambda_1^2 t_2} = \frac{\alpha\beta}{1-\alpha}. \quad (1.4.2)$$

By employing a similar method of approximations we can find  $t_3$  through the equation

$$e^{-\lambda_1^2 t_3} \left[ e^{\lambda_1^2 t_2} - e^{\lambda_1^2 t_1} + 1 \right] = \alpha,$$

which implies that

$$e^{-\lambda_1^2 t_3} = \frac{\alpha^2\beta}{(1-\alpha)(1-\beta)}. \quad (1.4.3)$$

For  $t_4$  and  $t_5$ , we obtain the explicit expressions

$$e^{-\lambda_1^2 t_4} = \frac{\alpha^2\beta^2}{(1-\alpha)^2(1-\beta)} \quad (1.4.4)$$

and

$$e^{-\lambda_1^2 t_5} = \frac{\alpha^3\beta^2}{(1-\alpha)^2(1-\beta)^2}. \quad (1.4.5)$$

Thus, we choose

$$e^{-\lambda_1^2 t_{2n}} = \frac{\alpha^n\beta^n}{(1-\alpha)^n(1-\beta)^{n-1}}, \quad n \geq 1, \quad (1.4.6)$$

and

$$e^{-\lambda_1^2 t_{2n+1}} = \frac{\alpha^{n+1}\beta^n}{(1-\alpha)^n(1-\beta)^n}, \quad n \geq 1. \quad (1.4.7)$$

By an induction argument similar to the one used in Section 3 we can show that (1.4.6) and (1.4.7) hold. Therefore, the consecutive time steps can be calculated by

$$t_{2n} - t_{2n-1} = \ln \frac{1-\alpha}{\beta} \quad (1.4.8)$$

and

$$t_{2n+1} - t_{2n} = \ln \frac{1-\beta}{\alpha} \quad (1.4.9)$$



where  $n \geq 1$ . For the special case when  $\alpha = \beta$ , the time intervals reduce that shown at the end of section 3.

## 1.5 Numerical Results

In this section, we use a finite difference technique along with the trapezoidal rule to get an approximate discrete solution  $U_j^n$  and the sequence  $\{T_m\}$  when the total mass hits one of the limits  $M$  or  $m$ .

We discretize the space and time by using

$$\text{i) } \Delta x = \frac{1}{J}, \quad X_j = j\Delta x, \quad j = 0, 1, \dots, J,$$

$$\text{ii) } \Delta t = \frac{T}{N}, \quad \tau_n = n\Delta t, \quad n = 0, \dots, N,$$

where  $J$  and  $N$  are positive integers and  $T$  is a positive real number. The integer  $N$  has to be chosen large enough so that the time step  $\Delta t$  is much smaller than the differences  $T_n - T_{n-1}$ .

We consider the backward implicit finite difference scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2}$$

as a discretized version of  $u_t = \alpha u_{xx}$ , where  $\alpha$  is a positive constant. The above scheme can be written in the form

$$-\beta U_{j-1}^{n+1} + (1 + 2\beta)U_j^{n+1} - \beta U_{j+1}^{n+1} = U_j^n \tag{1.5.1}$$

where  $j = 1, \dots, J - 1$  and  $n = 0, 1, \dots, N - 1$ . The initial data are set to be  $U_j^0 = 0$  for  $j = 1, \dots, J - 1$ , and the boundary conditions are  $U_0^n = U_J^n = \phi(\tau_n)$  for  $n = 0, 1, \dots, N$ . The function  $\phi(\tau_n)$  will be either 10 or 0 depending on the value of the mass which will be approximated by the trapezoidal rule

$$\mu_n = \frac{h}{2} \sum_{j=0}^{N-1} (U_j^{n+1} + U_{j+1}^n). \quad (1.5.2)$$

The numerical experiment is carried out in the following way. We start by setting the boundary conditions  $U_0^n = U_J^n = 10$  then we solve a tridiagonal system coming out of the difference method. We check the total mass  $\mu_n$  in (1.5.2). We keep doing that at each time step until the mass  $\mu_n$  exceeds or equals the upper limit  $M$ . Then we switch the boundary conditions to  $U_0^n = U_J^n = 0$ , and we continue the finite difference scheme for several time steps  $\Delta t$  until the total mass  $\mu_n$  decreases to  $m$ . At this moment we switch the boundary condition back to 10 and continue the process as we did before.

For the data specifications  $\Delta x = 0.02$ ,  $T = 20$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.05$ ,  $M = 7$ ,  $m = 3$ , Table (1.1) shows the times switches  $T_n$ . As we can see there, the duration of each stage turns out to be constant.

For the same set of data, figures (1.1) through (1.6) show the concentration versus the space. The figures are obtained for different stages, where at each stage the concentration is kept constant at the end points.

A profile of the concentrations at  $x = 0.5$  for various times is shown in figure (1.7) with the same specified data.

For a different set of upper and lower bounds on the mass  $M = 5$  and  $m = 2$  along with

Table 1.1: Time switches  $T_n$  corresponding to  $M = 7$ ,  $m = 3$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.05$ .

$n$	$T_n$	$T_n - T_{n-1}$	$n$	$T_n$	$T_n - T_{n-1}$
1	2.1000	2.1000	8	10.5000	1.2000
2	3.3000	1.2000	9	11.7000	1.2000
3	4.5000	1.2000	10	12.9000	1.2000
4	5.7000	1.2000	11	14.1000	1.2000
5	6.9000	1.2000	12	15.3000	1.2000
6	8.1000	1.2000	13	16.5000	1.2000
7	9.3000	1.2000	14	17.7000	1.2000

$\Delta x = 0.02$ ,  $T = 20$ ,  $\Delta t = 0.02$ ,  $\alpha = 0.05$ , Table (1.2) shows the time switches  $T_n$ . Durations of the time intervals fluctuates between 0.5, 1. Figure (1.8) is the concentration at  $x = 0.5$  for the same set of data.

CONCLUSION: From Table (1.1) and Table (1.2), we see that the theoretical estimates of  $t_{2n} - t_{2n-1}$  and  $t_{2n+1} - t_{2n}$  are exhibited in the numerical examples.

Table 1.2: Time switches  $T_n$  corresponding to  $M = 5$ ,  $m = 2$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.02$ ,  
 $\alpha = 0.05$

$n$	$T_n$	$T_n - T_{n-1}$	$n$	$T_n$	$T_n - T_{n-1}$
1	1.0000	1.0000	14	10.9400	1.0200
2	1.9400	0.9400	15	11.4200	0.4800
3	2.4200	0.4800	16	12.4400	1.0200
4	3.4400	1.0200	17	12.9200	0.4800
5	3.9200	0.4800	18	13.9400	1.0200
6	4.9400	1.0200	19	14.4200	0.4800
7	5.4200	0.4800	20	15.4400	1.0200
8	6.4400	1.0200	21	15.9200	0.4800
9	6.9200	0.4800	22	16.9400	1.0200
10	7.9400	1.0200	23	17.4200	0.4800
11	8.4200	0.4800	24	18.4400	1.0200
12	9.4400	1.0200	25	18.9200	0.4800
13	9.9200	0.4800	26	19.9400	1.0200

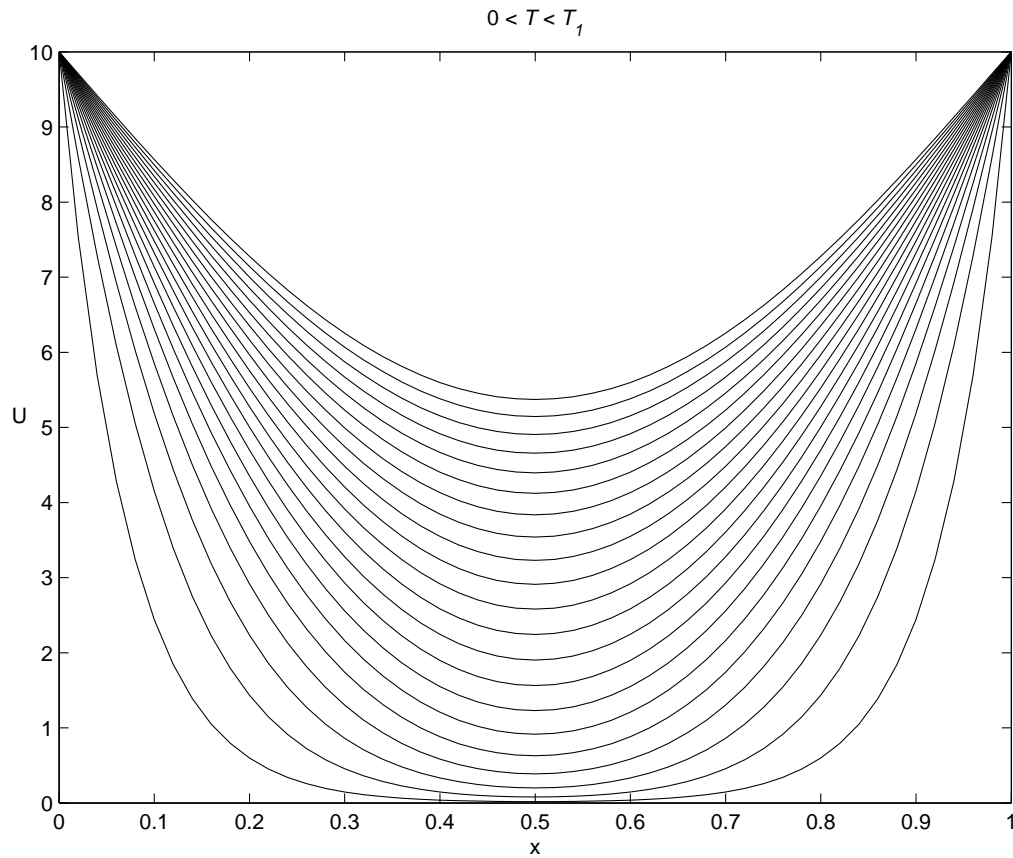


Figure 1.1: The first stage where the concentration  $U$  is held at 10 at the end points. Each curve shows the concentration profile at various discrete time steps  $t_n = n\Delta t$ . As the time goes on, the level of concentrations gets higher

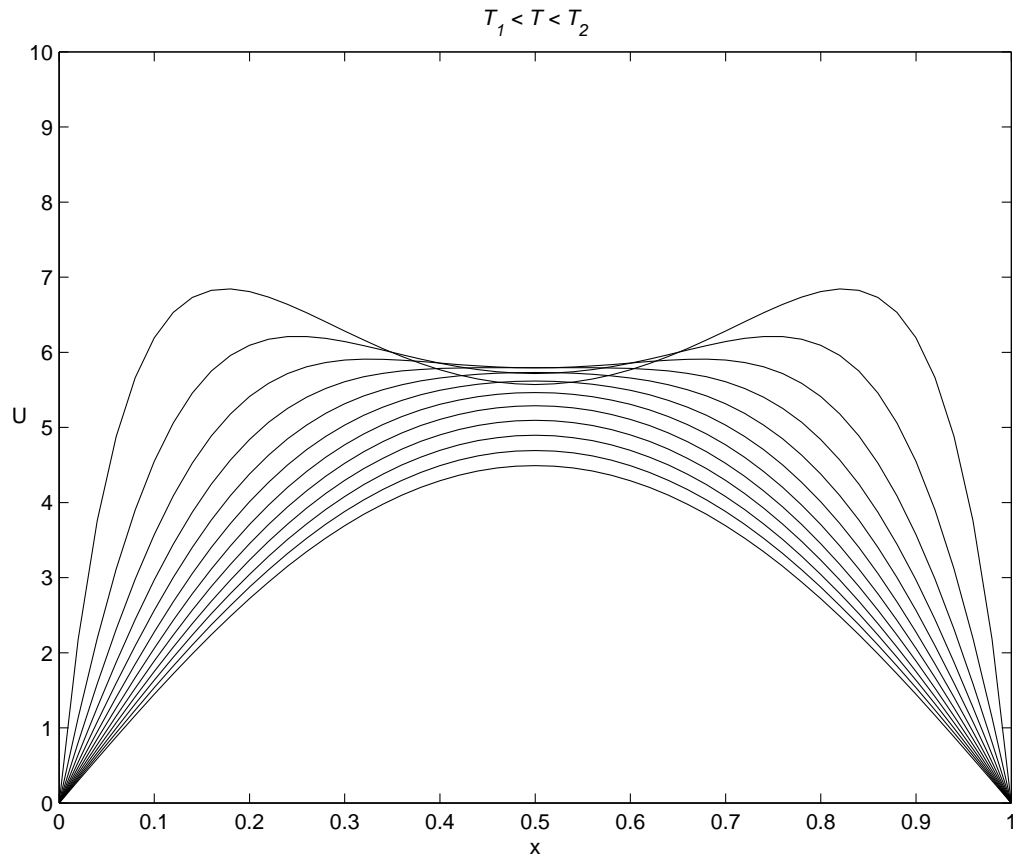


Figure 1.2: The second stage where the concentration  $U$  is held at 0 at the end points. As the time goes on, the level of concentrations decreases. Notice the fluctuations when the concentration is dropped suddenly to 0 at the beginning of the stage

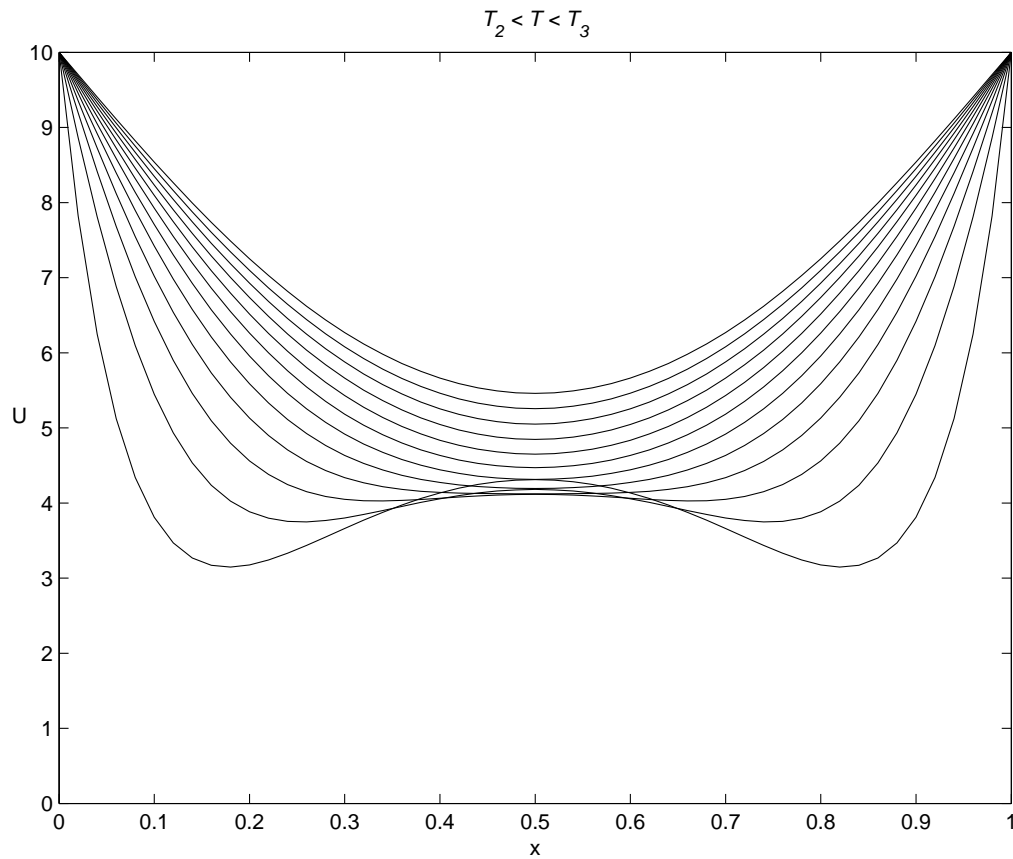


Figure 1.3: The third stage where the concentration  $U$  is switched to 10 at the end points. Each curve shows the concentration profile at various discrete time steps  $t_n = n\Delta t$ . Notice the fluctuations due to the sudden change on the concentrations. After a little while, the concentrations levels increase monotonically.

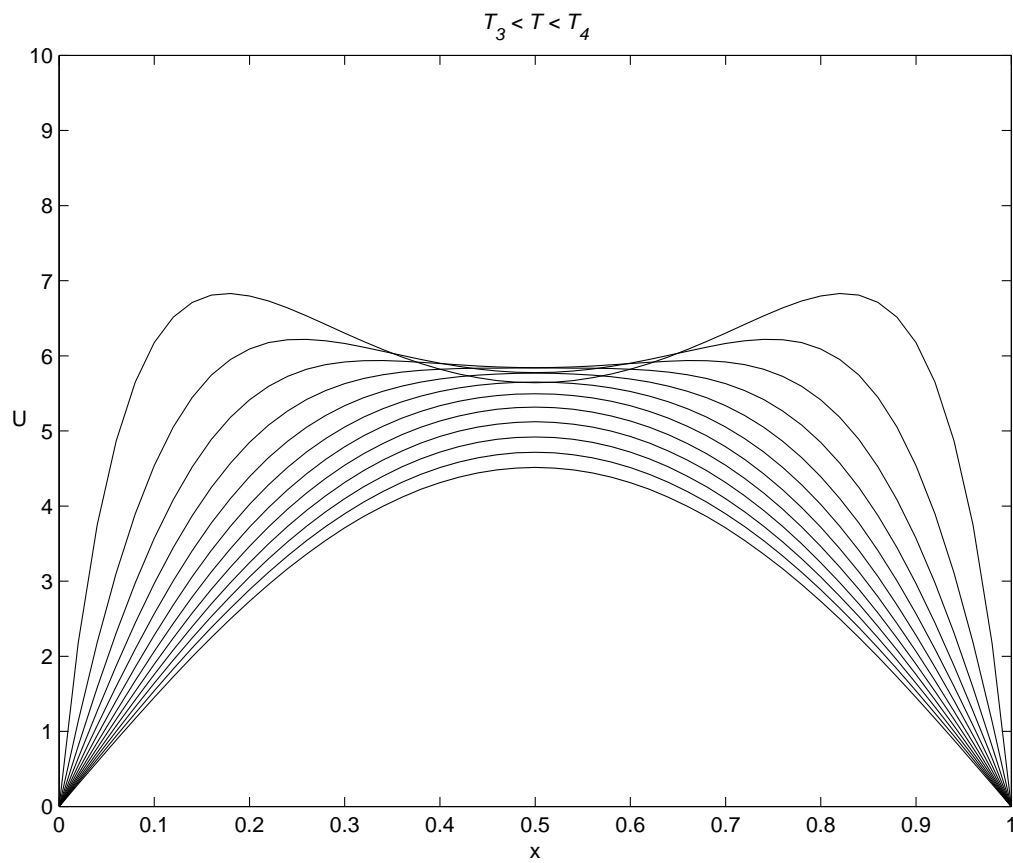


Figure 1.4: The fourth stage where the concentration  $U$  is switched to 0 at the end points.

