FINITE DIFFERENCE SCHEME FOR NUMERICAL SOLUTION OF A SINGLE PARTICLE PYROLYSIS MODEL

Mr. Damrongsak Yambangwai

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วิธีผลต่างอันตะสำหรับผลเฉลยเชิงตัวเลขของแบบจำลองการสลายตัวของอนุภาคเดี่ยวเมื่อถูกความร้อนสูง

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วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
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แบบจำลองเชิงคณิตศาสตร์ที่ใช้ศึกษาการสลายตัวของอนุภาคเมื่อถูกความร้อนสูงในงานวิจัยนี้ประกอบด้วยสมการสองสมการคือสมการอนุรักษ์มวลและสมการอนุรักษ์พลังงาน ภายใต้สมมติฐานที่ว่าอนุภาคมีรูปร่างเป็นทรงกลมทำให้สามารถแปลงปัญหานี้โดยใช้พิกัดทรงกลมได้ เนื่องจากเป็นการแปลงปัญหานี้ไปสู่ระบบพิกัดทรงกลม จึงจำเป็นที่จะต้องกำหนดเงื่อนไขขอบที่เหมาะสมที่จุดศูนย์กลางของอนุภาค วิทยานิพนธ์นี้จะเสนอวิธีผลต่างอันตะภายใต้กฎการอนุรักษ์สำหรับหาผลเฉลยเชิงตัวเลขและศึกษาอิทธิพลของเงื่อนไขขอบในกรณีสองกรณีที่จุดศูนย์กลางของอนุภาคที่มีต่อผลเฉลยของปัญหานี้ ในงานวิจัยนี้ได้แสดงให้เห็นว่าผลเฉลยเชิงตัวเลขที่คำนวณได้สอดคล้องกับข้อมูลของผลเฉลยเชิงตัวเลขของปัญหาการสลายตัวของขี้เลื่อย (Wagenaar, Kuipers, Prin, and Van Swaaij, 1994) ซึ่งได้จากวิธีเชิงตัวเลขอีกวิธีหนึ่ง

สาขาวิชาคณิตศาสตร์ ลายมือชื่อนักศึกษา.....

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DAMRONGSAK YAMBANGWAI : FINITE DIFFERENCE SCHEME FOR NUMERICAL SOLUTION OF A SINGLE PARTICLE PYROLYSIS MODEL

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PYROLYSIS/ CONSERVATIVE DISCRETIZATION/ CONSERVATIVE FORM/ CONSERVATIVE FINITE DIFFERENCE SCHEME

The mathematical model is used to simulate the pyrolysis reaction within the particle. This model consists of the coupled equation for conservation of mass and energy. Under the assumption that the particle has a spherical shape, we transform the problem by using the spherical coordinates system. Due to this transformation, we have to specify the proper boundary condition at the center of the particle. In this thesis, we present the finite difference method based on the conservation law to find the numerical solution of the problem. We study the influence of two kinds of boundary conditions at the center of the particle on the solution of the problem. The results of numerical simulation presented in this thesis are in good agreement with the numerical solutions of the pyrolysis problem of pine pinaster sawdust (Wagenaar, Kuipers, Prin, and Van Swaaij (1994)) obtained from another pproach.

School of Mathematics Signature of Student _____

Academic Year 2002 Signature of Advisor _____

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Damrongsak Yambangwai

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Chapter I

Introduction

1.1 Background and Objective

Pyrolysis is the thermal decomposition of organic material through the application of heat in the absence of oxygen. When the organic material is exposed to external heating in the absence of oxygen environment, a number of different processes proceed simultaneously in the reactor. Heat is first transferred to the particle surface by means of convection from gas flow. The temperature reaches the pyrolysis level, and thermal decomposition of the biomass occurs. Heat is transferred inside the particle by conduction and through the pores by volatile convection.

The mathematical model of the pyrolysis process within the particle is presented by coupled equations for conservation of mass and energy (Josette and Richard, 1998). For the gaseous chemical species, the equations for conservation of mass include both flow divergence terms and source terms proportional to the products of partial densities and reaction rate constant. For the solid and liquid species, only the source terms are included. The reaction is assumed to be irreversible and of *first order*. For modelling conservation of energy, all species are assumed to be in local thermal equilibrium state in the particle. The partial internal energy of each chemical species is assumed to be proportional to the product of its partial density, its specific heat at constant volume, and the local temperature. The rate of change of local internal energy present as the sum of

1. Heat release rates proportional to the chemical reaction constant multiplied by source terms.

2. Conduction proportional to the local gradient of temperature multiplied by the effective thermal conductivity.

3. Convection of heat via the flow of gaseous species.

In the present research, the mathematical model of the pyrolysis process used is simplified by the following assumptions

1. The particle is solid and homogeneous.

2. The particle has spherical shape with the assumption of spherical symmetry.

The problem to be solved is one dimensional in case of these assumption.

There are many papers such as Wagenaar, Kuipers, Prin, and Van Swaaij (1994), Buckmaster, Smooke and Giovangigli (1993), Weber, Mercer, and Sidhu (2000) describing the mathematical model of the pyrolysis process under these assumptions. The model of pyrolysis of biomass was applied in a parametric study of the effect of initial reactor temperature, heating rate, initial particle size, and conversion times in the pyrolysis of spherical biomass.

This thesis will offer and study the numerical method to find the approximate solution for the mathematical model of the pyrolysis process. The study of the influence of different numerical boundary conditions on the approximate solution are the main target of the present thesis. The data on the pyrolysis of pine pinaster sawdust in the rotating cone reaction (Wagenaar, Kuipers, Prin, and Van Swaaij, 1994) has been used to test the numerical algorithm used.

1.2 Notations and Terminology

This section provides main notations and information to make the thesis self-sufficient.

1.2.1 The Reaction Order

The relationship between the reaction rate (velocity, V) and the concentration is called the rate law (Mathews, Van Holde, and Ahern, 1994). In general terms the rate may be written

$$V = k[A]^{\alpha}[B]^{\beta},$$

where $[A]$ is the concentration of product A, $[B]$ is the concentration of product B, α is the order with respect to $[A]$ and β is the order with respect to $[B]$. The reaction is αth order in A, βth order in B and $\alpha + \beta th$ order overall.

First order reaction. For an irreversible reaction, $A \rightarrow B$, the reaction rate (velocity, V) is given by

$$V = \frac{d[B]}{dt}.$$

For the rate of appearance of the substrate A, these equations are equally valid for this reaction, so we can write

$$V = \frac{d[B]}{dt} = -\frac{dA}{at} = K_1[A],$$

where K_1 is called the reaction rate constant and for this reaction has the unit of $(second)^{-1}$. This type of a reaction is called a first order reaction, because its rate depends on the first power of the reactant concentration.

Second order reaction. A reaction of this type typically occurs when two molecules come together to form products. A simple example is

$$A + A = P,$$

with a the reaction rate constant given by K_2. The rate of such a reaction is proportional to the second power of the concentration of the reactant. Therefore,

$$V = \frac{-d[A]}{dt} = K_2[A]^2.$$

Here K_2 is the second-order rate constant.

1.2.2 Mass Conservation for the Pyrolysis of Biomass Particles

The conservation of mass for the pyrolysis of solid species of biomass particle under the assumption that the reaction is irreversible and of first order (Josette and Richard, 1998) was interpreted in terms of a simple first order differential equation

$$\frac{\partial C}{\partial t} = -KC,$$

where C is the concentration, t is time, K is the reaction rate constant. In the general case the reaction rate constant is given by the Arrhenius kinetic equation $K = Ae^{\frac{-E}{RT}}$ (see James Birk (1991)) where A is the rate frequency constant, E is the activation energy, R is the universal gas constant, and T is the absolute temperature. This equation describes the rate of mass loss.

1.2.3 The Spherical Coordinate System

The spherical coordinate system is the most important coordinate systems besides the Cartesian coordinate system. Many physical problem possess spherical symmetry. In such cases, the governing differential equations should be solved in the spherical coordinate system.

Difficulties arise when numerically solving boundary problems of heat transfer in complex computational domains. We have thus far considered problems in a rectangular domain (a regular computational domain). The simple

approach to the solution of problems in irregular domain is to use curvilinear coordinates in which the computational domain becomes regular.

In the physics of heat, much attention is paid to spherical coordinates when modelling thermal fields in spherical domains.

The relation between cartesian and spherical coordinates is illustrated in Figure 1.1 the inverse transformation is specified by

$$x = r\sin\theta\cos\phi,\ y = r\sin\theta\sin\phi,\ and\ z = r\cos\theta.$$

where $r \geq 0$, $0 \leq \phi \leq 2\pi$, and $0 \leq \theta \leq \pi$.

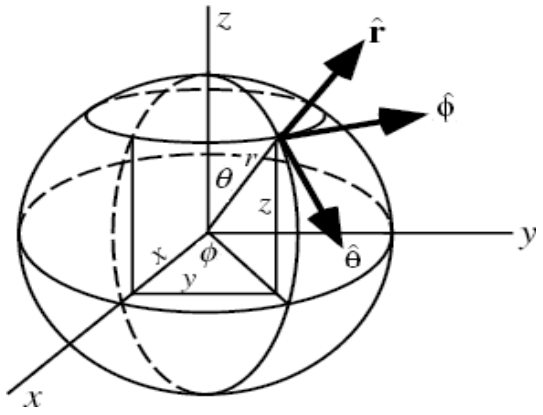

Figure 1.1: Spherical coordinate system

The gradient operator ∇f in spherical coordinate system is given by

$$\nabla f = i_r f_r + i_\theta \frac{1}{r} f_\theta + i_\phi \frac{1}{r\sin\theta} f_\phi,$$

where i_r, i_θ, and i_ϕ are unit vectors in the r, θ, and ϕ directions, respectively. The Laplacian operator $\nabla^2 f$ in spherical coordinate system is given by

$$\nabla^2 f = f_{rr} + \frac{2}{r} f_r + \frac{1}{r^2} f_{\theta\theta} + \frac{1}{r^2\tan\theta} f_\theta + \frac{1}{r^2\sin^2\theta} f_{\phi\phi}.$$

1.2.4 Conservation of Energy for the Pyrolysis of a Biomass Particle

The conservation of energy for the pyrolysis of solid species of biomass particle (Josette and Richard, 1998) is presented by this form

$$c_p C \frac{\partial T}{\partial t} = -\nabla \cdot q + f, \tag{1.1}$$

where C is the concentration of biomass, c_p is the specific heat capacity, t is time, T is temperature, λ is the thermal conductivity, $q = -\lambda \nabla T$ is the heat conduction flux, and $f = KCH_r$ represents the heat release rates, H_r is the term due to the chemical reaction, K is the reaction rate constant. This equation allows us to determine the temperature at different points of a solid particle. Equation (1.1) is known as heat equation. In the spherical coordinate system, equation (1.1) can be written as

$$\begin{aligned} c_p C \frac{\partial T}{\partial t} = & \frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda r^2 \frac{\partial T}{\partial r}\right) + \frac{1}{r \sin\theta}\frac{\partial}{\partial \theta}\left(\lambda \sin\theta \frac{1}{r}\frac{\partial T}{\partial \theta}\right) \\ & + \frac{1}{r \sin\theta}\frac{\partial}{\partial \phi}\left(\lambda \frac{1}{\sin\theta}\frac{\partial T}{\partial \phi}\right) + f. \end{aligned} \tag{1.2}$$

In case of spherical symmetry equation (1.2) becomes

$$c_p C \frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda r^2 \frac{\partial T}{\partial r}\right) + f. \tag{1.3}$$

1.2.5 Finite Difference Methods

We use the finite difference methods to solve the boundary value problem by discretizing the continuous solution domain and approximating the exact derivatives by finite difference approximation and substitute into the boundary value problem to obtain the finite difference equation. Four basic properties of the finite difference equation for the boundary value problem were identified as consistency, order of approximation, stability, convergence.

Consistency, Order of Approximation, Stability, and Convergence

Let us consider the boundary value problem

$$Lu = f. \tag{1.4}$$

and a finite difference scheme which corresponds to the boundary value problem (1.4)

$$L_h u^{(h)} = f^{(h)}. \tag{1.5}$$

Here, L is a differential operator, $L : \mathcal{C} \to F$, $\mathcal{C}$ and $\mathcal{F}$ are sets of sufficiently smooth functions, L_h is a difference operator, $L_h : \mathcal{C}_h \to F_h$, $\mathcal{C}_h$ and $\mathcal{F}_h$ are sets of grid functions, u is a solution of boundary value problem (1.4), and u_h is a solution of the finite difference scheme (1.5). Let us introduce the projection operator $\mathcal{P}_h$, $\mathcal{P}_h : \mathcal{C} \to \mathcal{C}_h$.

$$\begin{array}{rcl} L & : \mathcal{C} & \to F \\ & \downarrow \mathcal{P}_h & \\ L_h & : \mathcal{C}_h & \to F_h \end{array}$$

Definition (convergence) We say that a solution $u^{(h)}$ of the finite difference scheme (1.5) converges to the solution of boundary value problem (1.4) u if

$$\left\| \mathcal{P}_h(u) - u^{(h)} \right\|_{\mathcal{C}_h} \xrightarrow[h \to 0]{} 0.$$

where $\|\cdot\|_{\mathcal{C}_h}$ is norm on $\mathcal{C}_h$.

Definition (convergence with order m) We say that the finite difference scheme (1.5) converges with order m if

$$\left\| \mathcal{P}_h(u) - u^{(h)} \right\|_{\mathcal{C}_h} \leq c h^m,$$

where the constants c and m do not depend on h.

The study of the convergence of the finite difference scheme involves two fundamental properties of the finite difference scheme, consistency and stability. To define these properties we introduce a new grid function called residual

$$\psi^h = f^{(h)} - L_h\left(\mathcal{P}_h(u)\right).$$

Here we assume that u is a solution of boundary value problem (1.4).

Definition (consistency) The finite difference scheme defined by (1.5) is called consistent with the boundary value problem (1.4) if

$$\left\|\psi^h\right\|_{F_h} = \left\|f^{(h)} - L_h\left(\mathcal{P}_h(u)\right)\right\|_{F_h} \xrightarrow[h \to 0]{} 0,$$

where u is a solution of boundary value problem and $\|\cdot\|_{F_h}$ is norm on $\mathcal{F}_h$.

