# ON THE SOLUTION AND PARAMETER ESTIMATION PROBLEM OF A NONLINEAR INTEGRODIFFERENTIAL POPULATION BALANCE

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## Abstract

The prediction of crystal size distribution from a continuous crystallizer at steady state is important for the simulation, operation and design of crystallizers. In this research, we consider integrodifferential population balance equations (PBE) describing the crystal size distribution for a crystallizer with random growth dispersion and particle agglomeration. We first develop numerical schemes to solve the initial value problem after we establish the well-posedeness of this problem. We then test the performance of these schemes on examples with known solutions. The numerical results from the first scheme we offer are in excellent agreement with the analytical solutions. However, the other variations we examined appear to be inferior. We then examine the analytical solution of the physical model and study its convergence, positivity and monotonicity under certain conditions.

We then address the problem of parameter identification in the constant parameters case. The nature of the equation is that the solutions are oscillatory for certain ranges of the parameters that are of interest. In order to carry out the identification of parameters that would be physically meaningful, we are required to solve a boundary value problem coupled with an optimization procedure. We solve the BVP by the shooting method employing our numerical scheme for the IVP. We then couple it with the Marquadt-Levenberg algorithm to obtain optimal estimates for the parameters. We found out that the shooting method is rather sensitive to the initial guesses. To ensure the speedy convergence of the optimization, it is well known that "good" initial guesses are necessary. For this purpose, we derive the moments of the PB

and use them to obtain good initial estimates. Our algorithm performed well when applied on a made-up example, and to the physical problem for small parameter values. For large parameter values, or for larger domains of the independent variable, obtaining physically meaningful results was not possible due to the oscillating nature of the solution. This suggests that the implementation of a more refined shooting method is necessary.

# Chapter 1. Introduction

This research has two main goals: first, the development of a numerical method to solve the PB model Eq.(1.50); then to utilize this numerical method to estimate the parameters (crystallization kinetics) for the model given by Eq.(1.60). In the first part, we develop, analyze, and test a new numerical method to solve Eq.(1.50) — which is a variation of the predictor-corrector method of Khanh [K]. The second part, is devoted to the development and implementation of an optimization algorithm that combines a shooting algorithm and an optimization routine that utilizes the numerical scheme developed earlier to generate optimal parameter values.

## 1.1. Background

Crystallization is a major separation and purification process used by the chemical industry. It is utilized in the production of many commercial commodities such as salts, sugar, fertilizers, pharmaceuticals; and for the production of many important intermediate chemicals such as adipic acid, terephthalic acid, and alumina. The crystallization process consists mainly of nucleation (crystal birth) and crystal growth, and most often it is carried out from solution. One of the main objectives in modeling crystallizers is to describe the crystal size distribution (CSD). It is well known that the use of empirical statistical distribution may have parameters that may not be necessarily related to the factors influencing the process environment that produced the particle distribution. The population balance (PB) approach provides an excellent theoretical framework for the modeling and simulation of crystallizers. The PBE forms the model that relates the CSD to the operating variable in the crystallizer. It also can account for all sorts of "growth" phenomena such as agglomeration and growth rate dispersion (among others). Agglomeration is another process by which the size of particles is enlarged whereby particles aggregate and get cemented to form larger particles. The growth rate dispersion (GRD) phenomenon was recognized in 1969 by White and Wright [WW] in their study of the crystallization of sucrose. They have shown that crystals of the same size in the same constant environment grow at different rates. When particle agglomeration and growth rate dispersion are included into the PB model, and when only one characteristic size of the particles is of interest, the macroscopic population balance equation reduces to an integrodifferential equation (see Eq.(1.50)), whose solution is the particle density function. Furthermore, it is also very important to be able to reduce experimental data from laboratory or pilot plants, and to extract the process kinetics that are built into the population balance model and which are essential for the accurate simulation, design and the scale-up of crystallization processes.

## 1.2. Mathematical Models

In this section, we introduce the background and the development of our mathematical model. We consider an ensemble of large crystal population in suspension. This is needed to be able to represent the distribution in a continuous fashion (continuous particle size). This also justifies the use of a deterministic (versus a stochastic) approach to derive the population balance as a conservation equation for the number of particles in a population. The development of the population balance for crystallizers was initiated in the early sixties by A. D. Randolph and M. A. Larson [RL], and by H. M. Hulburt and S. Katz [HK] in view of Boltzmann's equation in statistical mechanics and Smoulchowski's coagulation equation.

Consider a region $R$ of the particle phase space, which is typically taken to have 3 spatial dimensions (external coordinates) and $m$ independent internal property coordinates. At any time $t$, define the $(m+3)$ dimensional crystal distribution function $n(R,t)$ over $R$. The number of particles existing at any time $t$ in a small incremental region of crystal phase space $dR$, can be represented by

$$dN = ndR,$$

while the total number of particles present in a finite subregion $R_1$ is

$$N(R_1) = \int_{R_1} ndR.$$

A PB for an ensemble of crystals in $R_1$ can be written from the Lagrangian perspective as

$$Accumulation = Net\ generation + (Input - Output)$$

$$\frac{d}{dt}\int_{R_1} ndR = \int_{R_1}(B-D)dR + zero,$$

where $B$ and $D$ represent birth and death density functions at a point in the phase space and $(B-D)dR$ is the net appearance rate of crystals.

Using Leibnitz's rule, then the left-hand side may be written as (a volume integral + a surface integral), and using the Divergence theorem, we get

$$\frac{d}{dt}\int_{R_1} ndR = \int_{R_1}\frac{\partial n}{\partial t}dR + \left(n\frac{d\mathbf{x}}{dt}\right)_{R_1} = \int_{R_1}\left[\frac{\partial n}{\partial t} + \nabla \bullet \left(\frac{d\mathbf{x}}{dt}n\right)\right]dR,$$

where $\mathbf{x}$ is the set of internal properties and external spatial coordinates comprising the phase space $R$.

Using the definition of crystal phase space velocity

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} = \mathbf{v}_e + \mathbf{v}_i,$$

where $\mathbf{v}$ is written as the sum of external velocities (cartesian components of the fluid velocities) and the internal velocities (like particle growth rate), the PBE from the Lagrangian viewpoint over $R_1$ becomes

$$\int_{R_1} \left[ \frac{\partial n}{\partial t} + \nabla \bullet (\mathbf{v}_e n) + \nabla \bullet (\mathbf{v}_i n) + D - B \right] dR = 0.$$

Since the $R_1$ was arbitrary, the integrand must vanish identically, and so we have the **microscopic** PB

$$\frac{\partial n}{\partial t} + \nabla \bullet (\mathbf{v}_e n) + \nabla \bullet (\mathbf{v}_i n) + D - B = 0.$$

This equation along with the momentum, mass and energy balances, appropriate kinetic models for rate processes, and the boundary conditions describe completely multidimensional crystal distributions. These equations are rather difficult to solve in distributed form.

In many problems, the suspension can be considered to be well mixed thus allowing us to ignore spatial variation and only worry about the internal phase space. Therefore, the PBE can be averaged over the external coordinates (it remains distributed in internal coordinates) to get the so called **macroscopic** PB

$$\frac{\partial n}{\partial t} + \frac{\partial Gn}{\partial y} = B - D + \sum_j \frac{Q_j n_j}{V},$$

where $y$ represents the particle size coordinate (we do assume that size coordinate is sufficient for describing the crystal),
$G$ is the overall growth rate of the crystals $(= \frac{dy}{dt})$,
$n$ is the population density function,
$V$ is the crystallizer volume,
$Q_j$ is the volumetric flow rate of the $j^{th}$ stream,
$B$ and $D$ are the birth and death rate functions (now assumed also independent of external coordinates), respectively.

As mentioned in the introduction, in certain systems (e.g., sucrose crystallization), growth rate dispersion has been observed. That is, it has been shown that crystals of the same size in the same constant environment grow at different rates. To account for the stochastic fluctuations in the growth rate of crystal faces, Melikov et al. [M] suggested the use of the generalized Fokker-Planck equation. Randolph and White [RW], by analogy with axial dispersion in columns and reactors, considered the modeling of size dispersion by adding to the conventional convective flux vector effective diffusivities representing flow and growth fluctuations, and proposed the following modified deterministic macro-distributed population balance

$$\frac{\partial n}{\partial t} + \frac{\partial (G(y)n)}{\partial y} + n\frac{\partial (\log V)}{\partial t} = \sum_j \frac{Q_j n_j}{V} + B - D + D_G \frac{\partial^2 n}{\partial y^2}, \qquad (1.10)$$

where $D_G$ is the growth rate diffusivity, which we assume herein that it is independent of $y$. In the Fokker-Planck equation $D_G$ represents the random noise added to the growth process of each particle.

Now to account for particle agglomeration, Hulburt and Katz [HK], using a statistical mechanical approach, and in view of Smoluchowski's coagulation equation, introduced the following forms for the birth and death functions (considering only binary collisional agglomeration — a diluteness assumption).

$$B(y) = \int_0^y \frac{\beta}{2} n(y-\varepsilon)n(\varepsilon)d\varepsilon, \text{ and } D(y) = \int_0^\infty \beta n(y)n(\varepsilon)d\varepsilon.$$

The function $\beta$ is called the agglomeration kernel and represents the frequency of collisions between particles of size $y - \varepsilon$ and of size $\varepsilon$ to produce a particle of size $y$. The factor $\frac{1}{2}$ ensures that the collisions are not counted twice.

For a self-seeding continuous crystallizer at steady state, equation (1.10) becomes

$$\begin{aligned} &- D_G n''(y) + (G(y)n(y))' + \frac{1}{\tau}n(y) \qquad (1.20)\\ &= \int_0^\infty \beta(y-\varepsilon, \varepsilon)n(y)n(\varepsilon)d\varepsilon - \frac{1}{2}\int_0^y \beta(y,\varepsilon)n(y-\varepsilon)n(\varepsilon)d\varepsilon, \end{aligned}$$

where $\tau := V/Q$ is the residence time.

Now, we first integrate equation (1.20) from 0 to $\infty$, then we integrate by parts on the left-hand side and change the order of integration on the right-hand side. We assume $G$ such that $G(y)(n(y)) \to 0$ as $y \to \infty$ (this is a statement about the asymptotic decay rate of $G$ relative to $n$), and we also make use of the physically justifiable assumptions $\lim_{y\to\infty} n(y) = 0, \lim_{y\to\infty} n'(y) = 0$. Moreover, we assume that $\beta(y-\varepsilon, \varepsilon)$ can be expressed in the separable multiplicative form $\gamma(y-\varepsilon)\gamma(\varepsilon)$ where $\gamma$ is an integrable function on $[0, \infty)$. Finally, let $N_T := \int_0^\infty n(y)dy$ and $N_\gamma := \int_0^\infty \gamma(y)n(y)dy$. Then, (1.20) becomes

$$\begin{aligned} &- D_G n''(y) + G(y)n'(y) + (\frac{1}{\tau} + G'(y) + N_\gamma \gamma(y))n(y) \\ &= \frac{1}{2}\int_0^y \beta(y,\varepsilon)n(y-\varepsilon)n(\varepsilon)d\varepsilon, \end{aligned} \tag{1.30}$$

where $N_\gamma = \sqrt{2\left(G(0)n(0) - D_G n'(0) - \frac{N_T}{\tau}\right)}$, with the restriction that $N_\gamma$ is a well defined real number.

Now let $A(y) = \int_0^y \frac{G(s)}{D_G}ds$ and $n(y) = e^{\frac{A(y)}{2}}v(y)$. Then equation (1.30) can be written as

$$\begin{aligned} &- D_G v''(y) + (\frac{1}{\tau} + \frac{G'(y)}{2} + N_\gamma \gamma(y))v(y) \\ &= \frac{1}{2}\int_0^y e^{[A(y-\varepsilon)+A(\varepsilon)-A(y)]/2}\gamma(y-\varepsilon)\gamma(\varepsilon)v(y)v(\varepsilon)d\varepsilon. \end{aligned} \tag{1.40}$$

Analytical solutions for special cases of equation (1.40) under appropriate boundary conditions were given in Saleeby and Lee [SL]. However, in general, one must solve equation (1.40) numerically. In Chapter 2, we will assume that we have a complete set of boundary conditions; that is, $n$ and $n'$ are given at the hypothetical zero particle size $y = 0$. This leads us to consider the following more general problem

$$\begin{aligned} f''(x) &= -\alpha(x)f(x) + \int_0^x \beta(x,\varepsilon)f(x-\varepsilon)f(\varepsilon)d\varepsilon + k(x), \\ f(0) &= f_0, f'(0) = f_0', \qquad x \in [0, L] \end{aligned} \tag{1.50}$$

where $f$ is the dimensionless density function, $L$ is an arbitrary positive number, $\alpha$, $\beta$ and $k$ are continuous functions, and $f_0, f_0'$ are constants.

Observe that (1.40) is not as general as (1.50), nevertheless it is still a sufficiently general special case that is still possible to carry out non-dimensionlization. Moreover, in Chapter 2, we will examine the well-posedness of this initial value problem, present a numerical method to solve it, and study the performance of variations of this method.

Motivated by the identification of crystallization kinetics for a basic steady state process, we will be interested in the special case of equation (1.10) where $G$ and $\beta$ are assumed to be constant. Towards this end, let $x = \frac{y}{G\tau}$, $f(x) = \frac{n(y)}{n_0}$, $\lambda = \frac{1}{2}n_0 GK\tau^2$ and $Pe = \frac{G(G\tau)}{D_G}$. Then (1.10) reduces to

$$f''(x) - Pef'(x) - Pef(x) = 2\lambda Pef(x)\int_0^\infty f(\varepsilon)d\varepsilon - \lambda Pe\int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon. \tag{1.60}$$

It turns out that, in the physical problem, we do end up with incomplete initial (or boundary) data to describe the nucleation process. Nucleation is well known to be difficult to characterize — especially in this instance.

Two common types of boundary conditions that have typically been considered are

(1) $f(0) - \frac{f'(0)}{Pe} = 1$, and

(2) $f(0) = 1$, $f'(0) = f_0'$ where $f_0'$ is an unknown constant.

Using the asymptotic conditions $\lim_{x\to\infty} f(x) = 0, \lim_{y\to\infty} f'(y) = 0$, type (1) boundary conditions and the transformation $f(x) = e^{(\frac{Pe}{2})x} g(x)$, (1.60) can be written as

$$g''(x) + \nu g(x) = \mu \int_0^x g(x-\varepsilon) g(\varepsilon) d\varepsilon, \tag{1.70}$$

where $\nu = -\frac{Pe^2}{4} - Pe\sqrt{1+4\lambda}$, and $\mu = -\lambda Pe$.

While using type (2) boundary conditions (1.60) can be written as

$$g''(x) + \widehat{\nu} g(x) = \mu \int_0^x g(x-\varepsilon) g(\varepsilon) d\varepsilon, \tag{1.80}$$

where $\widehat{\nu} = -\frac{Pe^2}{4} - Pe\sqrt{1 + \frac{4\lambda(Pe - f'(0))}{Pe}}$, and $\mu = -\lambda Pe$.

Note that equations (1.70) and (1.80) are special cases of (1.50).

For the rest of this investigation, we will limit ourselves to the study of the problem with type (2) boundary conditions. Similar analysis can be conducted for the other problem.

### 1.3. Outline

In Chapter Two, we will consider the initial value problem. We start by establishing its well-posedness, then develop a numerical scheme to solve it. To examine the performance of our method, we run tests on some examples and compare the results with those given by other methods and with the available analytical solutions.

In Chapter Three, we examine a boundary value problem that arises from the analysis of a crystallization operation. We present the analytical solution of this BVP and study some of its properties before solving this BVP numerically using the shooting method. The moments equations of the PB are then derived and solved in order to determine initial approximations for the parameters in the parameter estimation problem addressed in the last section.

# Chapter 2. Solution of the IVP

There are a number of different numerical schemes in the literature to solve integral and integrodifferential equations (see [B],[DM]). Khanh [K] developed a predictor-corrector method to solve first order integral and integro-differential equations that arose in the study of turbulent diffusion. In [ES], the method of Khanh was extended to the IVP given by Eq.(1.50). In this chapter, we develop different variations of the method of Khanh to solve numerically our second order model represented by Eq.(1.50), which also allow us to test the performance of another quadrature rule. We then apply these methods to also solve (1.60) and compare the results with the analytical solution given in [SL]. This comparison motivates us to consider the solution of a boundary value problem (BVP) whose solution will be addressed in Chapter 3.