Notice the similarity with the second stage



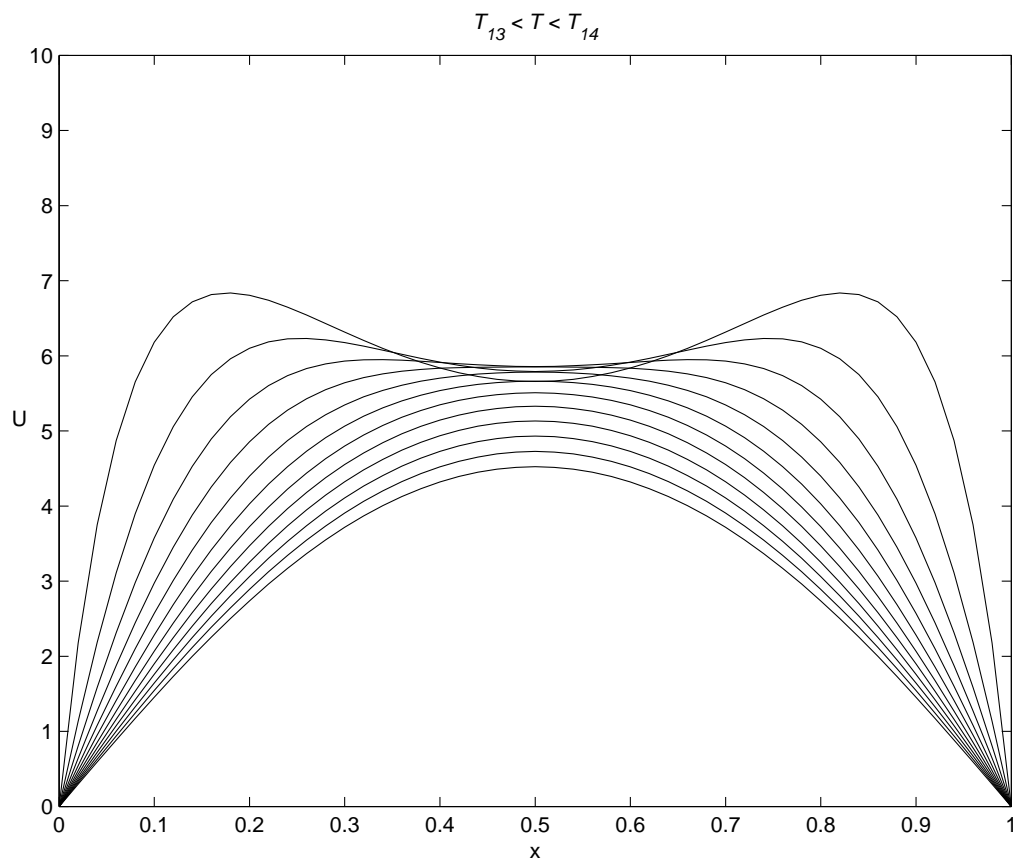


Figure 1.5: The fourteenth stage where the concentration  $U$  is held at 0 at the end points.

A similar pattern appears in all such stages.

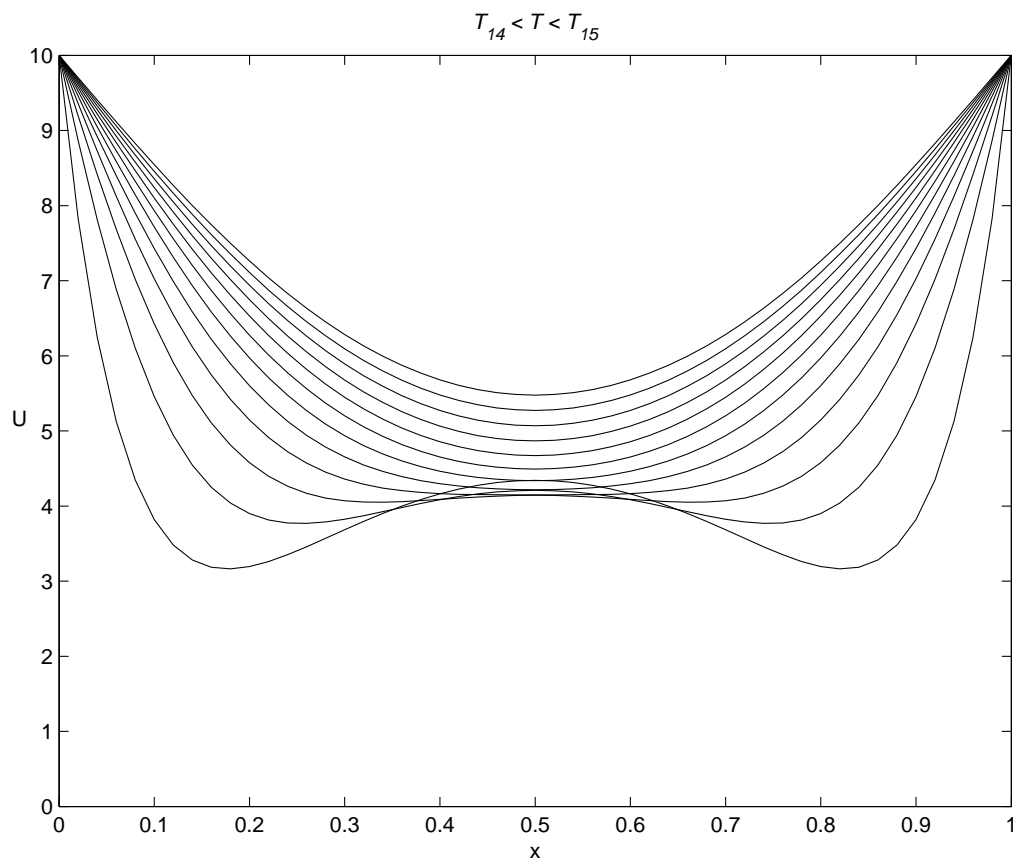


Figure 1.6: The fifteenth stage where the concentration  $U$  is held at 10 at the end points. A similar pattern appears in all such stages.

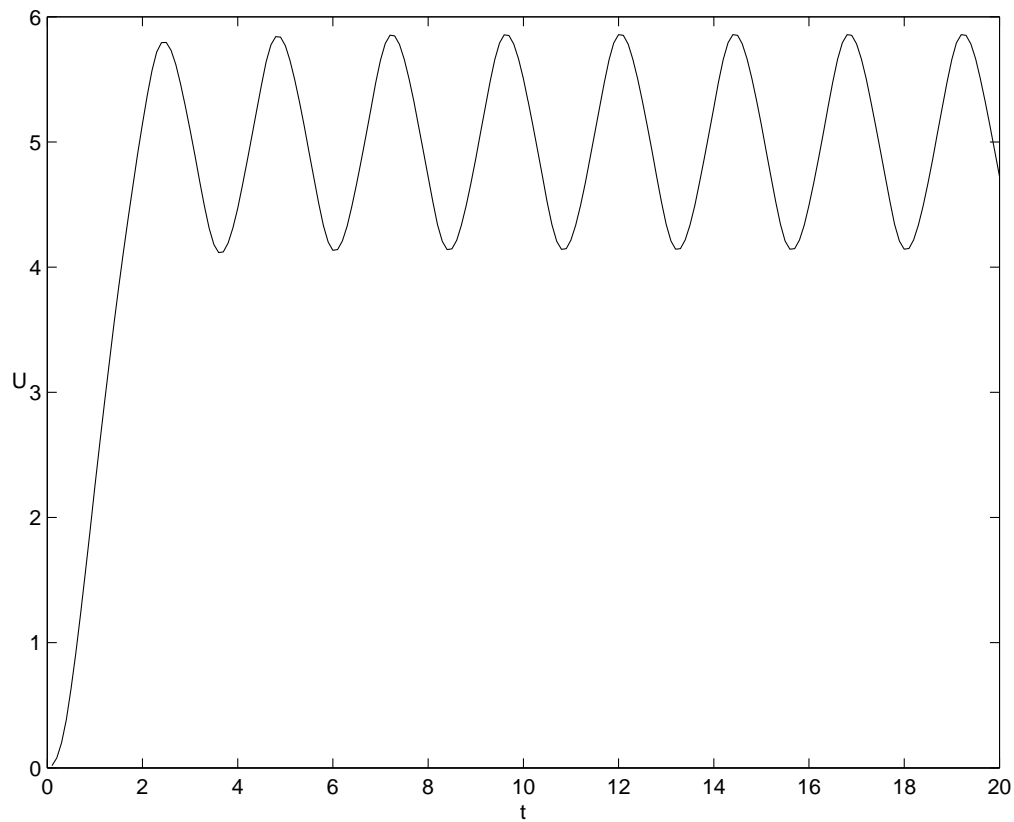


Figure 1.7: For the data  $M = 7$ ,  $m = 3$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.05$ , the concentration profile at  $x = 0.5$  for various times shows periodic behavior due to the change of the boundary conditions

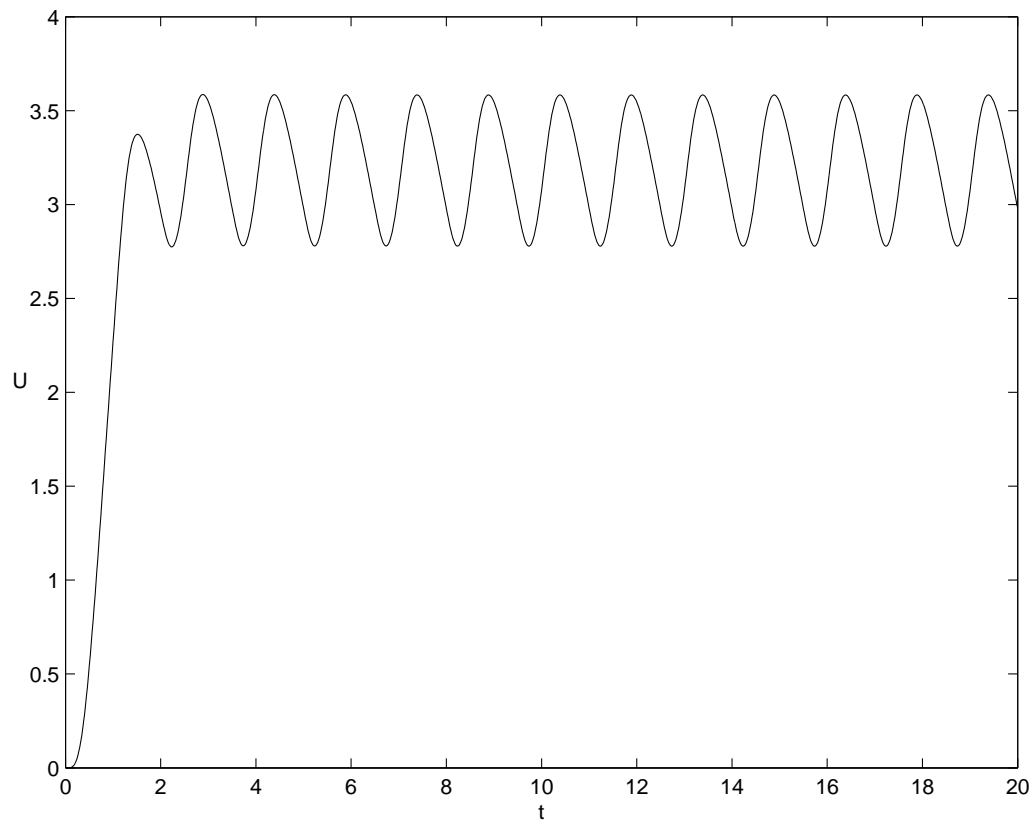


Figure 1.8: For the data  $M = 5$ ,  $m = 2$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.02$ ,  $\alpha = 0.05$ , the concentration profile at  $x = 0.5$  for various times shows periodic behavior due to the change of the boundary conditions

## CHAPTER 2

# A BOUNDARY CONTROL PROBLEM WITH A LINEAR REACTION TERM

### 2.1 Introduction

In this chapter we study the diffusion equation

$$u_t = u_{xx} - u, \quad 0 < x < 1, \quad t > 0, \quad (2.1.1)$$

subject to the initial concentration

$$u(x, 0) = 0, \quad 0 < x < 1,$$

and boundary conditions controlled by the total mass  $\mu(t) = \int_0^1 u(x, t) dx$ . We are going to begin by setting the concentration to be  $u = u_0$  at both boundary points  $x = 0$  and  $x = 1$ , where  $u_0$  is a positive constant. We shall watch the total mass  $\int_0^1 u(x, t) dx$  until it reaches a certain specified level  $M$  at time  $t = t_1$ , where  $0 < M$ . At this moment,  $t = t_1$  we switch the concentration to

$$u(0, t) = u(1, t) = 0 \quad t_1 < t.$$

We keep watching the total mass until it drops down to a prespecified level  $m$  at time  $t = t_2$ , where  $0 < m < M$ . We keep switching the concentration according to the level of the total mass so that we always have

$$m \leq \int_0^1 u(x, t) dx \leq M.$$

In other words, the boundary conditions will be

$$u(0, t) = u(1, t) = \begin{cases} u_0, & t_{2n} \leq t \leq t_{2n+1}, \\ 0, & t_{2n+1} \leq t \leq t_{2n+2} \end{cases} \quad (2.1.2)$$

where  $n = 0, 1, 2, \dots$ , and where the sequence  $\{t_n\}$  will be strictly increasing; i.e.

$$0 = t_0 < t_1 < t_2 < \dots,$$

and its terms  $t_n$  are defined by the equations

$$\begin{aligned} \int_0^1 u(x, t_n) dx &= M, & n = 1, 3, 5, \dots, \\ \int_0^1 u(x, t_n) dx &= m, & n = 2, 4, 6, \dots. \end{aligned}$$

In section 2.2 we shall consider the concentration boundary conditions with  $u_0 = 1$ . Existence and uniqueness will be discussed in section 2.3 and the estimate of  $t_n$  will be considered in section 2.4. We shall consider the flux boundary conditions in section 2.5, some numerical example in section 2.6.

## 2.2 Dirichlet Boundary Conditions

Consider the diffusion problem

$$\begin{aligned}u_t &= u_{xx} - u; & 0 < x < 1, & t > 0 \\u(0, t) &= u(1, t) = \psi(t); & t > 0 \\u(x, 0) &= 0\end{aligned}\tag{2.2.1}$$

where the function  $\psi(t)$  is either 1 or 0 depending on the total mass

$$\mu(t) := \int_0^1 u(x, t) dx.$$

More specifically, the function  $\psi(t)$  will be described by

$$\psi(t) = \begin{cases} 1, & t_{2n} < t < t_{2n+1} \\ 0, & t_{2n+1} < t < t_{2n+2} \end{cases}\tag{2.2.2}$$

where  $n = 0, 1, 2, \dots$  and the sequence  $\{t_n\}$  will be strictly increasing

$$0 = t_0 < t_1 < t_2 < \dots$$

and the  $t_n$  satisfy the equations

$$\int_0^1 u(x, t_n) dx = M, \quad n = 1, 3, 5, \dots\tag{2.2.3}$$

and

$$\int_0^1 u(x, t_n) dx = m, \quad n = 2, 4, 6, \dots\tag{2.2.4}$$

By using the substitution  $v = e^t u$ , problem (2.2.1) is transformed into

$$\begin{aligned} v_t &= v_{xx}, \quad 0 < x < 1, \quad t > 0, \\ v(0, t) &= v(1, t) = \phi(t), \quad t > 0, \\ v(x, 0) &= 0, \quad 0 < x < 1, \end{aligned} \tag{2.2.5}$$

where  $\phi(t) = e^t \psi(t)$ . The solution of (2.2.5) can be explicitly represented as [16, 46]

$$v(x, t) = 2 \int_0^t \left[ \frac{\partial \theta}{\partial x}(x-1, t-\tau) - \frac{\partial \theta}{\partial x}(x, t-\tau) \right] \phi(\tau) d\tau \tag{2.2.6}$$

where

$$\theta(x, t) = \frac{1}{2} + \sum_{n=1}^{\infty} e^{-n^2 \pi^2 t} \cos n\pi x. \tag{2.2.7}$$

Hence

$$u(x, t) = 2e^{-t} \int_0^t \left[ \frac{\partial \theta}{\partial x}(x-1, t-\tau) - \frac{\partial \theta}{\partial x}(x, t-\tau) \right] \phi(\tau) d\tau. \tag{2.2.8}$$

An explicit form for the total concentration can be obtained by integrating over  $x$ . Namely,

$$\begin{aligned} \mu(t) &= \int_0^1 u(x, t) dx \\ &= 4e^{-t} \int_0^t [\theta(0, t-\tau) - \theta(1, t-\tau)] \phi(\tau) d\tau \\ &= 8e^{-t} \int_0^t \phi(\tau) \left( \sum_{k=0}^{\infty} e^{-\lambda_{2k+1}^2 (t-\tau)} \right) d\tau \end{aligned} \tag{2.2.9}$$

where  $\lambda_k^2 = k^2 \pi^2$ .



### 2.3 Existence and Uniqueness

The existence and uniqueness of the solution will follow from the existence and unique determination of the sequence  $\{t_n\}$  when the total mass limits  $m$  and  $M$  are properly chosen.

Let  $t > 0$ , and choose  $\phi(t) \equiv e^t$ . Then

$$\mu(t) = 8 \sum_{k=0}^{\infty} \frac{1}{\lambda_{2k+1}^2 + 1} \left[ 1 - e^{-(\lambda_{2k+1}^2 + 1)t} \right] \quad (2.3.1)$$

which is an increasing function that ranges between zero and  $\mu_{\infty} = 2\frac{e-1}{e+1}$ . Then, for any  $0 < M < \mu_{\infty}$ , there exists  $t_1 > 0$  such that  $\mu(t_1) = M$ .