Definition (order of approximation l) The finite difference scheme defined by (1.5) is called a $l-th$ order approximation of boundary value problem (1.4) if

$$\left\|\psi^h\right\|_{F_h} = \left\|f^{(h)} - L_h\left(\mathcal{P}_h(u)\right)\right\|_{F_h} \leq ch^l,$$

where u is a solution of boundary value problem and the constants c and l do not depend on h and $f^{(h)}$.

Definition (stability) The finite difference scheme defined by (1.5) is called stable, if there exist $\delta > 0$ and $h_0 > 0$ such that for arbitrary $h < h_0$ and for a discrete function $\varphi^{(h)} \in F_h$ with property $\left\|\varphi^h\right\|_{F_h} < \delta$ solution of the finite difference scheme

$$L_h z^h = f^{(h)} + \varphi^{(h)},$$

exists, unique, and satisfies the inequality

$$\left\|z^{(h)} - u^{(h)}\right\|_{\mathcal{C}_h} \leq c\left\|\varphi^h\right\|_{F_h}.$$

Theorem (Lax equivalence theorem) The finite difference scheme is stable and consistent iff it is convergent.

Technics to Estimate the Order of Convergence

Let $error_1$ and $error_2$ be errors which correspond to grid systems with $N1$ nodes for mesh size h and $N2$ nodes for mesh size $\frac{h}{2}$, respectively. The definition of convergence with order m yields

$$error_1 = \| \mathcal{P}_h(u) - u^h \|_{\mathcal{C}_h} \leq ch^m,$$

and

$$error_2 = \| \mathcal{P}_{\frac{h}{2}}(u) - u^{\frac{h}{2}} \|_{\mathcal{C}_h} \leq c(\frac{h}{2})^m.$$

Dividing $error_1$ by $error_2$ we obtain

$$\frac{error_1}{error_2} \simeq 2^m.$$

Taking the natural logarithm on both sides, we get an approximate value for the rate of convergence

$$m \simeq \frac{ln(\frac{error_1}{error_2})}{ln2}. \tag{1.6}$$

Chapter II

Mathematical Model

2.1 Mathematical Model of Pyrolysis

The mathematical model of pyrolysis studied here consists of the coupled equations for conservation of mass and energy (Josette and Richard, 1998). The conservation of mass for the pyrolysis of a homogeneous solid of biomass particle under the assumption that the reaction be irreversible and of first order is

$$\frac{\partial C}{\partial t} = -KC, \text{ in } \Omega, \tag{2.1}$$

where C is the concentration of biomass, t is time, $K = Ae^{\frac{-E}{RT}}$ is the pyrolysis reaction rate constant, A is a rate frequency constant, E is the activation energy, R is the universal gas constant, and T is the temperature. The conservation of energy for the pyrolysis of a homogeneous solid particle of biomass is presented by the following equation

$$c_p C\frac{\partial T}{\partial t} = -\nabla \cdot q + f, \text{ in } \Omega, \tag{2.2}$$

where c_p is the specific heat capacity, T is temperature, $q = -\lambda\nabla T$ is the heat conduction flux, λ is the thermal conductivity, and $f = KCH_r$ represents the heat release rates, H_r is term due to the chemical reaction, K is the reaction rate constant. The first term on the right hand side is the thermal conductivity and the final term represents the capacity of the internal heat sources, for example: due to the chemical reaction.

For the sake of simplicity, let us required that the particle has a spherical shape with the assumption of spherical symmetry. Due to this assumption all unknown functions depend on r and t only. The system of equations (2.1), (2.2) can be rewritten in the spherical coordinate system as

$$\frac{\partial C}{\partial t} = -KC,\ 0 \le r \le r_p,\ 0 \le t \le \overline{t}, \tag{2.3}$$

$$c_p C \frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda r^2 \frac{\partial T}{\partial r}\right) + f,\ 0 < r < r_p,\ 0 \le t \le \overline{t}, \tag{2.4}$$

where r is the radial coordinate of the spherical coordinate system with origin at the center of the particle, and r_p is the radius of the particle. In these equations, concentration, temperature, the reaction rate constant, and heat release rates respectively are function of r and t. All other quantities are constants.

In order to specify a unique solution of the system of partial differential equations (2.3), (2.4) it is necessary to formulate boundary and initial conditions. The boundary condition at the particle center expresses a zero heat conduction flux from the particle center

$$\lim_{r\to 0}\left(-\lambda r^2 \cdot \frac{\partial T}{\partial r}\right) = 0,\ 0 \le t \le \overline{t}. \tag{2.5}$$

Three kind of the boundary conditions at the particle surface can be considered

$$T\mid_{r=r_p} = T_f,\ 0 \le t \le \overline{t}, \tag{2.6}$$

or

$$\lambda r^2 \cdot \frac{\partial T}{\partial r}\mid_{r=r_p} = T_f,\ 0 \le t \le \overline{t}, \tag{2.7}$$

or

$$-\lambda r^2 \cdot \frac{\partial T}{\partial r}\mid_{r=r_p} = \alpha \cdot \left(T\mid_{r=r_p} - T_f\right),\ 0 \le t \le \overline{t}. \tag{2.8}$$

Here α is the heat transfer coefficient. The boundary condition (2.8) simulates convective heat transfer between the surface of the solid particle and the environment which has the temperature T_f. The temperature and density fields have to

be specified at the initial moment of time

$$T(r,0) = T_0,\ 0 \le r \le r_p, \tag{2.9}$$

$$C(r,0) = C_0,\ 0 \le r \le r_p, \tag{2.10}$$

where T_0 is the initial temperature and C_0 is the initial concentration.

2.2 Dimensionless Problem

The method of dimensionless problem allows us to reduce the total number of parameters of the mathematical model, which is extremely important for numerical modelling. We can investigate the influence of a group of parameters on the solution by studying the influence of a smaller group of parameters on this solution.

The problem (2.3), (2.4) with initial and boundary conditions is characterized by the following set of parameters r_p, T_0, C_0, c_p, λ, T_f, H_r, α, E, A. The solution of the pyrolysis problem depends on ten parameters namely $T = T(r,t;r_p,T_0,C_0,c_p,\lambda,T_f,H_r,\alpha,E,A)$ and $C = C(r,t;r_p,T_0,C_0,c_p,\lambda,T_f,H_r,\alpha,E,A)$.

We should first choose characteristic quantities for scaling in order to pass to a dimensionless problem. This choice is not always obvious and depends on the specific problem. It is reasonable to use common techniques of scaling and call these methods as "making a problem dimensionless "(Samarskii and Vabishchevich (1995)).

In the considered problem we can take the length of radius of the particle r_p for scaling the spatial variable r. We use the same letters for dimensionless quantities but supply them with primes. Then $r = r_p r'$, where r' is a dimensionless variable. We can take the temperature of the medium T_f for scaling the

temperature, i.e. $T = T_f T'$, where T' is dimensionless temperature. We can take the concentration of the medium C_0 for scaling concentration, i.e. $C = C_0 C'$, where C' is dimensionless. Similarly, let $t = t_0 t'$, where a typical time interval t_0 is not yet defined.

We substitute these formulae into PDE (2.3) - (2.5) with boundary condition (2.8) and formulate problem in dimensionless variables, For simplicity, We will drop the apostophe in the non-dimensional variables.

$$
\begin{aligned}
&\frac{\partial C}{\partial t} = -\gamma_1 P C,\ 0 \le r \le 1, 0 \leqslant t \leqslant \Gamma, \\
&C\frac{\partial T}{\partial t} = \gamma_3 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) - \gamma_4 P C,\ 0 < r < 1, 0 \leqslant t \leqslant \Gamma, \\
&\lim_{r\to 0} r^2 \frac{\partial T}{\partial r} = 0,\ 0 \le t \le \Gamma, \\
&-\frac{\partial T}{\partial r} = \gamma_5 (T-1),\ r = 1,\ 0 \le t \le \Gamma, \\
&C(r,0) = 1, \\
&T(r,0) = \gamma_6,
\end{aligned}
\tag{2.11}
$$

where $\gamma_1 = At_0$, $P = e^{\frac{\gamma_2}{T}}$, $\gamma_2 = -\dfrac{E}{RT_f}$, $\Gamma = \dfrac{\bar{t}}{t_0}$, $\gamma_3 = \dfrac{\lambda t_0}{(r_p)^2 c_p C_0}$, $\gamma_4 = \dfrac{At_0 H_r}{c_p T_f}$, $\gamma_5 = \dfrac{\alpha r_p}{\lambda_s}$, and $\gamma_6 = \dfrac{T_0}{T_f}$.

The following set of deterministic parameters is used in [1]: the rate frequency constant A is $10^{13}\ s^{-1}$, the specific heat capacity c_p is 1335 $J \cdot kg^{-1} \cdot K^{-1}$, the thermal conductivity λ is 0.105 $W \cdot m^{-1} \cdot K^{-1}$, the activation energy E is 183,300 $J \cdot mol^{-1}$, the particle radius r_p varies between $70 - 125\ \mu m$, the temperature of gas the phase T_f is 873 K, the initial temperature T_0 is 298 K, the initial density ρ_0 is 500 $kg \cdot m^{-3}$, the heat of the pyrolysis reaction rate H_r is 500 $kJ \cdot kg^{-1}$.

The problem in dimensionless variables (2.11) is characterized by six dimensionless parameters, namely γ_1, γ_2, γ_3, γ_4, γ_5, and γ_6. Note that we have only six rather than ten parameters for the problem, i.e. $T = T(r, t; \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6)$

and $C = C(r, t; \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6)$. We reduce the total number of parameters of the mathematical model. Therefore we can investigate the influence of the group of parameters on the solution by studying the influence of the smaller group of the parameter on this solution. The dimensionless variables allow us to separate small and large parameters of the problem. It is in dimensionless variables that we can compare terms with one another. The small (large) parameters are used to construct simplified mathematical model and analyze the problem asymptotically (i.e. find an approximate solution).

Chapter III

Discretization and Analysis of Numerical Scheme

The basic difficulty in solving the problem (2.11) for C and T is that this system of equations is nonlinear. There are two different ways to overcome this difficulty. The first one is to solve the system of coupled equations by means of the iterative method. The second one is to uncouple the equations by "freezing" the nonlinear terms in small time intervals. For example, we can assume that the nonlinear terms do not change due to the time step. In this case, we do not need to find simultaneous solutions. It is possible to split this problem into two problems. In each time step from t_p to t_{p+1}, we can solve the following two problems to find a solution.

The first one is the Cauchy problem

$$\begin{aligned} &\frac{\partial C}{\partial t} = -\gamma_1 P(T(r,t_p))C, \quad 0 \le r \le 1,\ t_p \le t \le t_{p+1}, \\ &C(r,t_p) \text{ is known,} \end{aligned} \tag{3.1}$$

where $p = 0, 1, ..., [W]-1$, $W = \dfrac{\Gamma}{\Delta t}$, and $T(r,t_p)$ is known.

The second is the initial boundary value problem

$$\begin{aligned} &C(r,t_{p+1})\frac{\partial T}{\partial t} = \frac{\gamma_3}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) + \gamma_4 P\left(T(r,t_p)\right)C(r,t_{p+1}), 0 < r < 1, t_p \le t \le t_{p+1}, \\ &\lim_{r\to 0} r^2\frac{\partial T}{\partial r} = 0, \\ &-\frac{\partial T}{\partial r} = \gamma_5(T-1), \quad r = 1, \\ &T(r,t_p) \text{ is known,} \end{aligned} \tag{3.2}$$

where $p = 0, 1, ..., [W] - 1$, $W = \dfrac{\Gamma}{\Delta t}$, and $C(r, t_{p+1})$ is known.

3.1 Finite Difference Scheme for the Approximate Solution of the Continuity Equation

Let us consider a finite difference scheme to obtain the numerical solution of problem (3.1) on the grid $\omega_h = \{x_i / x_i = i\Delta x, i = 0, 1, ..., N\}$ where $\Delta x = 1/N$. We apply the Modified Euler method (Hoffman (1992)) to problem (3.1) and we get

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -\gamma_1 P(T_i^n) \left(\frac{C_i^{n+1} + C_i^n}{2} \right), \quad i = 0, ..., N,$$
$$C(i, 0) = U, \quad i = 0, ..., N, \tag{3.3}$$

where $n = 0, 1, ..., [W]-1$, $W = \dfrac{\Gamma}{\Delta t}$, the value $P(T_i^n)$ is known, and U is constant.

3.2 Finite Difference Scheme for the Approximate Solution of the Energy Equation

In this section, we introduce the important material to construct the formulation of finite difference scheme for problem (3.2).

3.2.1 Conservative Form

The terms conservative form, conservation law form, and divergence form are all synonymous. The conservative form has the property that the coefficients of the derivative terms are either constant or if variable, their derivative appears nowhere in the equation. Normally for the PDEs that represent a physical conservation statement, this means that the divergence of a physical quantity can be identified in the equation. An example is the conservation form of steady

state diffusion of u in a one dimensional case (John, Tannehill, Dale, Anderson, Richard, Pletcher (1978))

$$\frac{d}{dx}\left(H(x)\frac{du}{dx}\right) = 0, \tag{3.4}$$

where H is the diffusion coefficient. A nonconservative form would be

$$H\frac{d^2u}{dx^2} + \frac{dH}{dx}\frac{dT}{dx} = 0. \tag{3.5}$$

As a second example, we consider the one-dimensional heat equation. The conservative form of this equation is

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(G\frac{\partial T}{\partial x}\right) + Q, \tag{3.6}$$

where $T = T(x,t)$ is temperature, $G = G(x)$ is the conductivity coefficient, and $Q(x,t)$ is the volume heat source. The nonconservative form would be

$$\frac{\partial T}{\partial t} = G\frac{\partial^2 T}{\partial x^2} + \frac{\partial G}{\partial x}\frac{\partial T}{\partial x} + Q. \tag{3.7}$$

A finite difference formulation based on a PDE in nonconservative form may lead to numerical difficulties in situations where the coefficients are discontinuous. It was shown by John, Tannehill, Dale, Anderson, Richard, and Pletcher (1978) that the finite difference formulation of equation (3.5) diverges if the conductivity coefficient H is discontinuous.