## 2.1. Solution of the General IVP

In this section, we will develop a numerical method that allow us to examine and compare the performance of the use of the Hermite quadrature with the use of the Euler-Macluarin quadrature to solve IVP (2.10) given by

$$f''(x) = -\alpha(x)f(x) + \int_0^x \beta(x,\varepsilon)f(x-\varepsilon)f(\varepsilon)d\varepsilon + k(x), \qquad (2.10(a))$$

$$f(0) = f_0, f'(0) = f_0'. \qquad x \in [0, L] \qquad (2.10(b))$$

### 2.1.1. Well-Posedness

Before trying to solve problem (2.10) numerically, one should make sure that this problem has a unique solution on the interval of interest, and determine whether this solution is continuously dependent on the initial conditions or not. In other words, it is essential to establish the well-posedeness of this initial-value problem. As we mentioned above, one of our major objectives in this research is to use (1.60) for parameter estimation. We also noted that (1.60) is a special case of (2.10(a)), and that it describes a model of a physical problem in which the initial conditions are often measured quantities or inferred from related measured variables. Therefore, it is very desirable that any errors made in the measurements do not influence the solution very much. Continuous dependence of the solution on initial conditions will give the reassurance that these small errors produce a small error in the solution.

**Theorem 2.1.** Suppose that $\alpha$ and $k$ are continuous functions on $[0, L]$, and that $\beta$ is continuous function on the set $\{(x, \varepsilon) : 0 \leq \varepsilon \leq x \leq L\}$. Then (2.11) is well-posed.

The following theorem proved in [ES] will be used to establish the well-posedness of our IVP.

**Theorem 2.2.** Suppose that $\alpha$ and $k$ are continuous functions on $[0, L]$, and that $\beta$ is continuous function on the set $\{(x, \varepsilon) : 0 \leq \varepsilon \leq x \leq L\}$. Then (2.10) has a unique solution $f \in C^2([0, L])$ for any given constants $f_0$ and $f_0'$.

Before we give the proof of Theorem 2.1, we state the following result due to

E. Young (see [Y], Eq.(12)) where he established a sharp bound for solutions of an integral inequality of the Gronwall-Bellman type. The bound which is the exact solution of the corresponding integral equation was obtained by reducing the equation to a system of differential equations.

**Theorem 2.3.** Let $u$ be a non-negative continuous function satisfying

$$u(x) \leq b + a_o \int_0^x u ds + a_o a_1 \int_0^x \int_0^s u dt ds + a_0 a_1 a_2 \int_0^x \int_0^s \int_0^t u dr dt ds,$$

where $b, a_0, a_1$ and $a_2$ are positive constants, then

$$u(x) \leq b \left\{ \frac{a_1}{a_0 + a_1 + a_2} + \frac{a_2 e^{a_0 x}}{a_1 + a_2} + \frac{a_0 a_1 \exp(a_0 + a_1 + a_2)x}{(a_1 + a_2)(a_0 + a_1 + a_2)} \right\}.$$

**Proof of Theorem 2.1.** First, by an exponential transformation, we observe that (2.14) can be considered as a special case of (2.10). Thus, Theorem 2.2 gives us the existence and uniqueness of the solution of (2.14) on $[0, L]$. However, the proof of uniqueness in theorem 2 given in [ES] is rather tedious. We start by giving an alternative simpler proof of the uniqueness of the solution before proving that this solution is continuously dependent on the initial data.

Uniqueness.

Let $E'' := C^2([0, L])$ be the space of real-valued functions with continuous second derivative on $[0, L]$ and let $u$ and $v \in E''$ be two solutions of the IVP

(2.10), $w(x) = u(x) - v(x)$, and $z(x, \varepsilon) = \beta(x, x-\varepsilon)u(x-\varepsilon) + \beta(x, \varepsilon)v(x-\varepsilon)$. Then for all $x$ in $[0, L]$ we obtain that

$$w'(x) = -\int_0^x \alpha(\varepsilon)w(\varepsilon)d\varepsilon + \int_0^x \int_0^t z(t, \varepsilon)w(\varepsilon)d\varepsilon dt \ , \tag{2.11}$$
$$w(0) = 0, \qquad x \in [0, L].$$

Integrating (2.11) from 0 to $x$, we have

$$w(x) = -\int_0^x \int_0^t \alpha(\varepsilon)w(\varepsilon)d\varepsilon dt + \int_0^x \int_0^t \int_0^s z(s, \varepsilon)w(\varepsilon)d\varepsilon ds dt \ , \tag{2.12}$$

Let $M = \sup_{0 \le \varepsilon \le L} |w(\varepsilon)|, A = \sup_{0 \le \varepsilon \le L} |\alpha(\varepsilon)|, N = \sup_{0 \le s, \varepsilon \le L} |z(s, \varepsilon)|$, then

$$\begin{aligned} |w(x)| &\le AM \int_0^x \int_0^t d\varepsilon dt + NM \int_0^x \int_0^t \int_0^s d\varepsilon ds dt. \\ &= AM\frac{x^2}{2} + NM\frac{x^3}{3.2} \\ &= \frac{M}{3!}(3A + xN)x^2. \end{aligned} \tag{2.13}$$

Substituting (2.13) in the right-hand side of (2.12), we obtain

$$\begin{aligned} |w(x)| \le\ & A^2M \int_0^x \int_0^t \frac{\varepsilon^2}{2} d\varepsilon dt + ANM \int_0^x \int_0^t \frac{\varepsilon^3}{3.2} d\varepsilon dt \\ & + ANM \int_0^x \int_0^t \int_0^s \frac{\varepsilon^2}{3.2} d\varepsilon ds dt + N^2M \int_0^x \int_0^t \int_0^s \frac{\varepsilon^3}{3.2} d\varepsilon ds dt \\ =\ & A^2M\frac{x^4}{4!} + 2ANM\frac{x^5}{5!} + N^2M\frac{x^6}{6!} \\ =\ & \frac{M}{6!}(30A^2 + 12ANx + x^2N^2)x^4. \end{aligned}$$

Repeating again, we get

$$|w(x)| \leq A^3 M \frac{x^6}{6!} + 3A^2 NM \frac{x^7}{7!} + 3AN^2 M \frac{x^8}{8!} + N^3 M \frac{x^9}{9!}.$$
$$= \frac{M}{9!}(504A^3 + 216A^2 Nx + 27AN^2 x^2 + N^3 x^3)x^6.$$

In general we have,

$$|w(x)| \leq \frac{Mx^{2n}}{(3n)!} K^{2n}, \qquad n = 1, 2, 3, ...$$

where $K = \max(1, A, N, L)$.

Letting $n \to \infty$, we have that $w(x) \to 0$ on $[0, L]$ implying that $u(x) = v(x)$, and therefore, the solution is unique.

Continuous dependence on initial data.

To complete the proof of Theorem 2.1, all is needed now is to show the continuous dependence of the solution of (2.14) on the initial conditions.

Consider $\mathbf{R}$, the set of real numbers with metric $\rho(u, v) = |u - v|$, and $C([0, L])$ the space of continuous functions on $[0, L]$ with metric $\rho(f(x), g(x)) = \max_{0 \leq x \leq L} |f(x) - g(x)|$.

Let $T : \mathbf{R} \to C([0, L])$ be defined by $T(n_0, n_0') = \phi$ where $\phi$ is the solution of

$$D_G n''(y) - G(y)n'(y) - (\frac{1}{\tau} + G'(y) + N_\gamma \gamma(y))n(y) = -\frac{1}{2}\int_0^y \beta(y - \varepsilon, \varepsilon)n(y - \varepsilon)n(\varepsilon)d\varepsilon, \tag{2.14}$$

$n(0) = n_0, n'(0) = n_0'$.

We show that $T$ is a continuous mapping.

Rewrite (2.14) as

$$n''(y) - \frac{1}{D_G}[G(y)n'(y) + G'(y)n(y)] - \frac{1}{D_G}(\frac{1}{\tau} + N_\gamma \gamma(y))n(y) \tag{2.15}$$
$$= -\frac{1}{2D_G}\int_0^y \beta(y-\varepsilon,\varepsilon)n(y-\varepsilon)n(\varepsilon)d\varepsilon.$$

Integrate (2.15) from 0 to $y$, we have

$$\begin{aligned} & n'(y) - n_0' - \frac{1}{D_G}[G(y)n(y) - G(0)n(0)] \\ & - \frac{1}{D_G\tau}\int_0^y n(s)ds - \frac{N_\gamma}{D_G}\int_0^y \gamma(s)n(s)ds \\ & = -\frac{1}{2D_G}\int_0^y\int_0^t \beta(t-\varepsilon,\varepsilon)n(t-\varepsilon)n(\varepsilon)d\varepsilon dt. \end{aligned} \tag{2.16}$$

Now integrate (2.16) from 0 to $y$, we obtain

$$\begin{aligned} & n(y) - n_0 - n_0'y - \frac{1}{D_G}\int_0^y G(s)n(s)ds + \frac{G(0)n(0)}{D_G}y \\ & - \frac{1}{D_G\tau}\int_0^y\int_0^t n(s)dsdt - \frac{N_\gamma}{D_G}\int_0^y\int_0^t \gamma(s)n(s)dsdt \\ & = -\frac{1}{2D_G}\int_0^y\int_0^t\int_0^s \beta(s-\varepsilon,\varepsilon)n(s-\varepsilon)n(\varepsilon)d\varepsilon dsdt. \end{aligned}$$

Let $\varepsilon > 0$. Let $\varphi = T(\eta,\mu)$ and $\psi = T(\eta_n,\mu_n)$ where $|\eta - \eta_n| < \delta_1$ and $|\mu - \mu_n| < \delta_2$ (the subscript $n$ is a fixed label).

Choose $\delta_1 < \frac{\varepsilon}{2M\left|1+\frac{G(0)L}{D_G}+\frac{\|\psi\|_\infty\|\gamma\|_\infty G(0)L^2}{2D_G\sqrt{\varsigma}}\right|}$ and $\delta_2 < \frac{\varepsilon}{2M[\frac{\|\psi\|_\infty\|\gamma\|_\infty L}{2\sqrt{\varsigma}}+1]}$

where $\varsigma$ is a number between $\sqrt{2\left(G(0)\eta - D_G\mu - \frac{N_T}{\tau}\right)}$ and $\sqrt{2\left(G(0)\eta_n - D_G\mu_n - \frac{N_T}{\tau}\right)}$.

Let $S = \sqrt{2\left(G(0)\eta - D_G\mu - \frac{N_T}{\tau}\right)}$ , $S_n = \sqrt{2\left(G(0)\eta_n - D_G\mu_n - \frac{N_T}{\tau}\right)}$, and $H = \frac{\|\beta\|_\infty}{2D_G}(\|\varphi\|_\infty + \|\psi\|_\infty)$, and also let

$$M = \frac{\frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right]}{\frac{\|G\|_\infty}{D_G} + \frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right] + H} + \frac{\frac{\|\beta\|_\infty}{2D_G}(\|\varphi\|_\infty + \|\psi\|_\infty)e^{\frac{\|G\|_\infty}{D_G}L}}{\frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right] + H}$$
$$+ \frac{\frac{\|G\|_\infty}{D_G}\frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right] \exp\left[\frac{\|G\|_\infty}{D_G} + \frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right] + H\right] L}{\left[\frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right] + H\right]\left[\frac{\|G\|_\infty}{D_G} + \frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right] + H\right]}.$$

Then

$$\varphi(y) - \psi(y) - (\eta - \eta_n) - (\mu - \mu_n)y - \frac{1}{D_G}\int_0^y G(s)(\varphi(y) - \psi(y))ds$$
$$+ \frac{G(0)}{D_G}(\eta - \eta_n)y - \frac{1}{D_G\tau}\int_0^y \int_0^t (\varphi(y) - \psi(y))dsdt \tag{2.17}$$
$$- \frac{1}{D_G}\int_0^y \int_0^t \left[S\varphi(s) - S_n\psi(s)\right]\gamma(s)dsdt$$
$$= -\frac{1}{2D_G}\int_0^y \int_0^t \int_0^s \beta(s-\varepsilon,\varepsilon)[\varphi(s-\varepsilon)\varphi(\varepsilon) - \psi(s-\varepsilon)\psi(\varepsilon)]d\varepsilon dsdt.$$

Note that

$$S\varphi(s) - S_n\psi(s) = S\left(\varphi(s) - \psi(s)\right) + \left[S - S_n\right]\psi(s)$$
$$= S\left(\varphi(s) - \psi(s)\right) + \frac{1}{\sqrt{\varsigma}}\left|G(0)(\eta - \eta_n) - D_G(\mu - \mu_n)\right|\psi(s),$$

(by the Mean Value Theorem), and that

$$\varphi(s-\varepsilon)\varphi(\varepsilon)-\psi(s-\varepsilon)\psi(\varepsilon) = \varphi(s-\varepsilon)(\varphi(\varepsilon)-\psi(\varepsilon))+\psi(\varepsilon)(\varphi(s-\varepsilon)-\psi(s-\varepsilon)).$$

Then,

$$\int_0^y \int_0^t \int_0^s \beta(s-\varepsilon,\varepsilon)\left[\varphi(s-\varepsilon)\varphi(\varepsilon) - \psi(s-\varepsilon)\psi(\varepsilon)\right] d\varepsilon ds dt$$
$$= \int_0^x \int_0^t \int_0^s \beta(s-\varepsilon,\varepsilon)\varphi(s-\varepsilon)(\varphi(\varepsilon) - \psi(\varepsilon)) d\varepsilon ds dt$$
$$+ \int_0^x \int_0^t \int_0^s \beta(s-\varepsilon,\varepsilon)\psi(\varepsilon)\left[\varphi(s-\varepsilon) - \psi(s-\varepsilon)\right] d\varepsilon ds dt,$$

substituting $v = s - \varepsilon$in the second integral of the right hand side, we get

$$\int_0^x \int_0^t \int_0^s \left[\varphi(s-\varepsilon)\varphi(s) - \psi(s-\varepsilon)\psi(s)\right] d\varepsilon ds dt$$
$$= \int_0^x \int_0^t \int_0^s \varphi(s-\varepsilon)\left[\varphi(\varepsilon) - \psi(\varepsilon)\right] d\varepsilon ds dt$$
$$+ \int_0^x \int_0^t \int_0^s \beta(v, s-v)\psi(s-v)\left[\varphi(v) - \psi(v)\right] dv ds dt,$$

From (2.17) , we have

$$
\begin{aligned}
|\varphi(y)-\psi(y)| \leq & \left[|\eta-\eta_n|\left|1+\frac{G(0)L}{D_G}\right|+|\mu-\mu_n|\,L\right] \\
& +\frac{\|G\|_\infty}{D_G}\int_0^y|\varphi(s)-\psi(s)|\,ds+\frac{1}{D_G\tau}\int_0^y\int_0^t|\varphi(s)-\psi(s)|\,dsdt \\
& +\frac{\|\gamma\|_\infty}{D_G}\sqrt{2\left(G(0)\eta-D_G\mu-\frac{N_T}{\tau}\right)}\int_0^y\int_0^t|\varphi(s)-\psi(s)|\,dsdt \\
& +\frac{\|\gamma\|_\infty\|\psi\|_\infty}{D_G\sqrt{\varsigma}}\left[G(0)\,|\eta-\eta_n|+D_G\,|\mu-\mu_n|\right]\frac{L^2}{2} \\
& +H\int_0^x\int_0^t\int_0^s|\varphi(s)-\psi(s)|\,d\varepsilon dsdt,
\end{aligned}
$$

which gives

$$
\begin{aligned}
|\varphi(y)-\psi(y)| \leq & \left[\begin{array}{c} |\eta-\eta_n|\left|1+\frac{G(0)L}{D_G}+\frac{\|\gamma\|_\infty\|\psi\|_\infty}{D_G\sqrt{\varsigma}}G(0)\frac{L^2}{2}\right| \\ +|\mu-\mu_n|\left[L\frac{\|\gamma\|_\infty\|\psi\|_\infty}{2\sqrt{\varsigma}}L+1\right] \end{array}\right] \\
& +\frac{\|G\|_\infty}{D_G}\int_0^y|\varphi(s)-\psi(s)|\,ds \qquad (2.18) \\
& +\frac{1}{D_G}\left[\frac{1}{\tau}+\|\gamma\|_\infty S\right]\int_0^y\int_0^t|\varphi(s)-\psi(s)|\,dsdt \\
& +H\int_0^x\int_0^t\int_0^s|\varphi(s)-\psi(s)|\,d\varepsilon dsdt,
\end{aligned}
$$

where $\|\beta\|_\infty=\max_{0\leq\varepsilon\leq x\leq L}|\beta(x,\varepsilon)|$and$\|h\|_\infty=\max_{0\leq x\leq L}|h(x)|$for $h\equiv\varphi,\psi,G,\gamma$.