Next, we prove the existence of  $t_2$  by taking

$$\phi(t) = \begin{cases} e^t & 0 \leq t < t_1 \\ 0 & t_1 < t. \end{cases} \quad (2.3.2)$$

This implies

$$\mu(t) = 8 \sum_{k=0}^{\infty} \frac{e^{-(\lambda_{2k+1}^2 + 1)t}}{\lambda_{2k+1}^2 + 1} \left[ e^{(\lambda_{2k+1}^2 + 1)t_1} - 1 \right] \quad (2.3.3)$$

which is a decreasing function that falls from  $M$  to 0 as  $t$  ranges from  $t_1$  to  $\infty$ . Then, for any  $0 < m < M$ , there exists  $t_2$  such that  $\mu(t_2) = m$ .

For  $t \geq t_{2n}$  and  $\phi(t) = e^t$ , we have by induction

$$\mu(t) = \sum_{k=0}^{\infty} \frac{8}{1 + \lambda_{2k+1}^2} \left[ 1 - e^{-(1 + \lambda_{2k+1}^2)t} \sum_{j=0}^{2n} (-1)^j e^{(1 + \lambda_{2k+1}^2)t_j} \right] \quad (2.3.4)$$

which is an increasing function that ranges between  $m$  and  $\mu_{\infty}$  as  $t$  goes from  $t_{2n}$  to infinity.

This ensures the existence of  $t_{2n+1}$  such that  $\mu(t_{2n+1}) = M$ .

For  $t \geq t_{2n+1}$ ,  $\phi(t) \equiv 0$  which implies

$$\begin{aligned}\mu(t) &= 8 \sum_{k=0}^{\infty} \frac{e^{-(1+\lambda_{2k+1}^2)t}}{1 + \lambda_{2k+1}^2} \sum_{j=0}^n \left[ e^{t_{2j+1}(1+\lambda_{2k+1}^2)} - e^{t_{2j}(1+\lambda_{2k+1}^2)} \right] \\ &= 8 \sum_{k=0}^{\infty} \frac{e^{-(1+\lambda_{2k+1}^2)t}}{1 + \lambda_{2k+1}^2} \sum_{j=0}^{2n+1} (-1)^{j+1} e^{(1+\lambda_{2k+1}^2)t_j}\end{aligned}\tag{2.3.5}$$

which is a decreasing function that ranges from  $M$  to 0 as  $t$  goes from  $t_{2n+1}$  to infinity. Hence, there exists  $t_{2n+2}$  such that  $\mu(t_{2n+2}) = m$ . Thus, by induction, the existence and uniqueness of the  $t_n, n = 1, 2, \dots$  has been shown. Given the switching points, the existence and uniqueness of the solution  $u(x, t)$  follows immediately.

## 2.4 First Term Approximation of the Time Switching Points

In this section we will use the first term approximation of (2.2.9) to get an estimate of the sequence  $\{t_n\}$  in an explicit form.

For simplicity, let us assume

$$\begin{aligned}M &= \frac{8}{1 + \lambda_1^2}(1 - \alpha) \\ m &= \frac{8}{1 + \lambda_1^2}\beta\end{aligned}\tag{2.4.1}$$

where  $\alpha$  and  $\beta$  are positive numbers, with

$$0 < \beta < 1 - \alpha.$$

After we drop off all the terms of order  $e^{-\lambda_{2k+1}^2(t-\tau)}$ ,  $k \geq 1$ , equation (2.2.9) can be written as

$$\tilde{\mu}(t) = 8e^{-t} \int_0^t \phi(\tau) e^{-\lambda_1^2(t-\tau)} d\tau, \quad (2.4.2)$$

where

$$\phi(t) = \begin{cases} e^t, & t_{2n} \leq t \leq t_{2n+1}, \\ 0, & \text{elsewhere.} \end{cases} \quad (2.4.3)$$

To get  $t_1$ , we set  $\phi(t) = e^t$ ,  $0 < t < t_1$ , in (2.4.2) and solve the equation

$$\tilde{\mu}(t_1) = M.$$

This becomes

$$\frac{8e^{-(1+\lambda_1^2)t_1}}{1+\lambda_1^2} (e^{(1+\lambda_1^2)t_1} - 1) = M. \quad (2.4.4)$$

Thus,

$$e^{-(1+\lambda_1^2)t_1} = \alpha. \quad (2.4.5)$$

For the next time switch  $t_2$ , we insert

$$\phi(t) = \begin{cases} e^t, & 0 < t < t_1, \\ 0, & t_1 < t < t_2 \end{cases} \quad (2.4.6)$$

in (2.4.2) and solve the equation

$$\tilde{\mu}(t_2) = m. \quad (2.4.7)$$

From (2.4.1), (2.4.6) and (2.4.2),

$$\frac{8e^{-(1+\lambda_1^2)t}}{1+\lambda_1^2} [e^{(1+\lambda_1^2)t_1} - 1] = m \quad (2.4.8)$$

which implies

$$e^{-(1+\lambda_1^2)t_2} = \frac{\alpha\beta}{1-\alpha}. \quad (2.4.9)$$

We use a similar argument to obtain

$$\begin{aligned} e^{-(1+\lambda_1^2)t_3} &= \frac{\alpha^2\beta}{(1-\alpha)(1-\beta)}, \\ e^{-(1+\lambda_1^2)t_4} &= \frac{\alpha^2\beta^2}{(1-\alpha)^2(1-\beta)}. \end{aligned}$$

Using mathematical induction, we can show that

$$e^{-(1+\lambda_1^2)t_{2n}} = \frac{\alpha^n\beta^n}{(1-\alpha)^n(1-\beta)^{n-1}}, \quad n \geq 1, \quad (2.4.10)$$

and

$$e^{-(1+\lambda_1^2)t_{2n+1}} = \frac{\alpha^{n+1}\beta^n}{(1-\alpha)^n(1-\beta)^n}, \quad n \geq 0. \quad (2.4.11)$$

These two equations imply the estimates

$$t_{2n} - t_{2n-1} = \frac{1}{1+\lambda_1^2} \ln \left( \frac{1-\alpha}{\beta} \right), \quad n \geq 1 \quad (2.4.12)$$

and

$$t_{2n+1} - t_{2n} = \frac{1}{1+\lambda_1^2} \ln \left( \frac{1-\beta}{\alpha} \right), \quad n \geq 1. \quad (2.4.13)$$

Hence, the length of the consecutive time intervals is always alternating between the two constants.

## 2.5 Neumann Boundary Conditions

In this section, we consider the diffusion problem

$$\begin{aligned}
 u_t &= u_{xx} - u & 0 < x < 1, \quad t > 0, \\
 u_x(0, t) &= -\psi(t), \quad u_x(1, t) = \psi(t), & t > 0 \\
 u(x, 0) &= 0, & 0 < x < 1,
 \end{aligned} \tag{2.5.1}$$

where  $\psi(t)$  is either 1 or 0 depending on the total mass  $\mu(t) = \int_0^1 u(x, t) dx$ . In other words, the flux  $\psi(t)$  will be described by

$$\psi(t) = \begin{cases} 1, & t_{2n} < t \leq t_{2n+1}, \\ 0, & t_{2n+1} < t \leq t_{2n+2}, \end{cases} \tag{2.5.2}$$

where  $n = 0, 1, 2, \dots$ , and the sequence  $\{t_n\}$  will be strictly increasing, i.e.

$$0 = t_0 < t_1 < t_2 < \dots \tag{2.5.3}$$

and it satisfies

$$\begin{aligned}
 \int_0^1 u(x, t_n) dx &= M, & n = 1, 3, 5, \dots, \\
 \int_0^1 u(x, t_n) dx &= m, & n = 2, 4, 6, \dots
 \end{aligned}$$

By using the transformation  $v = e^t u$ , we obtain the equivalent problem

$$\begin{aligned}
 v_t &= v_{xx}, & 0 < x < 1, \quad t > 0, \\
 -v_x(0, t) &= v_x(1, t) = \phi(t), & t > 0, \\
 v(x, 0) &= 0, & 0 < x < 1,
 \end{aligned} \tag{2.5.4}$$

where  $\phi(t) = e^t \psi(t)$ . For  $0 \leq t$ , the solution of (2.5.4) can be written explicitly [16, 46] as

$$v(x, t) = 2 \int_0^t \theta(x, t - \tau) \phi(\tau) d\tau + 2 \int_0^t \theta(x - 1, t - \tau) \phi(\tau) d\tau \quad (2.5.5)$$

where

$$\theta(x, t) = \frac{1}{2} + \sum_{n=1}^{\infty} e^{-n^2 \pi^2 t} \cos n\pi x. \quad (2.5.6)$$

From (2.5.5) and (2.5.6), we obtain an explicit form for the total mass

$$\begin{aligned} \mu(t) &= \int_0^1 u(x, t) dx \\ &= 2e^{-t} \int_0^t \int_0^1 [\theta(x, t - \tau) + \theta(x - 1, t - \tau)] \phi(\tau) dx d\tau. \end{aligned}$$

Carrying out the  $x$  integrals, we get

$$\int_0^1 \theta(x, t) dx = \int_0^1 \left[ \frac{1}{2} + \sum_1^{\infty} e^{-n^2 \pi^2 t} \cos n\pi x \right] dx = \frac{1}{2} \quad (2.5.7)$$

and

$$\int_0^1 \theta(x - 1, t) dx = \frac{1}{2}. \quad (2.5.8)$$

Thus

$$\mu(t) = 2e^{-t} \int_0^t \phi(\tau) d\tau. \quad (2.5.9)$$

**Remark:** If we leave  $\psi(t) \equiv 1$  for all  $t > 0$  then the asymptotic solution of (2.5.1) will be

$$u_{\infty} = (e - 1)^{-1} (e^x + e^{1-x})$$

which has

$$\mu = \int_0^1 u_{\infty} dx = 2.$$

This suggests that the upper threshold has to satisfy  $M < 2$ .

Formula (2.5.9) can be used to find  $\{t_n\}$  exactly. For simplicity of computations, we shall assume

$$M = 2(1 - \alpha), \quad (2.5.10)$$

and

$$m = 2\beta, \quad (2.5.11)$$

for some positive numbers  $\alpha$  and  $\beta$ , where

$$0 < \beta < (1 - \alpha) < 1. \quad (2.5.12)$$

To find  $t_1$ , we solve  $\mu(t_1) = M$ , where  $\phi(t) = e^t, 0 < t < t_1$ . That is

$$2e^{-t_1} \int_0^{t_1} e^\tau d\tau = 2(1 - \alpha). \quad (2.5.13)$$

This simplifies to

$$e^{-t_1} = \alpha. \quad (2.5.14)$$

To compute  $t_2$ , we solve the equation

$$\mu(t_2) = 2e^{-t_2} \int_0^{t_2} \phi(\tau) d\tau = m, \quad t_1 \leq t \leq t_2, \quad (2.5.15)$$

where

$$\phi(t) = \begin{cases} e^t, & 0 < t < t_1, \\ 0, & t_1 < t < t_2. \end{cases}$$

This reduces (2.5.15) to

$$2e^{-t_2}[e^{t_1} - 1] = 2\beta \quad (2.5.16)$$

which gives

$$e^{-t_2} = \frac{\alpha\beta}{1-\alpha}. \quad (2.5.17)$$

In a similar fashion, we find  $t_3$  by solving

$$2e^{-t_3} \int_0^{t_3} \phi(\tau) d\tau = M \quad (2.5.18)$$

where

$$\phi(t) = \begin{cases} e^t, & 0 < t < t_1 \quad \text{and} \quad t_2 < t < t_3, \\ 0, & t_1 < t < t_2. \end{cases}$$

For  $t_4$  and  $t_5$ , we find that

$$e^{-t_4} = \frac{\alpha^2\beta^2}{(1-\alpha)^2(1-\beta)} \quad (2.5.19)$$

and that

$$e^{-t_5} = \frac{\alpha^3\beta^2}{(1-\alpha)^2(1-\beta)^2}. \quad (2.5.20)$$

Using mathematical induction, we can show

$$e^{-t_{2n}} = \frac{\alpha^n\beta^n}{(1-\alpha)^n(1-\beta)^{n-1}}, \quad n \geq 1, \quad (2.5.21)$$

and

$$e^{-t_{2n+1}} = \frac{\alpha^{n+1}\beta^n}{(1-\alpha)^n(1-\beta)^n}, \quad n \geq 0. \quad (2.5.22)$$

Expressions (2.5.21) and (2.5.22) imply that

$$t_{2n+1} - t_{2n} = \ln \frac{1-\beta}{\alpha}, \quad n \geq 1$$

and

$$t_{2n+2} - t_{2n+1} = \ln \frac{1-\alpha}{\beta}, \quad n \geq 0.$$



## 2.6 Numerical Results

In this section, we use a finite difference technique along with the trapezoidal rule to get an approximate discrete solution  $U_j^n$  and the sequence  $\{T_n\}$  when the total mass hits one of the limits  $M$  or  $m$ .

We discretize the space and time by using

$$\text{i) } \Delta x = \frac{1}{J}, \quad X_j = j\Delta x, \quad j = 0, 1, \dots, J$$

$$\text{ii) } \Delta t = \frac{T}{N}, \quad \tau_n = n\Delta t, \quad n = 0, \dots, N$$

where  $J$  and  $N$  are positive integers and  $T$  is a positive real number. The integer  $N$  has to be chosen large enough so that the time step  $\Delta t$  is much smaller than the differences  $T_n - T_{n-1}$ .

We consider the backward implicit finite difference scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2} - U_j^{n+1}$$

as a discretized version of  $u_t = \alpha u_{xx} - u$ , where  $\alpha$  is a positive constant. The above scheme can be written in the form

$$-\beta U_{j-1}^{n+1} + (1 + \Delta t + 2\beta)U_j^{n+1} - \beta U_{j+1}^{n+1} = U_j^n \tag{2.6.1}$$

where  $j = 1, \dots, J - 1$  and  $n = 0, 1, \dots, N - 1$  and  $\beta = \alpha\Delta t/(\Delta x)^2$ . The initial data are set to be  $U_j^0 = 0$  for  $j = 1, \dots, J - 1$ , and the boundary conditions are  $U_0^n = U_J^n = \phi(\tau_n)$  for  $n = 0, 1, \dots, N$ . The function  $\phi(\tau_n)$  will be either 10 or 0 depending on the value of the

mass which will be approximated by the trapezoidal rule

$$\mu_n = \frac{h}{2} \sum_{j=0}^{N-1} (U_j^{n+1} + U_{j+1}^n). \quad (2.6.2)$$

The numerical experiment is carried out in the following way. We start by setting the boundary conditions  $U_0^n = U_j^n = 10$  then we solve a tridiagonal system coming out of the difference method. We check the total mass  $\mu_n$  in (2.6.2). We keep doing that at each time step until the mass  $\mu_n$  exceeds or equals the upper limit  $M$ . Then we switch the boundary conditions to  $U_0^n = U_j^n = 0$ , and we iterate by solving a tridiagonal system after each time steps  $\Delta t$  until the total mass  $\mu_n$  decreases to  $m$ . At this moment we switch the boundary condition back to 10 and continue the process as we did before.

For the data specifications  $\Delta x = 0.02$ ,  $T = 20$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.01$ ,  $M = 1.8$ ,  $m = 0.2$ , Table (2.1) shows the times switches  $T_n$ . As we can see there, the duration of each stage is either 1.18 or 1.20.

For the same set of data, figures (2.1) through (2.5) show the concentration versus the space. The figures are obtained for different stages, where at each stage the concentration is kept constant at the end points.

A profile of the concentrations at  $x = 0.5$  for various times is shown in figure (2.6) with the same specified data.

For a different set of upper and lower bounds on the mass  $M = 5$  and  $m = 2$  along with  $\Delta x = 0.02$ ,  $T = 20$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.01$ , Table (2.2) shows the time switches  $T_n$ . Durations of the time intervals fluctuates between 0.6, 1.1. Figure (2.7) is the concentration at  $x = 0.5$  for the same set of data.

Table 2.1: Time switches  $T_n$  corresponding to  $\Delta x = 0.02$ ,  $T = 20$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.01$ ,  
 $M = 1.8$ ,  $m = 0.2$

$n$	$T_n$	$T_n - T_{n-1}$	$n$	$T_n$	$T_n - T_{n-1}$
1	1.3400	1.3200	9	10.8600	1.1800
2	2.5400	1.2000	10	12.0600	1.2000
3	3.7200	1.1800	11	13.2400	1.1800
4	4.9200	1.2000	12	14.4400	1.2000
5	6.1000	1.1800	13	15.6200	1.1800
6	7.3000	1.2000	14	16.8200	1.2000
7	8.4800	1.1800	15	18.0000	1.1800
8	9.6800	1.2000	16	19.2000	1.2000

Table 2.2: Time switches  $T_n$  corresponding to  $M = 1.5$ ,  $m = 0.2$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.01$

$n$	$T_n$	$T_n - T_{n-1}$	$n$	$T_n$	$T_n - T_{n-1}$
1	0.8000	0.7000	12	10.4000	1.1000
2	1.9000	1.1000	13	11.0000	0.6000
3	2.5000	0.6000	14	12.1000	1.1000
4	3.6000	1.1000	15	12.7000	0.6000
5	4.2000	0.6000	16	13.8000	1.1000
6	5.3000	1.1000	17	14.4000	0.6000
7	5.9000	0.6000	18	15.5000	1.1000
8	7.0000	1.1000	19	16.1000	0.6000
9	7.6000	0.6000	20	17.2000	1.1000
10	8.7000	1.1000	21	17.8000	0.6000
11	9.3000	0.6000	22	18.9000	1.1000