3.2.2 Conservative Discretization

Let us consider the one-dimensional heat equation (3.6) in the conservative form with a central difference applied to the stencil of Figure 3.1. The following discretized equation is obtained at point i

$$\left(\frac{\partial T}{\partial t}\right)_i = \frac{\left(G\frac{\partial T}{\partial x}\right)_{i+\frac{1}{2}} - \left(G\frac{\partial T}{\partial x}\right)_{i-\frac{1}{2}}}{\Delta x} + Q_i. \tag{3.8}$$

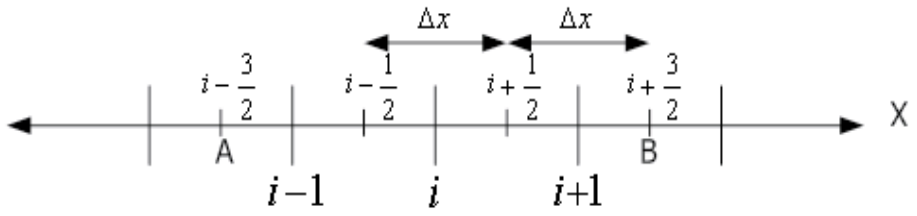

Figure 3.1: Subdivision of the one dimensional space into mesh cell.

The same discretization applied to point $(i+1)$ will give

$$\left(\frac{\partial T}{\partial t}\right)_{i+1} = \frac{\left(G\frac{\partial T}{\partial x}\right)_{i+\frac{3}{2}} - \left(G\frac{\partial T}{\partial x}\right)_{i+\frac{1}{2}}}{\Delta x} + Q_{i+1}, \tag{3.9}$$

and for $(i-1)$,

$$\left(\frac{\partial T}{\partial t}\right)_{i-1} = \frac{\left(G\frac{\partial T}{\partial x}\right)_{i-\frac{1}{2}} - \left(G\frac{\partial T}{\partial x}\right)_{i-\frac{3}{2}}}{\Delta x} + Q_{i-1}. \tag{3.10}$$

The sum of these three equations is a consistent discretization of the conservation law for the cell $AB \equiv \left(i-\frac{3}{2}, i+\frac{3}{2}\right)$

$$\frac{\left(\frac{\partial T}{\partial t}\right)_{i+1} + \left(\frac{\partial T}{\partial t}\right)_{i} + \left(\frac{\partial T}{\partial t}\right)_{i-1}}{3} - \frac{(Q_{i+1} + Q_i + Q_{i-1})}{3} = \frac{\left(G\frac{\partial T}{\partial x}\right)_{i+\frac{3}{2}} - \left(G\frac{\partial T}{\partial x}\right)_{i-\frac{3}{2}}}{3\Delta x}. \tag{3.11}$$

On the left side, we have an approximation of $\dfrac{\partial T}{\partial t}$ on the interval $\left(i-\frac{3}{2}, i+\frac{3}{2}\right)$. Since the flux contributions at the internal points $i-\frac{1}{2}$ and $i+\frac{1}{2}$ have cancelled out in the right hand side, this is sometimes called the " telescoping property "for the flux terms (Mikhail Shashkov (1996)).

3.2.3 Construction of Conservative Finite Difference Scheme

Basic differential equations are derived by applying conservation laws (in the integral form) to elementary volumes and then tending these volumes to zero. This passage to the limit gives the differential form of the conservation laws. The method of finite difference is actually the inverse transition from the differential model to the difference model. It is logical to require that the conservation laws be satisfied after this transition. Difference scheme that express the conservation laws on a grid are called conservative finite difference scheme. The conservation laws for the whole grid should be an algebraic conclusion of the difference equation.

When constructing conservative finite difference scheme, it is logical to start with conservation (balance) laws for separate cell of difference grid. This method of constructing conservative finite difference scheme is called the integro interpolation method.

Let us consider the one dimensional heat equation on a bounded interval $[0, 1]$ whose temperature $T(x, t)$ depends on time and varies in only one direction, say, along the x coordinate, thermal conductivity $G(x)$ varies with position and $Q(x, t)$ represents the capacity of the internal heat sources. The conservation law of energy has the following conservative form

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(G(x)\frac{\partial T}{\partial x}\right) + Q(x,t), \qquad 0 < x < 1, 0 < t < \Gamma. \tag{3.12}$$

We impose the boundary conditions

$$\lim_{x\to 0} G(x)\frac{\partial T}{\partial x} = 0, \tag{3.13}$$

$$T(1,t) = M, \tag{3.14}$$

where $G(x) \geq 0$ and $G(x) = 0$ if $x = 0$, and the initial condition

$$T(x, 0) = T_0. \tag{3.15}$$

Next we will show how the integro interpolation method is applied for constructing a conservative finite difference scheme for a conservative form of one-dimensional heat equation (3.12). Let us denote the heat flux $q = G(x)\dfrac{\partial T}{\partial x}$. We construct the difference scheme on the grid $\omega_h = \{x_i / x_i = i\Delta x, i = 0, 1, ..., N\}$ where $\Delta x = 1/N$. We integrate the one dimensional heat equation (3.12) over the interval $x_{i-\frac{1}{2}} \leq x \leq x_{i+\frac{1}{2}}$ to get

$$\begin{aligned} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial T}{\partial t} dx &= \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(G\frac{\partial T}{\partial x}\right) dx + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} Q dx \\ &= q_{i+\frac{1}{2}} - q_{i-\frac{1}{2}} + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} Q dx. \end{aligned} \tag{3.16}$$

The quantity $q_{i-\frac{1}{2}}$ is the amount of heat coming through the cross section $x_{i-\frac{1}{2}}$ and $q_{i+\frac{1}{2}}$ is the amount heat outgoing through the section $x_{i+\frac{1}{2}}$. The unbalance of this flux is due to the distributes sources (the right hand side).

Integration of the one-dimensional heat equation (3.12) over a finite number of control interval intervals $x_{i-\frac{1}{2}} \leq x \leq x_{i+\frac{1}{2}}$, $i = 1, 2, ..., N-1$ yields a set of discretized conservation equation involving fluxes of the transported T through the boundary of control intervals. To ensure conservation of T for the whole solution domain the flux of T leaving a control interval across a certain boundary must be equal to the flux of T entering the adjacent control interval through the same boundary. To achieve this, the flux through a common face must be represented in a consistent manner (by one and the same expression) in adjacent control intervals.

For the next level of integration, we take advantage of the mean-value theorem to estimate integrals. The mean-value theorem assures us that for a

continuous function $f(y)$,

$$\int_{y}^{y+\Delta y} f(y)dy = f(\bar{y})\Delta y, \tag{3.17}$$

where $\bar{y}$ is some value of y in the interval $y \leq \bar{y} \leq y + \Delta y$. Any value of $\hat{y}$ on this interval will provide an approximation to the integral, and we can write

$$\int_{y}^{y+\Delta y} f(y)dy \approx f(\hat{y})\Delta y \qquad y \leq \hat{y} \leq y + \Delta y. \tag{3.18}$$

We use the mean-value theorem to further simplification of equation (3.16). We select x_i on the left hand and right hand side as the location within the intervals of integration at which to evaluate the integrand and multiply by Δx, equation (3.16) can be written as

$$\left(\frac{\partial T}{\partial t}\right)_i = \frac{1}{\Delta x}\left(q_{i+\frac{1}{2}} - q_{i+\frac{1}{2}}\right) + Q_i. \tag{3.19}$$

Let us integrate the expression $q = G(x)\dfrac{\partial T}{\partial x}$ over the interval $x_{i-1} \leq x \leq x_i$ and get

$$T_i - T_{i-1} = \int_{x_{i-1}}^{x_i} \frac{q}{G(x)}dx \approx q_{i-\frac{1}{2}} \int_{x_{i-1}}^{x_i} \frac{1}{G(x)}dx.$$

Let us denote $a_i = 1/\displaystyle\int_{x_{i-1}}^{x_i} \frac{1}{G(x)}dx$. So we get $q_{i-\frac{1}{2}} \approx a_i(T_i - T_{i-1})$, $q_{i+\frac{1}{2}} \approx a_{i+1}(T_{i+1} - T_i)$. After we substituting these equations into equation (3.19), this equation becomes

$$\left(\frac{\partial T}{\partial t}\right)_i = \frac{1}{\Delta x}\left(a_{i+1}T_{i+1} - (a_{i+1} + a_i)T_i + a_i T_{i-1})\right) + Q_i. \tag{3.20}$$

Let us introduce the following notations

$$T_i^{\sigma} = (1-\sigma)T_i^n + \sigma T_i^{n+1}, \tag{3.21}$$

$$t^{\sigma} = (1-\sigma)t^n + \sigma t^{n+1}, \tag{3.22}$$

$$Q_i^\sigma = Q(x_i, t^\sigma). \tag{3.23}$$

Then using the integro interpolation method, we get the following conservative finite difference scheme for

$$\begin{aligned}\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{\Delta x}\left(a_{i+1}T_{i+1}^\sigma - (a_{i+1} + a_i)T_i^\sigma + a_i T_{i-1}^\sigma\right) \\ + Q_i^\sigma, \quad i = 1, 2, ..., N-1,\end{aligned} \tag{3.24}$$

or

$$\begin{aligned}\frac{T_i^{n+1} - T_i^n}{\Delta t} = (1-\sigma)\frac{\left(a_{i+1}T_{i+1}^n - (a_{i+1} + a_i)T_i^n + a_i T_{i-1}^n\right)}{\Delta x} \\ + \sigma\frac{\left(a_{i+1}T_{i+1}^{n+1} - (a_{i+1} + a_i)T_i^{n+1} + a_i T_{i-1}^{n+1}\right)}{\Delta x} \\ + Q(x_i, t^\sigma), \quad i = 1, 2, ..., N-1.\end{aligned} \tag{3.25}$$

The Approximation of Boundary Condition

Let us now consider the case of the boundary condition (3.13). We use the integro interpolation method to construct the finite difference approximation of this boundary condition. To ensure that conservation of T for the whole solution domain is satisfied, we have to require that the flux of T leaving a control interval $[\frac{\Delta x}{2}, \frac{3\Delta x}{2}]$ across a boundary $x = \frac{\Delta x}{2}$ must be equal to the flux of T entering the control interval $[0, \frac{\Delta x}{2}]$ through the same boundary. To achieve this we should integrate equation (3.12) over the interval $0 \le x \le \frac{\Delta x}{2}$ (see Figure 3.2) to get.

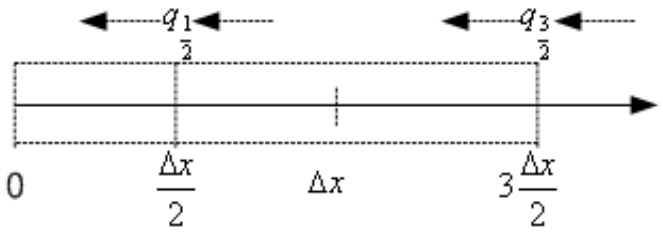

Figure 3.2: Subdivision over the interval $0 \le x \le \frac{\Delta x}{2}$

$$\int_0^{\frac{\Delta x}{2}} \frac{\partial T}{\partial t} dx = \int_0^{\frac{\Delta x}{2}} \frac{\partial}{\partial x}\left(G\frac{\partial T}{\partial x}\right) dx + \int_0^{\frac{\Delta x}{2}} Q dx$$

$$= q_{\frac{1}{2}} - q_0 + \int_0^{\frac{\Delta x}{2}} Q dx. \tag{3.26}$$

As we use the mean value theorem to simplify equation (3.26), we select points $x = 0$ on the left and right hand sides as the location within the intervals of integration at which to evaluate the integrand and multiply by $\frac{\Delta x}{2}$, equation (3.26) can be written as

$$\left(\frac{\partial T}{\partial t}\right)_0 = \frac{2}{\Delta x}\left(q_{\frac{1}{2}} - q_0\right) + Q_0. \tag{3.27}$$

The flux q_0 is equal to zero because of condition (3.13). Equation (3.27) becomes

$$\left(\frac{\partial T}{\partial t}\right)_0 = \frac{2}{\Delta x} q_{\frac{1}{2}} + Q_0,$$

and

$$\left(\frac{\partial T}{\partial t}\right)_0 = \frac{2}{\Delta x} a_1 (T_1 - T_0) + Q_0. \tag{3.28}$$

where $a_1 = 1/\int_0^{\Delta x} \frac{1}{G(x)} dx$.

By using the notation (3.21)-(3.23), equation (3.28) becomes

$$\frac{T_0^{n+1} - T_0^n}{\Delta t} = \frac{2}{\Delta x} a_1 (T_1^\sigma - T_0^\sigma) + Q_0^\sigma.$$

or

$$\frac{T_0^{n+1} - T_0^n}{\Delta t} = \frac{2}{\Delta x} a_1 ((1-\sigma)(T_1^{n+1} - T_0^{n+1}) + \sigma(T_1^n - T_0^n)) + Q_0^\sigma. \tag{3.29}$$

For the Dirichlet condition (3.14), we have

$$T_N^{n+1} = M. \tag{3.30}$$

Order of Approximation of the Finite Difference Scheme

Now let us investigate the error which is a difference between the solution of the discrete one dimensional heat equation and the projections of the solution of the one dimensional heat equation by the discrete equation (3.25) on the solution of the differential problem

$$Z_i^n = T_i^n - (\mathcal{P}_h^n T)_i^n = T_i^n - T(x_i, t^n).$$

To obtain the formula for the error, we express T_i^n from the previous equation as follows:

$$T_i^n = T(x_i, t^n) + Z_i^n, \tag{3.31}$$

and substitute the formula (3.31) into equation (3.25) for the difference equation

$$\begin{aligned}\frac{Z_i^{n+1} - Z_i^n}{\Delta t} = (1-\sigma)&\frac{(a_{i+1}Z_{i+1}^n - (a_{i+1}+a_i)Z_i^n + a_i Z_{i-1}^n)}{\Delta x} \\ &\sigma\frac{(a_{i+1}Z_{i+1}^{n+1} - (a_{i+1}+a_i)Z_i^{n+1} + a_i Z_{i-1}^{n+1})}{\Delta x} \\ &+ \varphi_i^n, \quad i = 1, ..., N-1,\end{aligned}$$

where φ_i^n is the residual:

$$\begin{aligned}\varphi_i^n = (1-\sigma)&\frac{a_{i+1}T(x_{i+1}, t^n) - (a_{i+1}+a_i)\,T(x_i, t^n) + a_i T(x_{i-1}, t^n)}{\Delta x^2} \\ &+ \sigma\frac{a_{i+1}T(x_{i+1}, t^{n+1}) - (a_{i+1}+a_i)\,T(x_i, t^{n+1}) + a_i T(x_{i-1}, t^{n+1})}{\Delta x^2} \\ &+ Q(x_i, t^\sigma) - \frac{T(x_i, t^{n+1}) - T(x_i, t^n)}{\Delta t}, \quad i = 1, ..., N-1.\end{aligned}$$

That is, we can separate the truncation error related to the space and time discretization, and the residual is the sum of the truncation error for the conduction term and for the first time derivative and for the function Q. By making the Taylor expansion to this formula, we can see that for ($\sigma \neq 0.5$), the truncation error is $O(\Delta x^2, \Delta t)$. For ($\sigma = 0.5$), the truncation error is $O(\Delta x^2, \Delta t^2)$ (Mikhail Shashkov (1996)).