Let $u(x)=|\varphi(x)-\psi(x)|$, then (2.18) gives

$$\begin{aligned}
u(x) \leq |\eta - \eta_n| &\left|1 + \frac{G(0)L}{D_G} + \frac{\|\gamma\|_\infty \|\psi\|_\infty}{D_G\sqrt{\varsigma}} G(0)\frac{L^2}{2}\right| \\
&+ |\mu - \mu_n| \left[L\frac{\|\gamma\|_\infty \|\psi\|_\infty}{2\sqrt{\varsigma}} L + 1\right] + \frac{\|G\|_\infty}{D_G}\int_0^y u(s)ds \\
&+ \frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right]\int_0^y \int_0^t u(s)dsdt \\
&+ H\int_0^x \int_0^t \int_0^s u(s)d\varepsilon dsdt.
\end{aligned}$$

Applying Theorem 2.3 with
$b = |\eta - \eta_n| \left|1 + \frac{G(0)L}{D_G} + \frac{\|\gamma\|_\infty \|\psi\|_\infty}{D_G\sqrt{\varsigma}} G(0)\frac{L^2}{2}\right| + |\mu - \mu_n| \left[L\frac{\|\gamma\|_\infty \|\psi\|_\infty}{2\sqrt{\varsigma}} L + 1\right]$,
$a_0 = \frac{\|G\|_\infty}{D_G}$, $a_1 = \frac{1}{D_G}\left[\frac{1}{\tau} + \|\gamma\|_\infty S\right]$, and $a_2 = H$, we obtain

$$u(x) \leq bM,$$

which is equivalent to

$$\begin{aligned}
|T(\eta,\mu)(y) - T(\eta_n,\mu_n)(y)| \leq |\eta - \eta_n| &\left|1 + \frac{G(0)L}{D_G} + \frac{\|\gamma\|_\infty \|\psi\|_\infty}{D_G\sqrt{\varsigma}} G(0)\frac{L^2}{2}\right| M \\
&+ |\mu - \mu_n| \left[L\frac{\|\gamma\|_\infty \|\psi\|_\infty}{2\sqrt{\varsigma}} L + 1\right] M \\
&< \varepsilon \qquad \forall y \in [0, L].
\end{aligned}$$

Since $T(\eta,\mu)(y) - T(\eta_n,\mu_n)(y)$ is a continuous function of $y$, the maximum on the left hand side occurs on $[0, L]$, so

$$\rho(T(\eta,\mu), T(\eta_n,\mu_n)) < \varepsilon,$$

and hence $T$ is a continuous mapping. This completes the proof.

This result gives the continuous dependence of the solution of the IVP on initial conditions, or in other words, that the solution is a continuous function of the initial conditions.

### 2.1.2. Numerical Method

Using the result of Theorem 2.2, it is straight forward to obtain the necessary degree of smoothness of $f$ that we will need in developing high-order numerical methods. We have

**Theorem 2.4.** If $\alpha(x), k(x) \in C^m([0,L])$, $\frac{\partial^{(i)}\beta(x,\varepsilon)}{\partial x^{i-j}\partial\varepsilon^j}$, $0 \leq j \leq i \leq m$, are continuous for $0 \leq \varepsilon \leq x \leq L$, then (2.10) possesses a solution $f \in C^{m+1}([0,L])$.

As we will see in Section 2.1.3, when estimating the discretization error, Theorem 2.4 allows us to replace $f \in C^{m+1}([0,L])$ by the Lipschitz continuity of the $m^{th}$ derivative on $[0,L]$. This simply follows by applying the Mean Value Theorem.

Take a uniform partition of the interval $[0,L]$ :

$$0 = x_0 < x_1 < \cdots < x_n < \cdots < x_{N-1} < x_N = L,$$
$$h := x_n - x_{n-1} = \frac{L}{N}, 1 \leq n \leq N.$$

Consider a point $x_n$, and evaluate the equation in (2.10(a)) at $x_n$, we obtain

$$f''(x_n) = -\alpha(x_n)f(x_n) + \int_0^{x_n} \beta(x_n,\varepsilon)f(x_n-\varepsilon)f(\varepsilon)d\varepsilon + k(x_n). \quad (2.21)$$

Integrate (2.21) between 0 and $x_n$, we obtain

$$f'(x_n) = f_0' - \int_0^{x_n} \alpha(s) f(s)\, ds + \int_0^{x_n}\int_0^{t} \beta(t,\varepsilon) f(t-\varepsilon) f(\varepsilon)\, d\varepsilon dt + \int_0^{x_n} k(s)\, ds. \tag{2.22}$$

Integrate (2.22) between 0 and $x_n$, we obtain

$$f(x_n) = f_0 + f_0' x_n - \int_0^{x_n}\int_0^{t} \alpha(s) f(s)\, dsdt \tag{2.23}$$
$$+ \int_0^{x_n}\int_0^{t}\int_0^{s} \beta(s,\varepsilon) f(s-\varepsilon) f(\varepsilon)\, d\varepsilon dsdt + \int_0^{x_n}\int_0^{t} k(s)\, dsdt.$$

Differentiate (2.10(a)) and evaluate at $x_n$, we obtain

$$\begin{aligned} f^{(3)}(x_n) &= -\alpha'(x_n) f(x_n) - \alpha(x_n) f'(x_n) + k'(x_n) \\ &+ \beta(x_n, x_n) f(0) f(x_n) \qquad (2.24) \\ &+ \int_0^{x_n} [\beta'(x_n,\epsilon) f(x_n-\epsilon) f(\epsilon) + \beta(x_n,\epsilon) f'(x_n-\epsilon) f(\epsilon)] d\epsilon. \end{aligned}$$

Now we use quadrature rules to replace the integrals in equations (2.21), (2.22) ,(2.23) and (2.24).

Let $g(s) = \alpha(s) f(s)$.

Set $\phi_0(\varepsilon) = \beta(x_n, \varepsilon) f(x_n - \varepsilon) f(\varepsilon)$,

$\phi_{0i}(\varepsilon) = \beta(x_i, \varepsilon) f(x_i - \varepsilon) f(\varepsilon), 1 \le i \le n-1$,

$\phi_1(\varepsilon) = \frac{\partial}{\partial x}(\beta(x,\varepsilon) f(x-\varepsilon) f(\varepsilon))_{x=x_n}$,

$\phi_{1i}(\varepsilon) = \frac{\partial}{\partial x}(\beta(x,\varepsilon) f(x-\varepsilon) f(\varepsilon))_{x=x_i}, 1 \le i \le n-1$.

In equations (2.21) (2.22) (2.23) and (2.24), replace the outer integrals by the Euler-Maclaurin formula [B, p. 113]

$$\int_{x_0}^{x_r} \phi(x)\,dx = h\left[\frac{1}{2}\phi(x_0) + \phi(x_1) + \cdots + \phi(x_{r-1}) + \frac{1}{2}\phi(x_r)\right] \qquad (2.25)$$
$$- \frac{h^2}{12}\left[\phi'(x_r) - \phi'(x_0)\right] + O\left(h^4\right).$$

Then the inner integral by the Hermite formula [K, Eq. (1.10), p.306]

$$\int_0^{x_n} \phi(x)\,dx = \sum_{i=1}^{n} \int_{x_{j-1}}^{x_j} \phi(x)dx = \sum_{i=1}^{n}\sum_{j=1}^{q} C_{j,q} h^j [\phi^{(j-1)}(x_{i-1}) + (-1)^{j-1}\phi^{(j-1)}(x_i)], \qquad (2.26)$$

with the maximal error given by $\left\|\phi^{(2q)}\right\|_\infty \frac{T(h)^{2q}}{2q+1}\left[\frac{q!}{(2q)!}\right]^2$ ( $\left\|\phi^{(2q)}\right\|_\infty$ being the supremum of $\left\|\phi^{(2q)}\right\|$ ); where the coefficients are expressed recursively as $C_{1,q} = \frac{1}{2}, C_{j+1,q} = \frac{(q-j)C_{j,q}}{(2q-j)(j+1)}, 1 \le j \le q-1$, and $\phi$ is assumed to have continuous derivatives up to order $q$.

Taking $q = 4$, let

$$Q(i,\zeta) = \tfrac{1}{2}h\left(\zeta(x_{i-1}) + \zeta(x_i)\right) + \tfrac{3}{28}h^2\left(\zeta'(x_{i-1}) - \zeta'(x_i)\right)$$
$$+ \tfrac{1}{84}h^3\left(\zeta''(x_{i-1}) + \zeta''(x_i)\right) + \tfrac{1}{1680}h^4\left(\zeta^{(3)}(x_{i-1}) - \zeta^{(3)}(x_i)\right),$$

and taking $q = 3$, let

$$Q_1(i,\zeta) = \tfrac{1}{2}h\left(\zeta(x_{i-1}) + \zeta(x_i)\right) + \tfrac{1}{10}h^2\left(\zeta'(x_{i-1}) - \zeta'(x_i)\right)$$
$$+ \tfrac{1}{120}h^3\left(\zeta''(x_{i-1}) + \zeta''(x_i)\right),$$

Equation (2.23) becomes

$$
\begin{aligned}
f(x_n) &= f_0 + f_0' x_n + \frac{h^2}{12}\left[g(x_n) - g(0)\right] - \frac{h^2}{12}\left[k(x_n) - k(0)\right] \\
&+ \frac{h^3}{24}\left[\beta(x_n, x_n) f(0) f(x_n) - \beta(0,0) f(0)^2\right] \\
&+ \frac{h}{2}\sum_{i=1}^{n}\left[\begin{array}{c} -Q(i,g) + Q(i,k) + \frac{h}{3}Q(i,\phi_0) - \frac{h^2}{12}Q_1(i,\phi_1) \\ -\frac{h^2}{6}\left[\beta(x_i,x_i) f(0) f(x_i) - \beta(0,0) f(0)^2\right] \end{array}\right] \qquad (2.27) \\
&+ h\sum_{i=1}^{n-1}\sum_{j=1}^{i}\left[-Q(j,g) + Q(j,k) + hQ(j,\phi_{0i}) - \frac{h^2}{12}Q_1(j,\phi_{1i})\right] \\
&+ h^2\sum_{i=2}^{n-1}\sum_{j=1}^{i-1}\sum_{k=1}^{j} Q(k,\phi_{0j}).
\end{aligned}
$$

Similarly equation (2.22) becomes

$$
\begin{aligned}
f'(x_n) &= f_0' + \sum_{i=1}^{n} Q(i,k) - \sum_{i=1}^{n} Q(i,g) \qquad (2.28) \\
&+ h\sum_{i=1}^{n-1}\sum_{j=1}^{i} Q(j,\phi_{0i}) + \frac{h}{2}\sum_{i=1}^{n} Q(i,\phi_0) \\
&- \frac{h^2}{12}\left[\beta(x_n,x_n) f(0) f(x_n) - \beta(x_0,x_0) f(0)^2 + \sum_{i=1}^{n} Q_1(i,\phi_1)\right],
\end{aligned}
$$

equation (2.21) with $q = 4$ in the Hermite formula becomes

$$
f''(x_n) = -a(x_n)f(x_n) + k(x_n) + \sum_{i=1}^{n} Q(i,\phi_0), \qquad (2.29)
$$

and equation (2.24) with $q = 3$ in the Hermite formula becomes

$$f'''(x_n) = -a'(x_n) f(x_n) - a(x_n) f'(x_n) + k'(x_n) \qquad (2.30)$$
$$+ \beta(x_n, x_n) f(0) f(x_n) + \sum_{i=1}^{n} Q_1(i, \phi_1).$$

Now, the non-linear system of equations (2.27) to (2.30) can be solved numerically to find the unknowns $f(x_n)$,$f'(x_n)$,$f''(x_n)$,$f'''(x_n)$, $1 \leq n \leq N$. Note that we have suppressed the error terms in writing out equations (2.27) to (2.30), and that we have kept the same functional notation for the approximation.

### 2.1.3. Convergence Analysis

Let $f_n \cong f(x_n)$, $f'_n \cong f'(x_n)$, $f''_n \cong f''(x_n)$, $f'''_n \cong f'''(x_n)$ be the solution of the system of equations (2.27),(2.28),(2.29) and (2.30), and for $0 \leq i \leq n$, let $\varepsilon_i = f(x_i) - f_i$, $\varepsilon'_i = f'(x_i) - f'_i$, $\varepsilon''_i = f''(x_i) - f''_i$, $\varepsilon'''_i = f'''(x_i) - f'''_i$. Obviously, $\varepsilon_0 = 0$, $\varepsilon'_0 = 0$, $\varepsilon''_0 = 0$, and $\varepsilon'''_0 = 0$.

In this section, we show, under the regularity conditions mentioned in Section 2.1.2 above, that the global error tends to zero as we refine the discretization, and that the speed of convergence is fourth order. First observe that equation

(2.23) can be considered as a special case of the more general equation

$$f(x_n) = f_0 + f'_0.x_n + \int_0^{x_n}\int_0^t G(s, f(s))\,ds + \int_0^{x_n}\int_0^t\int_0^s K(t, s, f(s))\,dsdt,$$

where $G(s, f(s)) = k(s) - \alpha(s) f(s)$ and $K(t, s, f(s)) = \beta(t, s) f(t-s) f(s)$.

Let

$$
\begin{aligned}
Q_G(i) &= \tfrac{h}{2}\left[G(x_{i-1}, f(x_{i-1})) + G(x_i, f(x_i))\right] \\
&\quad + \tfrac{3h^2}{28}\left[G'(x_{i-1}, f(x_{i-1})) - G'(x_i, f(x_i))\right] \\
&\quad + \tfrac{h^3}{84}\left[G''(x_{i-1}, f(x_{i-1})) + G''(x_i, f(x_i))\right] \\
&\quad + \tfrac{h^4}{1680}\left[G'''(x_{i-1}, f(x_{i-1})) - G'''(x_i, f(x_i))\right], \\
Q_K(i,j) &= \tfrac{h}{2}[K(x_i, x_{j-1}, f(x_{j-1})) + K(x_i, x_j, f(x_j))] \\
&\quad + \tfrac{3h^2}{28}[K'(x_i, x_{j-1}, f(x_{j-1})) - K'(x_i, x_j, f(x_j))] \\
&\quad + \tfrac{h^3}{84}[K''(x_i, x_{j-1}, f(x_{j-1})) + K''(x_i, x_j, f(x_j))] \\
&\quad + \tfrac{h^4}{1680}[K'''(x_i, x_{j-1}, f(x_{j-1})) - K'''(x_i, x_j, f(x_j))], \\
Q_{K_1}(i,j) &= \tfrac{h}{2}[K_1(x_i, x_{j-1}, f(x_{j-1})) + K_1(x_i, x_j, f(x_j))] \\
&\quad + \tfrac{h^2}{10}[K_1'(x_i, x_{j-1}, f(x_{j-1})) - K_1'(x_i, x_j, f(x_j))] \\
&\quad + \tfrac{h^3}{120}[K_1''(x_i, x_{j-1}, f(x_{j-1})) + K_1''(x_i, x_j, f(x_j))].
\end{aligned}
$$

Using the quadrature formulae approximating (2.23) by (2.27), we have

$$
\begin{aligned}
f(x_n) &\cong f_0 + f_0' x_n - \frac{h^2}{12}[G(x_n, f(x_n)) - G(0, f(0))] \\
&\quad + \frac{h^3}{24}[K(x_n, x_n, f(x_n)) - K(0,0,f(0))] \\
&\quad + \frac{h}{2}\sum_{1\le i\le n} Q_G(i) + \frac{h}{3}\sum_{1\le i\le n} Q_K(n,i) - \frac{h^2}{12}\sum_{1\le i\le n} Q_{K_1}(n,i) \qquad (2.31) \\
&\quad - \frac{h^2}{6}\sum_{1\le i\le n}[K(x_i, x_i, f(x_i)) - K(0,0,f(0))] \\
&\quad + h\sum_{1\le i\le n-1}\sum_{1\le j\le i} Q_G(j) + h\sum_{1\le i\le n-1}\sum_{1\le j\le i} Q_K(i,j) - \frac{h^2}{12}\sum_{1\le i\le n-1}\sum_{1\le j\le i} Q_{K_1}(i,j) \\
&\quad + h^2\sum_{2\le i\le n-1}\sum_{1\le j\le i-1}\sum_{1\le k\le j} Q_K(j,k),
\end{aligned}
$$

where $K_1(t, s, f(s)) = \frac{\partial}{\partial t} K(t, s, f(s))$.