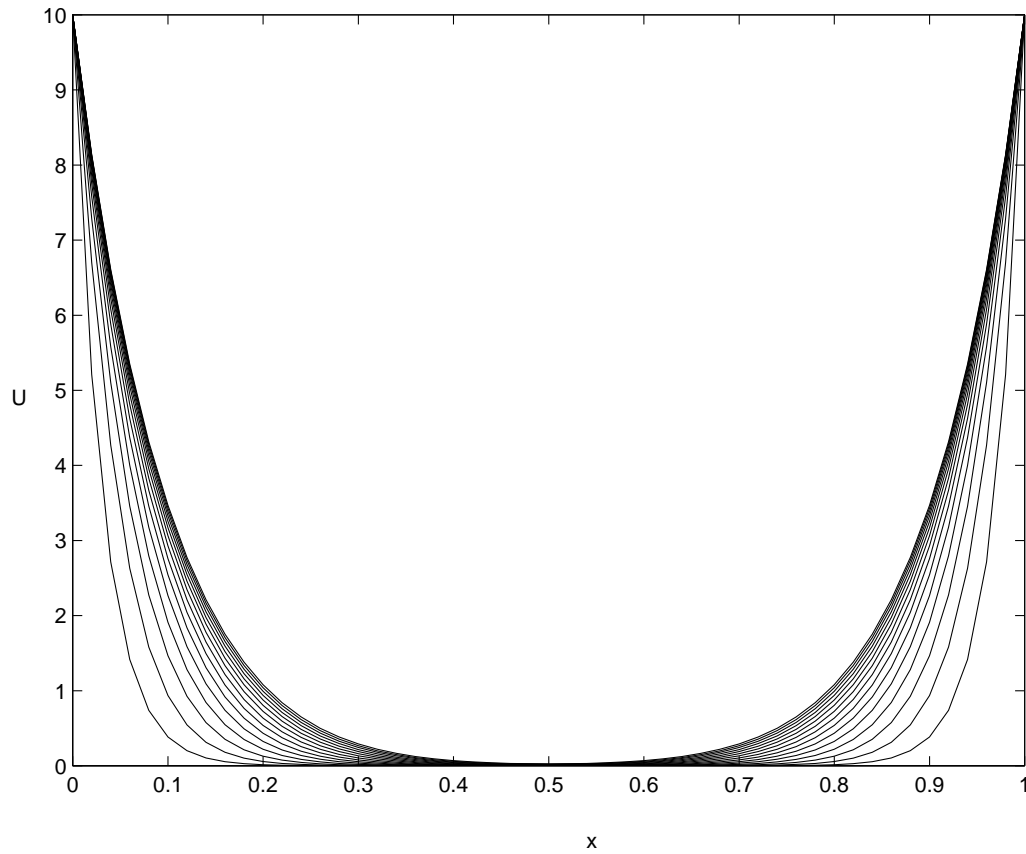


Figure 2.1: The first stage where the concentration  $U$  is held at 10 at the end points. Each curve shows the concentration profile at various discrete time steps  $t_n = n\Delta t$ . As the time goes on, the level of concentrations gets higher

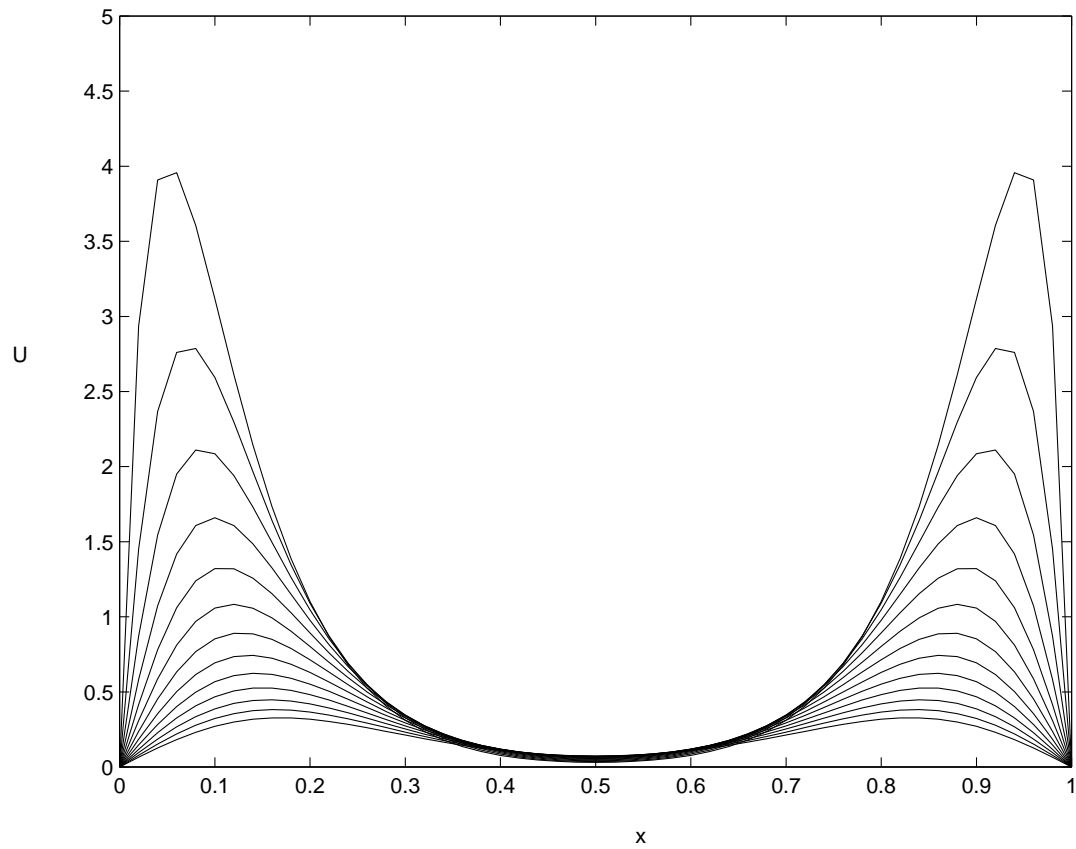


Figure 2.2: The second stage where the concentration  $U$  is held at 0 at the end points. As the time goes on, the level of concentrations decreases. Notice the fluctuations when the concentration is dropped suddenly to 0 at the beginning of the stage

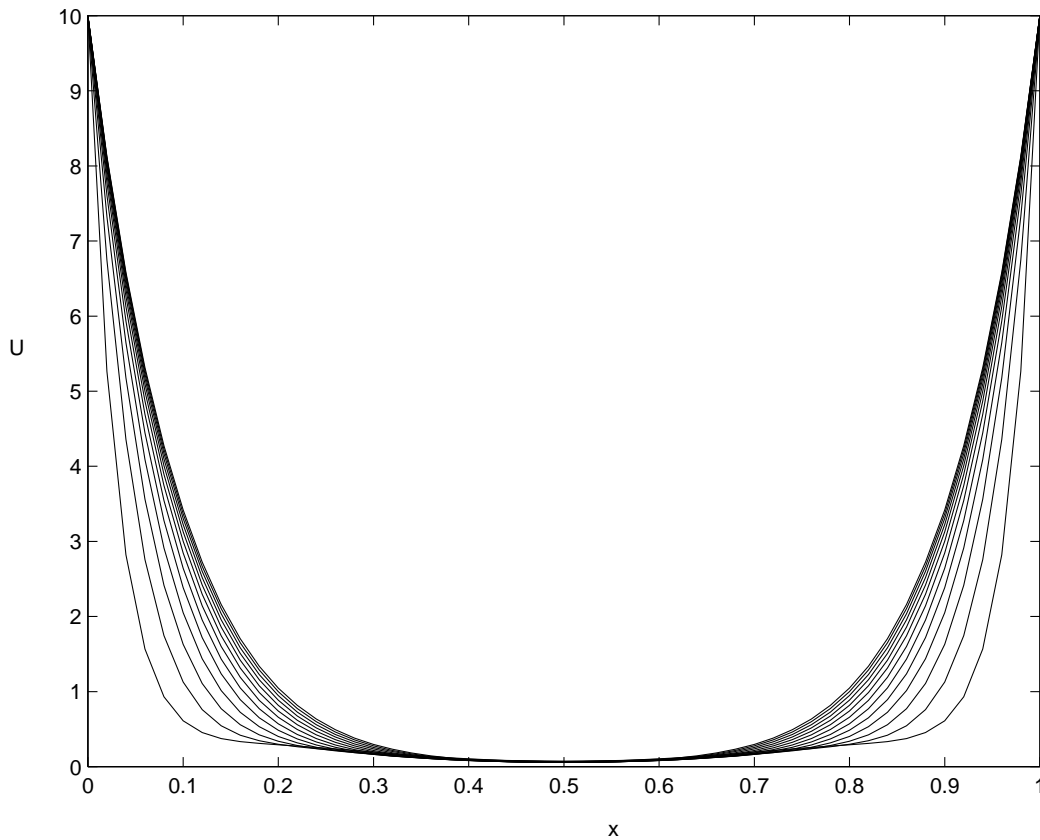


Figure 2.3: The third stage where the concentration  $U$  is switched to 10 at the end points. Each curve shows the concentration profile at various discrete time steps  $t_n = n\Delta t$ . Notice the fluctuations due to the sudden change on the concentrations. After a little while, the concentrations levels increase monotonically.

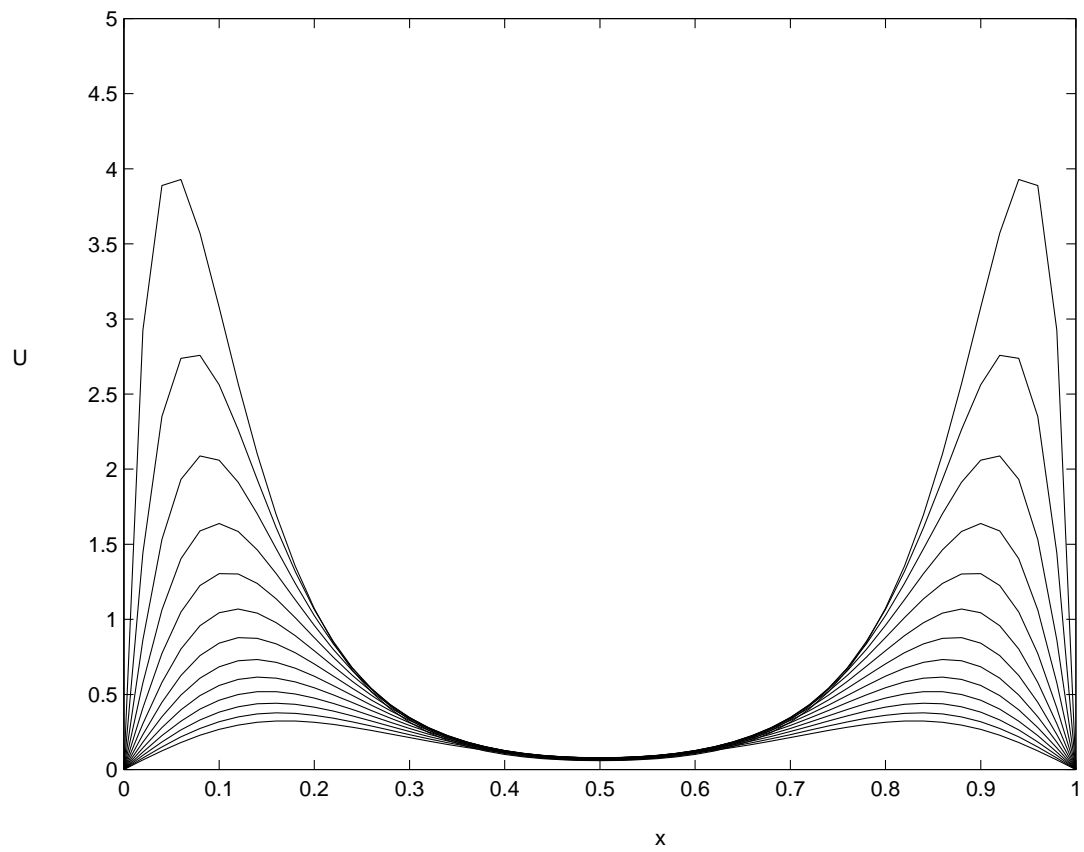


Figure 2.4: The fourth stage where the concentration  $U$  is switched to 0 at the end points. Notice the similarity with the second stage.



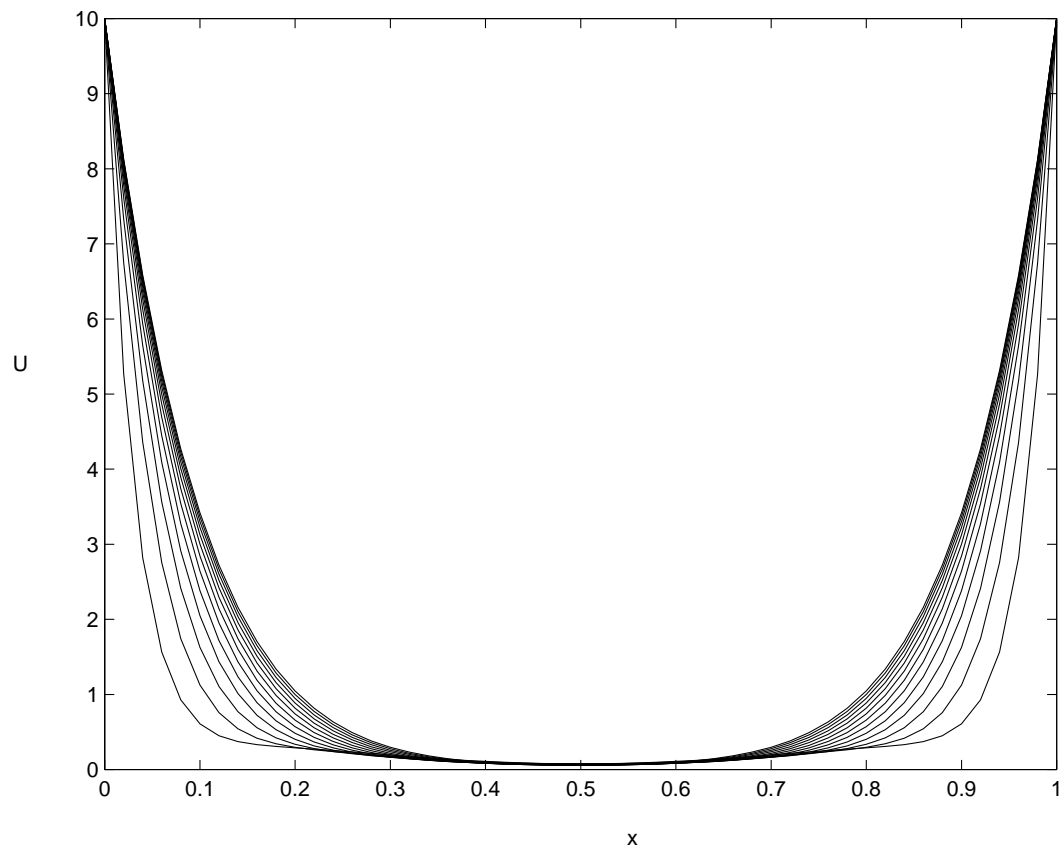


Figure 2.5: The fifth stage where the concentration  $U$  is held at 10 at the end points. Notice the similarity with the third stage.

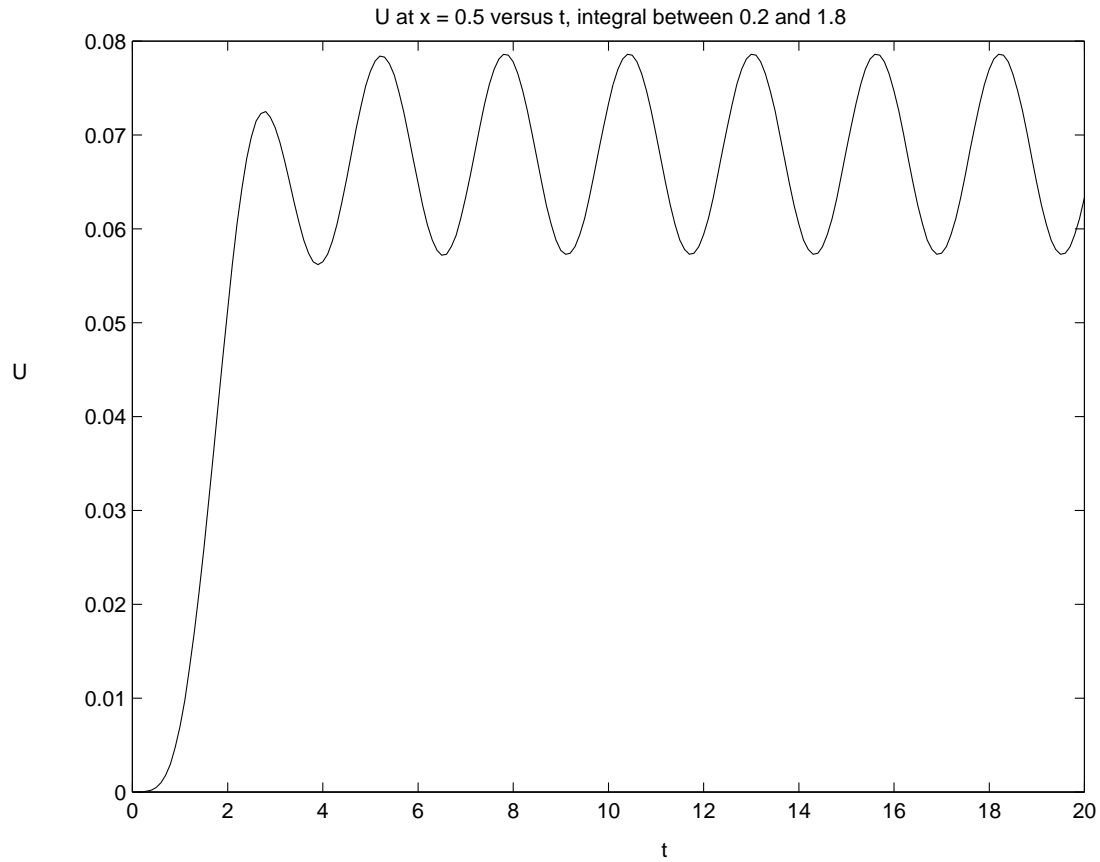


Figure 2.6: For the data  $M = 1.8$ ,  $m = 0.2$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.01$ , the concentration profile at  $x = 0.5$  for various times shows periodic behavior due to the periodic change of the boundary conditions