Order of Approximation of Boundary Condition

Let us consider the order of approximation of the boundary condition. We consider the order of approximation only on equation (3.29). We substitute the formula (3.31) into equation (3.29) for the difference equation

$$\frac{Z_0^{n+1} + Z_0^n}{\Delta t} = \frac{2}{\Delta x} a_1((1-\sigma)(Z_1^{n+1} - Z_0^{n+1}) + \sigma(Z_1^n - Z_0^n)) + \chi,$$

where χ is the residual:

$$\chi = \frac{2}{\Delta x} a_1((1-\sigma)(T(\Delta x, t^{n+1}) - T(0, t^{n+1})) + \sigma(T(\Delta x, t^n) - T(0, t^n)) + Q(0, t^\sigma) - \left(\frac{T_0^{n+1} + T_0^{n+1}}{\Delta t}\right).$$

We can separate the truncation error related to the space and time discretization. Making the Taylor expansion to this formula we can see that for ($\sigma \neq 0.5$), the truncation error is $O(\Delta x, \Delta t)$. For ($\sigma = 0.5$), the truncation error is $O(\Delta x, \Delta t^2)$.

Stability of the Finite Difference Scheme

Let us consider the fully explicit finite difference scheme for equation (3.12) with variable coefficient $G(x) \geq 0$. Now to investigate stability, we use the method of frozen coefficients. Let us take arbitrary an inner point $\tilde{x}\ \epsilon\ [0, 1]$. We will " freeze "the coefficient $G(x) = G(\tilde{x})$ in some neighborhood of point $\tilde{x}$. The method of frozen coefficients together with the von Neumann method (Hoffman (1992)) gives us the following stability condition

$$\Delta t \leq \Delta x^2 / \left(2 \max_{0 \leq x \leq 1} G(x)\right). \tag{3.32}$$

It is well known that in the case of $\sigma \geq \frac{1}{2}$ the scheme is unconditionally stable (Hoffman (1992)) and in case of $\sigma = \frac{1}{2}$ we have the Crank - Nicholson approximation.

3.2.4 Conservation Laws and the Iterative Process

Here we want to consider the important question relating to the implementation of the finite difference schemes. Suppose a conservative finite

difference scheme is constructed, and the system of linear equation is solved by an iteration method. The result of the iteration process is some discrete function which satisfies the equations related to the finite difference scheme with some accuracy. Consequently, even if the finite difference scheme is conservative, the solution obtained by the iterative method may not satisfy the conservation law. Then the important question is how much the magnitude of the resulting energy imbalances depends on the accuracy of the iteration process, and how much it depends on the parameter of the finite difference scheme itself (e.g., on the time and space steps).

Let us consider the example of a nonconservative iteration process. For the purpose of this demonstration, we consider the Neumann problem for the one dimensional heat equation.

$$\begin{aligned} &\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \qquad 0 < x < 1, \\ &\frac{\partial T}{\partial x} \mid_{x=0} = \zeta_1(t), \ \frac{\partial T}{\partial x} \mid_{x=1} = \zeta_2(t), \\ &T \mid_{t=0} = T_0(x), \end{aligned}$$

where ζ_1, ζ_2 and T_0 are given function.

The amount of heat Q contained in the system at the instant of time t is given by

$$Q(t) = \int_0^1 T(x,t)dt.$$

From the statement of this problem, we get

$$\frac{dQ}{dt} = \zeta_2(t) - \zeta_1(t). \tag{3.33}$$

This equation expresses the fact that the change in the amount of heat in the entire system occurs because of the heat inflow through the boundary of the region.

The conservative implicit-finite difference scheme has truncation error $O(\Delta t, \Delta h^2)$ as follows

$$\begin{aligned}
&\frac{T_1^{n+1} - T_0^{n+1}}{\Delta h} - \frac{\Delta h}{2}\frac{T_0^{n+1} - T_0^n}{\Delta t} = \zeta_1(t^{n+1}),\\
&\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta h^2}, \qquad i = 1, 2, ..., N-1,\\
&\frac{T_N^{n+1} - T_{N-1}^{n+1}}{\Delta h} + \frac{\Delta h}{2}\frac{T_N^{n+1} - T_N^n}{\Delta t} = \zeta_2(t^{n+1}),
\end{aligned}$$

which can be written in the matrix form $Ax = b$ as follows

$$\begin{bmatrix}
-\frac{1}{\Delta h} - \frac{\Delta h}{2\Delta t} & \frac{1}{\Delta h} & 0 & \dots & 0 & 0 & 0\\
-\frac{\Delta t}{\Delta h^2} & \frac{2\Delta t}{\Delta h^2} & 1 - \frac{\Delta t}{\Delta h^2} & \dots & 0 & 0 & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots\\
0 & 0 & 0 & \dots & -\frac{\Delta t}{\Delta h^2} & \frac{2\Delta t}{\Delta h^2} & 1 - \frac{\Delta t}{\Delta h^2}\\
0 & 0 & 0 & \dots & 0 & -\frac{1}{\Delta h} & \frac{1}{\Delta h} + \frac{\Delta h}{2\Delta t}
\end{bmatrix}
\begin{bmatrix} T_0^{n+1}\\ T_1^{n+1}\\ \vdots\\ T_{N-1}^{n+1}\\ T_N^{n+1} \end{bmatrix}$$

$$= \begin{bmatrix} \gamma_1(t^{n+1}) - \frac{\Delta h}{2\Delta t}T_0^n\\ T_1^n\\ \vdots\\ T_{N-1}^n\\ \gamma_2(t^{n+1}) + \frac{\Delta h}{2\Delta t}T_N^n \end{bmatrix}.$$

The discrete analogue for the amount of heat Q has the following form

$$Q = \sum_{i=0}^{N-1} \Delta h \frac{T_{i+1} + T_i}{2} = \frac{\Delta h}{2}T_0 + \sum_{i=1}^{N-1} \Delta h T_i + \frac{\Delta h}{2}T_N.$$

Using the equation for the finite difference scheme, we get

$$\frac{Q^{n+1} - Q^n}{\Delta t} = \zeta_2(t^{n+1}) - \zeta_1(t^{n+1}).$$

This equation is the discrete analogue of (3.33) expressing the fact that the finite difference scheme is conservative and no additional discrete input or outflows of heat are present.

Now let us consider what happens if we solve the system of difference equations by the usual Gauss-Siedel method. The Gauss-Siedel algorithms for matrix $Ax = b$ is

$$T_i^{s+1} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} T_j^{s+1} - \sum_{j=i+1}^{n} a_{ij} T_j^s \right), \qquad i = 1, .., n. \tag{3.34}$$

By equation (3.34) the formulas for the Gauss-Siedel method are

$$\begin{aligned}
&\frac{T_1^s - T_0^{s+1}}{\Delta h} - \frac{\Delta h}{2} \frac{T_0^{s+1} - T_0^n}{\Delta t} = \zeta_1(t^{n+1}), \\
&\frac{T_i^{s+1} - T_i^n}{\Delta t} = \frac{T_{i+1}^s - 2T_i^{s+1} + T_{i-1}^{s+1}}{\Delta h^2}, \qquad i = 1, 2, ..., N-1, \\
&\frac{T_N^{s+1} - T_{N-1}^{s+1}}{\Delta h} + \frac{\Delta h}{2} \frac{T_N^{s+1} - T_N^n}{\Delta t} = \zeta_2(t^{n+1}),
\end{aligned}$$

where s is the iteration number.

We can write these equations in the form of analogue of the finite difference scheme

$$\frac{T_1^{s+1} - T_0^{s+1}}{\Delta h} - \frac{\Delta h}{2} \frac{T_0^{s+1} - T_0^n}{\Delta t} = \zeta_1(t^{n+1}) + \frac{T_1^{s+1} - T_1^s}{\Delta h}, \tag{3.35}$$

$$\frac{T_i^{s+1} - T_i^n}{\Delta t} = \frac{T_{i+1}^s - 2T_i^{s+1} + T_{i-1}^{s+1}}{\Delta h^2} + \frac{T_{i+1}^s - T_{i+1}^{s+1}}{\Delta h^2}, \qquad i = 1, 2, ..., N-1, \tag{3.36}$$

$$\frac{T_N^{s+1} - T_{N-1}^{s+1}}{\Delta h} + \frac{\Delta h}{2} \frac{T_N^{s+1} - T_N^n}{\Delta t} = \zeta_2(t^{n+1}), \tag{3.37}$$

After carrying out a certain number of iterations necessary to satisfy the chosen criterion of convergence, the process is terminated, and T_i^{s+1} is taken as the value of temperature on the next time t^{n+1}. Thus $T_i^{s+1} \equiv T_i^{n+1}$, obtained by the iteration process, satisfies equations (3.35)-(3.37) which are the same as original conservative finite difference scheme with the exception that the right hand side contains terms that are in addition to the original equations and can also be regarded as heat sources and heat sinks.

Let the condition of the termination of the iteration process have the form

$$\max_i \mid T_i^{s+1} - T_i^s \mid \; < \varepsilon,$$

where ε is a given small number. Let us estimate the imbalance in the amount of heat caused by using the Gauss-Siedel method with this termination condition. From equations (3.35)-(3.37) and the definition of Q in discrete case, we get

$$\frac{Q^{n+1}-Q^n}{\Delta t}=\zeta_2^{n+1}-\zeta_1^{n+1}+\sum_{i=1}^{N}\frac{T_i^s-T_i^{s+1}}{\Delta h^2}\Delta h.$$

Therefore, the imbalance in the amount of heat is

$$\Delta Q=\Delta t\sum_{i=1}^{N}\frac{T_i^s-T_i^{s+1}}{\Delta h^2}\Delta h.$$

Now using the termination condition, we can estimate this imbalance as follows

$$|\Delta Q|\leq\frac{\varepsilon}{\Delta h^2}N\Delta h\Delta t=\frac{\varepsilon\Delta t}{\Delta h^2}.$$

The expression on the right hand side gives the upper limit of the imbalance occurring at the one time step.

This estimation must be taken into account when using the Gauss-Siedel method for the solution of difference equation. For example, in order for the Law of change in the amount of heat for the difference scheme for an instant of time t^k to be satisfied with accuracy h^2, i.e., with the accuracy of the finite difference scheme, the quantity, ε, should be chosen from the condition

$$\sum_{p=1}^{k}\frac{\varepsilon\Delta t}{\Delta h^2}\sim\Delta h^2$$

or

$$\varepsilon\sim\frac{\Delta h^4}{\Delta t(k-1)}$$

3.3 Numerical Solution for Test Problem

In this section, we present the exact solution of the test problem and present the results of the numerical solution to the test problem with different boundary conditions.

3.3.1 Exact Solution for the Test Problem

Let us consider the test problem about heat propagation in the bounded domain as

$$\begin{aligned} &u_t - a^2\Delta u = f(\overline{x},t),\ in\ \Omega,\ t \geq 0, \\ &u(\overline{x},0) = \varphi(\overline{x}),\ \overline{x}\ \epsilon\ \Omega, \\ &u\ |_{\Sigma} = \mu_0, \end{aligned} \tag{3.38}$$

where a is constant, $u = u(\overline{x},t)$ is solution, Σ is the boundary of Ω. Let $\widehat{u} = u - \mu_0$ where μ_0 is constant. Then problem (3.38) can be written as a problem with homogeneous boundary condition

$$\begin{aligned} &\widehat{u}_t - a^2\Delta\widehat{u} = f(\overline{x},t),\ in\ \Omega,\ t \geq 0, \\ &\widehat{u}(\overline{x},0) = \varphi(\overline{x}) - \mu_0 = \widehat{\varphi}(\overline{x}),\ \overline{x}\ \epsilon\ \Omega, \\ &\widehat{u}\ |_{\Sigma} = 0. \end{aligned} \tag{3.39}$$

Now we can split problem (3.39) into two problems when

$$\widehat{u}(\overline{x},t) = v(\overline{x},t) + w(\overline{x},t),$$

where v is a solution of homogeneous equation with inhomogeneous initial data

$$\begin{aligned} &v_t - a^2\Delta v = 0,\ in\ \Omega,\ t \geq 0, \\ &v(\overline{x},0) = \widehat{\varphi}(\overline{x}), \\ &v\ |_{\Sigma} = 0, \end{aligned} \tag{3.40}$$

and w is a solution of the inhomogeneous equation with homogeneous initial condition

$$\begin{aligned} &w_t - a^2\Delta\widehat{w} = f(\overline{x},t),\ in\ \Omega,\ t \geq 0, \\ &w(\overline{x},0) = 0, \\ &w\ |_{\Sigma} = 0. \end{aligned} \tag{3.41}$$

Solution of the Homogeneous Equation with Inhomogeneous Initial Data

Let us solve problem (3.40). To find a solution, we can use the method of separation of variables by assumeing that

$$v(\overline{x},t) = X(\overline{x})T(t), \tag{3.42}$$

and substitute equation (3.42) into equation (3.40). We get the following problems to determine function $X(\overline{x})$ and $T(t)$

$$\begin{aligned} &\Delta X(\overline{x}) + \lambda X(\overline{x}) = 0,\ in\ \Omega,\ X(\overline{x}) \neq 0, \\ &X(\overline{x})\mid_{\Sigma} = 0,\ on\ \Sigma, \end{aligned} \tag{3.43}$$

and

$$T_t(t) + a^2\lambda T(t) = 0. \tag{3.44}$$

Let $\lambda_1, \lambda_2, ..., \lambda_n, ...$ be the eigenvalues of problem (3.43) and $X_1, X_2, ..., X_n, ...$ be the eigenfunctions of problem (3.43). The functions $\{X_n\}_1^\infty$ form an orthogonal basis (system of functions). The corresponding solutions of equation (3.44) are

$$T_n(t) = c_n e^{-a^2\lambda_n t}. \tag{3.45}$$

There are nontrivial solutions of the problem

$$\begin{aligned} &v_t - a^2\Delta v = 0, \\ &v\mid_{\Sigma} = 0. \end{aligned}$$

These solutions are

$$v_n(\overline{x},t) = c_n X_n(\overline{x}) e^{-a^2\lambda_n t}, \quad n = 1, 2, ... \tag{3.46}$$

The general solution of problem (3.40) can be represented in the form

$$v(\overline{x},t)=\sum_{n=1}^{\infty}c_n e^{-a^2\lambda_n t}X_n(\overline{x}). \tag{3.47}$$

To satisfy the initial condition

$$v(\overline{x},0)=\widehat{\varphi}(\overline{x})=\sum_{n=1}^{\infty}c_n X_n(\overline{x}), \tag{3.48}$$

we have to choose

$$c_n=\frac{\int_\Omega \widehat{\varphi}(\overline{x})X_n(\overline{x})dV_{\overline{x}}}{\|X_n(\overline{x})\|^2},$$

where $V_{\overline{x}}$ is the volume that contains $\overline{x}$ and

$$\|X_n(\overline{x})\|^2=\int_\Omega (X_n(\overline{x}))^2 dV_{\overline{x}}.$$

Under this choice function (3.47), the solution of the problem (3.40) is obtained.