Eq. (2.31) can be written as

$$f\left(x_n\right) \cong f_0 + f_0' x_n + h^2 M_1 + h^3 M_2 + h^4 M_3 + h^5 M_4 + h^6 M_5, \qquad (2.32)$$

where

$$\begin{aligned}
M_1 = & \sum_{0\le i\le n} A_i G(x_i, f(x_i)) + \sum_{1\le i\le n-1}\sum_{0\le j\le i} A_{ij} G(x_j, f(x_j)) \\
& - \frac{1}{12}[G(x_n, f(x_n)) - G(0, f(0))], \\
M_2 = & \sum_{0\le i\le n} B_i \frac{d}{ds} G(x_i, f(x_i)) + \sum_{0\le i\le n} E_i K\left(x_n, x_i, f\left(x_i\right)\right) + \sum_{0\le i\le n} L_i K\left(x_i, x_i, f\left(x_i\right)\right) \\
& + \sum_{0\le i\le n} M_i K\left(0, 0, f\left(0\right)\right) + \sum_{1\le i\le n-1}\sum_{0\le j\le i} B_{ij} \frac{d}{ds} G(x_j, f(x_j)) \\
& + \sum_{1\le i\le n-1}\sum_{0\le j\le i} E_{ij} K\left(x_i, x_j, f\left(x_j\right)\right) + \sum_{2\le i\le n-1}\sum_{1\le j\le i-1}\sum_{0\le k\le j} A_{ijk} K(x_j, x_k, f\left(x_k\right)) \\
& + \frac{1}{24}[K\left(x_n, x_n, f\left(x_n\right)\right) - K\left(0, 0, f\left(0\right)\right)],
\end{aligned}$$

$$M_3 = \sum_{0\le i\le n} C_i \frac{d^2}{ds^2} G(x_i, f(x_i)) + \sum_{0\le i\le n} F_i \frac{d}{ds} K\left(x_n, x_i, f\left(x_i\right)\right) + \sum_{0\le i\le n} I_i K_1\left(x_n, x_i, f\left(x_i\right)\right)$$

$$+ \sum_{1\le i\le n-1} \sum_{0\le j\le i} C_{ij} \frac{d^2}{ds^2} G(x_j, f(x_j)) + \sum_{1\le i\le n-1} \sum_{0\le j\le i} F_{ij} \frac{d}{ds} K(x_i, x_j, f\left(x_j\right))$$

$$+ \sum_{1\le i\le n-1} \sum_{0\le j\le i} I_{ij} K_1(x_i, x_j, f(x_j)) + \sum_{2\le i\le n-1} \sum_{1\le j\le i-1} \sum_{0\le k\le j} B_{ijk} \frac{d}{ds} K(x_j, x_k, f\left(x_k\right)),$$

$$M_4 = \sum_{0\le i\le n} D_i \frac{d^3}{ds^3} G(x_i, f(x_i)) + \sum_{0\le i\le n} G_i \frac{d^2}{ds^2} K\left(x_n, x_i, f\left(x_i\right)\right) + \sum_{0\le i\le n} J_i \frac{d}{ds} K_1\left(x_n, x_i, f\left(x_i\right)\right)$$

$$+ \sum_{1\le i\le n-1} \sum_{0\le j\le i} D_{ij} \frac{d^3}{ds^3} G(x_j, f(x_j)) + \sum_{1\le i\le n-1} \sum_{0\le j\le i} G_{ij} \frac{d^2}{ds^2} K(x_i, x_j, f\left(x_j\right))$$

$$+ \sum_{1\le i\le n-1} \sum_{0\le j\le i} J_{ij} \frac{d}{ds} K_1(x_i, x_j, f\left(x_j\right)) + \sum_{2\le i\le n-1} \sum_{1\le j\le i-1} \sum_{0\le k\le j} C_{ijk} \frac{d^2}{ds^2} K(x_j, x_k, f\left(x_k\right)),$$

$$M_5 = \sum_{0\le i\le n} H_i \frac{d^3}{ds^3} K\left(x_n, x_i, f\left(x_i\right)\right) + \sum_{0\le i\le n} K_i \frac{d^2}{ds^2} K_1\left(x_n, x_i, f\left(x_i\right)\right)$$

$$+ \sum_{1\le i\le n-1} \sum_{0\le j\le i} H_{ij} \frac{d^3}{ds^3} K(x_i, x_j, f\left(x_j\right)) + \sum_{1\le i\le n-1} \sum_{0\le j\le i} K_{ij} \frac{d^2}{ds^2} K_1(x_i, x_j, f\left(x_j\right))$$

$$+ \sum_{2\le i\le n-1} \sum_{1\le j\le i-1} \sum_{0\le k\le j} D_{ijk} \frac{d^3}{ds^3} K(x_j, x_k, f\left(x_k\right)),$$

and

$A_i$,$B_i$,$C_i$, $D_i$, $E_i$, $F_i$, $G_i$, $H_i$, $I_i$, $J_i$, $K_i$, $L_i$, $M_i$, $0 \le i \le n$,

$A_{ij}$, $B_{ij}$,$C_{ij}$,$D_{ij}$,$E_{ij}$, $F_{ij}$, $G_{ij}$,$H_{ij}$,$I_{ij}$,$J_{ij}$, $K_{ij}$, $1 \le i \le n-1, 0 \le j \le i$,and

$A_{ijk}$, $B_{ijk}$,$C_{ijk}$,$D_{ijk}$ $1 \le i \le n-1, 0 \le j \le i-1, 0 \le k \le j$ are constant coefficients.

Likewise, we get

$$f_n \cong f_0 + f_0^{'} x_n \tag{2.33}$$

$$+ \text{ right-hand side of (2.32) with } f\left(x_n\right) \text{ replaced by } f_n.$$

Let

$\Delta_G(i) = G(x_i, f(x_i)) - G(x_i, f_i)$,

$\Delta_K(i,j) = K(x_i, x_j, f(x_j)) - K(x_i, x_j, f_j)$, and

$\Delta_{K_1}(i) = K_1(x_n, x_i, f(x_i)) - K_1(x_n, x_i, f_i)$, then (2.32) and (2.33) yield

$$
\begin{aligned}
|\varepsilon_n| = |f(x_n) - f_n| \le & h^2 \Delta M_1 + h^3 \Delta M_2 + h^4 \Delta M_3 \\
& + h^5 \Delta M_4 + h^6 \Delta M_5 + \left\| G^{(2p)} \right\|_\infty \frac{T(h)^{2p}}{2p+1} \left[ \frac{p!}{(2p)!} \right]^2 \\
& + h \left\| K^{(2p)} \right\|_\infty \frac{T(h)^{2p}}{2p+1} \left[ \frac{p!}{(2p)!} \right]^2 \\
& + h^2 \left\| K_1^{(2q)} \right\|_\infty \frac{T(h)^{2q}}{2q+1} \left[ \frac{q!}{(2q)!} \right]^2 + O(h^4),
\end{aligned} \tag{2.34}
$$

where

$$
\begin{aligned}
\Delta M_1 = & \sum_{0 \le i \le n} |A_i| |\Delta_G(i)| + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |A_{ij}| |\Delta_G(j)| - \tfrac{1}{12} |\Delta_G(n)|, \\
\Delta M_2 = & \sum_{0 \le i \le n} |B_i| |\Delta_G(i)| + \sum_{0 \le i \le n} |E_i| |\Delta_K(n,i)| + \sum_{0 \le i \le n} |L_i| |\Delta_K(i,i)| \\
& + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |B_{ij}| \left| \tfrac{d}{ds} \Delta_G(j) \right| + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |E_{ij}| |\Delta_K(i,j)| \\
& + \sum_{2 \le i \le n-1} \sum_{1 \le j \le i-1} \sum_{0 \le k \le j} |A_{ijk}| |\Delta_K(j,k)| + \tfrac{1}{24} |\Delta_K(n,n)|, \\
\Delta M_3 = & \sum_{0 \le i \le n} |C_i| \left| \tfrac{d^2}{ds^2} \Delta_G(i) \right| + \sum_{0 \le i \le n} |F_i| \left| \tfrac{d}{ds} \Delta_K(n,i) \right| + \sum_{0 \le i \le n} |I_i| |\Delta_{K_1}(n,i)| \\
& + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |C_{ij}| \left| \tfrac{d^2}{ds^2} \Delta_G(j) \right| + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |F_{ij}| \left| \tfrac{d}{ds} \Delta_K(i,j) \right| \\
& + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |I_{ij}| |\Delta_{K_1}(i,j)| + \sum_{2 \le i \le n-1} \sum_{1 \le j \le i-1} \sum_{0 \le k \le j} |B_{ijk}| \left| \tfrac{d}{ds} \Delta_K(j,k) \right|, \\
\Delta M_4 = & \sum_{0 \le i \le n} |D_i| \left| \tfrac{d^3}{ds^3} \Delta_G(i) \right| + \sum_{0 \le i \le n} |G_i| \left| \tfrac{d^2}{ds^2} \Delta_K(n,i) \right| + \sum_{0 \le i \le n} |J_i| \left| \tfrac{d}{ds} \Delta_{K_1}(n,i) \right| \\
& + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |D_{ij}| \left| \tfrac{d^3}{ds^3} \Delta_G(j) \right| + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |G_{ij}| \left| \tfrac{d^2}{ds^2} \Delta_K(i,j) \right| \\
& + \sum_{1 \le i \le n-1} \sum_{0 \le j \le i} |J_{ij}| \left| \tfrac{d}{ds} \Delta_{K_1}(i,j) \right| + \sum_{2 \le i \le n-1} \sum_{1 \le j \le i-1} \sum_{0 \le k \le j} |C_{ijk}| \left| \tfrac{d^2}{ds^2} \Delta_K(j,k) \right|,
\end{aligned}
$$

$$\Delta M_5 = \sum_{0\le i\le n} |H_i| \left|\frac{d^3}{ds^3}\Delta_K(n,i)\right| + \sum_{0\le i\le n} |K_i| \left|\frac{d^2}{ds^2}\Delta_{K_1}(n,i)\right| + \sum_{1\le i\le n-1}\sum_{0\le j\le i} |H_{ij}| \left|\frac{d^3}{ds^3}\Delta_K(i,j)\right|$$
$$+ \sum_{1\le i\le n-1}\sum_{0\le j\le i} |K_{ij}| \left|\frac{d^2}{ds^2}\Delta_{K_1}(i,j)\right| + \sum_{2\le i\le n-1}\sum_{1\le j\le i-1}\sum_{0\le k\le j} |D_{ijk}| \left|\frac{d^3}{ds^3}\Delta_K(j,k)\right|.$$

The term $O(h^4)$ is due to the error term resulting from the Euler-Maclaurin formula.

Then by using the Lipschitz property of $G(s, f(s))$ and $K(t, s, f(s))$ and the chain rule in several variables we have that

$$|\Delta_G(i)| \le L_1 |\varepsilon_i|$$
$$|\Delta_K(i,j)| \le L_2 |\varepsilon_j|$$
$$|\Delta_{K_1}(i,j)| \le L_3 |\varepsilon_j|,$$

$$\left|\frac{d}{ds}\Delta_G(i)\right| \le L_4 |\varepsilon_i| + L_5 |\varepsilon_i'|$$
$$\left|\frac{d^2}{ds^2}\Delta_G(i)\right| \le L_6 |\varepsilon_i| + L_7 |\varepsilon_i'| + L_8 |\varepsilon_i''|$$
$$\left|\frac{d^3}{ds^3}\Delta_G(i)\right| \le L_9 |\varepsilon_i| + L_{10} |\varepsilon_i'| + L_{11} |\varepsilon_i''| + L_{12} |\varepsilon_i'''|,$$

$$\left|\frac{d}{ds}\Delta_K(i,j)\right| \le M_1 |\varepsilon_j| + M_2 |\varepsilon_j'|$$
$$\left|\frac{d^2}{ds^2}\Delta_K(i,j)\right| \le M_3 |\varepsilon_j| + M_4 |\varepsilon_j'| + M_5 |\varepsilon_j''|$$
$$\left|\frac{d^3}{ds^3}\Delta_K(i,j)\right| \le M_6 |\varepsilon_j| + M_7 |\varepsilon_j'| + M_8 |\varepsilon_j''| + M_9 |\varepsilon_j'''|,$$

and

$$\left|\frac{d}{ds}\Delta_{K_1}(i,j)\right| \le N_1 |\varepsilon_j| + N_2 |\varepsilon_j'|$$
$$\left|\frac{d^2}{ds^2}\Delta_{K_1}(i,j)\right| \le N_3 |\varepsilon_j| + N_4 |\varepsilon_j'| + N_5 |\varepsilon_j''|,$$

where $L_i, M_j$and $N_k$ are positive constants for $1 \le i \le 12,\ \ 1 \le j \le 9$, and $1 \le k \le 5$.

Therefore, for a sufficiently small $h$, (2.35) yields

$$
\begin{aligned}
|\varepsilon_n| \le P_0 h^8 + P_1 h^2 \sum_{0\le i\le n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right) \\
+ P_2 h^2 \sum_{1\le i\le n} \sum_{0\le j\le i} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right) \\
+ P_3 h^3 \sum_{2\le i\le n-1} \sum_{1\le j\le i-1} \sum_{0\le k\le j} \left( |\varepsilon_k| + |\varepsilon_k'| + |\varepsilon_k''| + \left|\varepsilon_k^{(3)}\right| \right) + O\left(h^4\right),
\end{aligned}
\tag{2.35}
$$

where $P_0$, $P_1$, $P_2$and $P_3$ are positive constants.

Replacing the double summation in (2.35) by $(n-1) \sum_{0\le j\le i} \left( |\varepsilon_j| + |\varepsilon_j'| + |\varepsilon_j''| + \left|\varepsilon_j^{(3)}\right| \right)$ and the triple summation by $\frac{(n-1)(n-2)}{2} \sum_{0\le k\le j} \left( |\varepsilon_k| + |\varepsilon_k'| + |\varepsilon_k''| + \left|\varepsilon_k^{(3)}\right| \right)$ yields

$$
\begin{aligned}
|\varepsilon_n| \le P_0 h^8 + P_1 h^2 \sum_{0\le i\le n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right) \\
+ P_2 h^2 n \sum_{0\le j\le i} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right) \\
+ P_3 h^3 \frac{n^2}{2} \sum_{0\le k\le j} \left( |\varepsilon_k| + |\varepsilon_k'| + |\varepsilon_k''| + \left|\varepsilon_k^{(3)}\right| \right) + O\left(h^4\right),
\end{aligned}
$$

which reduces to

$$
|\varepsilon_n| \le P_4 h^4 + T_1 h \sum_{0\le i\le n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right),
$$

where $T_1 = P_1 + P_2 L + P_3 \frac{L^2}{2}$.

Applying a similar analysis to the equations (2.28), (2.29) and (2.30), we obtain

$$\left|\varepsilon_n^{'}\right| \leq N_1 h^4 + R_1 h \sum_{0 \leq i \leq n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right)$$

$$\left|\varepsilon_n^{''}\right| \leq N_2 h^8 + R_2 h \sum_{0 \leq i \leq n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right)$$

$$\left|\varepsilon_n^{(3)}\right| \leq N_3 h^6 + R_3 h \sum_{0 \leq i \leq n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right),$$

where $N_1$, $N_2$, $N_3$, $R_1$, $R_2$, and $R_3$ are positive constants.

Summing up, we thus have

$$|\varepsilon_n| + |\varepsilon_n'| + \left|\varepsilon_n^{''}\right| + \left|\varepsilon_n^{(3)}\right| \leq N h^4 + R h \sum_{0 \leq i \leq n} \left( |\varepsilon_i| + |\varepsilon_i'| + |\varepsilon_i''| + \left|\varepsilon_i^{(3)}\right| \right),$$

where $N$, and $R$ are positive constants.