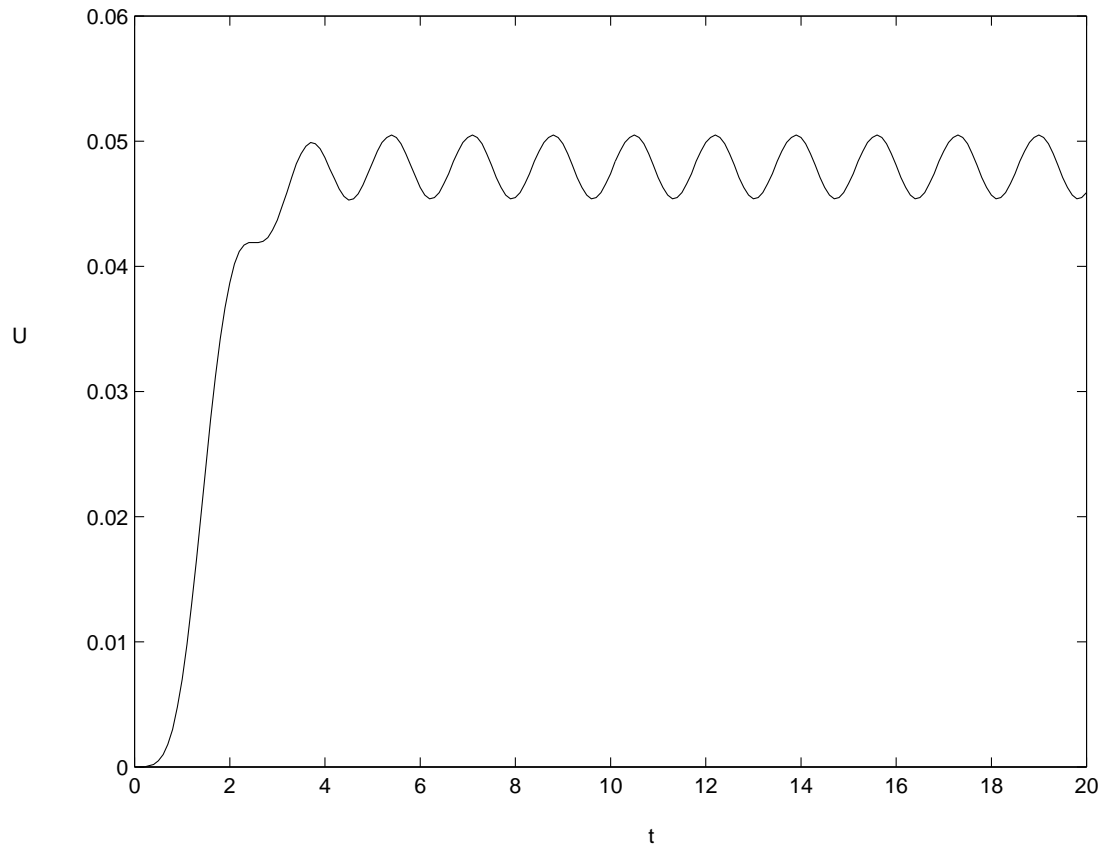


Figure 2.7: For the data  $M = 1.5$ ,  $m = 0.2$ ,  $\Delta x = 0.02$ ,  $\Delta t = 0.1$ ,  $\alpha = 0.05$ , the concentration profile at  $x = 0.5$  for various times shows periodic behavior due to the periodic change of the boundary conditions

## CHAPTER 3

### DIFFUSION PROBLEM WITH NEUMANN

#### BOUNDARY CONTROL

##### 3.1 Definition of the Problem

We consider the heat problem

$$\begin{aligned} u_t &= u_{xx}, & t > 0, \quad 0 < x < 1, \\ u(x, 0) &= 0 & 0 < x < 1, \\ u_x(0, t) &= -\phi(t) & t > 0, \\ u_x(1, t) &= \phi(t) & t > 0. \end{aligned} \tag{3.1.1}$$

where the flux  $\phi(t)$  is set in such a way to control the level of the total energy  $\mu(t) = \int_0^1 u(x, t) dx$ . Namely,

$$\phi(t) = \begin{cases} 1 & \text{if } t_{2n} < t < t_{2n+1}, \\ -1 & \text{if } t_{2n+1} < t < t_{2n+2}, \end{cases}$$

where the sequence

$$0 = t_0 < t_1 < t_2 < \dots,$$

satisfies

$$\begin{aligned}\mu(t_{2n}) &= m, & n = 1, 2, 3, \dots, \\ \mu(t_{2n+1}) &= M, & n = 0, 1, 2, \dots,\end{aligned}$$

where  $m$  and  $M$  are certain positive threshold to ensure  $m < \mu < M$ . The total energy has a time derivative equal to

$$\begin{aligned}\mu'(t) &= \int_0^1 u_t(x, t) dx & (3.1.2) \\ &= \int_0^1 u_{xx}(x, t) dx \\ &= u_x(1, t) - u_x(0, t) \\ &= 2\phi(t).\end{aligned}$$

where we use the fact that  $u(x, t)$  satisfies (3.1.1). This relationship will allow us to explicitly find the time switches  $t_n$ .

Since the flux  $\phi(t)$  is initially set at 1, and  $\mu(0) = 0$  due to the initial condition on  $u$ , then

$$\mu(t) = 2t, \quad 0 \leq t \leq t_1.$$

where  $t_1$  can be calculated as a solution of  $\mu(t_1) = M$ , which implies  $t_1 = M/2$ .

At the second time interval  $t_1 < t < t_2$ , the flux is reversed, that is  $\phi(t) = -1$ , therefore the total energy will be

$$\mu(t) = -2t + M + 2t_1, \quad t_1 \leq t \leq t_2,$$

where due to the continuity of  $\mu(t)$  at  $t_1$ . The second time switch  $t_2$  will be calculated as a solution of  $\mu(t_2) = m$ , this gives

$$\begin{aligned} t_2 &= t_1 + \left(\frac{M}{2} - \frac{m}{2}\right) \\ &= M - \frac{m}{2}, \end{aligned}$$

Now, if we bring the flux back to  $\phi(t) = 1$ , where  $t_2 \leq t \leq t_3$ , we will find

$$\mu(t) = 2t + m - 2t_2, \quad t_2 \leq t \leq t_3.$$

Setting  $\mu(t_3) = M$  yields

$$\begin{aligned} t_3 &= t_2 + \left(\frac{M}{2} - \frac{m}{2}\right) \\ &= \frac{3M}{2} - m, \end{aligned}$$

Following the same pattern, we will successively get

$$\mu(t) = -2t + M + 2t_3, \quad t_3 \leq t \leq t_4,$$

$$\begin{aligned} t_4 &= t_3 + \left(\frac{M}{2} - \frac{m}{2}\right) \\ &= 2M - \frac{3m}{2}, \end{aligned}$$

$$\mu(t) = 2t + m - 2t_4, \quad t_4 \leq t \leq t_5,$$

$$\begin{aligned} t_5 &= t_4 + \left(\frac{M}{2} - \frac{m}{2}\right) \\ &= \frac{5M}{2} - 2m, \end{aligned}$$

$\vdots$

$$\mu(t) = \begin{cases} 2t + m - 2t_{2n} & \text{if } t_{2n} < t < t_{2n+1} \\ -2t + M + 2t_{2n+1} & \text{if } t_{2n+1} < t < t_{2n+2} \end{cases}$$

$$\begin{aligned} t_n &= t_{n-1} + \left(\frac{M}{2} - \frac{m}{2}\right) \\ &= \frac{nM}{2} - \frac{(n-1)m}{2}, \end{aligned}$$

where  $n \geq 1$ . We infer from these calculations that the time switches  $t_n$  are equi-spaced with  $t_n - t_{n-1} = 0.5M - 0.5m$ . Since the control flux is now fully identified, our control problem turns out to an initial boundary value problem with a prescribed Neumann condition.

### 3.2 Finite difference analysis

We study a finite difference discretization for the control problem (3.1.1). We consider the implicit backward scheme

$$\begin{aligned} \frac{U_j^{n+1} - U_j^n}{\Delta t} &= \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2}, & j = 1, \dots, J-1, \quad n = 0, 1, 2, \dots \\ U_j^0 &= 0, & j = 0, \dots, J \\ \frac{U_1^{n+1} - U_0^{n+1}}{\Delta x} &= -\phi(\tau_{n+1}), & n = 0, 1, 2, \dots \\ \frac{U_J^{n+1} - U_{J-1}^{n+1}}{\Delta x} &= \phi(\tau_{n+1}), & n = 0, 1, 2, \dots \end{aligned}$$

where  $\tau_n$  is not necessarily a uniform grid. The total mass can be computed by the following Riemann type sum

$$\mu_n = \Delta x \sum_{j=1}^{J-1} U_j^n$$

A discrete version of (3.1.2) may look like

$$\begin{aligned} \frac{\mu_{n+1} - \mu_n}{\Delta t} &= \Delta x \sum_{j=1}^{J-1} \frac{U_j^{n+1} - U_j^n}{\Delta t}, \\ &= \Delta x \sum_{j=1}^{J-1} \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2}, \\ &= \frac{U_J^{n+1} - U_{J-1}^{n+1}}{\Delta x} - \frac{U_1^{n+1} - U_0^{n+1}}{\Delta x}, \\ &= 2\phi(\tau_{n+1}). \end{aligned} \tag{3.2.1}$$

Next we shall explicitly find  $\mu_n$  and the time switches  $t_n$  with some restriction on the mesh size. In the first subinterval  $0 < \tau_n < t_1$ , we choose  $\Delta t = \Delta t_0 = \frac{M}{2N_0}$ , where  $N_0$  is a positive integer, along with the flux  $\phi(\tau_n) = 1$ . We obtain

$$\mu_n = 2n\Delta t_0 = 2\tau_n, \quad 0 \leq \tau_n \leq t_1$$

This special choice for  $\Delta t_0$  leads to

$$\mu_{N_0} = M$$

i.e.  $N_0$  specifies the first time switch

$$t_1 = \tau_{N_0} = \frac{M}{2}$$

which coincides with the one computed analytically. Next, we reverse the flux, i.e.  $\phi(\tau_n) = -1$ , for  $n > N_0$ , and define  $\Delta t = \frac{M - m}{2N}$ , for some positive integer  $N$ . Then in view of (3.2.1),



we obtain

$$\mu_n = M - 2(n - N_0)\Delta t, \quad n \geq N_0.$$

Notice that in the second stage, the time mesh size is not necessarily equal to the one at the first stage. With this carefully chosen  $\Delta t$ , we can easily get

$$\mu_{N_0+N} = m$$

with the second time switch equal to

$$\begin{aligned} t_2 &= N_0\Delta t_0 + N\Delta t \\ &= t_1 + \left(\frac{M}{2} - \frac{m}{2}\right). \end{aligned}$$

This result is in agreement with the one computed analytically.

For the next upcoming stages, we keep the time mesh size as  $\Delta t = \frac{M - m}{2N}$ . The following are the total mass and the time switches for the third and the fourth stages respectively

$$\mu_n = m + 2(n - N_0 - N)\Delta t, \quad n \geq N_0 + N,$$

$$\begin{aligned} t_3 &= N_0\Delta t_0 + 2N\Delta t, \\ &= t_2 + \left(\frac{M}{2} - \frac{m}{2}\right), \end{aligned}$$

$$\mu_n = M - 2(n - N_0 - 2N)\Delta t, \quad n \geq N_0 + 2N,$$

$$\begin{aligned} t_4 &= N_0\Delta t_0 + 3N\Delta t, \\ &= t_3 + \left(\frac{M}{2} - \frac{m}{2}\right), \end{aligned}$$

This inductively gives

$$\mu_n = \begin{cases} M - 2(n - N_0 - kN)\Delta t, & \text{if } N_0 + kN \leq n \leq N_0 + (k+1)N, \quad k \text{ is even} \\ m + 2(n - N_0 - kN)\Delta t, & \text{if } N_0 + kN \leq n \leq N_0 + (k+1)N, \quad k \text{ is odd} \end{cases}$$

$$\begin{aligned} t_k &= N_0\Delta t_0 + (k-1)N\Delta t, \\ &= t_{k-1} + \left(\frac{M}{2} - \frac{m}{2}\right). \end{aligned}$$

The above calculations shows that if the time grid is chosen properly, the time switches computed by the above difference scheme coincides with those computed analytically.

**Remark:** The situation when the  $\tau_n$  is equispaced does not, in general, generate to the exact time switches  $t_n$ . However, if we take the switching criteria as,  $\mu_n \geq M$ , and  $\mu_n \leq m$  instead of  $\mu_n = M$  and  $\mu_n = m$ , respectively, where  $n$  is the least integer that satisfies such

inequalities, we obtain a new set of switching points, say  $T_n$ , with the errors

$$\begin{aligned}
 0 &\leq T_1 - t_1 < \Delta t, \\
 0 &\leq T_2 - t_2 < 2\Delta t, \\
 0 &\leq T_3 - t_3 < 3\Delta t, \\
 &\vdots \\
 0 &\leq T_k - t_k < k\Delta t.
 \end{aligned}$$

If the maximum time limit  $T$  is finite, with  $\Delta t = T/N$ , for some integer  $n$ , then for a fixed integer  $k$ , we will have  $T_k - t_k < k\Delta t = kT/N$  convergent to 0 as  $N \rightarrow \infty$ .

### 3.3 Numerical Example

In this section, we consider a finite difference method to discretize the problem

$$\begin{aligned}
 u_t &= \alpha u_{xx}, & 0 < x < 1, & \quad 0 < t \leq T \\
 -u_x(0, t) &= u_x(1, t) = \phi(t), & & \quad 0 < t \leq T \\
 u(x, 0) &= 0, & & \quad 0 < x < 1
 \end{aligned}$$

where the boundary control function is

$$\phi(t) = \begin{cases} 1, & t_{2n} \leq t \leq t_{2n+1} \\ -1, & \text{elsewhere} \end{cases}$$

and  $\{t_n\}$  depends on

$$\mu(t) = \int_0^1 u(x, t) dx$$

where

$$\mu(t_{2n}) = 0.1, \quad n = 1, 2, \dots$$

$$\mu(t_{2n+1}) = 0.2, \quad n = 0, 1, \dots$$

The time limit and the diffusivity constant are taken as  $T = 10$  and  $\alpha = 0.05$ .

Let's consider the space and time discretization

$$\text{i) } \Delta x = \frac{1}{J}, \quad x_j = j\Delta x, \quad j = 0, 1, \dots, J$$

$$\text{ii) } \Delta t = \frac{T}{N}, \quad \tau_n = n\Delta t, \quad n = 0, \dots, N$$

where  $J = 50$  and  $N = 200$ . The integer  $N$  is chosen large enough so that the time step  $\Delta t$  is much smaller than an estimated differences between two consecutive values of the time switches.

We consider the backward implicit finite difference scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2}$$

which can be written as

$$-\nu U_{j-1}^{n+1} + (1 + 2\nu)U_j^{n+1} - \nu U_{j+1}^{n+1} = U_j^n \quad (3.3.1)$$

where  $\nu = \alpha\Delta t/(\Delta x)^2$ ,  $j = 1, \dots, J - 1$  and  $n = 0, 1, \dots, N - 1$ . The initial condition is

$U_j^0 = 0$  for  $j = 1, \dots, J - 1$ , and the boundary conditions are

$$-\frac{U_1^n - U_0^n}{\Delta x} = \frac{U_J^n - U_{J-1}^n}{\Delta x} = \phi(\tau_n) \quad (3.3.2)$$

for  $n = 0, 1, \dots, N$ . The total mass integral is calculated by the following trapezoidal rule

$$\mu_n = \frac{h}{2} \sum_{j=0}^{N-1} (U_j^{n+1} + U_{j+1}^n). \quad (3.3.3)$$

The numerical experiment is carried out in the following way. We start by setting the flux at  $\phi = 1$  then we solve a tridiagonal system coming out of the difference method. We evaluate the total mass  $\mu_n$  and compare it with the upper threshold  $M = 0.2$ . We move to the next time step while keeping the flux at  $\phi = 1$ , if  $\mu_n < M$ , or switch it to  $\phi = -1$ , if  $\mu_n \geq M$ . At the moment, say  $\tau_{n_1}$ , for some integer  $n_1$ , when the total mass exceeds  $M$  for the first time, we take  $T_1 = \tau_{n_1}$  as an approximation for the first time switch. With  $\phi = -1$ , we move on our solution through the time, as long as  $\mu_n$  does not fall below the threshold  $m = 0.1$ . By the moment, when  $\mu_{n_2} \leq m$ , for some integer  $n_2$ , we set  $T_2 = \tau_{n_2}$ , and we switch the flux back to  $\phi = 1$  at the next step. We keep switching the flux between ( $\phi = 1$ ) and ( $\phi = -1$ ) and calculating the time switches  $T_k$  until the end of the run when  $\tau_n = 10$ .

Table (3.1) shows the times switches  $T_n$ . As we can see there, the difference between any two consecutive time switches tend to 0.95. For the same set of data, figures (3.1) through (3.4) show the concentration versus the space at consecutive time steps. The figures are obtained for different stages, where at each stage the flux is kept constant at the end points. A profile of the concentrations at  $x = 0.5$  for various times is shown in figure (3.5) with the same specified data. Figure (3.6) shows the total mass computed analytically and numerically .

Table 3.1: The Time switches  $T_n$  and the differences  $T_n - T_{n-1}$ . Note the differences between any two consecutive times tends to 0.95.