Solution of the Inhomogeneous Equation with Homogeneous Initial Data

The problem (3.41) can be solved by the separation of variables method. As usual, we assume that

$$w(\overline{x},t)=\sum_{n=1}^{\infty}T_n(t)X_n(\overline{x}). \tag{3.49}$$

Now expand the function $f(\overline{x},t)$ with respect to eigenfunction $X_n(\overline{x}),\ n=1,2,...,$ we get

$$f(\overline{x},t)=\sum_{n=1}^{\infty}f_n(t)X_n(\overline{x})$$

where

$$f_n(t)=\frac{\int_\Omega f(\overline{x},t)X_n(\overline{x})dV_{\overline{x}}}{\|X_n(\overline{x})\|^2}. \tag{3.50}$$

Equations (3.49) and (3.50) give the relationship for $T_n(t)$

$$T_n(t)+a^2\lambda T_n(t)=0,$$

$$T_n(0)=0. \tag{3.51}$$

The solution of problem (3.51) is

$$T_n(t) = \int_0^t e^{-a^2\lambda_n(t-\tau)} f_n(\tau) d\tau. \tag{3.52}$$

So we have

$$w(\overline{x},t) = \int_0^t \int_\Omega \{\sum_{n=1}^{\infty} e^{-a^2\lambda_n(t-\tau)} \frac{(X_n(\overline{x}))^2}{\|X_n(\overline{x})\|^2}\} f(\overline{x},t) d\tau dV_{\overline{x}}. \tag{3.53}$$

The solution for problem (3.38) is $u(\overline{x},t) = v(\overline{x},t) + w(\overline{x},t) + \mu_0$. So, we can see that if we know the solution of eigenvalue-eigenvector problem (3.43) then we can present solution of (3.38) in terms of infinite series.

Example

Let us consider the problem

$$\begin{aligned}
&u_t - a^2\Delta u = f(r,t),\ in\ 0 < r < r_0,\ t \geq 0,\\
&\mid u(r,t) \mid < \infty,\ 0 \leq r \leq r_0,\ t \geq 0,\\
&u(r,0) = u_0,\\
&u(r_0,t) = \mu_0,\ t \geq 0,
\end{aligned} \tag{3.54}$$

where $\Delta u = \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial u}{\partial r}\right)$.

Let $\widehat{u} = u - \mu_0$, we can write problem (3.54) as

$$\begin{aligned}
&\widehat{u}_t - a^2\Delta\widehat{u} = f(r,t),\ in\ 0 < r < r_0,\ t \geq 0,\\
&\mid \widehat{u}(r,t) \mid < \infty,\ 0 \leq r \leq r_0,\ t \geq 0,\\
&\widehat{u}(r,0) = u_0 - \mu_0,\\
&\widehat{u}(r_0,t) = 0,\ t \geq 0,
\end{aligned} \tag{3.55}$$

So, now we can split problem (3.55) into two problems

$$\widehat{u}(r,t) = v(r,t) + w(r,t),$$

where v is a solution of the homogeneous equation with inhomogeneous initial data

$$\begin{aligned} & v_t - a^2 \Delta v = 0, \ in \ 0 < r < r_0, \ t \geq 0, \\ & \mid v(r,t) \mid < \infty, \ 0 \leq r \leq r_0, \ t \geq 0, \\ & v(r,0) = u_0 - \mu_0 = c_0, \\ & v(r_0,t) = 0, \ t \geq 0, \end{aligned} \tag{3.56}$$

and w is a solution of the inhomogeneous equation with homogeneous initial condition

$$\begin{aligned} & w_t - a^2 \Delta w = f(r,t), \ in \ 0 < r < r_0, \ t \geq 0, \\ & \mid w(r,t) \mid < \infty, \ 0 \leq r \leq r_0, \ t \geq 0, \\ & w(r,0) = 0, \\ & w(r_0,t) = 0, \ t \geq 0, \end{aligned} \tag{3.57}$$

Solution of the Homogeneous Equation with Inhomogeneous Initial Data

Let us solve problem (3.56). To find a solution we can use the method of separation of variables by assuming that

$$v(r,t) = R(r)T(t), \tag{3.58}$$

and substitute equation (3.58) into equation (3.56). We get the following problems to determine function $R(r)$ and $T(t)$

$$\begin{aligned} & \Delta R(r) + \lambda R(r) = 0, \ in \ 0 < r < r_0, \ R(r) \neq 0, \\ & R(r_0) = 0, \quad \mid R(0) \mid < \infty, \end{aligned} \tag{3.59}$$

and

$$T_t(t) + a^2 \lambda T(t) = 0. \tag{3.60}$$

In the particular case where the domain is a ball and R is a function only of r, we have the problem

$$\begin{aligned} &\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) + \lambda R(r) = 0,\ in\ 0 < r < r_0,\ R(r) \neq 0, \\ &R(r_0) = 0,\ |R(0)| < \infty. \end{aligned} \tag{3.61}$$

By a change variables

$$\begin{aligned} x = \lambda^{\frac{1}{2}} r\ ,\ r = x/\lambda^{\frac{1}{2}}, \\ y(x) = R x^{\frac{1}{2}}\ ,\ R = y(x)/x^{\frac{1}{2}}, \end{aligned}$$

and using the chain rule we get

$$\begin{aligned} &\frac{d}{dx}\frac{dx}{dr} = \lambda^{\frac{1}{2}}\frac{d}{dx},\ \frac{d^2}{dr^2} = \lambda \frac{d^2}{dx^2}, \\ &\frac{dR}{dr} = \lambda\left(\frac{y'}{x^{\frac{1}{2}}} - \frac{1}{2}\frac{y}{x^{\frac{3}{2}}}\right),\ \frac{d^2R}{dr^2} = \lambda\left(\frac{y''}{x^{\frac{1}{2}}} - \frac{y'}{x^{\frac{3}{2}}} + \frac{3}{4}\frac{y'}{x^{\frac{5}{2}}}\right). \end{aligned}$$

Problem (3.61) becomes

$$\begin{aligned} &\frac{2}{r}\frac{dR}{dr} + \frac{d^2R}{dr^2} + \lambda R(r) = 0,\ in\ 0 < r < r_0,\ R(r) \neq 0, \\ &R(r_0) = 0,\ |R(0)| < \infty \end{aligned} \tag{3.62}$$

or

$$\begin{aligned} y'' + \frac{1}{x}y' + \left(1 - \frac{\left(\frac{1}{2}\right)^2}{x^2}\right) y = 0, \\ y(\lambda^{\frac{1}{2}} r_0) = 0. \end{aligned} \tag{3.63}$$

Equation (3.63) is Bessel's equation of half order and the general solution is in the form [14]

$$y(x) = c_1 \xi_\nu(x) + c_2 \xi_{-\nu}(x),$$

where $\xi_\nu(x)$, $\xi_{-\nu}(x)$ are Bessel function of order $\nu = \frac{1}{2}$.

Function $\xi_{-\nu}(x)$ has a pole of order ν at the point $r = 0$, must be excluded on physical grounds. The desired solution of equation (3.60) has the form

$$y(x) = c_1 \xi_\nu(x).$$

Bessel's functions of half order are given by relations (Stanley (1994))

$$\xi_{\frac{1}{2}}(x) = \left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \sum_{m=0}^{\infty} \frac{(-1^m)}{(2m+1)!} x^{2m+1} = \left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \sin\ x,$$
$$\xi_{-\frac{1}{2}}(x) = \left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \sum_{m=0}^{\infty} \frac{(-1^m)}{(2m)!} x^{2m} = \left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \cos\ x.$$

So, we have

$$y(x) = c_1 \left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \sin\ x.$$

The boundary condition

$$y(x_0) = y(\lambda^{\frac{1}{2}} r_0),$$

implies that λ must be one of the positive zeroes λ_n of $\xi_{\frac{1}{2}}(\lambda^{\frac{1}{2}} r_0) = 0$ or

$$\sin(\lambda_n^{\frac{1}{2}} r_0) = 0,$$
$$\lambda_n^{\frac{1}{2}} r_0 = n\pi,\ n = 1, 2, \ldots,$$
$$\lambda_n = \left(\frac{n\pi}{r_0}\right)^2,\ n = 1, 2, \ldots.$$

The acceptable solutions of problem (3.61)are

$$R_n(r) = c_1 \left(\frac{2\pi}{\lambda_n}\right)^{\frac{1}{2}} \frac{1}{r} \sin(\lambda_n^{\frac{1}{2}} r).$$

The corresponding solution of equation (3.60) are

$$T_n(t) = c_n e^{-a^2 \lambda_n t}. \tag{3.64}$$

The general solution of problem (3.56) may be represented in the form

$$v(r,t) = \sum_{n=1}^{\infty} c_n e^{-a^2\lambda_n t} R_n(r). \tag{3.65}$$

To satisfy the initial condition

$$v_n(r,0) = c_0 = \sum_{n=1}^{\infty} c_n R_n(r). \tag{3.66}$$

We have to choose

$$c_n = \frac{\int_0^{r_0} c_0 R_n(r) dr}{\|R_n(r\|^2},$$

where

$$\|R_n(r)\|^2 = \int_0^{r_0} (R_n(r))^2 r^2 dr.$$

Under this choice function (3.65) gives a solution of the problem (3.56).

Solution of the Inhomogeneous Equation with Homogeneous Initial Data

The problem (3.57) can be solved by the separation of variables method. Assume, as usual

$$w(r,t) = \sum_{n=1}^{\infty} T_n(t) R_n(r). \tag{3.67}$$

Expanding function $f(r,t)$ with respect to eigenfunctions $R_n(r)$, and get

$$f(r,t) = \sum_{n=1}^{\infty} f_n(t) R_n(r)$$

then

$$f_n(t) = \frac{\int_0^{r_0} f(r,t) R_n(r) r^2 dr}{\|R_n(r)\|^2}. \tag{3.68}$$

Equations (3.67) and (3.68) give a relationship to $T_n(t)$

$$T_n(t) + a^2 \lambda T(t) = 0,$$

$$T_n(0) = 0. \tag{3.69}$$

The solution of problem (3.69) is

$$T_n(t) = \int_0^t e^{-a^2\lambda_n(t-\tau)} f_n(\tau) d\tau.$$

So we have

$$w(\overline{r},t) = \int_0^t \int_0^{r_0} \{\sum_{n=1}^{\infty} e^{-a^2\lambda_n(t-\tau)} \frac{(R_n(r))^2}{\|R_n(r)\|^2}\} f(r,\tau) r^2 dr d\tau. \tag{3.70}$$

The solution for problem (3.54) is $u(r,t) = v(r,t) + w(r,t) + \mu_0$.

3.3.2 Numerical Solution for the Test Problem

Let us consider the numerical solution of the test problem on heat propagation in the bounded domain

$$\begin{aligned} &\frac{\partial T}{\partial t} - \Delta T = 0, \ in\ 0 < r < 1, \ t \geq 0, \\ &\mid T(r,t) \mid < \infty, \ in\ 0 \leq r \leq 1, \ t \geq 0, \\ &T(r,0) = 0, \\ &T(r,t) \mid_{r=1} = 1, \ t \geq 0, \end{aligned} \tag{3.71}$$

where $\Delta T = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right)$ and the exact solution for these problem is obtained by the separation of variables approach

$$T(r,t) = 1 + \Sigma_{n=1}^{\infty} \frac{2 \cdot (\lambda_n^{\frac{1}{2}} \cos(\lambda_n^{\frac{1}{2}})) - \sin(\lambda_n^{\frac{1}{2}})}{\lambda_n^{\frac{1}{2}} \cdot (\lambda_n^{\frac{1}{2}} - \frac{1}{2}\sin(2\lambda_n^{\frac{1}{2}}))} \cdot e^{-\lambda_n t} \cdot \frac{\sin(\lambda_n^{\frac{1}{2}} r)}{r}, \ 0 < r \leq 1,$$

or

$$T(r,t) = \begin{cases} 1 + \Sigma_{n=1}^{\infty} \frac{2 \cdot (\lambda_n^{\frac{1}{2}} \cos(\lambda_n^{\frac{1}{2}})) - \sin(\lambda_n^{\frac{1}{2}})}{\lambda_n^{\frac{1}{2}} \cdot (\lambda_n^{\frac{1}{2}} - \frac{1}{2}\sin(2\lambda_n^{\frac{1}{2}}))} \cdot e^{-\lambda_n t} \cdot \frac{\sin(\lambda_n^{\frac{1}{2}} r)}{r} & \text{if } 0 < r \leq 1 \\ 1 + \Sigma_{n=1}^{\infty} \frac{2 \cdot (\lambda_n^{\frac{1}{2}} \cos(\lambda_n^{\frac{1}{2}})) - \sin(\lambda_n^{\frac{1}{2}})}{\lambda_n^{\frac{1}{2}} - \frac{1}{2}\sin(2\lambda_n^{\frac{1}{2}})} \cdot e^{-\lambda_n t} & \text{if } r = 0 \end{cases} \tag{3.72}$$

where $\lambda_n = (n\pi)^2$.