By the discrete version of Gronwall's inequality, we obtain

$$|\varepsilon_n| + |\varepsilon_n'| + \left|\varepsilon_n^{''}\right| + \left|\varepsilon_n^{(3)}\right| \leq \frac{h^4 L}{1 - Rh} \exp\left(\frac{RL}{1 - Rh}\right).$$

Hence, $\varepsilon_n$, $\varepsilon_n^{'}$, $\varepsilon_n^{''}$, and $\varepsilon_n^{(3)}$ go to zero as $h$ goes to zero.

### 2.1.4. Numerical Experiments

To evaluate the performance of our numerical scheme, we tested it on the following example

$$f''(x) = -(x-1) f(x) + 4 \int_0^x f(x-t) f(t)\, dt + (x-4)\sin x + 2x \cos x, \tag{2.40}$$

$$f(0) = 0, f^{'}(0) = 0, \qquad 0 \leq x \leq 2,$$

whose exact solution is $f(x) = \sin x$.

We compute $f(x_n)$,$f'(x_n)$,$f''(x_n)$,$f'''(x_n)$ using equations (2.27),(2.28),(2.29) and (2.30). To solve these equations, we use the Newton-Raphson method for a non-linear system of equations as implemented in the subroutine mnewt given in Press et al. (see [P], page 374). We supplied the analytic expression for the Jacobian.We wrote the program in FORTRAN 95 using double precision.The results are shown in Table 1 that displays the errors $e_n$ at the mesh points $x_n$ for different step size $h$.
Note that $e_n = f(x_n) - f_n$ where $f(x_n)$ and $f_n$ are respectively the exact and approximate values of $f$ at $x_n$.

| $x_n$ | $h = 0.1$ | $h = 0.05$ | $h = 0.025$ | $h = 0.01$ |
|---|---|---|---|---|
| 0.5 | $4.57 \times 10^{-8}$ | $2.87 \times 10^{-9}$ | $1.80 \times 10^{-10}$ | $4.61 \times 10^{-12}$ |
| 1.0 | $4.00 \times 10^{-8}$ | $2.46 \times 10^{-9}$ | $1.53 \times 10^{-10}$ | $3.91 \times 10^{-12}$ |
| 1.5 | $3.33 \times 10^{-7}$ | $2.07 \times 10^{-8}$ | $1.29 \times 10^{-9}$ | $3.31 \times 10^{-11}$ |
| 2.0 | $8.18 \times 10^{-7}$ | $5.10 \times 10^{-8}$ | $3.19 \times 10^{-9}$ | $8.15 \times 10^{-11}$ |

Table 1: Errors for problem (2.40)

These results show that our numerical scheme yields very good approximations in comparison to results given for first order integrodifferential equations of this sort reported by Khanh in [K].

Moreover, we further evaluate the accuracy of our method by comparing the above results with those reported in [ES] for their method given in Table 2 below

| $x_n$ | $h = 0.1$ | $h = 0.05$ | $h = 0.025$ | $h = 0.01$ |
|---|---|---|---|---|
| 0.5 | $2.34 \times 10^{-8}$ | $1.44 \times 10^{-9}$ | $8.96 \times 10^{-11}$ | $2.29 \times 10^{-12}$ |
| 1.0 | $1.77 \times 10^{-7}$ | $1.10 \times 10^{-8}$ | $6.90 \times 10^{-11}$ | $1.76 \times 10^{-11}$ |
| 1.5 | $5.57 \times 10^{-7}$ | $3.47 \times 10^{-8}$ | $2.17 \times 10^{-9}$ | $5.56 \times 10^{-11}$ |
| 2.0 | $1.21 \times 10^{-6}$ | $7.54 \times 10^{-8}$ | $4.71 \times 10^{-9}$ | $1.21 \times 10^{-10}$ |

Table 2: Errors for problem (2.40)

The comparison of the two tables shows that both methods give similar results. Based on this test, our method seems to perform slightly better for larger $x$ values.

### 2.1.5. Comparison with Two Other Numerical Schemes

In this section, we develop two other numerical schemes derived similarly but with some variations in the use of the quadrature formulae. In the first method, we evaluate the inner integral in Eqs.(2.21), (2.22), (2.23), and (2.24) using a higher order Euler-Maclaurin formula instead of the Hermite quadrature formula. In the second method, instead of evaluating the middle integral in Eq.(2.25) using the Euler-Maclaurin formula, we carry out the approximation using the Hermite formula.

**Method 1.** The general Euler-Maclaurin formula is given by

$$\int_{x_0}^{x_r} \phi(x)\,dx = h\left[\frac{1}{2}\phi(x_0) + \phi(x_1) + \cdots + \phi(x_{r-1}) + \frac{1}{2}\phi(x_r)\right] - \sum_{k=1}^{N} h^{2k}\frac{B_{2k}}{(2k)!}\left[\phi^{(2k-1)}(x_r) - \phi^{(2k-1)}(x_0)\right] + E,$$

where $E = O(h^{2N+1})$ if $\phi^{(2N+1)}(x)$ is continuous, and $E = O(h^{2N+2})$ if $\phi^{(2N+2)}(x)$ is continuous, and where $B_j$ are the Bernoulli numbers [B, p. 113].

Note that in the Euler-Maclaurin formula, derivatives of even order are missing. Note also that when $N = 1$, this formula gives formula (2.25) adopted so far.

In the derivation of this method we proceed in a similar fashion as we did above when deriving our first scheme. That is, we replace the outer integrals in equations (2.21), (2.22), (2.23), and (2.24) by the Euler-Maclaurin formula (2.25), but instead now we will replace the inner integral by the Euler-Maclaurin formula of order 8

$$\begin{aligned}\int_{x_0}^{x_r} \phi(x)\, dx = h\left[\frac{1}{2}\phi(x_0) + \phi(x_1) + \cdots + \phi(x_{r-1}) + \frac{1}{2}\phi(x_r)\right] \\ - \frac{h^2}{12}\left[\phi'(x_r) - \phi'(x_0)\right] + \frac{h^4}{720}\left[\phi^{(3)}(x_r) - \phi^{(3)}(x_0)\right] \\ - \frac{h^6}{30240}\left[\phi^{(5)}(x_r) - \phi^{(5)}(x_0)\right] + O\left(h^8\right),\end{aligned}$$

which was obtained from the general Euler-Maclaurin formula with $N = 3$.

Taking $N = 3$, let

$$\begin{aligned}Q(i,\zeta) = \tfrac{h}{2}[\zeta(0) + \zeta(x_i)] - \tfrac{h^2}{12}[\zeta'(x_i) - \zeta'(0)] \\ + \tfrac{1}{720}h^4[\zeta^{(3)}(x_i) - \zeta^{(3)}(0)] - \tfrac{1}{30240}h^6[\zeta^{(5)}(x_i) - \zeta^{(5)}(0)] + O(h^8),\end{aligned}$$

taking $N = 2$, let

$$Q_1(i,\zeta) = \tfrac{1}{2}h[\zeta(0) + \zeta(x_i)] - \tfrac{1}{12}h^2[\zeta'(x_i) - \zeta'(0)]$$

$$+\tfrac{1}{720}h^4[\zeta^{(3)}(x_i)-\zeta^{(3)}(0)]+O(h^6)$$

and taking $N=1$, let

$$Q_3(i,\zeta)=\tfrac{1}{2}h[\zeta(0)+\zeta(x_i)]-\tfrac{1}{12}h^2[\zeta'(x_i)-\zeta'(0)]+O(h^4)$$

Set

$$\begin{aligned}
\phi_0(s) &= \beta(x_n,s)\,f(x_n-s)\,f(s),\\
\phi_{0i}(s) &= \beta(x_i,s)\,f(x_i-s)\,f(s),\, 1\le i\le n-1,\\
\phi_1(s) &= \frac{\partial}{\partial x}\left(\beta(x,s)\,f(x-s)\,f(s)\right)_{x=x_n},\\
\phi_{1i}(s) &= \frac{\partial}{\partial x}\left(\beta(x,s)\,f(x-s)\,f(s)\right)_{x=x_i},\, 1\le i\le n-1,\\
\phi_2(s) &= \frac{\partial^2}{\partial x^2}\left(\beta(x,s)\,f(x-s)\,f(s)\right)_{x=x_n},\\
\phi_{2i}(s) &= \frac{\partial^2}{\partial x^2}\left(\beta(x,s)\,f(x-s)\,f(s)\right)_{x=x_i},\, 1\le i\le n-1,\\
\phi_3(s) &= \frac{\partial^3}{\partial x^3}\left(\beta(x,s)\,f(x-s)\,f(s)\right)_{x=x_n},\\
\phi_{3i}(s) &= \frac{\partial^3}{\partial x^3}\left(\beta(x,s)\,f(x-s)\,f(s)\right)_{x=x_i},\, 1\le i\le n-1.
\end{aligned}$$

Equation (2.23) becomes

$$f(x_n) = f_0 + f_0' x_n + \frac{h}{2}\left[\begin{array}{c} \frac{h}{3}Q(n,\phi_0) - \frac{h^2}{12}Q_1(n,\phi_1) + Q(n,k) - Q(n,g) \\ -\frac{h^2}{12}\left[\beta(x_n,x_n) f(0) f(x_n) - \beta(0,0) f(0)^2\right] \\ -\frac{h}{6}[k(x_n) - k(0)] + \frac{h}{6}[g(x_n) - g(0)] \end{array}\right]$$

$$+ h\sum_{i=1}^{n-1}\left[\begin{array}{c} Q(i,k) - Q(i,g) + hQ(i,\phi_{0i}) - \frac{h^2}{12}Q_1(i,\phi_{1i}) \\ +\frac{h^2}{6}\phi_0(x_i) - \frac{h^3}{24}\phi_1(x_i) \\ -\frac{h^2}{12}\left[\beta(x_i,x_i) f(0) f(x_i) - \beta(0,0) f(0)^2\right] + \frac{h}{2}[k(x_i) - g(x_i)] \end{array}\right] \tag{2.41}$$

$$+ h^2\sum_{i=2}^{n-1}\sum_{j=1}^{i-1}\left[Q(j,\phi_{0j}) + h\phi_{0i}(x_j) - \frac{h^2}{12}\phi_{1i}(x_j) + [k(x_j) - g(x_j)]\right]$$

$$+ h^3\sum_{i=2}^{n-1}\sum_{j=2}^{i-1}\sum_{k=1}^{j-1}\phi_{0j}(x_k).$$

Similarly equation (2.22) becomes

$$f'(x_n) = f_0' + h^2\sum_{i=2}^{n-1}\sum_{j=1}^{i-1}\phi_{0i}(x_j) + \frac{h^2}{2}\sum_{i=1}^{n-1}\phi_0(x_i) - \frac{h^3}{12}\sum_{i=1}^{n-1}\phi_1(x_i) + h\sum_{i=1}^{n-1}Q(i,\phi_{0i})$$

$$+ h\sum_{i=1}^{n-1}k(x_i) - h\sum_{i=1}^{n-1}g(x_i) + \frac{h}{2}Q(n,\phi_0) - \frac{h^2}{12}Q_1(n,\phi_1) + Q(n,k) - Q(n,g) \tag{2.42}$$

$$- \frac{h^2}{12}\left[\beta(x_n,x_n) f(0) f(x_n) - \beta(0,0) f(0)^2\right] + O(h^4),$$

equation (2.21) becomes

$$f''(x_n) = k(x_n) - g(x_n) + h\sum_{i=1}^{n-1}\phi_0(x_i) + Q(n,\phi_0) + O(h^4), \tag{2.43}$$

and equation (2.24) becomes

$$f^{(3)}(x_n) = k'(x_n) - g'(x_n) + \beta(x_n,x_n) f(0) f(x_n) \tag{2.44}$$

$$+ h\sum_{i=1}^{n-1}\phi_1(x_i) + Q_1(n,\phi_1) + O(h^4).$$

In this case, we need two more equations to be able to solve the system. Differentiating (2.24) and conducting a similar analysis, we get

$$\begin{aligned} f^{(4)}(x_n) &= k''(x_n) - g''(x_n) + \frac{d}{dx}(\beta(x,x))_{x=x_n} f(0) f(x_n) \\ &+ \beta(x_n,x_n) f(0) f'(x_n) + \frac{d}{dx}(\beta(x,\varepsilon))_{\varepsilon,x=x_n} f(0) f(x_n) \\ &+ \beta(x_n,x_n) f'(0) f(x_n) + h\sum_{i=1}^{n-1}\phi_2(x_i) + Q_1(n,\phi_2) + O(h^4). \end{aligned} \tag{2.45}$$

Differentiating one more time and proceeding the same way, we get

$$\begin{aligned} f^{(5)}(x_n) &= k^{(3)}(x_n) - g^{(3)}(x_n) + \frac{d^2}{dx^2}(\beta(x,x))_{x=x_n} f(0) f(x_n) \\ &+ 2\frac{d}{dx}(\beta(x,x))_{x=x_n} f(0) f(x_n) + \beta(x_n,x_n) f(0) f''(x_n) \\ &+ \frac{d}{dx}\left(\frac{d}{dx}((\beta(x,\varepsilon))_{\varepsilon=x})_{x=x_n} f(0) f(x_n)\right) \\ &+ \frac{d}{dx}(\beta(x,\varepsilon))_{\varepsilon,x=x_n} f(0) f'(x_n) + \frac{d}{dx}(\beta(x,x))_{x=x_n} f'(0) f(x_n) \\ &+ \beta(x_n,x_n) f'(0) f'(x_n) + \frac{d^2}{dx^2}(\beta(x,\varepsilon))_{\varepsilon,x=x_n} f(0) f(x_n) \\ &+ 2\frac{d}{dx}(\beta(x,\varepsilon))_{\varepsilon,x=x_n} f'(0) f(x_n) + \beta(x_n,x_n) f''(0) f(x_n) \\ &+ h\sum_{i=1}^{n-1}\phi_3(x_i) + Q_3(n,\phi_3) + O(h^4). \end{aligned} \tag{2.46}$$

Now, the non-linear system of equations (2.41) to (2.46) can be solved numerically to find the unknowns $f(x_n)$,$f'(x_n)$,$f''(x_n)$,$f'''(x_n)$, $f^{(4)}(x_n)$, $f^{(5)}(x_n)$ $1 \leq n \leq N$.

We evaluated the performance of this new scheme on example (2.40) given above. Our implementation in code for this example did not produce satisfactory results. We can tentatively conclude that using the Euler-Maclaurin quadrature for the inner integral instead of the Hermite quadrature has no advantages.

**Method 2.**

In this method we proceed similarly as in section 2.1.2. First, as we did above, we replace the outer integral in equations (2.21), (2.22), (2.23), and (2.24) by the Euler-Maclaurin formula, but in this instance we replace all inner integrals by the Hermite formula (2.26).