$n$	$T_n$	$T_n - T_{n-1}$
1	1.9500	1.9000
2	2.9000	0.9500
3	3.8500	0.9500
4	4.8000	0.9500
5	5.7500	0.9500
6	6.7000	0.9500
7	7.6500	0.9500
8	8.6000	0.9500
9	9.5500	0.9500

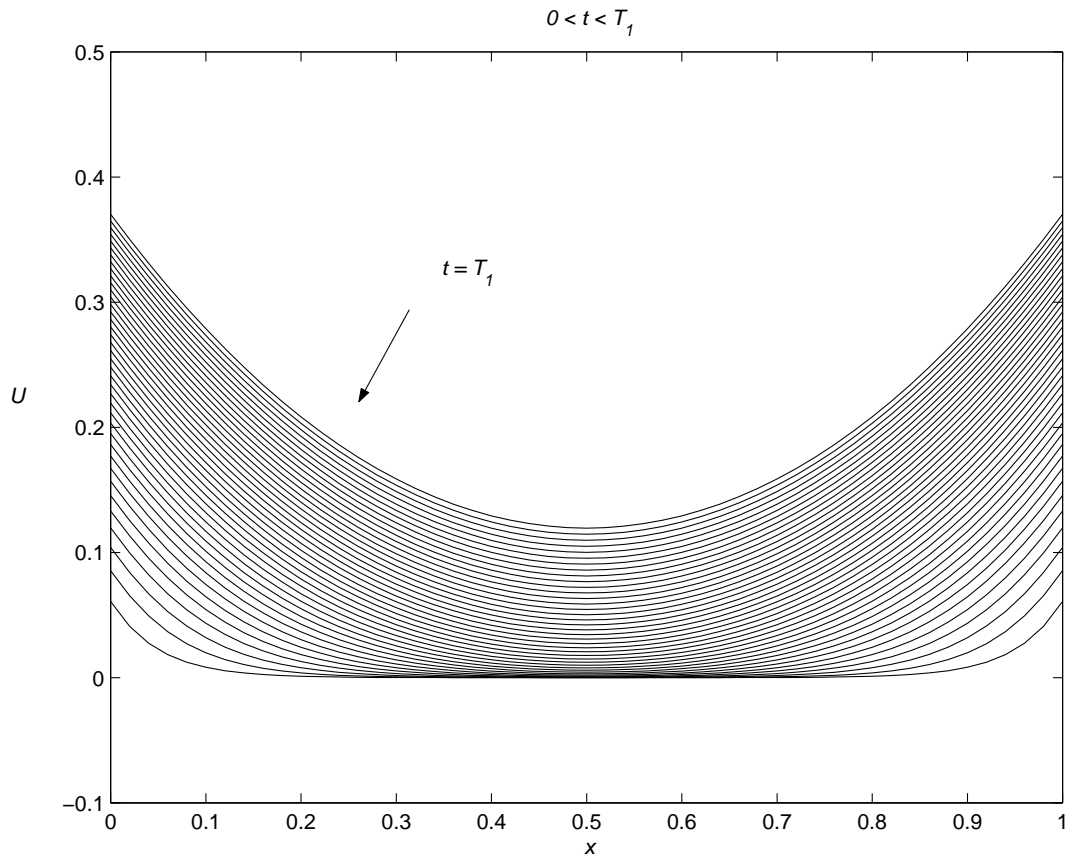


Figure 3.1: The first stage where the flux  $\phi$  is held at 1 at the end points. Each curve shows the concentration profile at various discrete time steps  $\tau_n = n\Delta t$ . As the time goes on, the level of concentrations gets higher

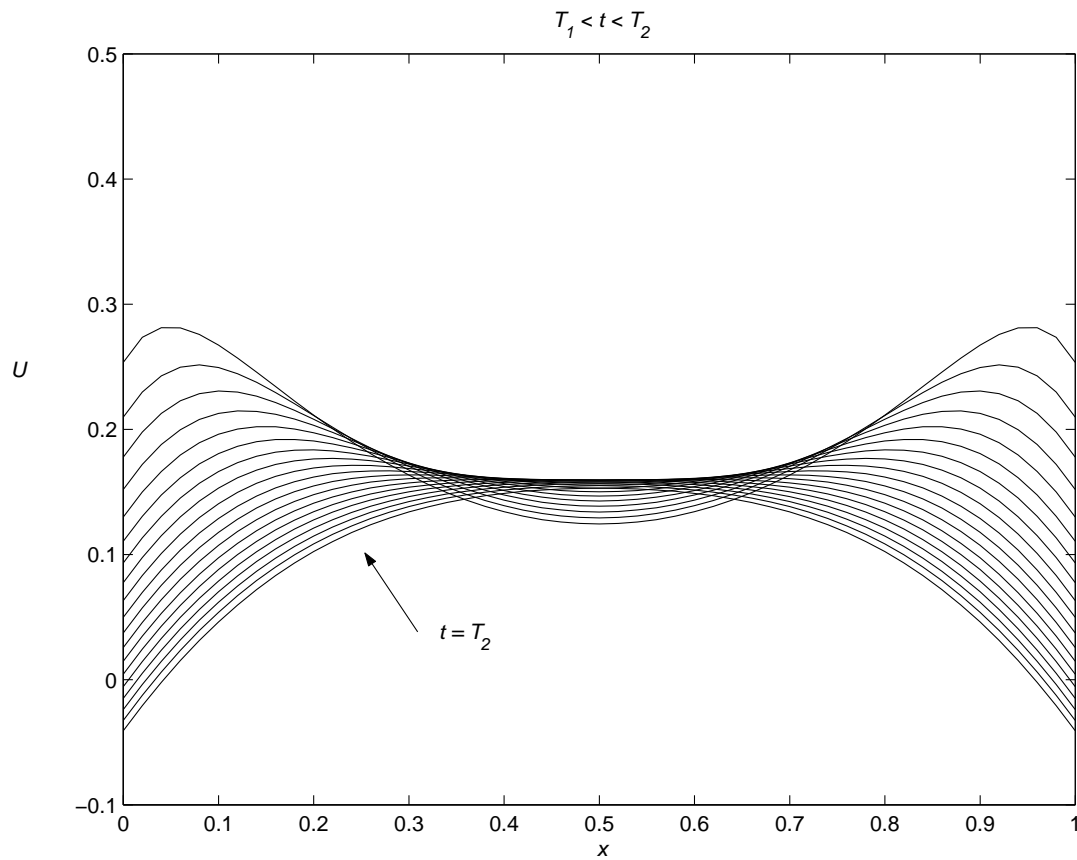


Figure 3.2: The second stage where the flux  $\phi$  is held at -1 at the end points. As the time goes on, the level of concentrations decreases. Notice the fluctuations when the flux is dropped suddenly to -1 at the beginning of the stage.



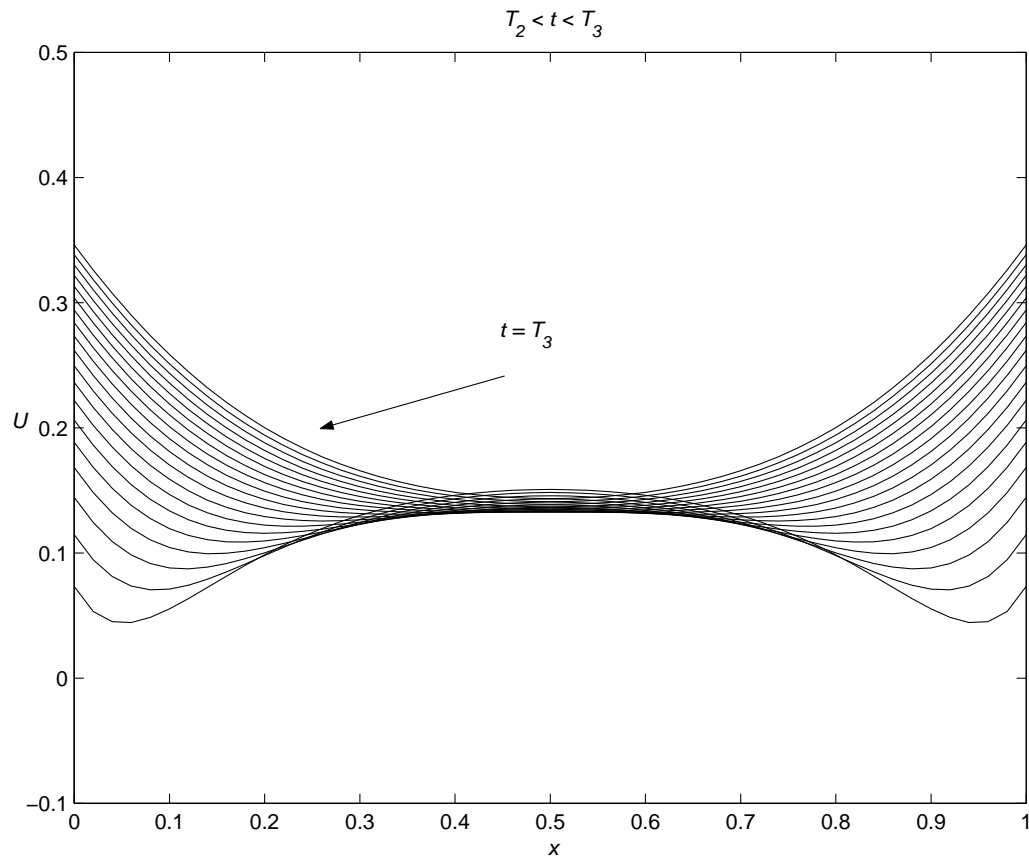


Figure 3.3: The third stage where the flux  $\phi$  is switched to 1 at the end points. Each curve shows the concentration profile at various discrete time steps. Notice the fluctuations due to the sudden change of the flux. After a little while, the concentrations levels increase monotonically.

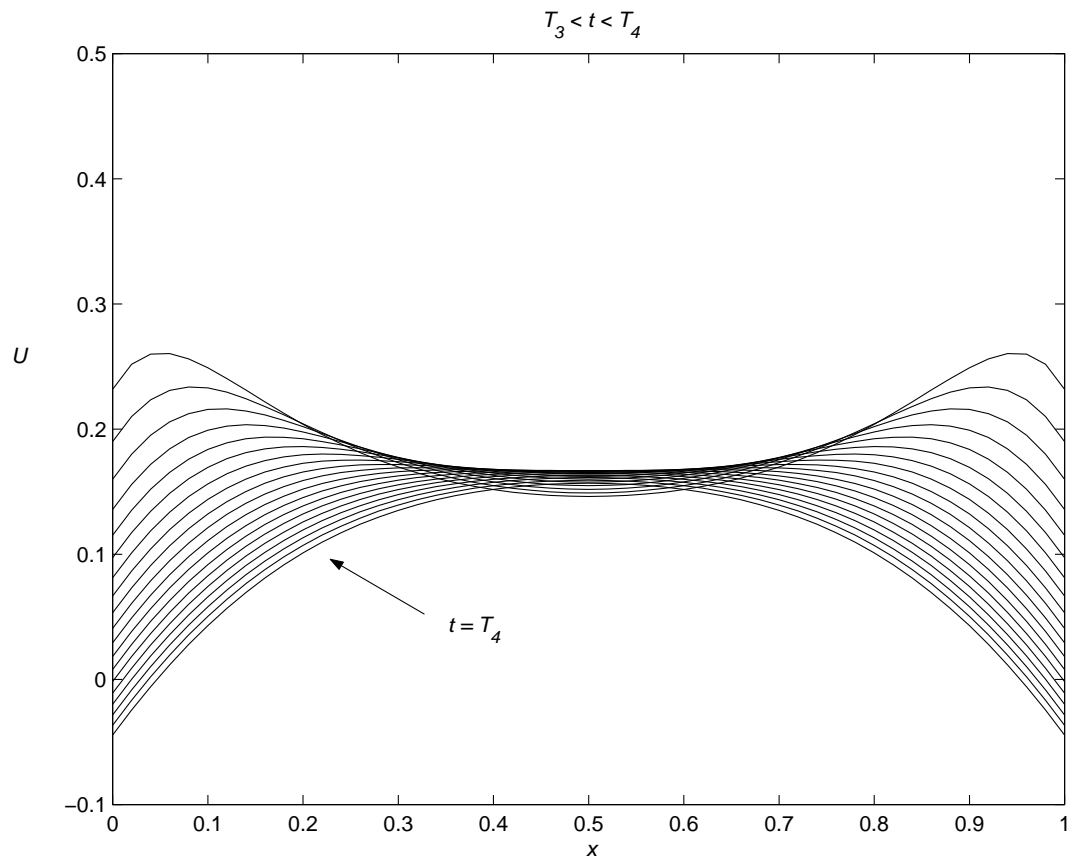


Figure 3.4: The fourth stage where the flux  $\phi$  is switched to -1 at the end points. Notice the similarity with the second stage.

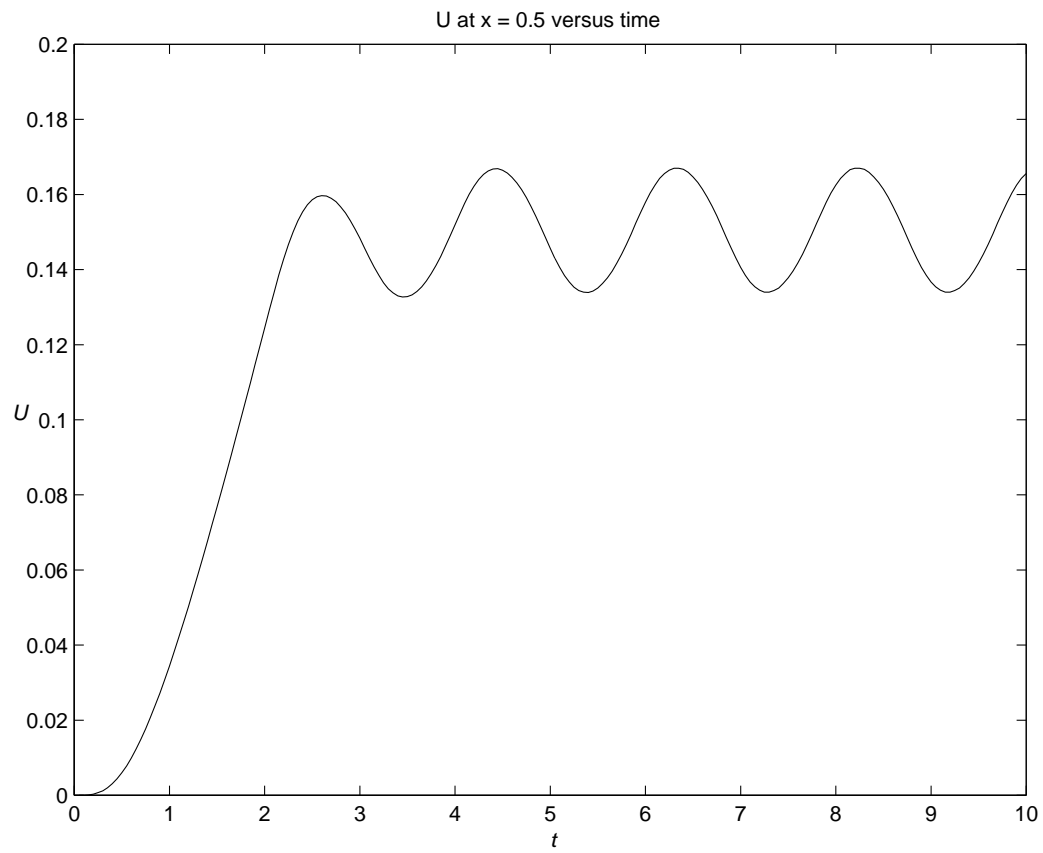


Figure 3.5: The concentration profile  $U$  at  $x = 0.5$  versus the time shows periodic behavior due to the periodic change of the boundary conditions

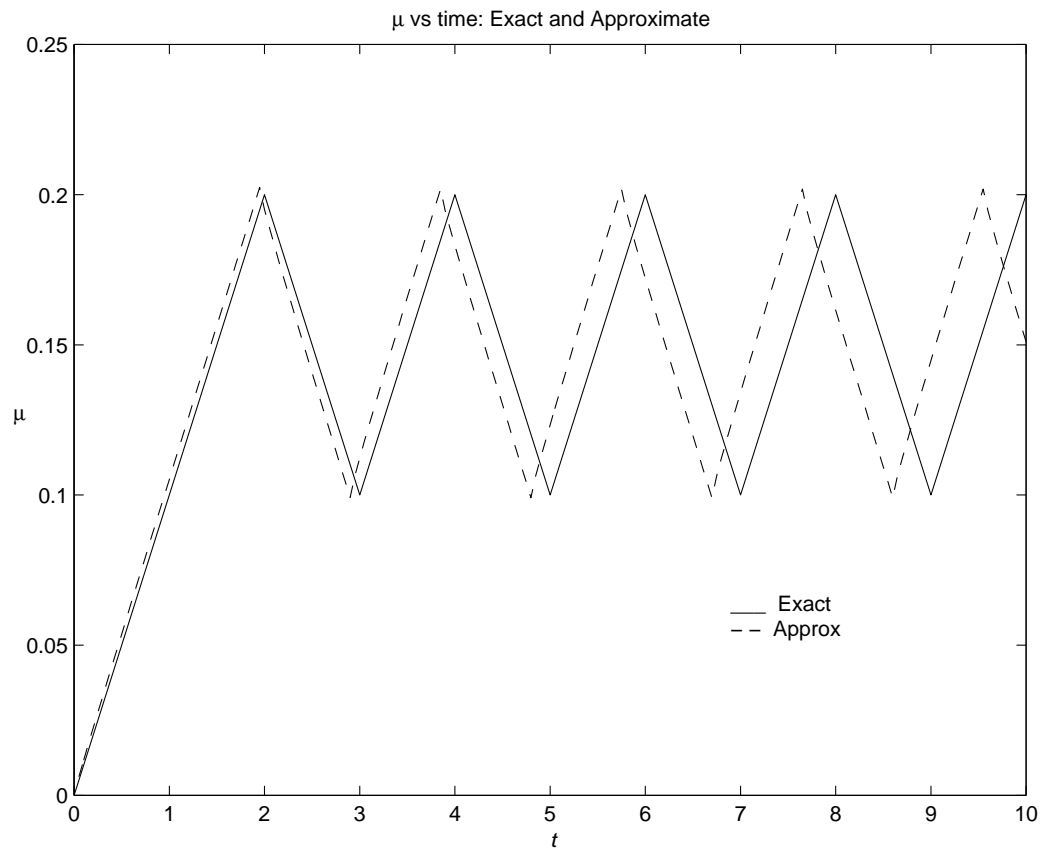


Figure 3.6: The total mass computed analytically and numerically. Note how the error in calculating the time switches accumulates as the time gets large.

## CHAPTER 4

# A BOUNDARY CONTROL PROBLEM WITH A NONLINEAR REACTION TERM

### 4.1 Introduction

In this chapter, we consider the problem

$$\begin{aligned}u_t &= u_{xx} - a(x, t, u)u, & 0 < x < 1, & \quad t > 0 \\-u_x(0, t) &= u_x(1, t) = \phi(t), & t > 0 \\u(x, 0) &= 0, & 0 < x < 1\end{aligned}\tag{4.1.1}$$

where  $a(x, t, u)$  is a continuous function and satisfies the following condition

$$0 < \alpha \leq a(x, t, u) \leq \beta\tag{H1}$$

$(x, t) \in [0, 1] \times [0, T]$  and  $u \in \mathbb{R}$ , and

$$\phi(t) = \begin{cases} 1, & t_{2n} \leq t \leq t_{2n+1} \\ 0, & t_{2n+1} \leq t \leq t_{2n+2} \end{cases}\tag{4.1.2}$$

where  $\{t_n\}$  depends on

$$\mu(t) = \int_0^1 u(x, t) dx \quad (4.1.3)$$

where

$$\begin{aligned} \mu(t_{2n}) &= m, \quad n = 1, 2, \dots \\ \mu(t_{2n+1}) &= M, \quad n = 0, 1, \dots \end{aligned}$$

with  $0 < m < M$ .

## 4.2 Existence of solution

We study the existence of a solution  $u(x, t)$  to (4.1.1) for a given stepwise boundary conditions  $\phi(t)$ . We assume that

$$|ua_u(x, t, u)| \leq C, \quad (\text{H2})$$

uniformly for all  $x, t, u$ , which insures that the source term  $F(x, t, u) = -a(x, t, u)u$  is uniformly Lipschitz with respect to  $u$ , i.e.

$$|F(x, t, u_1) - F(x, t, u_2)| \leq C |u_1 - u_2|,$$

for all  $x, t, u_1, u_2$ . The constants  $C$ 's in the above inequalities or that come in the sequel aren't necessarily the same.