It is natural to require a boundary condition at the point $r = 0$ when we solve this problem by the finite difference technique. In the numerical technique we assume that the flux of temperature is zero on physical grounds, $\lim\limits_{r\to 0} r^2 \dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$. In many research papers, scientist instead this boundary condition by the stronger boundary condition $\dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$. We would like to study the influence of these two boundary conditions on the approximate solution. We will consider two finite difference schemes.

The first finite difference scheme is

$$\begin{aligned}
&\frac{T_1^{n+1} + T_0^{n+1}}{\Delta t} - \frac{T_1^n + T_0^n}{\Delta t} = \frac{2}{(\Delta r)^2}((T_1^{n+1} + T_1^n) + (T_0^{n+1} + T_0^n)),\\
&\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{2r_i^2}\frac{\left(a_{i+1}T_{i+1}^n - (a_{i+1} + a_i)T_i^n + a_i T_{i-1}^n\right)}{\Delta r}\\
&\qquad + \frac{1}{2r_i^2}\frac{\left(a_{i+1}T_{i+1}^{n+1} - (a_{i+1} + a_i)T_i^{n+1} + a_i T_{i-1}^{n+1}\right)}{\Delta r}, \quad i = 1, 2, ..., N-1,
\end{aligned} \tag{3.73}$$

$T_N = 1.$

The second finite difference scheme is

$$\begin{aligned}
&T_0^{n+1} = T_1^{n+1},\\
&\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{2r_i^2}\frac{\left(a_{i+1}T_{i+1}^n - (a_{i+1} + a_i)T_i^n + a_i T_{i-1}^n\right)}{\Delta r}\\
&\qquad + \frac{1}{2r_i^2}\frac{\left(a_{i+1}T_{i+1}^{n+1} - (a_{i+1} + a_i)T_i^{n+1} + a_i T_{i-1}^{n+1}\right)}{\Delta r}, \quad i = 1, 2, ..., N-1,
\end{aligned} \tag{3.74}$$

$T_N = 1.$

The finite difference scheme (3.73) is a conservative approximation of test problem (3.71) with conservative approximation of the boundary condition $\lim\limits_{r\to 0} r^2 \dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$. The finite difference scheme (3.74) corresponds to the boundary condition $\dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$.

The comparison of the exact and numerical solutions of the test problem (3.71) are presented in Figures 3.3 and 3.4. Figure 3.3 shows the graph of the

exact solution of problem (3.71) and the numerical solution of the finite difference scheme (3.73). Figure 3.4 shows the graph of the exact solution of problem (3.71) and the numerical solution of the finite difference scheme (3.74). In these figures the sign " $-$ "corresponds to the exact solution, " o "corresponds to the approximate solution with 11 nodes, " $\triangleleft$ "corresponds to the approximate solution with 21 nodes, " $\times$ "corresponds to the approximate solution with 41 nodes. Figures 3.3 and 3.4 show that when the grid sizes decreases (the number of points increases) the numerical solution tends to the exact solution.

Convergence analysis of the finite difference scheme (3.73) and the finite difference scheme (3.74) are shown by the numerical results presented in Tables 3.1, 3.2 respectively. Table 3.1 shows the L_2 norm of the difference between the exact solution of problem (3.71) and the numerical solution of the finite difference scheme (3.73). That is,

$$\|T - \tilde{T}\|_{L_2} = \frac{1}{N}\left(\sum_{i=0}^{N}(T_i^j - \tilde{T}_i^j)^2\right)^{\frac{1}{2}}$$

where T is the exact solution and $\tilde{T}$ is the numerical solution. Table 3.2 shows the L_2 norm of difference between the exact solution of problem (3.71) and the numerical solution of the finite difference scheme (3.74). To estimate the order of convergence, we use the data from the second column of Tables 3.1, 3.2 and the techniques to estimate the order of convergence presented in Section 1.2.5. We can see that the finite difference scheme (3.73) and finite difference scheme (3.74) converge with second order.

The behavior of the approximate solution of the finite difference scheme (3.73) and finite difference scheme (3.74) at point zero is shown in Figure 3.5. In these Figure the sign " $-$ "corresponds to the exact solution, " $\cdot\cdot$ "corresponds to the approximate solution of finite difference scheme (3.73), " $--$ "corresponds to the approximate solution of finite difference scheme (3.74). We can see that

the approximated solution of finite difference scheme (3.73) is closer to the exact solution than the solution of (3.74).

The relation between errors of the finite difference scheme (3.73) and the finite difference scheme (3.74) on the test problem (3.71) are shown in Table 3.3. In Table 3.3, we demonstrate $relative\ error = \dfrac{(error2) - (error1)}{(error2)} \times 100$ where $error_1$ is the maximum absolute error between the exact solution of test problem (3.71) and the approximate solution of finite difference scheme (3.73) at the point zero and $error_2$ is the maximum absolute error between the exact solution of test problem (3.71) and the approximate solution of finite difference scheme (3.74) at the point zero. We can see that the approximate solution of finite difference scheme (3.74) at point zero is larger than the numerical solution for test problem (3.71) with boundary condition (a) by about 15 percent.

We do not need any boundary condition at $r = 0$ for the exact solution (3.72) of problem (3.71). To find the approximate solution, we have to specify the boundary condition at point $r = 0$. On physical grounds, we have to require that the solution of the problem (3.71) be bounded at $r = 0$ which corresponds to the requirement $\lim_{r\to 0} r^2 \dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$ and corresponds to the absence of thermal flux for $r = 0$. In many research papers, the scientists specify the boundary condition at point $r = 0$ by the stronger boundary condition $\dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$ and overlook the correspondence of the exact solution. We can get some information about the proper boundary condition using exact solution (3.72). Let us consider equation (3.72) which is the solution for test problem (3.71). We can see that $T(r,t)$ includes the summation of $\dfrac{1}{r}\sin(\lambda_n^{\frac{1}{2}} r)$ which depends on r and if we differentiate only this term, we can see that

$$\frac{\partial T}{\partial r} \mid_{r=0} = \frac{1}{r^2}\left(r\lambda_n^{\frac{1}{2}}\cos(\lambda_n^{\frac{1}{2}} r) + \sin(\lambda_n^{\frac{1}{2}} r)\right), \tag{3.75}$$

$$r^2 \frac{\partial T}{\partial r} \mid_{r=0} = r\lambda_n^{\frac{1}{2}}\cos(\lambda_n^{\frac{1}{2}} r) + \sin(\lambda_n^{\frac{1}{2}} r) = 0. \tag{3.76}$$

We can see that the right hand side of equation (3.75) is unbounded as $r \longrightarrow 0$ and the homogeneous Neumann boundary condition $\dfrac{\partial T}{\partial r} \mid_{r=0} = 0,\ t > 0$ does not satisfy the exact solution.

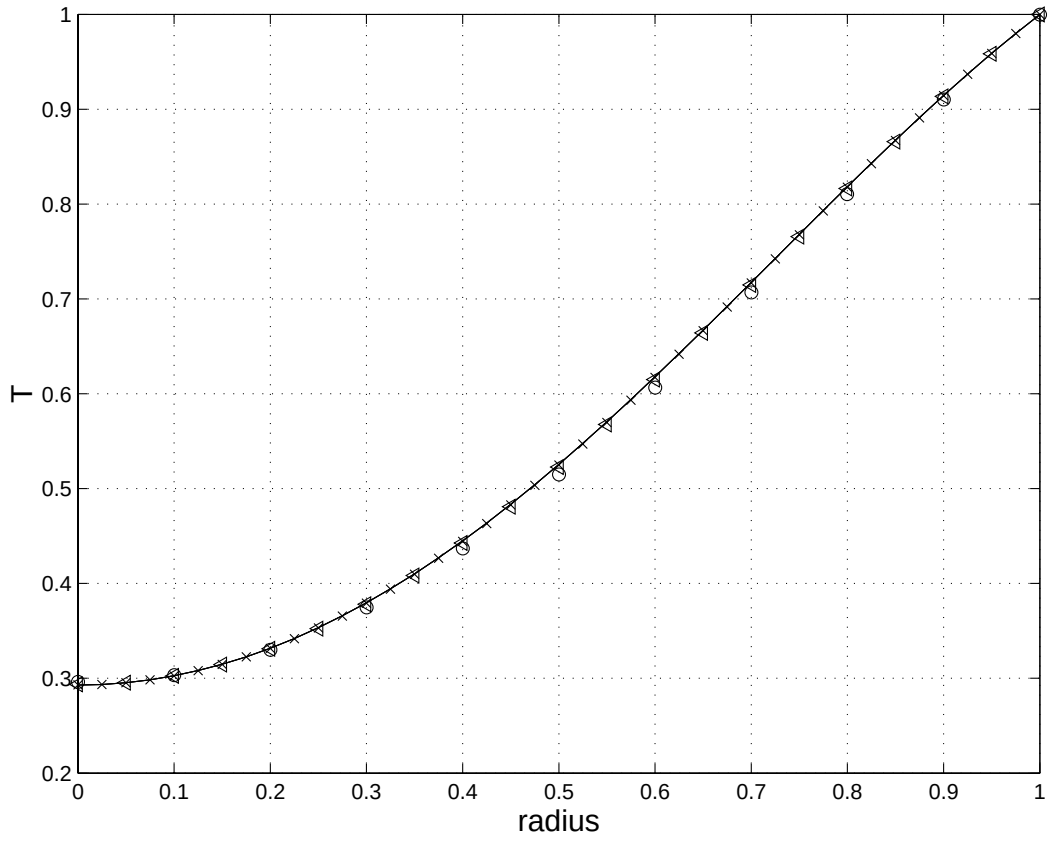

Figure 3.3: ***Graph of the exact solution of problem (3.71) and the numerical solution of finite difference scheme (3.73) where*** $-$ ***corresponds to the exact solution,*** o, $\triangleleft$, $\times$ ***corresponds to the approximate solution with*** $11,\ 21,$ ***and*** 41 ***nodes respectively.***

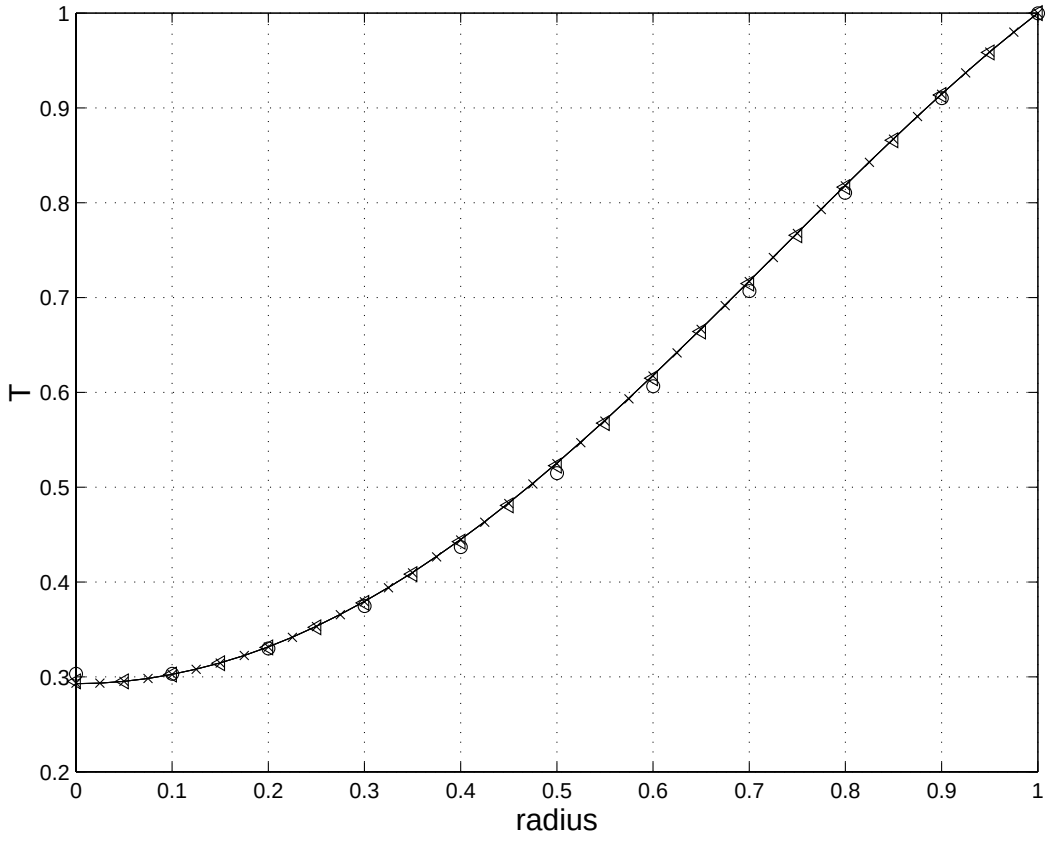

Figure 3.4: ***Graph of the exact solution of problem (3.71) and the numerical solution of finite difference scheme (3.74) where*** $-$ ***corresponds to the exact solution,*** o, $\triangleleft$, $\times$ ***corresponds to the approximate solution with*** $11,\ 21,$ ***and*** 41 ***nodes respectively.***