Taking $q = 4$, let

$$\begin{aligned} Q(i,\zeta) &= \tfrac{1}{2}h\left(\zeta(x_{i-1}) + \zeta(x_i)\right) + \tfrac{3}{28}h^2\left(\zeta'(x_{i-1}) - \zeta'(x_i)\right) \\ &\quad + \tfrac{1}{84}h^3\left(\zeta''(x_{i-1}) + \zeta''(x_i)\right) + \tfrac{1}{1680}h^4\left(\zeta^{(3)}(x_{i-1}) - \zeta^{(3)}(x_i)\right), \end{aligned}$$

and taking $q = 3$, let

$$\begin{aligned} Q_1(i,\zeta) &= \tfrac{1}{2}h\left(\zeta(x_{i-1}) + \zeta(x_i)\right) + \tfrac{1}{10}h^2\left(\zeta'(x_{i-1}) - \zeta'(x_i)\right) \\ &\quad + \tfrac{1}{120}h^3\left(\zeta''(x_{i-1}) + \zeta''(x_i)\right), \end{aligned}$$

and $q = 4$, let

$$Q_2(i,\zeta) = \tfrac{1}{2}h\left(\zeta(x_{i-1}) + \zeta(x_i)\right) + \tfrac{1}{12}h^2\left(\zeta'(x_{i-1}) - \zeta'(x_i)\right)$$

Equation (2.23) becomes

$$
\begin{aligned}
f(x_n) = & \frac{h^2}{2}\sum_{i=2}^{n-1}\sum_{j=2}^{i}\sum_{k=1}^{j-1}\left[Q\left(k,\phi_{0(j-1)}\right)+\frac{h}{5}Q_1\left(k,\phi_{1(j-1)}\right)+\frac{h^2}{60}Q_2\left(k,\phi_{2(j-1)}\right)\right] \\
& +\frac{h^2}{2}\sum_{i=1}^{n-1}\sum_{j=2}^{i}\sum_{k=1}^{j-1}\left[Q\left(k,\phi_{0j}\right)-\frac{h}{5}Q_1\left(k,\phi_{1j}\right)+\frac{h^2}{60}Q_2\left(k,\phi_{2j}\right)\right] \\
& +h\sum_{i=1}^{n-1}\sum_{j=1}^{i}\left[\begin{array}{c}
\frac{h^2}{10}\left[\beta\left(x_{j-1},x_{j-1}\right)f(0)f\left(x_{j-1}\right)-\beta(x_j,x_j)f(0)f(x_j)\right] \\
+\frac{h^3}{120}\left[\begin{array}{c}
\left(\frac{d}{ds}\beta(s,s)\right)_{s=x_{j-1}}f(0)f\left(x_{j-1}\right)+\left(\frac{d}{ds}\beta(s,s)\right)_{s=x_j}f(0)f\left(x_j\right) \\
+\left(\frac{d}{ds}\beta(s,\varepsilon)\right)_{s,\varepsilon=x_{j-1}}f(0)f\left(x_{j-1}\right)+\left(\frac{d}{ds}\beta(s,\varepsilon)\right)_{s,\varepsilon=x_j}f(0)f\left(x_j\right)
\end{array}\right] \\
+\frac{h^3}{120}\left[\begin{array}{c}
\beta\left(x_{j-1},x_{j-1}\right)f'(0)f\left(x_{j-1}\right)+\beta\left(x_j,x_j\right)f'(0)f\left(x_j\right) \\
+\beta\left(x_{j-1},x_{j-1}\right)f(0)f'\left(x_{j-1}\right)+\beta\left(x_j,x_j\right)f(0)f'\left(x_j\right)
\end{array}\right] \\
+Q(j,k)-Q(j,g)
\end{array}\right] \\
& +\frac{h^2}{4}\sum_{i=2}^{n}\sum_{j=1}^{i-1}\left[Q\left(j,\phi_{0(i-1)}\right)+\frac{h}{5}Q_1\left(j,\phi_{1(i-1)}\right)+\frac{h^2}{60}Q_2\left(j,\phi_{2(i-1)}\right)\right] \\
& +\frac{h^2}{4}\sum_{i=1}^{n}\sum_{j=1}^{i}\left[Q\left(j,\phi_{0i}\right)+\frac{h}{5}Q_1\left(j,\phi_{1i}\right)+\frac{h^2}{60}Q_2\left(j,\phi_{2i}\right)\right] \\
& +h\sum_{i=1}^{n}\left[\begin{array}{c}
\frac{h^2}{10}\left[\beta\left(x_{i-1},x_{i-1}\right)f(0)f\left(x_{i-1}\right)-\beta(x_i,x_i)f(0)f(x_i)\right] \\
+\frac{h^3}{120}\left[\begin{array}{c}
\left(\frac{d}{ds}\beta(s,s)\right)_{s=x_{i-1}}f(0)f\left(x_{i-1}\right)+\left(\frac{d}{ds}\beta(s,s)\right)_{s=x_i}f(0)f(xi) \\
+\left(\frac{d}{ds}\beta(s,\varepsilon)\right)_{s,\varepsilon=x_{i-1}}f(0)f\left(x_{i-1}\right)+\left(\frac{d}{ds}\beta(s,\varepsilon)\right)_{s,\varepsilon=x_i}f(0)f\left(x_i\right)
\end{array}\right] \\
+\frac{h^3}{120}\left[\begin{array}{c}
\beta\left(x_{i-1},x_{i-1}\right)f'(0)f\left(x_{i-1}\right)+\beta\left(x_i,x_i\right)f'(0)f\left(x_i\right) \\
+\beta\left(x_{i-1},x_{i-1}\right)f(0)f'\left(x_{i-1}\right)+\beta\left(x_i,x_i\right)f(0)f'\left(x_i\right)
\end{array}\right] \\
+Q(i,k)-Q(i,g)-\frac{h}{6}Q\left(i,\phi_0\right)
\end{array}\right] \\
& +f_0+f_0'x_n-\frac{h^2}{12}\left[\left[k(x_n)-k(0)\right]-\left[g(x_n)-g(0)\right]\right].
\end{aligned}
\tag{2.47}
$$

Similarly equation (2.22) becomes

$$\begin{aligned} f'(x_n) &= f'_0 + \sum_{i=1}^{n} Q(i,k) - \sum_{i=1}^{n} Q(i,g) \\ &+ h \sum_{i=1}^{n-1} \sum_{j=1}^{i} Q(j,\phi_{0i}) + \frac{h}{2} \sum_{i=1}^{n} Q(i,\phi_0) \\ &- \frac{h^2}{12} \left[ \beta(x_n,x_n) f(0) f(x_n) - \beta(x_0,x_0) f(0)^2 + \sum_{i=1}^{n} Q_1(i,\phi_1) \right], \end{aligned} \tag{2.48}$$

equation (2.21) with $q = 4$ in the Hermite formula becomes

$$f''(x_n) = -a(x_n)f(x_n) + k(x_n) + \sum_{i=1}^{n} Q(i,\phi_0), \tag{2.49}$$

and equation (2.24) with $q = 3$ in the Hermite formula becomes

$$\begin{aligned} f'''(x_n) &= -a'(x_n) f(x_n) - a(x_n) f'(x_n) + k'(x_n) \\ &+ \beta(x_n,x_n) f(0) f(x_n) + \sum_{i=1}^{n} Q_1(i,\phi_1). \end{aligned} \tag{2.50}$$

Now, the non-linear system of equations (2.47) to (2.50) can be solved numerically to find the unknowns $f(x_n)$,$f'(x_n)$,$f''(x_n)$,$f'''(x_n)$, $1 \le n \le N$.

To evaluate the performance of this scheme we test it on the same example (2.40).
Preliminary results are shown in the following table,

| $x_n$ | $h = 0.001$ |
| --- | --- |
| 0.5 | $6.68 \times 10^{-5}$ |
| 1.0 | $3.21 \times 10^{-5}$ |
| 1.5 | $9.02 \times 10^{-5}$ |
| 2.0 | $2.00 \times 10^{-3}$ |

Table 3: Errors for problem (2.40)

The results shown are acceptable but are of low accuracy when compared to our initial method developed in section 2.1.2. At this point, the reasons for this are not clear. Further analysis and testing of the program implementing this scheme is necessary before making any definite conclusions.

## 2.2. Solution of the Physical Problem

### 2.2.1. Analytical Solution

As seen before, our physical problem can be modeled by the following IVP

$$f''(x) - Pef'(x) - Pef(x) = 2\lambda Pef(x)\int_0^\infty f(\varepsilon)d\varepsilon - \lambda Pe\int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon, \quad (2.51)$$

$$f(0) = 1, \quad f(0) = f_0',$$

where $f_0'$ is an unknown constant.

An analytical solution for this problem was given in Saleeby and Lee [SL]. We will present it briefly before tackling the problem numerically.

Consider problem (2.51). Using an Inverse Transform method (Laplace Transform coupled with series reversion — an operational calculus type method), the solution of (2.51) can be shown to be

$$
f(x) = e^{\left(\frac{Pe}{2}+\widehat{b}\right)x} \left\{ \begin{array}{c} \frac{1}{2} + \frac{d}{2\widehat{b}} + \sum_{j=2}^{\infty} \frac{\mu^{j-1}}{(j-1)!(2j-2)!} \\ \cdot \sum_{i=0}^{j} \binom{2j-2}{j-i} \frac{\left(d+\widehat{b}\right)^{i}}{i!} \sum_{m=0}^{2j-2} \binom{2j-2}{m} \\ \cdot \sum_{k=0}^{3j+i-m-4} \frac{(-1)^{5j+i-2m-6+k}(3j+i-m-4)!x^{m+k}}{k!\left(2\widehat{b}\right)^{3j+i-m-3-k}} \end{array} \right\} \tag{2.52}
$$

$$
+ e^{\left(\frac{Pe}{2}-\widehat{b}\right)x} \left\{ \begin{array}{c} \frac{1}{2} - \frac{d}{2\widehat{b}} + \sum_{j=2}^{\infty} \frac{\mu^{j-1}}{(j-1)!(2j-2)!} \sum_{i=0}^{j} \binom{2j-2}{j-i} \frac{\left(d+\widehat{b}\right)^{i}}{i!} \\ \cdot \sum_{m=0}^{2j-2} \binom{2j-2}{m} \frac{(-1)^{5j+i-2m-5}(3j+i-m-4)!x^{m}}{\left(2\widehat{b}\right)^{3j+i-m-3}} \end{array} \right\},
$$

where

$d = f'(0) - \frac{Pe}{2}$,

$\widehat{b} = \sqrt{-\widehat{\nu}} = \frac{Pe}{2}\sqrt{1 + \frac{4}{Pe}\sqrt{1 + \frac{4\lambda(Pe - f'(0))}{Pe}}}$, and

$\mu = -\lambda Pe.$

### 2.2.2. Comparison Between Analytical Solution and Numerical Solution

In this section, we plot the graphs of the analytical solution given by (2.52) for different values of $f'(0), Pe$ and $\lambda$.

Fig.(2.21) and Fig.(2.22) display the analytical solutions on a logarithmic scale.

Fig.(2.21) shows a plot of $\log(f(x))$ whenever $f(x) > 0$ whereas Fig.(2.22) shows a plot of $-\log(-f(x))$ to account for the negative values of $f(x)$.

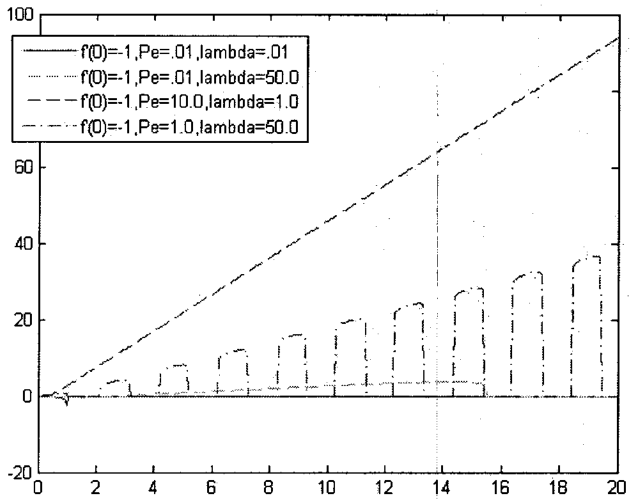



Fig.(2.21): Plot of $\log(f(x))$ when $f(x) > 0$.. $f(x)$ represents the analytical solution of the IVP.

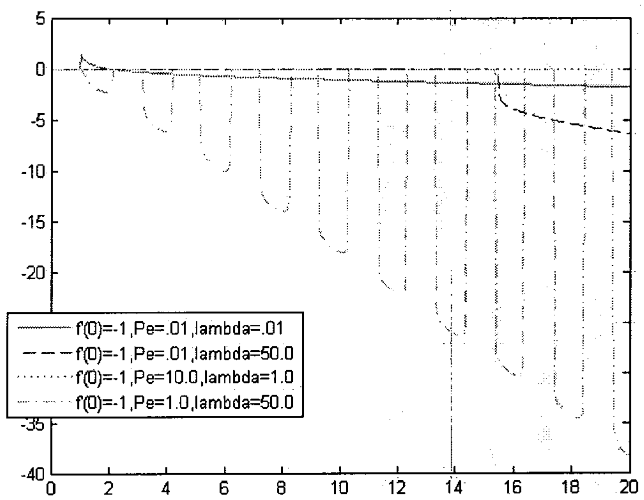



Fig.(2.22): Plot of $-\log(-f(x))$ when $f(x) < 0$. $f(x)$ represents the analytical solution of the IVP.

The numerical solution was in perfect match with the analytical solution (with only 9 terms used in the infinite series).

We notice from the graphs above, that we do have oscillating solutions, and solutions that could go to infinity, and this is highly influenced by the choice of initial conditions. So in order to enforce $\lim_{x\to\infty} f(x) = 0$ as needed by the physical setting, we are required to solve the following BVP

$$f''(x) - Pef'(x) - Pe\sqrt{1 + \frac{4\lambda\,(Pe - f'(0))}{Pe}}f(x) = -\lambda Pe \int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon,$$
$$f(0) = 1,$$
$$f(L) = 0.$$

Note that (3.0) is obtained from (1.60) by using $\int_0^x f(\varepsilon)d\varepsilon = \frac{-1+\sqrt{1+\frac{4\lambda(Pe-f'(0))}{Pe}}}{2\lambda}$.

Physically, $f(x)$ represents the dimensionless number of particles of size $x$. Therefore, for large $x$, $f(x)$ should tend to 0. To account for this, we consider in this chapter the following BVP (3.0)

$$f''(x) - Pef'(x) - Pe\sqrt{1 + \frac{4\lambda\left(Pe - f'(0)\right)}{Pe}}f(x) = -\lambda Pe\int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon, \tag{3.0(a)}$$

$$f(0) = 1, \tag{3.0(b)}$$

$$f(L) = 0, \qquad 0 \leq x \leq L. \tag{3.0(c)}$$

We start by presenting its analytical solution with some of its properties, then solve it numerically using the shooting method which employs our numerical solution of the IVP. In the last section, we couple the shooting technique with an optimization technique to find optimal estimates for the parameters.

## 3.1. Analytical Solution

### 3.1.1. Analytical Expression of the Solution

We have seen in section 2.2.3, that we could have oscillations in the solution of (2.51). It is clear from the analytical expression of the solution given by (2.52), that these oscillations are caused by the term $e^{\left(\frac{Pe}{2}+\widehat{b}\right)x}(\cdot)$. So in order that $\lim_{x\to\infty} f(x) = 0$, the term multiplying $e^{\left(\frac{Pe}{2}+\widehat{b}\right)x}$ in (2.52) should be set equal to zero, and therefore, the solution reduces to

$$f(x) = e^{\left(\frac{Pe}{2}-\widehat{b}\right)x} \left\{ \begin{array}{c} \frac{1}{2} - \frac{d}{2\widehat{b}} + \sum_{j=2}^{\infty} \frac{\mu^{j-1}}{(j-1)!(2j-2)!} \sum_{i=0}^{j} \binom{2j-2}{j-i} \frac{\left(d+\widehat{b}\right)^i}{i!} \\ \cdot \sum_{m=0}^{2j-2} \binom{2j-2}{m} \frac{(-1)^{5j+i-2m-5}(3j+i-m-4)!x^m}{\left(2\widehat{b}\right)^{3j+i-m-3}} \end{array} \right\}. \tag{3.11}$$

Conducting further analysis (see [SL]), and to obtain real solutions, it can be shown that

$$\frac{Pe}{2}\left[1-\sqrt{1+\frac{4}{Pe}\sqrt{1+\frac{4\lambda\left(Pe-f'(0)\right)}{Pe}}}\right] < f'(0) \leq Pe. \tag{3.12}$$

Note that the upper bound in (3.12) was set to 0 in [SL]. This was determined based primarily on numerical experiments, some heuristic physical reasoning, and considerations of limiting cases. In section 3.1.4 we actually justify this upper bound mathematically (see Proposition 3.4). For more details see Saleeby and Lee [SL].

### 3.1.2. Convergence of the Solution

It was shown in section 3.1.1 above that the analytic solution of (2.52) with $\lim_{x\to\infty} f(x) = 0$ is given by

$$f(x) = e^{\left(\frac{Pe}{2}-\widehat{b}\right)x} \left\{ \begin{array}{c} \frac{1}{2} - \frac{d}{2\widehat{b}} + \sum_{j=2}^{\infty} \frac{\mu^{j-1}}{(j-1)!(2j-2)!} \sum_{i=0}^{j} \binom{2j-2}{j-i} \frac{\left(d+\widehat{b}\right)^i}{i!} \\ \cdot \sum_{m=0}^{2j-2} \binom{2j-2}{m} \frac{(-1)^{5j+i-2m-5}(3j+i-m-4)!x^m}{\left(2\widehat{b}\right)^{3j+i-m-3}} \end{array} \right\}.$$

Let

$$S = \sum_{j=2}^{\infty} \frac{\mu^{j-1}}{(j-1)!\,(2j-2)!} \sum_{i=0}^{j} \binom{2j-2}{j-i} \frac{\left(d+\widehat{b}\right)^i}{i!} \cdot \sum_{m=0}^{2j-2} \binom{2j-2}{m} \frac{(-1)^{5j+i-2m-5}\,(3j+i-m-4)!x^m}{\left(2\widehat{b}\right)^{3j+i-m-3}}, \tag{3.13}$$

then,

$$f(x) = e^{\left(\frac{Pe}{2}-\widehat{b}\right)x} \left[\frac{1}{2} - \frac{d}{2\widehat{b}} + S\right]. \tag{3.14}$$

It follows that if the series $S$ is convergent, then $f$ will also be convergent. Since $S$ is a positive series, we will show that it is convergent by showing that it is bounded above by a convergent series.