Under certain smoothness conditions on  $u(x, t)$ ,  $a(x, t, u)$ , problem (4.1.1) is equivalent to

$$u(x, t) = 2 \int_0^t [\theta(x, t - \tau) + \theta(1 - x, t - \tau)] \phi(\tau) d\tau + \int_0^t \int_0^1 [\theta(x - \xi, t - \tau) + \theta(x + \xi, t - \tau)] F(\xi, \tau, u(\xi, \tau)) d\xi d\tau. \quad (4.2.1)$$

Let us show that the integral equation (4.2.1) has a solution by considering the operator

$$Hu = 2 \int_0^t [\theta(x, t - \tau) + \theta(1 - x, t - \tau)] \phi(\tau) d\tau + \int_0^t \int_0^1 [\theta(x - \xi, t - \tau) + \theta(x + \xi, t - \tau)] F(\xi, \tau, u(\xi, \tau)) d\xi d\tau,$$

on the set of functions

$$B_\eta = \{u(x, t) \in C([0, 1] \times [0, \eta]), \|u\|_\eta < \infty\},$$

where

$$\|u\|_\eta = \sup_{\substack{0 \leq x \leq 1 \\ 0 \leq t \leq \eta}} |u(x, t)|.$$

The set  $B_\eta$  is a Banach space. The mapping  $H$  maps  $B_\eta$  into itself [16]. Furthermore,

$$\|Hu_1 - Hu_2\|_t \leq Ct \|u_1 - u_2\|_t,$$

which implies

$$\|Hu_1 - Hu_2\|_\eta \leq C\eta \|u_1 - u_2\|_\eta.$$

If we select  $\eta < 1/C$ , then  $H$  is a contraction map on  $B_\eta$ , Thus  $H$  has a unique fixed point  $u \in B_\eta$ , which solves (4.2.1). Since  $F$  is uniformly Lipschitz, the solution  $u$  can be extended on any time interval  $[0, T]$  (see [16]).

### 4.3 Maximum Principle

In this section, we use the maximum principle to prove that problem (4.1.1) has a nonnegative solution. To achieve this we establish the following lemmas.

**Lemma 4.3.1.** *Let  $D = \{(x, t) : 0 < x < 1; 0 \leq t \leq T\}$  and  $a(x, t, u)$  satisfy condition (H1).*

*The solution  $u$  of*

$$\begin{aligned} u_t &= u_{xx} - a(x, t, u)u, & (x, t) \in D \\ u(x, 0) &\geq 0, & 0 < x < 1 \\ -u_x(0, t) &= u_x(1, t) = 1, & 0 < t \leq T \end{aligned} \tag{4.3.1}$$

*is nonnegative on  $\bar{D}$ .*

*Proof.* To prove that  $u(x, t) \geq 0$  in  $\bar{D}$ , let us assume the converse, i.e.  $u(x, t) < 0$  at some point in  $\bar{D}$ . The continuity of  $u(x, t)$  on  $\bar{D}$  implies the existence of a negative minimum in  $\bar{D}$ . If  $\min_{\bar{D}} u = u(0, \bar{t})$ , for some  $0 < \bar{t} \leq T$ , then the boundary condition  $u_x(0, t) = -1$  implies  $u_x < 0$  in neighborhood of  $(0, \bar{t})$ , so  $u(x, \bar{t}) < u(0, \bar{t})$  for some small  $x$ , which contradicts the fact that  $u(0, \bar{t})$  is the minimum.

A similar argument can be used to prove that the minimum can never happen at  $x = 1$ . So,  $u$  has its negative minimum at  $(\bar{x}, \bar{t})$  in the interior of  $D$ . This implies  $u_t(\bar{x}, \bar{t}) \leq 0$  and  $u_{xx}(\bar{x}, \bar{t}) \geq 0$ . Therefore,  $u_t - u_{xx} + au$  is negative at  $(\bar{x}, \bar{t})$ , which is a contradiction.

Thus, we proved the lemma. □



Next, we consider the problem

$$\begin{aligned}
u_t &= u_{xx} - a(x, t, u)u, & (x, t) &\in D \\
u_x(0, t) &= u_x(1, t) = 0 & 0 < t &\leq T \\
u(x, 0) &\geq 0 & 0 < x &< 1
\end{aligned} \tag{4.3.2}$$

and  $a(x, t, u)$  satisfies condition (H1). We establish the following lemma for a closely related problem.

**Lemma 4.3.2.** *For a positive constant  $\gamma$ , the solution  $v(x, t; \gamma)$  of*

$$\begin{aligned}
v_t &= v_{xx} - \gamma v, & (x, t) &\in D \\
v_x(0, t) &= v_x(1, t) = 0 \\
v(x, 0) &> 0
\end{aligned}$$

*is positive for all  $(x, t) \in \overline{D}$  where  $\gamma$  is a positive constant.*

*Proof.* Let  $w = e^{\gamma t}v$ . Then

$$\begin{aligned}
w_t &= w_{xx} & \text{in } D \\
w_x(0, t) &= w_x(1, t) = 0 & t > 0 \\
w(x, 0) &= v(x, 0) > 0, & 0 \leq x \leq 1.
\end{aligned}$$

If  $w \leq 0$ , then  $w$  has a minimum that's not positive either at  $x = 0$  or  $x = 1$  for some  $t = t_0 \in (0, T]$ , which implies by the strong maximum principle [61],  $w_x(0, t_0) > 0$  or  $w_x(1, t_0) < 0$  which is a contradiction. Hence  $w > 0$  which implies  $v > 0$ .  $\square$

**Lemma 4.3.3.** *The solution  $z(x, t, \epsilon)$  of*

$$\begin{aligned} z_t &= z_{xx} && \text{in } D \\ z_x(0, t) &= \epsilon && 0 < t \leq T \\ z_x(1, t) &= -\epsilon && 0 < t \leq T \\ z(x, 0) &= 0 && 0 < x < 1 \end{aligned}$$

*satisfies the inequality*

$$-C\epsilon < z(x, t) \leq 0 \quad \text{in } \bar{D}$$

*where the positive constant  $C$  is a function of  $T$ .*

*Proof.* This is a straightforward application of the representation of the solution  $z(x, t)$ .  $\square$

**Lemma 4.3.4.** *The solution  $u$  of (4.3.2) satisfies the inequality*

$$0 < v(x, t; \beta) \leq u(x, t) \leq v(x, t; \alpha) \quad \text{in } \bar{D}$$

*where  $\alpha$  and  $\beta$  are the lower and upper bound of  $a(x, t, u)$ , respectively.*

*Proof.* First consider  $v(x, t; \beta) + z(x, t; \epsilon)$ . For a fixed  $T$ , we can chose  $\epsilon$  sufficiently small so that  $v + z > 0$  in  $\bar{D}$ . Consider  $w = u - v - z$ . Clearly,  $w$  satisfies

$$\begin{aligned} w_t &= w_{xx} - aw - (a - \beta)v - az && \text{in } D \\ w_x(0, t) &= -\epsilon, && 0 < t \leq T \\ w_x(1, t) &= \epsilon, && 0 < t \leq T \\ w(x, 0) &= 0, && 0 \leq x \leq 1. \end{aligned}$$

Suppose  $w < 0$  somewhere in  $\overline{D}$ . Then the boundary conditions force a negative minimum in  $D$ , where

$$w_t - w_{xx} + aw + (a - \beta)v + az < 0$$

which contradicts the equation

$$w_t - w_{xx} + aw + (a - \beta)v + az = 0 \quad \text{in } D.$$

Thus  $w \geq 0$  which implies that

$$u(x, t) \geq v(x, t, \beta) + z(x, t, \epsilon)$$

for all  $\epsilon > 0$  sufficiently small. Hence

$$u(x, t) \geq v(x, t; \beta).$$

Likewise, by considering  $w = v - z - u$ , the inequality

$$v(x, t; \alpha) \geq u(x, t)$$

follows by a similar argument. □

**Theorem 4.3.5.** *The solution  $u$  of (4.1.1) is nonnegative.*

*Proof.* By applying, successively, Lemma (4.3.1) and (4.3.4) on each time stage where we keep the flux  $u_x$  either zero or one. The result follows. □

## 4.4 Existence of the Time Switches

If we formally differentiate (4.1.3), we obtain

$$\mu'(t) = 2\phi(t) - \int_0^1 a(x, t, u)u dx. \quad (4.4.1)$$

To prove the existence of  $t_1$ , let  $\phi(t) = 1$  for  $t > 0$ . In view of hypothesis (H1), equation (4.4.1) implies the estimate

$$\mu'(t) \geq 2 - \beta \int_0^1 u dx$$

that is

$$\mu'(t) \geq 2 - \beta\mu(t), \quad t \geq 0.$$

By applying Gronwall's inequality, we get

$$\mu(t) \geq \frac{2}{\beta}[1 - e^{-\beta t}].$$

Since  $\mu(t)$  is continuous, then there exists a  $t_1 > 0$  such that

$$\mu(t_1) = M,$$

for any  $0 < M < \frac{2}{\beta}$ .

Next, we prove the existence of  $t_2$  by taking  $\phi(t) = 0$  for  $t > t_1$ . This implies

$$\mu'(t) = - \int_0^1 a(x, t, u)u(x, t)dx, \quad t > t_1.$$

Using the estimate on  $a(x, t, u)$ , we obtain

$$\mu'(t) \leq -\alpha\mu(t), \quad t \geq t_1.$$

Gronwall's inequality implies

$$\begin{aligned}\mu(t) &\leq \mu(t_1)e^{-\alpha(t-t_1)} \\ &= Me^{-\alpha(t-t_1)}, \quad t \geq t_1.\end{aligned}$$

Since  $\mu(t)$  is continuous, then there exists a  $t_2 > t_1$  such that

$$\mu(t_2) = m$$

where  $0 < m < M$ .

For  $t > t_2$ , we take  $\phi(t) = 1$ . This gives the estimate

$$\mu'(t) \geq 2 - \beta\mu(t), \quad t \geq t_2.$$

Using the condition  $\mu(t_2) = m$  and Gronwall's inequality, we get

$$\mu(t) \geq \frac{2}{\beta} - \left(\frac{2}{\beta} - m\right) e^{-\beta(t-t_2)}, \quad t \geq t_2.$$

Note that the coefficient  $\frac{2}{\beta} - m$  is positive, then this implies the existence of  $t_3 > t_2$  such that

$$\mu(t_3) = M.$$

We inductively get for  $t > t_{2n}$  and  $\phi(t) = 1$ ,

$$\mu(t) \geq \frac{2}{\beta} - \left(\frac{2}{\beta} - m\right) e^{-\beta(t-t_{2n})}, \quad t \geq t_{2n}, \quad (4.4.2)$$

which implies the existence of  $t_{2n+1}$  such that  $\mu(t_{2n+1}) = M$ .

Also, for  $t > t_{2n+1}$  and  $\phi(t) = 0$ , we have,

$$\mu(t) \leq Me^{-\alpha(t-t_{2n+1})}, \quad t \geq t_{2n+1}, \quad (4.4.3)$$

which ensures the existence of  $t_{2n+2}$  such that  $\mu(t_{2n+2}) = m$ .

Estimate (4.4.2) implies

$$M = \mu(t_{2n+1}) \geq \frac{2}{\beta} - \left( \frac{2}{\beta} - m \right) e^{-\beta(t_{2n+1}-t_{2n})}$$

which gives rise

$$t_{2n+1} - t_{2n} \leq \frac{1}{\beta} \ln \frac{2 - m\beta}{2 - M\beta}. \quad (4.4.4)$$

Similarly, if we employ (4.4.3), we can get

$$t_{2n+2} - t_{2n+1} \leq \frac{1}{\alpha} \ln \frac{M}{m}.$$

## 4.5 Numerical Example

In this section, we consider a finite difference method to discretize the problem

$$u_t = \alpha u_{xx} - \sin u, \quad 0 < x < 1, \quad 0 < t \leq T$$

$$-u_x(0, t) = u_x(1, t) = \phi(t), \quad 0 < t \leq T$$

$$u(x, 0) = 0, \quad 0 < x < 1$$

where the boundary control function is

$$\phi(t) = \begin{cases} 10, & t_{2n} \leq t \leq t_{2n+1} \\ 0, & \text{elsewhere} \end{cases}$$

and  $\{t_n\}$  depends on

$$\mu(t) = \int_0^1 u(x, t) dx,$$

where

$$\mu(t_{2n}) = 1, \quad n = 1, 2, \dots$$

$$\mu(t_{2n+1}) = 2, \quad n = 0, 1, \dots$$

The time limit and the diffusivity constant are taken as  $T = 40$  and  $\alpha = 0.05$ .

Let's consider the space and time discretization

$$\text{i) } \Delta x = \frac{1}{J}, \quad x_j = j\Delta x, \quad j = 0, 1, \dots, J$$

$$\text{ii) } \Delta t = \frac{T}{N}, \quad \tau_n = n\Delta t, \quad n = 0, \dots, N$$

where  $J = 50$  and  $N = 400$ . The integer  $N$  is chosen large enough so that the time step  $\Delta t$  is much smaller than an estimated differences between two consecutive values of the time switches.

We consider the backward implicit finite difference scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2} - \sin U_j^n$$

which can be written as

$$-\nu U_{j-1}^{n+1} + (1 + 2\nu)U_j^{n+1} - \nu U_{j+1}^{n+1} = U_j^n - \Delta t \sin U_j^n \quad (4.5.1)$$

where  $\nu = \alpha\Delta t/(\Delta x)^2$ ,  $j = 1, \dots, J - 1$  and  $n = 0, 1, \dots, N - 1$ . The initial condition is

$U_j^0 = 0$  for  $j = 1, \dots, J - 1$ , and the boundary conditions are

$$-\frac{U_1^n - U_0^n}{\Delta x} = \frac{U_J^n - U_{J-1}^n}{\Delta x} = \phi(\tau_n) \quad (4.5.2)$$

for  $n = 0, 1, \dots, N$ . The total mass integral is calculated by the following trapezoidal rule

$$\mu_n = \frac{h}{2} \sum_{j=0}^{N-1} (U_j^{n+1} + U_{j+1}^n). \quad (4.5.3)$$

The numerical experiment is carried out in the following way. We start by setting the flux at  $\phi = 10$  then we solve a tridiagonal system coming out of the difference method. We evaluate the total mass  $\mu_n$  and compare it with the upper threshold  $M = 2$ . We move to the next time step while keeping the flux at  $\phi = 10$ , if  $\mu_n < M$ , or switch it to  $\phi = 0$ , if  $\mu_n \geq M$ . At the moment, say  $\tau_{n_1}$ , for some integer  $n_1$ , when the total mass exceeds  $M$  for the first time, we take  $T_1 = \tau_{n_1}$  as an approximation for the first time switch. With  $\phi = 0$ , we move on our solution through the time, as long as  $\mu_n$  does not fall below the threshold  $m = 1$ . By the moment, when  $\mu_{n_2} \leq m$ , for some integer  $n_2$ , we set  $T_2 = \tau_{n_2}$ , and we switch the flux back to  $\phi = 10$  at the next step. We keep switching the flux on ( $\phi = 10$ ) and off ( $\phi = 0$ ) and calculating the time switches  $T_k$  until the end of the run when  $\tau_n = 40$ .

Table (4.1) shows the times switches  $T_n$ . As we can see there, the difference between any two consecutive time switches has a tendency to alternate between 3.8, 3.9 and 1.2. For the same set of data, figures (4.1) through (4.5) show the concentration versus the space at consecutive time steps. The figures are obtained for different stages, where at each stage the flux is kept constant at the end points. A profile of the concentrations at  $x = 0.5$  for various times is shown in figure (4.6) with the same specified data. Figure (4.7) shows the total mass computed through (4.5.3) versus the time. Note the slow increase and the sharp fall in the figure due to the sink term  $\sin U_j^n$ .



Table 4.1: The Time switches  $T_n$  and the differences  $T_n - T_{n-1}$ . Note the differences between any two consecutive times tend to alternate between 1.2 and 3.8 or 3.9.

$n$	$T_n$	$T_n - T_{n-1}$	$n$	$T_n$	$T_n - T_{n-1}$
1	5.2000	5.1000	8	21.6000	1.2000
2	6.4000	1.2000	9	25.5000	3.9000
3	10.2000	3.8000	10	26.7000	1.2000
4	11.4000	1.2000	11	30.6000	3.9000
5	15.3000	3.9000	12	31.8000	1.2000
6	16.5000	1.2000	13	35.6000	3.8000
7	20.4000	3.9000	14	36.8000	1.2000

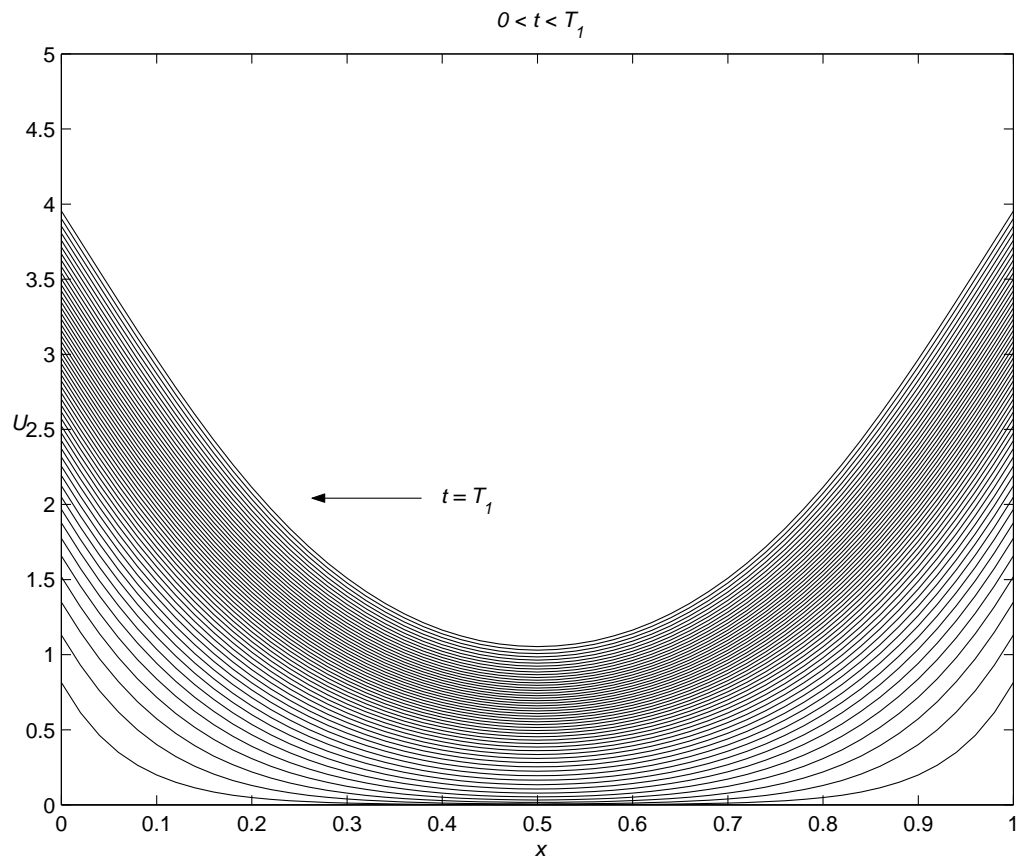


Figure 4.1: The first stage where the flux  $\phi$  is held at 10 at the end points. Each curve shows the concentration profile at various discrete time steps  $\tau_n = n\Delta t$ . As the time goes on, the level of concentrations gets higher