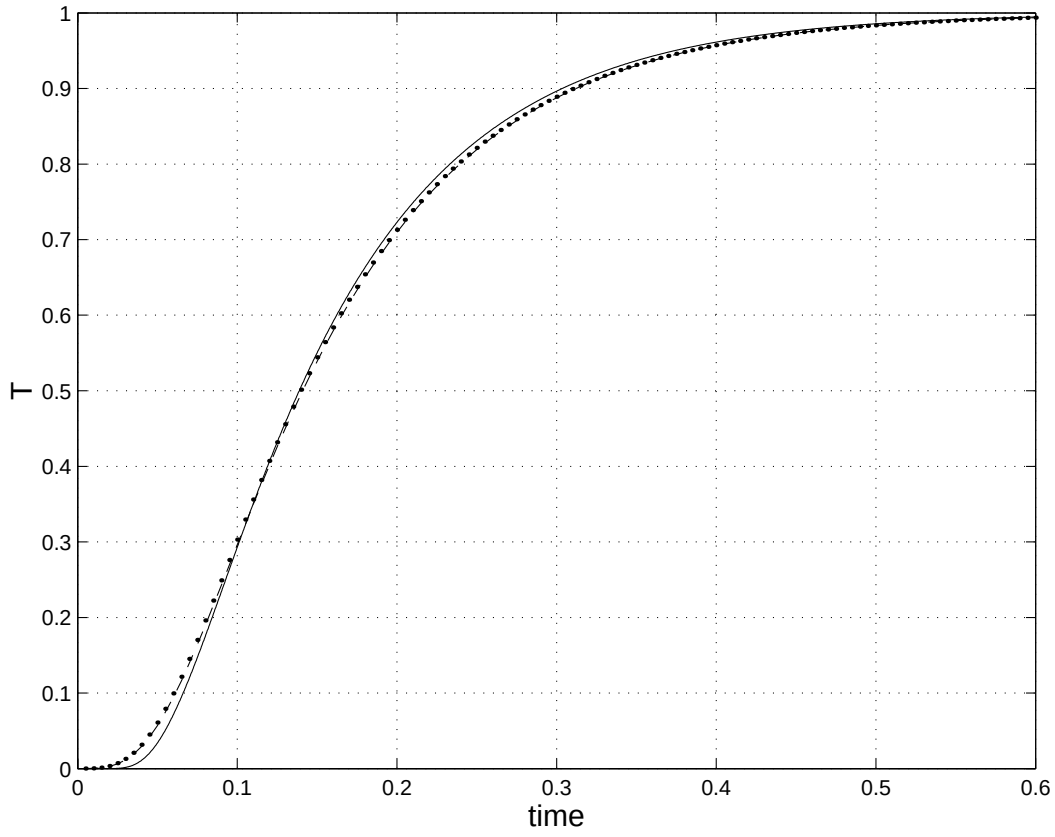

Figure 3.5: *Exact solution of test problem (3.71), numerical solution of the finite difference scheme (3.73), and numerical solution of the finite difference scheme (3.74) where – corresponds to the exact solution of test problem (3.71), · ·, –– corresponds to the numerical solution of finite difference scheme (3.73) and (3.74) respectively.*

number of grid points	L_2 norm	order of convergence
11	.746790100E-02	-
21	.191575400E-02	1.962790484
41	.483829900E-03	1.985340484

Table 3.1: Convergence analysis of finite difference scheme (3.73).

number of grid points	L_2 norm	order of convergence
11	.805333900E-02	-
21	.198843000E-02	2.017957289
41	.492770500E-03	2.012641979

Table 3.2: Convergence analysis of finite difference scheme (3.74).

number of point	error_1 FDS (3.73)	error_2 FDS (3.74)	relative error
11	.235908300E-01	.280116700E-01	15.78213652
21	.679798100E-02	.794643500E-02	14.45244314
41	.177168800E-02	.206337100E-02	14.13623629

Table 3.3: Relative error at point zero of finite difference scheme (3.73) and finite difference scheme (3.74) on the approximate solution.

Chapter IV

Numerical Solution for Pyrolysis of Sawdust

In this Chapter, the data on the pyrolysis of pine pinaster sawdust in a rotating cone reactor (Wagenaar, Kuipers, Prin, and Van Swaaij (1994)) has been used to test the numerical algorithm discussed.

The data from Wagenaar, Kuipers, Prin, and Van Swaaij (1994) is compared with the approximate solution of the mathematical model of pyrolysis which is described by the coupled equations for conservation of mass and energy

$$\frac{\partial C}{\partial t} = -K(T)C, \quad 0 \le r \le r_p, \ 0 \le t \le \bar{t}, \tag{4.1}$$

$$(0.1C_0 + 0.9C)c_p\frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\ (\lambda r^2\frac{\partial T}{\partial r}) - K(T)CH_r, \quad 0 < r < r_p, \quad 0 \le t \le \bar{t}, \tag{4.2}$$

where T is the temperature, C is the concentration of sawdust, $K(T) = Ae^{\frac{-E}{RT}}$ is the pyrolysis reaction rate constant, A is the rate frequency constant, E is the activation energy, R is the gas constant, c_p is the specific heat capacity, λ is the thermal conductivity, r is the radius, t is the time, r_p is the radius of particle, $\bar{t}$ is the residence time, and H_r is the heat of the pyrolysis reaction.

The initial temperature and concentration at the initial moment of time are

$$T(r,0) = T_0, \tag{4.3}$$

$$C(r,0) = C_0. \tag{4.4}$$

The boundary condition at the particle center expresses a zero heat conduction

flux

$$\lim_{r\to 0}\left(-\lambda 4\pi r^2\cdot\frac{\partial T}{\partial r}\right)=0,\quad 0\le t\le \bar{t}. \tag{4.5}$$

The boundary condition on the particle surface couples the heat transport conduction inside the particle with the external heat transfer

$$-\lambda\cdot\frac{\partial T}{\partial r}\mid_{r=r_p}=\alpha\cdot\left(T\mid_{r=r_p}-T_f\right),\quad 0\le t\le \bar{t}. \tag{4.6}$$

Here α is the external heat transfer coefficient and T_f is the temperature of the gas phase. This boundary condition simulates the convective heat transfer between the surface of the solid particle and the environment which has the temperature T_f. Rewriting problem (4.1) - (4.6) in dimensionless variables, we obtain

$$\frac{\partial C}{\partial t}=-\gamma_1 PC,\quad 0<r<1,\quad 0\leqslant t\leqslant\Gamma, \tag{4.7}$$

$$(0.1+0.9C)\frac{\partial T}{\partial t}=\gamma_3\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)-\gamma_4 PC,\quad 0<r<1,\quad 0\leqslant t\leqslant\Gamma, \tag{4.8}$$

$$\lim_{r\to 0} r^2\frac{\partial T}{\partial r}=0,\quad 0\le t\le\Gamma, \tag{4.9}$$

$$-\frac{\partial T}{\partial r}=\gamma_5(T-1),\quad r=1,\quad 0\le t\le\Gamma, \tag{4.10}$$

$$C(r,0)=1, \tag{4.11}$$

$$T(r,0)=\gamma_6, \tag{4.12}$$

where $\gamma_1=At_0$, $P=e^{\frac{\gamma_2}{T}}$, $\gamma_2=-\frac{E}{RT_f}$, $\Gamma=\dfrac{\bar{t}}{t_0}$, $\gamma_3=\dfrac{\lambda t_0}{(r_p)^2c_pC_0}$, $\gamma_4=\dfrac{At_0H_r}{c_pT_f}$, $\gamma_5=\dfrac{\alpha r_p}{\lambda_s}$, and $\gamma_6=\dfrac{T_0}{T_f}$. The value of the dimensionless parameters γ_1, γ_2, γ_3, γ_4, γ_5, and Γ are chosen according to the physical properties of pine waste from [1]. For example, in case of $t_0=1\ s$, $E=1.83\times10^5\ J\cdot mol^{-1}$, $R=8.3145\ J\cdot mol^{-1}\cdot K^{-1}$, $A=1\times10^{13}\ s^{-1}$, $r_p=70\ \mu m$, $T_0=298\ K$, $c_p=1335\ J\cdot kg^{-1}\cdot K^{-1}$, $C_0=500\ kg\cdot m^{-3}$, $\lambda=0.105\ W\cdot m^{-1}\cdot K^{-1}$, $T_f=873\ K$, $H_r=500\ kJ\cdot kg^{-1}$, $\alpha=1.65\times10^2\ W\cdot m^{-2}K^{-1}$, and $\bar{t}=0.3553816\ s$, the dimensionless parameters $\gamma_1=1\times10^{13}$, $\gamma_2=25.21313365$ $\gamma_3=3.2103$, $\gamma_4=0.42902$, $\gamma_5=1.1$, and $\gamma_6=0.3413516609$.

To solve the problem (4.7) - (4.12), we assume that the nonlinear terms do not change within one time step t^n to t^{n+1}, so we use the method of freezing the nonlinear terms in small time interval that we presented in Chapter III. It is possible to split the problem (4.7) - (4.12) into two problem. In each time step from t_n to t_{n+1}, we can solve the following two problems to find a solution.
The first one is the Cauchy problem

$$\begin{aligned} &\frac{\partial C}{\partial t} = -\gamma_1 P(T(r,t^n))C, \quad 0 \le r \le 1,\ t^n < t < t^{n+1}, \\ &C(r,t^n) \text{ is known,} \end{aligned} \tag{4.13}$$

where $n = 0, 1, ..., [W]-1$, $W = \dfrac{\Gamma}{\Delta t}$, and $T(r,t_p)$ is known.
The second one is the initial boundary value problem

$$\begin{aligned} (0.1 + 0.9C(r,t^{n+1}))\frac{\partial T}{\partial t} &= \gamma_3 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) \\ &\quad + \gamma_4 P\left(T(r,t^n)\right) C(r,t^{n+1}), \quad 0 < r < 1,\ t^n < t < t^{n+1}, \\ \lim_{r\to 0} r^2 \frac{\partial T}{\partial r} &= 0, \\ -\frac{\partial T}{\partial r} &= \gamma_5 (T-1), \quad r = 1, \\ T(r,t^n) &\text{ is known,} \end{aligned} \tag{4.14}$$

where $n = 0, 1, ..., [W]-1$, $W = \dfrac{\Gamma}{\Delta t}$, and $C(r,t^{n+1})$ is known.

We use the notations from Sections 3.1, 3.2 to construct the finite difference scheme for problem (4.13), (4.14). The two steps of following finite difference scheme are presented to find the approximate solution for problem (4.7) - (4.12). The first step is

$$C_i^{n+1} = \frac{(1-\gamma_1 P(T_i^n))}{(1+\gamma_1 P(T_i^n))} C_i^n, \quad i = 0, 1, ..., N, \tag{4.15}$$

The second step is

$$(0.1+0.9C_0^{n+1})\left(\frac{T_1^{n+1}+T_0^{n+1}}{\Delta t}-\frac{T_1^n+T_0^n}{\Delta t}\right)=\frac{2\gamma_3}{\Delta r^2}((T_1^{n+1}+T_1^n)$$
$$-(T_0^{n+1}+T_0^n))+\gamma_4 K_0^n C_0^{n+1},$$
$$A_iT_{i-1}^{n+1}-D_iT_i^{n+1}+B_iT_{i+1}^{n+1}=F_i,\qquad i=1,2,...,N-1, \tag{4.16}$$
$$\frac{T_N^{n+1}-T_{N-1}^{n+1}}{\Delta r}=-\gamma_5(T_N^{n+1}-1),$$

where $n=0,1,...,[W]-1$, $C_i^0=1$, $T_i^0=\gamma_6$, $\gamma_1=At_0$ $\gamma_3=\dfrac{\lambda t_0}{r_p^2c_pC_0}$, $\gamma_4=\dfrac{At_0H_r}{c_pT_f}$, $\gamma_5=\dfrac{\alpha r_p}{\lambda}$, $\gamma_6=\dfrac{T_0}{T_f}$, $A_i=\dfrac{\gamma_3\Delta t a_i}{2}$, $B_i=\dfrac{\gamma_3\Delta t a_{i+1}}{2}$, $a_i=1/\displaystyle\int_{r_{i-1}}^{r_i}\frac{1}{r^2}dr$, $D_i=A_i+B_i+E_i$, $E_i=0.1+0.9C_i^{n+1}$, $F_i=-\gamma_4\Delta tK_i^nC_i^{n+1}-A_iT_{i-1}^n-C_iT_i^n-B_iT_{i+1}^n-E_iT_i^n$.

The finite difference scheme (4.16) can be written in matrix form with a tri-diagonal matrix and we can find the approximate solution by using the sweep method (Hoffman (1992)).

The cone rotational frequency is used to control the residence time of the particle when we feed the particle into the rotating cone reactor (Wagenaar, Kuipers, Prin, and Van Swaaij (1994)) which is a novel reactor type for flash pyrolysis of biomass, in which rapid heating and short residence time of the particle can be realized. As expected, the particle residence time decreases rapidly with an increasing cone rotational frequency because of increased velocities of the particles.

The conversion of mass $\xi(\Gamma)$ due to pyrolysis of the particle can be defined in terms of mass of wood evaporated relative to the initial wood mass as follows Wagenaar, Kuipers, Prin, and Van Swaaij (1994)

$$\xi(\Gamma)=1-3\int_0^1 r^2C(r,\Gamma)dr. \tag{4.17}$$

We can approximate equation (4.17) by using the trapezoid rule and

$$\xi^\Gamma=1-\frac{3}{2}\sum_{i=0}^{k-1}\left(r_i^2C_i^\Gamma+r_{i+1}^2C_{i+1}^\Gamma\right). \tag{4.18}$$

The conversion of mass versus the cone rotational frequency for different particle

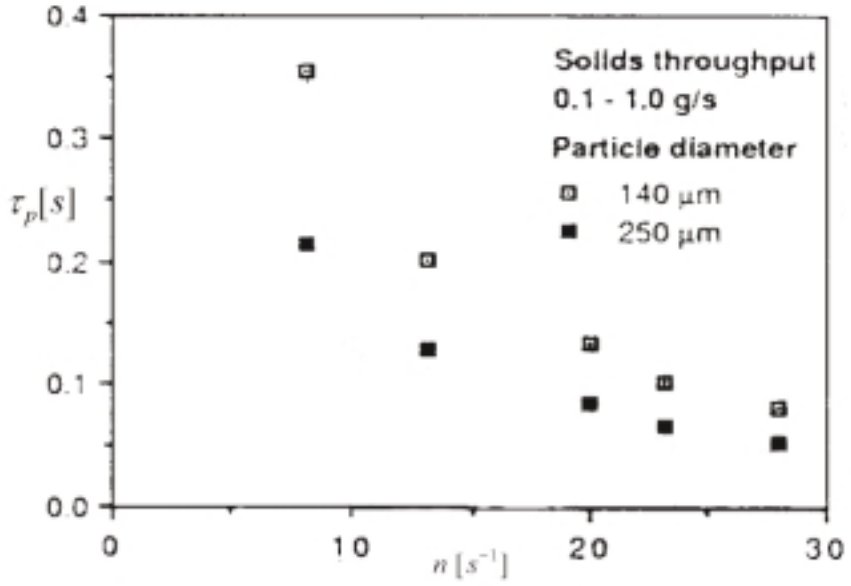

Figure 4.1: The particle residence time versus the cone rotational frequency (reproduce from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994))

diameter is shown by graph in Figures 4.2 and 4.3. The relation between the residence time and cone rotation frequency for different particle diameters are shown in Figure 4.1. This Figure is reproduced from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994). The numerical solution from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994) and the numerical solution of this thesis for different external heat transfer coefficient α for particle diameter 140 μm and 250 μm are shown in Figures 4.2 and 4.3. In the Figure 4.2 the particle diameter is equal to 140 μm. The data from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994) are presented by the cross sign " $\times$ ", the sign " $\lhd$ "corresponds to the numerical solution with $\alpha = 4{\times}10^2$, the sign " o "corresponds

to the numerical solution with $\alpha = 8 \times 10^2$, the sign " $\triangle$ "corresponds to the numerical solution with $\alpha = 1.65 \times 10^3$, the sign " ∇ "corresponds to the numerical solution with $\alpha = 3 \times 10^3$, the sign " $\triangleright$ "corresponds to the numerical solution with $\alpha = 5 \times 10^3$. In the Figure 4.3 the particle diameter is equal to 250 μm. The data from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994) are presented by cross sign "$\times$ ", the sign " $\triangleleft$ "corresponds to the numerical solution with $\alpha = 1 \times 10^2$, the sign " Δ "corresponds to the numerical solution with $\alpha = 1.65 \times 10^2$, the sign " o "corresponds to the numerical solution with $\alpha = 3 \times 10^3$, the sign " $\triangleright$ "corresponds to the numerical solution with $\alpha = 5 \times 10^3$. We can see that our numerical solution is close to the numerical solution from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994) when $\alpha = 1.65 \times 10^3$.