Let $\mu = -\delta$, where $\delta > 0$ then

$$S = \sum_{j=2}^{\infty} \frac{\delta^{j-1}}{(j-1)!\,(2j-2)!} \sum_{i=0}^{j} \binom{2j-2}{j-i} \frac{(-1)^i\left(d+\widehat{b}\right)^i}{i!} \cdot \sum_{m=0}^{2j-2} \binom{2j-2}{m} \frac{(3j+i-m-4)!x^m}{\left(2\widehat{b}\right)^{3j+i-m-3}}. \tag{3.15}$$

Considering that

$$\begin{aligned}
&\frac{1}{(j-1)!\,(2j-2)!} \binom{2j-2}{j-i} \frac{1}{i!} \binom{2j-2}{m} (3j+i-m-4)! \\
&= \frac{1}{(j-1)!\,(2j-2)!} \frac{(2j-2)!}{(j-i)!(j+i-2)!} \frac{1}{i!} \frac{(2j-2)!}{m!(2j-2-m)!} \\
&\cdot k(2j-2-m)!\,(j+i-2)! \frac{j!}{j!} \\
&= k \frac{(2j-2)!}{(j-1)!j!} \frac{1}{m!} \frac{j!}{(j-i)!i!},
\end{aligned}$$

where $k$ is a positive constant.

$S$ can be written as

$$S = k\sum_{j=2}^{\infty}\left(\frac{\delta}{8\widehat{b}^3}\right)^{j-1}\frac{(2j-2)!}{(j-1)!j!}\sum_{i=0}^{j}\left(\begin{array}{c} j \\ i \end{array}\right)(-1)^i\left(\frac{d+\widehat{b}}{2\widehat{b}}\right)^i\sum_{m=0}^{2j-2}\frac{(2\widehat{b}x)^m}{m!}.$$

From Eq.(3.12) we have that

$$d < \widehat{b} \qquad \text{and that} \qquad d+\widehat{b} > 0, \tag{3.16}$$

implying that

$$0 < 1 - \frac{d+\widehat{b}}{2\widehat{b}} < 1. \tag{3.17}$$

Using (3.17) and the binomial expansion formula

$$\sum_{k=0}^{n}\left(\begin{array}{c} n \\ k \end{array}\right)a^k b^{n-k} = (a+b)^n,$$

we get

$$S \leq ke^{2\widehat{b}x}\sum_{j=2}^{\infty}\left(\frac{\delta}{8\widehat{b}^3}\right)^{j-1}\frac{(2j-2)!}{(j-1)!j!}\left(1-\frac{d+\widehat{b}}{2\widehat{b}}\right)^j e^{2\widehat{b}x}.$$

For the series to be convergent, we need that

$$\frac{\delta}{8\widehat{b}^3} < 1 \qquad \text{i.e} \qquad \mu > -8\widehat{b}^3, \tag{3.18}$$

so that

$$\sum_{j=2}^{\infty}\left(\frac{\delta}{8\widehat{b}^3}\right)^{j-1}\frac{(2j-2)!}{(j-1)!j!}\left(1-\frac{d+\widehat{b}}{2\widehat{b}}\right)^j \to 0 \quad \text{as} \quad j \to \infty.$$

In this case, applying the ratio test

$$\lim_{j\to\infty}\frac{a_{j+1}}{a_j} = \lim_{j\to\infty}\frac{\left(\frac{\delta}{8\widehat{b}^3}\right)^j \frac{(2j)!}{j!(j+1)!}\left(1-\frac{d+\widehat{b}}{2\widehat{b}}\right)^{j+1}}{\left(\frac{\delta}{8\widehat{b}^3}\right)^{j-1} \frac{(2j-2)!}{(j-1)!j!}\left(1-\frac{d+\widehat{b}}{2\widehat{b}}\right)^{j}}$$

$$= \lim_{j\to\infty}\frac{\delta}{8\widehat{b}^3}\frac{(2j)(2j-1)}{j(j+1)}\left(1-\frac{d+\widehat{b}}{2\widehat{b}}\right)$$

$$= \frac{\delta}{2\widehat{b}^3}\left(1-\frac{d+\widehat{b}}{2\widehat{b}}\right).$$

For this limit to be less than 1, $\frac{\delta}{2\widehat{b}^3}$ should be less than 1

$$\frac{\delta}{2\widehat{b}^3} < 1 \qquad \text{i.e} \qquad \mu > -2\widehat{b}^3. \tag{3.19}$$

From Ineq.(3.18) and (3.19), we can conclude that $S$, and subsequently $f$, is convergent whenever $\mu > -2\widehat{b}^3$.

### 3.1.3. Positivity of the Solution

Since $f$ is a density function (although not necessarily normalized), then it should be positive. In this section, we show that $f$ is positive by showing that it is bounded below by a positive function.

It was shown in section 3.1.2, that

$$f(x) = e^{\left(\frac{Pe}{2}-\widehat{b}\right)x}\left[\frac{1}{2}-\frac{d}{2\widehat{b}}+S\right],$$

where

$$S = \sum_{j=2}^{\infty}\frac{\delta^{j-1}}{(j-1)!\,(2j-2)!}\sum_{i=0}^{j}\binom{2j-2}{j-i}\frac{(-1)^i\left(d+\widehat{b}\right)^i}{i!} \cdot\sum_{m=0}^{2j-2}\binom{2j-2}{m}\frac{(3j+i-m-4)!x^m}{\left(2\widehat{b}\right)^{3j+i-m-3}}.$$

Considering that

$$\frac{1}{(j-1)!\,(2j-2)!}\left(\begin{array}{c}2j-2\\ j-i\end{array}\right)\frac{1}{i!}\left(\begin{array}{c}2j-2\\ m\end{array}\right)(3j+i-m-4)!$$
$$=\frac{1}{(j-1)!\,(2j-2)!}\frac{(2j-2)!}{(j-i)!(j+i-2)!}\frac{1}{i!}\left(\begin{array}{c}2j-2\\ m\end{array}\right)$$
$$\cdot\, k(2j-2-m)!\,(j+i-2)!$$
$$=\frac{k}{(j-1)!j!}\left(\begin{array}{c}j\\ i\end{array}\right)\left(\begin{array}{c}2j-2\\ m\end{array}\right)(2j-2-m)!$$

$S$ can be written as

$$S=k\sum_{j=2}^{\infty}\left(\frac{1}{2\widehat{b}}\right)^{3j-3}\frac{\delta^{j-1}}{(j-1)!j!}\sum_{i=0}^{j}\left(\begin{array}{c}j\\ i\end{array}\right)(-1)^{i}\left(\frac{d+\widehat{b}}{2\widehat{b}}\right)^{i}$$
$$\cdot\sum_{m=0}^{2j-2}\left(\begin{array}{c}2j-2\\ m\end{array}\right)(2j-2-m)!(2\widehat{b}x)^{m},$$

using that $n!\geq 2^{n+1}$ and that

$$1-\frac{d+\widehat{b}}{2\widehat{b}}>0,$$

we have that

$$S \geq 2k \sum_{j=2}^{\infty} \left( \frac{\delta}{8\widehat{b}^3} \right)^{j-1} \frac{1}{(j-1)!j!} \left( 1 - \frac{d+\widehat{b}}{2\widehat{b}} \right)^j$$

$$\cdot \sum_{m=0}^{2j-2} \left( \begin{array}{c} 2j-2 \\ m \end{array} \right) 2^{2j-2-m} (2\widehat{b}x)^m,$$

$$= 2k \sum_{j=2}^{\infty} \left( \frac{\delta}{8\widehat{b}^3} \right)^{j-1} \frac{1}{(j-1)!j!} \left( 1 - \frac{d+\widehat{b}}{2\widehat{b}} \right)^j (2 + 2\widehat{b}x)^{2j-2}$$

$$= 2k \sum_{j=2}^{\infty} \left( \frac{\delta}{2\widehat{b}^3} \right)^{j-1} \frac{1}{(j-1)!j!} \left( 1 - \frac{d+\widehat{b}}{2\widehat{b}} \right)^j (1 + \widehat{b}x)^{2j-2} > 0,$$

where $k$ is a positive constant.

We know from Eq.(3.14) that

$$f(x) = e^{\left(\frac{Pe}{2} - \widehat{b}\right)x} \left[ \frac{1}{2} - \frac{d}{2\widehat{b}} + S \right].$$

So in order that

$$f(x) > 0 \quad \forall\, x,$$

all we still need to prove is that $\frac{1}{2} - \frac{d}{2\widehat{b}} > 0$. This follows immediately from $d < \widehat{b}$.

### 3.1.4. Monotonicity of the Solution

Given that in a previous section we have established that the solution given in (3.11) converged, it is natural to attempt to examine the monotone behavior of the solution by finding a representation for its derivative. However, in order to do this, even at $x = 0$, it is then necessary to solve an infinite series implicit inequality, which appears to be a difficult task. Alternatively, in this section we obtain the result we are seeking by considering the equation of our model coupled with the constraints under which we have obtained the convergence and positivity of the series representation of solution.

Differentiate Eq.(3.0), we obtain

$$f'''(x) - Pef''(x) - \rho f'(x) + \lambda Pef(x) = -\lambda Pe \int_0^x f(x-\varepsilon)f'(\varepsilon)d\varepsilon, \quad (3.21)$$

where $\rho = Pe\sqrt{1 + \frac{4\lambda\left(Pe - f_0'\right)}{Pe}}$.

Let $g(x) = f'(x)$. Then (3.21) can be written as

$$g''(x) - Peg'(x) - \rho g(x) + \lambda Pef(x) = -\lambda Pe \int_0^x f(x-\varepsilon)g(\varepsilon)d\varepsilon. \quad (3.22)$$

Integrate (3.22) from 0 to $x$ and exchange the order of integration, we obtain

$$\begin{aligned} g'(x) = Peg(x) &+ \int_0^x \left(\rho - \lambda Pe \int_\varepsilon^x f(s-\varepsilon)\, ds\right) g(\varepsilon)\, d\varepsilon \qquad (3.23) \\ &- \lambda Pe \int_0^x f(\varepsilon)\, d\varepsilon + g'(0) - Peg(0). \end{aligned}$$

Again, integrate (3.23) from 0 to $x$ and exchange the order of integration, we obtain

$$\begin{aligned} g(x) = &\int_0^x \int_0^t \left[\rho - \lambda Pe \int_\varepsilon^t f(s-\varepsilon)\, ds\right] g(\varepsilon)\, d\varepsilon dt + Pe \int_0^x g(\varepsilon)\, d\varepsilon \\ &- \lambda Pe \int_0^x \int_0^s f(\varepsilon)\, d\varepsilon ds + (g'(0) - Peg(0))x + g(0), \end{aligned}$$

which can be written as

$$g(x) = \int_0^x \left( Pe + \int_\varepsilon^x \left[ \rho - \lambda Pe \int_\varepsilon^t f(s-\varepsilon)\, ds \right] dt \right) g(\varepsilon)\, d\varepsilon \qquad (3.24)$$
$$- \lambda Pe \int_0^x \int_0^s f(\varepsilon)\, d\varepsilon ds + (g'(0) - Peg(0))x + g(0),$$

which can in turn be written as

$$g(x) = \int_0^x K(x-\varepsilon)\, g(\varepsilon)\, d\varepsilon + k(x). \qquad (3.25)$$

Then, from (3.24) we see that

$$K(x-\varepsilon) = Pe + \int_\varepsilon^x \left[ \rho - \lambda Pe \int_\varepsilon^t f(s-\varepsilon)\, ds \right] dt.$$

Recall that from the expression of the solution (3.11), and under the constraints $\frac{Pe}{2}\left[1 - \sqrt{1 + \frac{4}{Pe}\sqrt{1 + \frac{4\lambda(Pe - f'(0))}{Pe}}}\right] < f'(0) \leq Pe$, and $\mu > -2\widehat{b}^3$, it was shown in section 3.1.3 that $f(x) > 0$ on $[0, \infty)$. This implies that

$$K(x-\varepsilon) \geq Pe + \int_\varepsilon^x \left[ \rho - \lambda Pe \int_0^\infty f(s-\varepsilon)\, ds \right] dt \qquad (3.26)$$
$$= Pe + \left( \rho - \lambda Pe \left( \frac{-1 + \frac{\rho}{Pe}}{2\lambda} \right) \right) (x-\varepsilon)$$
$$= Pe + \left( \frac{1}{2}\rho + \frac{1}{2}Pe \right) (x-\varepsilon) > 0.$$

The expression of $k(x)$ is

$$k(x) = -\lambda Pe \int_0^x \int_0^s f(\varepsilon)\, d\varepsilon ds + (g'(0) - Peg(0))x + g(0), \tag{3.27}$$

where $g(0) = f_0'$, and $g'(0) = Pef_0' + \rho$.

Now, we are interested in showing (under the constraints stated above) that $g(x) = f'(x) < 0$ on $[0, \infty)$. Towards this end we need the following results, from [GLS] and Naito et al. [NSMN], that characterize positive solutions of equation (3.25). Recall that $L^1_{loc}([0,\infty), \mathbf{R})$ is the space of functions that are locally integrable.

**Theorem 3.1.** (see [GLS]) Let $K \in L^1_{loc}([0,\infty), \mathbf{R})$. Then for every $k \in L^1_{loc}([0,\infty), \mathbf{R})$, there exists a unique solution $G(x) \in L^1_{loc}([0,\infty), \mathbf{R})$ of (3.25) given by the variation of parameters formula

$$G(x) = k(x) + (r * k)(x), \; x \geq 0, \tag{3.28}$$

where $r$ is the resolvent of $K$.

**Definition.** (Definition 3.3 in [NSMN]) Equation (3.25) is called positive if for every $k \in L^1_{loc}([0,\infty), \mathbf{R})$ being nonnegative, the corresponding solution $g$ is also nonnegative.

**Theorem 3.2.** (Theorem 3.4 in [NSMN]) Equation (3.25) is positive if and only if the resolvent $r$ of $K$ is nonnegative.

**Corollary 3.3.** (Corollary 3.7 in [NSMN]) If $K$ is nonnegative, then Equation (3.25) is positive.

In order to employ these results, multiply (3.25) by $-1$, and let $G(x) = -g(x), h(x) = -k(x)$. Then (3.25) can be written as

$$G(x) = \int_0^x K(x-\varepsilon) G(\varepsilon) d\varepsilon + h(x). \tag{3.29}$$

Given $K$ non-negative, then by Theorem 3.2, Eq.(3.28) and Corollary 3.3, it follows that (3.29) is positive (or $f'(x) < 0$) if and only if $h(x)$ is nonnegative ($k(x)$ is nonpositive).

Now we obtain a necessary condition for $k(x)$ to be nonpositive.

Consider the expression of $k(x)$ given in (3.27), then

$$k'(x) = -\lambda Pe \int_0^x f(\varepsilon) d\varepsilon + \rho,$$

and

$$k''(x) = -\lambda Pe f(x).$$

Under our assumptions, we immediately obtain that $k''(x) < 0$ on $[0, \infty)$. Now suppose that $k'(x) \leq 0$ on $[0, \infty)$, then

$$\int_0^x f(\varepsilon) d\varepsilon \geq \frac{\rho}{\lambda Pe}.$$

But then by the positivity of $f$ we have that

$\int_0^\infty f(\varepsilon) d\varepsilon = \frac{-1+\frac{\rho}{Pe}}{2\lambda} > \int_0^x f(\varepsilon) d\varepsilon \geq \frac{\rho}{\lambda Pe}$, which is impossible.

Therefore, we have that $k(x)$ is a concave down monotone increasing function on $[0, \infty)$. Hence, a necessary (but not sufficient) condition for $k(x)$ to be nonpositive is that $k(0) = f_0'$ is nonpositive.