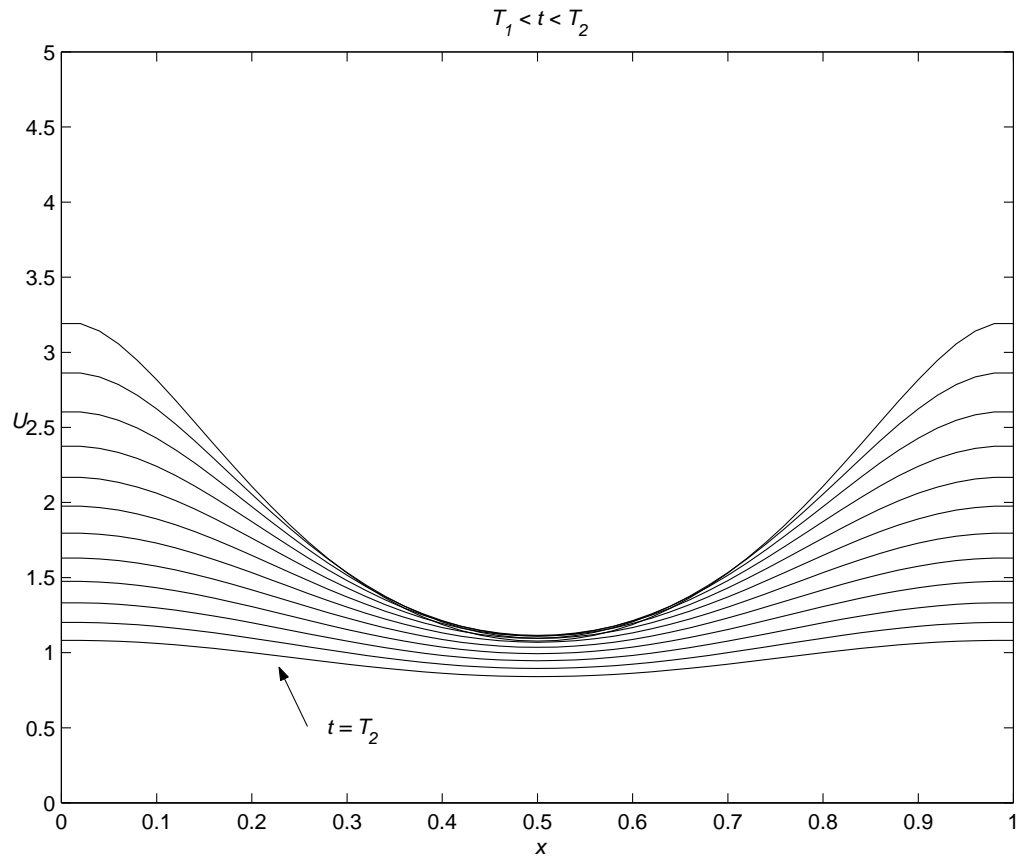


Figure 4.2: The second stage where the flux  $\phi$  is held at 0 at the end points. As the time goes on, the level of concentrations decreases. Notice the fluctuations when the concentration is dropped suddenly to 0 at the beginning of the stage.

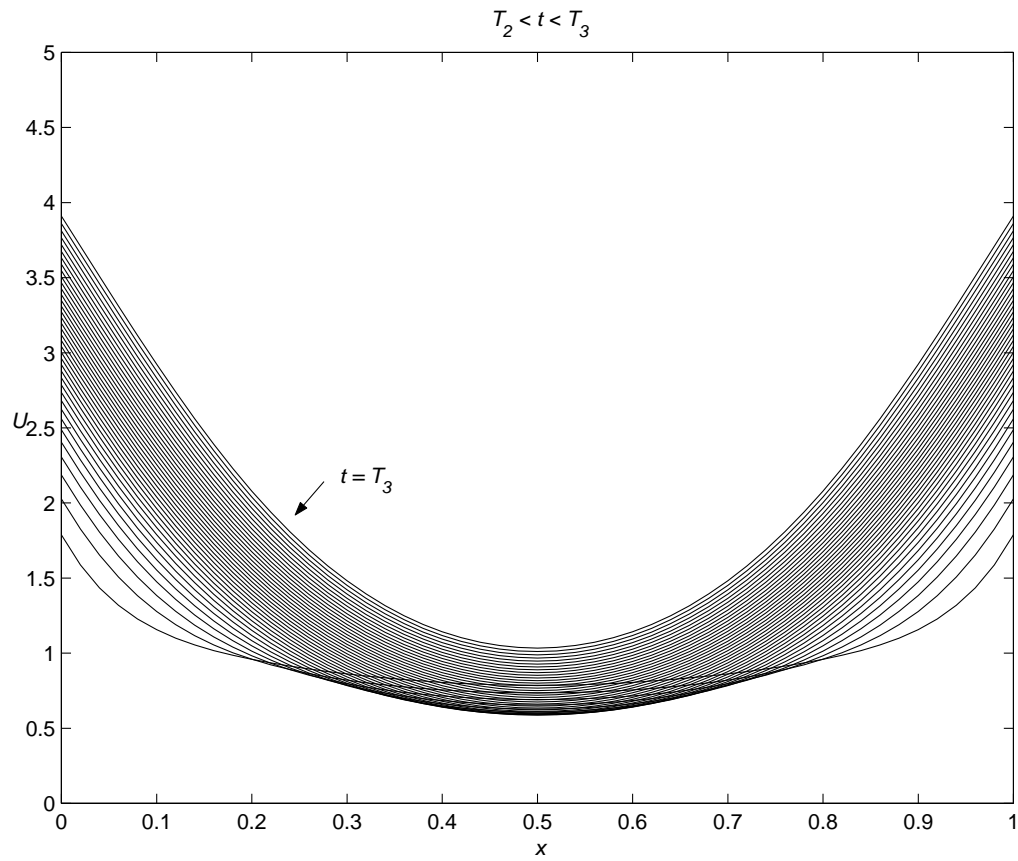


Figure 4.3: The third stage where the flux  $\phi$  is switched to 10 at the end points. Each curve shows the concentration profile at various discrete time steps. Notice the fluctuations due to the sudden change on the concentrations. After a little while, the concentrations levels increase monotonically.

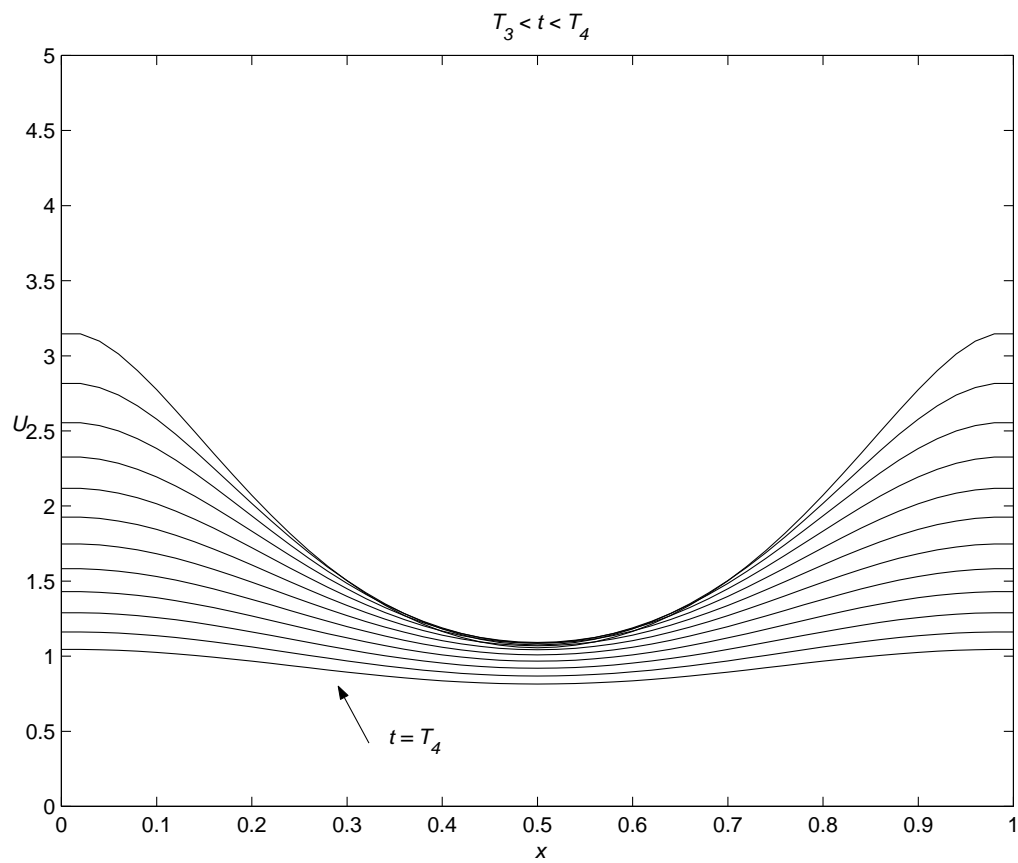


Figure 4.4: The fourth stage where the flux  $\phi$  is switched to 0 at the end points. Notice the similarity with the second stage.

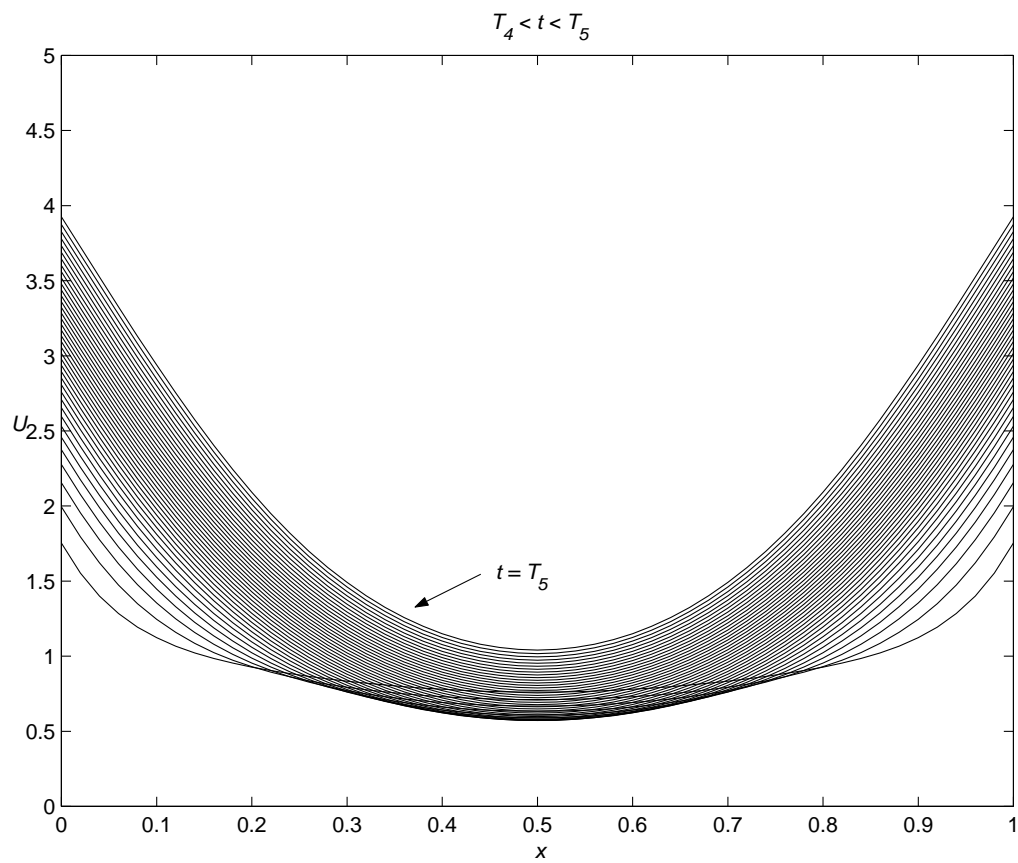


Figure 4.5: The fifth stage where the flux  $\phi$  is switched to 10 at the end points. Notice the similarity with the third stage.

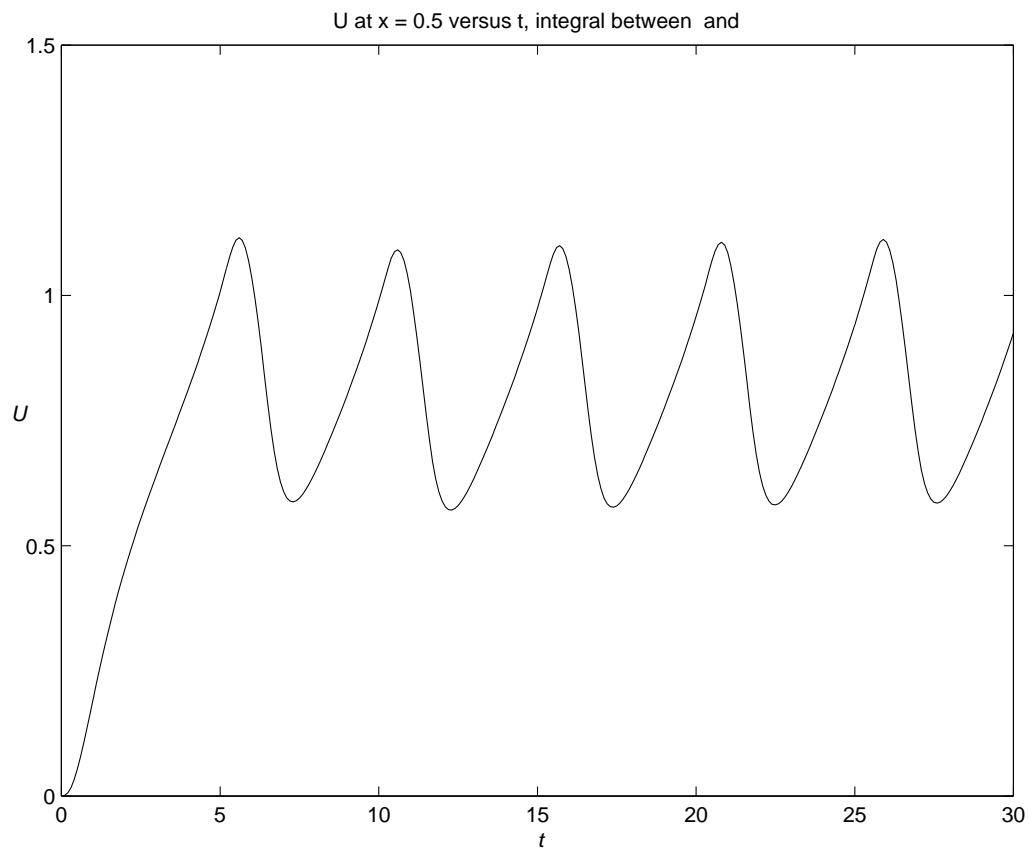


Figure 4.6: The concentration profile  $U$  at  $x = 0.5$  versus the time shows periodic behavior due to the periodic change of the boundary conditions

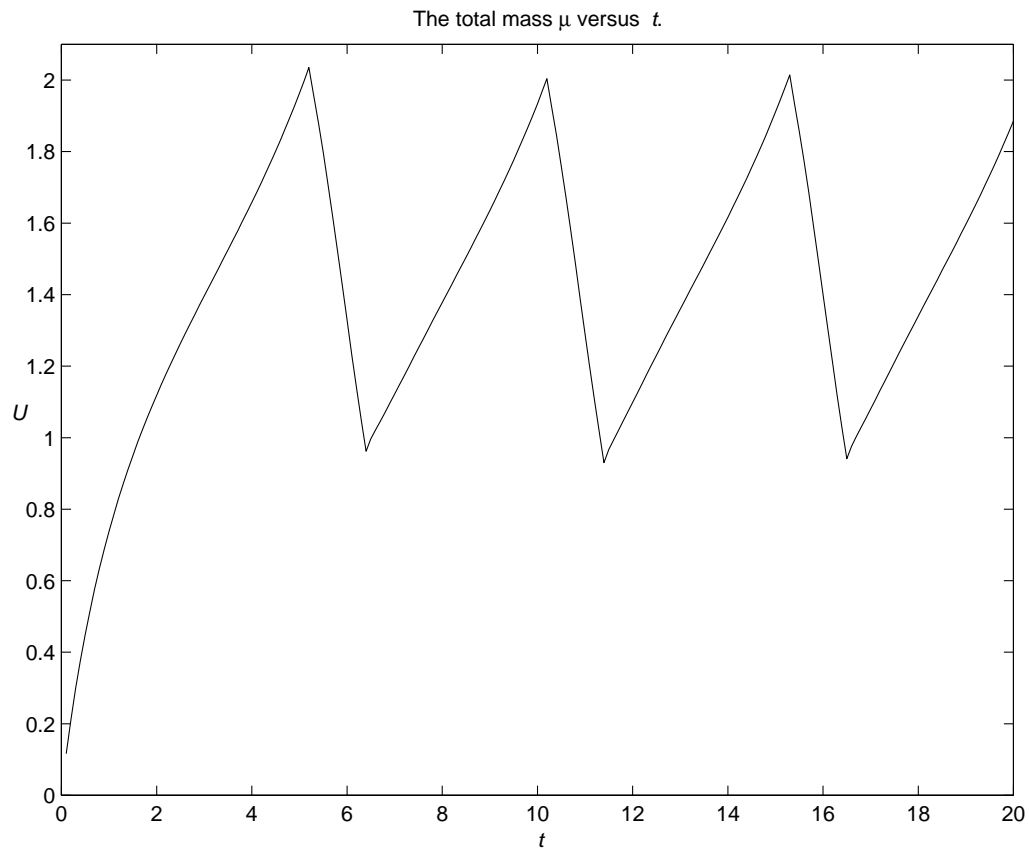


Figure 4.7: The total mass computed via equation (4.5.3) versus the time. Note the slow increase and the sharp fall in the figure due to the sink term  $\sin U_j^n$ .



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