Let us consider the boundary condition (4.12) when α tend to zero and α tend to ∞. In case where α tends to zero, the Neumann boundary condition will be received

$$\frac{\partial T}{\partial r} = 0. \tag{4.19}$$

The two steps of the following finite difference scheme are presented to find the approximate solution for problem (4.7) - (4.11) and (4.19).

The first step is

$$C_i^{n+1} = \frac{(1 - \gamma_1 P(T_i^n))}{(1 + \gamma_1 P(T_i^n))} C_i^n, \quad i = 0, 1, ..., N. \tag{4.20}$$

The second step is

$$\begin{aligned}
&(0.1 + 0.9C_0^{n+1}) \left(\frac{T_1^{n+1} + T_0^{n+1}}{\Delta t} - \frac{T_1^n + T_0^n}{\Delta t} \right) = \frac{2\gamma_3}{\Delta r^2} ((T_1^{n+1} + T_1^n) \\
&\qquad\qquad - (T_0^{n+1} + T_0^n)) + \gamma_4 K_0^n C_0^{n+1}, \\
&A_i T_{i-1}^{n+1} - D_i T_i^{n+1} + B_i T_{i+1}^{n+1} = F_i, \qquad i = 1, 2, ..., N-1, \\
&T_{N-1}^{n+1} = T_N^{n+1},
\end{aligned} \tag{4.21}$$

where $n = 0, 1, ..., [W] - 1$, $C_i^0 = 1$, $T_i^0 = \gamma_6$.

In case where α tend to ∞, the Dirichlet boundary condition will be received

$$T(1, t) = 1. \tag{4.22}$$

The two steps of the following finite difference scheme are presented to find the approximate solution for problem (4.7) - (4.11) and (4.22).

The first step is

$$C_i^{n+1} = \frac{(1 - \gamma_1 P(T_i^n))}{(1 + \gamma_1 P(T_i^n))} C_i^n, \quad i = 0, 1, ..., N. \tag{4.23}$$

The second step is

$$\begin{aligned}
&(0.1 + 0.9C_0^{n+1}) \left(\frac{T_1^{n+1} + T_0^{n+1}}{\Delta t} - \frac{T_1^n + T_0^n}{\Delta t} \right) = \frac{2\gamma_3}{\Delta r^2} ((T_1^{n+1} + T_1^n) \\
&\qquad\qquad - (T_0^{n+1} + T_0^n)) + \gamma_4 K_0^n C_0^{n+1}, \\
&A_i T_{i-1}^{n+1} - D_i T_i^{n+1} + B_i T_{i+1}^{n+1} = F_i, \qquad i = 1, 2, ..., N - 1, \\
&T_N^{n+1} = 1,
\end{aligned} \tag{4.24}$$

where $n = 0, 1, ..., [W] - 1$, $C_i^0 = 1$, $T_i^0 = \gamma_6$.

Next, we will show that the numerical solution of problem (4.7) - (4.12) corresponds to the numerical solution of problem (4.7) - (4.11) with Neumann boundary condition (4.19) when α tends to zero and the numerical solution of problem (4.7) - (4.12) corresponds to the numerical solution of problem (4.7) - (4.11) with Dirichlet boundary condition (4.22) when α tends to ∞. We presented the data for the particle diameter $r_p = 140\ \mu m$ and cone rotational frequency $20.0414\ s^{-1}$ in Table 4.1. The conversion of mass which corresponds to the problem (4.20) - (4.21) (Neumann boundary condition (4.19)) is equal $0.312596600E - 03$ and the conversion of mass which correspond to the problem (4.23) - (4.24) (Dirichlet

boundary condition (4.22)) is equal 0.999958400. Table 4.1 shows that the numerical solution of problem (4.7) - (4.12) corresponds to the numerical solution of problem (4.7) - (4.11) with Neumann boundary condition (4.19) when α tend to zero and the numerical solution of problem (4.7) - (4.12) corresponds to the numerical solution of problem (4.7) - (4.11) with Dirichlet boundary condition (4.22) when α tend to ∞.

α	conversion
$\alpha = 0 \left(\frac{\partial T}{\partial r} = 0\right)$	.312596600E-03
1×10^{-1}	.312596600E-03
1	.312596600E-03
1×10^{1}	.312596600E-03
1×10^{2}	.296682100E-03
1×10^{3}	.780116300E+00
1×10^{4}	.999837500E+00
1×10^{5}	.999952300E+00
1×10^{6}	.999957800E+00
1×10^{7}	.999958300E+00
1×10^{8}	.999958400E+00
$\alpha = \infty$ $(T = 1)$	.999958400E+00

Table 4.1: The calculation of conversion of mass with the influence of α

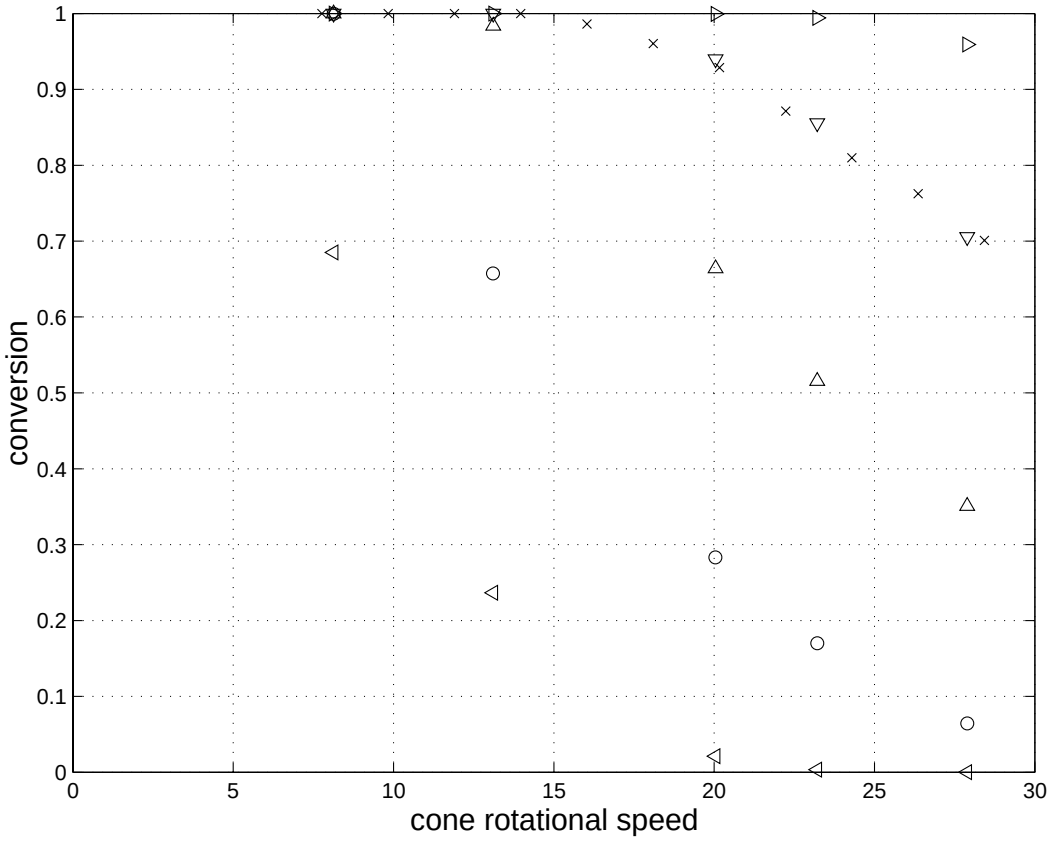

Figure 4.2: ***The calculated conversion versus the cone rotational speed for particle diameters*** $140\ \mu m$ ***and*** $\times$ ***corresponding to the numerical solution from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994),*** $\triangleleft$, o, $\triangle$, ∇, $\triangleright$ ***corresponding to the numerical solution of FDS (4.15), (4.16) with*** $\alpha = 4 \times 10^2,\ 8 \times 10^2,\ 1.65 \times 10^3,\ 3 \times 10^3,\ 5 \times 10^3$ ***respectively.***

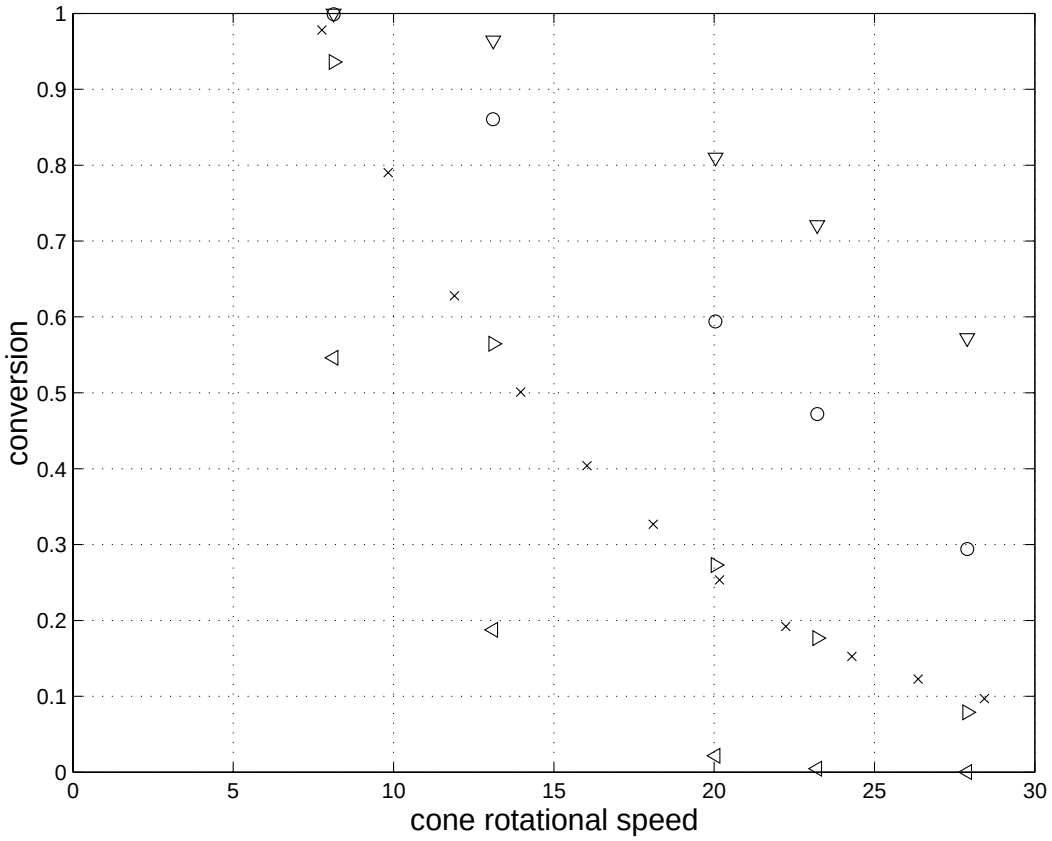

Figure 4.3: ***The calculated conversion versus the cone rotational speed for particle diameters*** $250\ \mu m$ ***and*** $\times$ ***corresponding to the numerical solution from the article of Wagenaar, Kuipers, Prin, and Van Swaaij (1994),*** $\triangleleft$, Δ, o, $\triangleright$ ***corresponding to the numerical solution of FDS (4.15), (4.16) with*** $\alpha = 1 \times 10^2,\ 1.65 \times 10^2,\ 3 \times 10^3,\ 5 \times 10^3$ ***respectively.***

Chapter V

Conclusion

The main goal of this research is to suggest a finite difference method to find the approximate solution for the mathematical model of single particle pyrolysis and to study the influence of different approximations of boundary conditions. The knowledge on conservation law, the method of dimensionless problem, the modified Euler method, conservative discretization, conservative finite difference scheme, and the integro interpolation method are utilized to construct the finite difference scheme to find the approximate solution for the mathematical model of a single particle pyrolysis model. We use the data for the pyrolysis of pine pinaster sawdust (Wagenaar, Kuipers, Prin, and Van Swaaij (1994)) to test the suggested finite difference scheme. The resulting is the numerical solution presented in this thesis which agrees with the numerical solution for pyrolysis of pine pinaster sawdust (Wagenaar, Kuipers, Prin, and Van Swaaij (1994)). Two kinds of boundary conditions at the particle center due to the transformation to spherical coordinates are studied. The difference between conservative and nonconservative boundary condition is 15 percent. The result of this research is intended to be used as a tool for constructing the numerical method for solving the mathematical models for the pyrolysis process.

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Curriculum Vitae

FIRST NAME: Damrongsak

LAST NAME: Yambangwai

GENDER: Male

NATIONALITY: Thai

DATE OF BIRTH: April 28, 1978.

EDUCATIONAL BACKGROUND:

- Bachelor of Science in Mathematics, June 1996-March 2000, Kasetsart University, Bangkok, Thailand.