Thus we have proved that

**Proposition 3.4.** A necessary condition for $f(x)$ to be monotone decreasing positive on $[0, \infty)$ is that

$$\frac{Pe}{2}\left[1-\sqrt{1+\frac{4}{Pe}\sqrt{1+\frac{4\lambda\left(Pe-f'(0)\right)}{Pe}}}\right] < f'(0) \leq 0, \text{ and } \mu > -2\widehat{b}^{3}.$$

.

### 3.2. Numerical Solution:Shooting Method

In this section, we consider the following BVP

$$f''(x) - Pef'(x) - Pe\sqrt{1+\frac{4\lambda\left(Pe-f'(0)\right)}{Pe}}f(x) = -\lambda Pe\int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon,$$
$$f(0) = 1,$$
$$f(L) = \gamma,$$

and show how to solve it numerically.

Note that for $\gamma = 0$, this BVP reduces to problem (3.0) that we are interested in solving.

In the literature, there exist several different methods to solve such a problem. The primary methods used are the finite difference method, the collocation method and the shooting method. To make use of our numerical scheme we will employ the shooting method, which replaces the given BVP by a sequence of IVPs (3.3) of the form

$$f''(x) - Pef'(x) - Pe\sqrt{1 + \frac{4\lambda\,(Pe - f'(0))}{Pe}}f(x) = -\lambda Pe \int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon, \tag{3.3(a)}$$

$$f(0) = 1, \tag{3.3(b)}$$

$$f'(0) = s, \tag{3.3(c)}$$

where $s$ is a guessed initial value that is successively refined until the desired boundary condition at $L$ is satisfied.

Since the solution of this IVP depends on $s$, we will denote it by $f(s,x)$, and the problem reduces to finding the value $s^*$ of $s$, such that $f(s^*,L) - \gamma = 0$. (3.3) with $s = s^*$ and $\gamma = 0$ is then equivalent to (3.0).

We start by guessing a value $s_0$ of $s$ in (3.3(c)) and then solve the resulting IVP using our numerical method to find $f(s_0,x)$, then we examine its value at $x = L$. If $f(s_0,L) - \gamma$ is not sufficiently close to 0, we choose another value $s_1$ for $s$, then again solve the resulting IVP and compare $f(s_1,L)$ to $\gamma$. We repeat until $f(s^*,L) - \gamma$ is sufficiently close to "hitting" 0 within a specified tolerance $\varepsilon$.

To find $s^*$ we can use a root-finding method such as Newton's method or the secant method. For example, using the secant method, after choosing two good initial approximations $s_0$ and $s_1$, the successive approximations given by

$$s_n = s_{n-1} - \frac{[f(s_{n-1},L) - \gamma]\,(s_{n-1} - s_{n-2})}{f(s_{n-1},L) - f(s_{n-2},L)} \qquad n = 2, 3, \ldots$$

converge to $s^*$.

But for the method to converge, $s_0$ and $s_1$ should be close to $s^*$ whose value is unknown. To overcome this problem, we derive the moments of the PB, which will give us good initial guesses for $s_0$ and $s_1$.
Note that it is not a simple matter to implement the Newton method in this setting as this would involve finding the derivative of a functional.

Example:

To examine the performance of the method, we first carry out a test on the following problem

$$f''(x) = -(x-1) f(x) + 4 \int_0^x f(x-t) f(t)\, dt + (x-4)\sin x + 2x \cos x,$$
$$f(0) = 0, f(\pi) = 0, \qquad 0 \le x \le \pi, \tag{3.40}$$

whose exact solution is $f(x) = \sin x$.

Case1:

We start with $s_0 = 0.4$, and choose $\varepsilon = 10^{-4}$. We obtain $|f(s_0, \pi)| = 5.0920 > \varepsilon$, then we have to apply the shooting method in order to find a value $s^*$ such that $|f(s^*, \pi)| < \varepsilon$. So we guess another value $s_1 = 3.6710$ of $s$ and apply the secant method with the two initial guesses $s_0$ and $s_1$. The successive values of $s_n$ given by the secant method were as follows:
$s_2 = 0.4841, s_3 = 0.5540, s_4 = 1.7168, s_5 = 0.7652, s_6 = 0.8881,$
$s_7 = 1.0320, s_8 = 0.9964, s_9 = 0.9998, s_{10} = s^* = 0.9999$,with $|f(s^*, \pi)| < \varepsilon$
Since $f'(0) = \cos(0) = 1$, it is clear that the shooting method converges to the exact solution. This is illustrated in Fig.(3.21) below

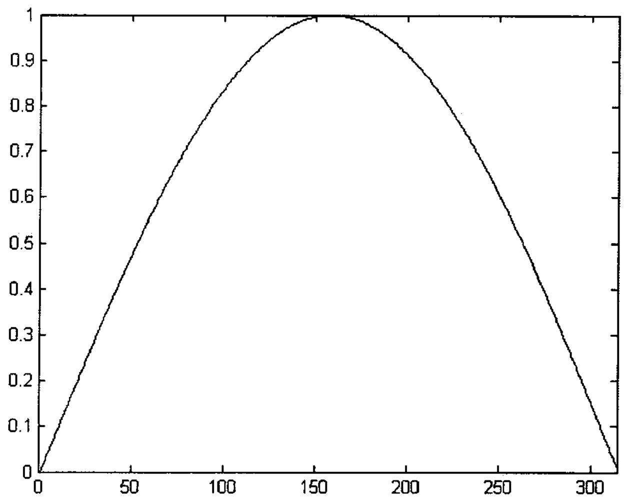



Fig.(3.21): The solution of (3.4) given by the shooting algorithm, using $s_0 =$ 0.4 as initial guess.

Case 2:

Now, we start with $s_0 = 0.05$, and choose $\varepsilon = 10^{-4}$.We obtain $|f(s_0, \pi)| =$ $4.4771 > \varepsilon$, so we also need to apply the shooting method. In this case, we choose $s_1$ to be $s_1 = -0.9267$, and apply the secant method with $s_0$ and $s_1$as initial guesses. The successive values of $s_n$ resulting from applying the secant method were as follows:

$s_2 = -0.4078, s_3 = -0.4952, s_4 = -0.5061, s_5 = s^* = -0.5057$ with $|f(s^*, \pi)| <$ $\varepsilon$.

In this case, the shooting method fails to find the exact solution. This is clearly illustrated in Fig.(3.22)

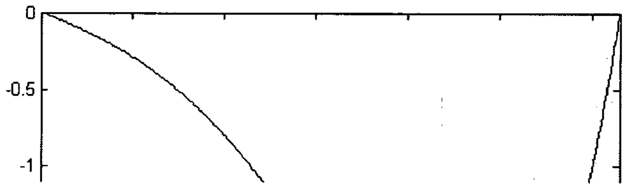



Fig.(3.22): The solution of (3.4) given by the shooting algorithm, using $s_0 = 0.05$ as initial guess.

The observation of the two cases, shows that the shooting method converges to the exact solution of the problem only if the initial guess $s_0$ is close to the actual one. This emphasizes the need for deriving the moments equations that will give good initial guess.

### 3.3. Moments Equations

It is well known that the method of moments can be applied to compute estimates of the parameters in population balances of first order integrodifferential equations(see [HK] &[RL]). It is then possible that these moments could be of some help to obtain reasonable initial estimates for our optimization algorithm. Our numerical experiments show that this is the case for small parameter values. However, a more detailed investigation is needed to assess how useful these initial estimates can be in our case for large parameter values. In this section, we derive the moments of (3.50).

Consider the equation

$$D_G n''(y) - Gn'(y) - \frac{1}{\tau}n(y) = Kn(y)\int_0^\infty n(\varepsilon)d\varepsilon - \frac{K}{2}\int_0^y n(y-\varepsilon)n(\varepsilon)d\varepsilon. \tag{3.50}$$

Its moment transformation is

$$\begin{aligned} &D_G\int_0^\infty y^j n''(y)dy - G\int_0^\infty y^j n'(y)dy - \frac{1}{\tau}\int_0^\infty y^j n(y)dy \\ &= K\int_0^\infty y^j n(y)\int_0^\infty n(\varepsilon)d\varepsilon dy - \frac{K}{2}\int_0^\infty y^j\int_0^y n(y-\varepsilon)n(\varepsilon)d\varepsilon dy. \end{aligned} \tag{3.51}$$

The terms in the above equation can be integrated separately

$$D_G\int_0^\infty y^j n''(y)dy = \begin{cases} -D_G n'(0), & for \quad j=0 \\ D_G n(0), & for \quad j=1 \\ D_G j(j-1)\mu_{j-2}, & for \quad j\geq 2 \end{cases},$$

$$G\int_0^\infty y^j n'(y)dy = \begin{cases} -Gn(0) \\ -Gj\mu_{j-1} \end{cases},$$

$$\frac{1}{\tau}\int_0^\infty y^j n(y)dy = \frac{1}{\tau}\mu_j,$$

$$K\int_0^\infty y^j n(y)\int_0^\infty n(\varepsilon)d\varepsilon dy = K\mu_0\mu_j,$$

$$\frac{K}{2}\int_0^\infty y^j\int_0^y n(y-\varepsilon)n(\varepsilon)d\varepsilon dy = \frac{K}{2}\sum_{i=0}^{j}\binom{j}{i}\mu_i\mu_{j-i},$$

where

$$m_j = \sum_{i=1}^{N} n_i y_i^j \Delta y.$$

Replacing in Eq.(3.51), the moment form of the population balance Eq.(3.50) is given as

$$\begin{cases} -D_G n'(0) + Gn(0) - \frac{1}{\tau}m_0 = \frac{K}{2}m_0^2, & for \quad j=0 \\ D_G n(0) + Gm_0 - \frac{1}{\tau}m_1 = 0, & for \quad j=1 \\ D_G j(j-1)m_{j-2} + Gjm_{j-1} - \frac{1}{\tau}m_j = Km_0m_j - \frac{K}{2}\sum_{i=0}^{j}\binom{j}{i}m_i m_{j-i}, & for \quad j\geq 2. \end{cases}$$

The parameters $D_G, G, \tau$ and $K$ can then be determined by solving the following system of nonlinear equations

$$\frac{1}{\tau}m_0 = -D_G n'(0) + Gn(0) - \frac{K}{2}m_0^2,$$
$$\frac{1}{\tau}m_1 = D_G n(0) + Gm_0,$$
$$\frac{1}{\tau}m_2 = 2D_G m_0 + 2Gm_1 + Km_1^2,$$
$$\frac{1}{\tau}m_3 = 6D_G m_1 + 3Gm_2 + 3Km_1m_2.$$

Using the dimensionless variables introduced in section 1.2, we see that $\mu_j = \frac{m_j}{n(0)(G_T)^{j+1}}, j = 1, 2, 3, \cdots$, and we then have the dimensionless moments equations

$$\mu_0 = -\frac{1}{Pe} f_0' + f_0 - \lambda \mu_0^2,$$
$$\mu_1 = \frac{f_0}{Pe} + \mu_0,$$
$$\mu_2 = \frac{2}{Pe}\mu_0 + 2\mu_1 + 2\lambda\mu_1^2,$$
$$\mu_3 = \frac{6}{Pe}\mu_1 + 3\mu_2 + 6\lambda\mu_1\mu_2.$$

To estimate the moments $\mu_j$ from the discrete data, we define $\mu_j := \sum_{i=1}^{N} f(x_i^*) x_i^{*j} \Delta x_i$, where $x_i^* = x_{i-1+} \frac{x_i - x_{i-1}}{2}, \Delta x_i = h$, and $f(x_i^*) = \frac{f(x_{i-1}) + f(x_i)}{2}$.

The following exact solution can be obtained for these equations

$$Pe = -6 \frac{\mu_2\mu_0 - \mu_1^2}{-3\mu_2^2 + 3\mu_1\mu_2 + \mu_3\mu_1},$$
$$\lambda = -\frac{1}{6\mu_1} \frac{3\mu_1\mu_2 + 3\mu_2\mu_0 - \mu_0\mu_3 - 6\mu_1^2}{\mu_2\mu_0 - \mu_1^2},$$

Let

$$I = 9\mu_0^2\mu_1\mu_2^3 - 27\mu_0^2\mu_1^2\mu_2^2 - 3\mu_0^2\mu_1^2\mu_2\mu_3 - 18\mu_0\mu_1^3\mu_2^2$$
$$+ 90\mu_0\mu_1^4\mu_2 + 6\mu_0\mu_1^4\mu_3 - 36\mu_1^6 + 45\mu_0^3\mu_1\mu_2^2 - 90\mu_0^2\mu_1^3\mu_2$$
$$+ 36\mu_0\mu_1^5 - 9\mu_0^3\mu_2^3 + 3\mu_0^3\mu_3\mu_2^2 - \mu_0^3\mu_3^2\mu_1 - 6\mu_0^2\mu_1^3\mu_3$$

$$f_0' = -\frac{I}{\left(-3\mu_2^2 + 3\mu_1\mu_2 + \mu_3\mu_1\right)^2 \mu_1},$$
$$f_0 = 6\left(\mu_2\mu_0 - \mu_1^2\right)\frac{-\mu_1 + \mu_0}{-3\mu_2^2 + 3\mu_1\mu_2 + \mu_3\mu_1}.$$

## 3.4. Parameter Estimation and Optimization

As was mentioned in the introduction, equations of the type of (1.10) arise in crystallization. Such models are used for predicting the crystal size distribution knowing the kinetics. Present theoretical knowledge does not permit the prediction of crystallization kinetics for a particular substance a priori. Hence we have the inverse problem for estimating the parameters from experimental data.

Given a set of data, the objective of the inverse problem is to find the model parameters that reproduce the experimental results in the best possible way. The inverse problem is then posed as an optimization problem that uses iterative techniques to minimize an objective function measuring the goodness of fit of the model with respect to experimental data.

The inverse problem can be divided into two phases:

In the first phase, the unknown parameters are guessed and the direct problem is solved.

In the second phase, an optimization algorithm such as in Newton method and gradient search methods (conjugate gradient method, quasi-Newton updates, Levenberg-Marquardt method or modified Gauss-Newton method) is used to minimize the objective function which is defined as an error norm between the experimental data and the data calculated for the guessed parameters. This gives new parameters values that are substituted for the unknown parameters, and the process repeats.

We apply in our case, the optimization routine lsqnonlin of Matlab Optimization Toolbox that uses the Levenberg-Marquardt algorithm to minimize the sum of squares $S(p) = \sum_{i=1}^{n}[f_i - f(x_i, p)]^2$, where $f_i$ is the measured value, $f(x_i, p)$ is the value obtained from the solution of the direct problem with estimated parameters, and $p$ is the vector of unknown parameters, and solve the direct IVPs using our numerical scheme.

It turns out that in our problem, $f_0'$ is one of the parameters to be estimated, and this parameter is subject to another constraint, since $f_0'$ should be chosen to satisfy $f(L, f_0') = 0$. To account for this constraint, the optimization algorithm should be coupled with the shooting algorithm as described in section 3.4.1. below.

### 3.4.1 Algorithm

*1/ Generation of a synthetic data set.*

Let $p = [c_0, c_1, c_{3,}c_{4,}c_5]$ be the vector of unknown parameters.

Specify values $c_i^*$ for $c_i$, $i = 0, 1, 3, 4, 5$ . Apply the shooting method to the IVP with the specified parameters to get a value $c_0^*$ of $f_0'$ such that $f(c_0^*, L) = 0$.

Let $p^* = [c_0^*, c_1^*, c_3^*, c_4^*, c_5^*]$. Use $p^*$ to generate a synthetic data set.

*2/ Shooting method and optimization.*

*Step 1*:

Guess two values $s_0^{(0)}$ and $s_1^{(0)}$ for $f_0'$ and values $c_i^{(0)}$ for $c_i$, $i = 1, 3, 4, 5$.

*Step 2*:

Apply the shooting method to the IVP with the above guesses to get a new value $c_0^{(0)}$ of $f_0'$, such that $f(c_0^{(0)}, L) = 0$.

Let $p^{(0)} = [c_0^{(0)}, c_1^{(0)}, c_3^{(0)}, c_4^{(0)}, c_5^{(0)}]$.

*Step 3*:

Consider now the IVP with $p = p^{(0)}$ and the synthetic data set generated earlier. Apply the optimization routine *lsqnonlin.*

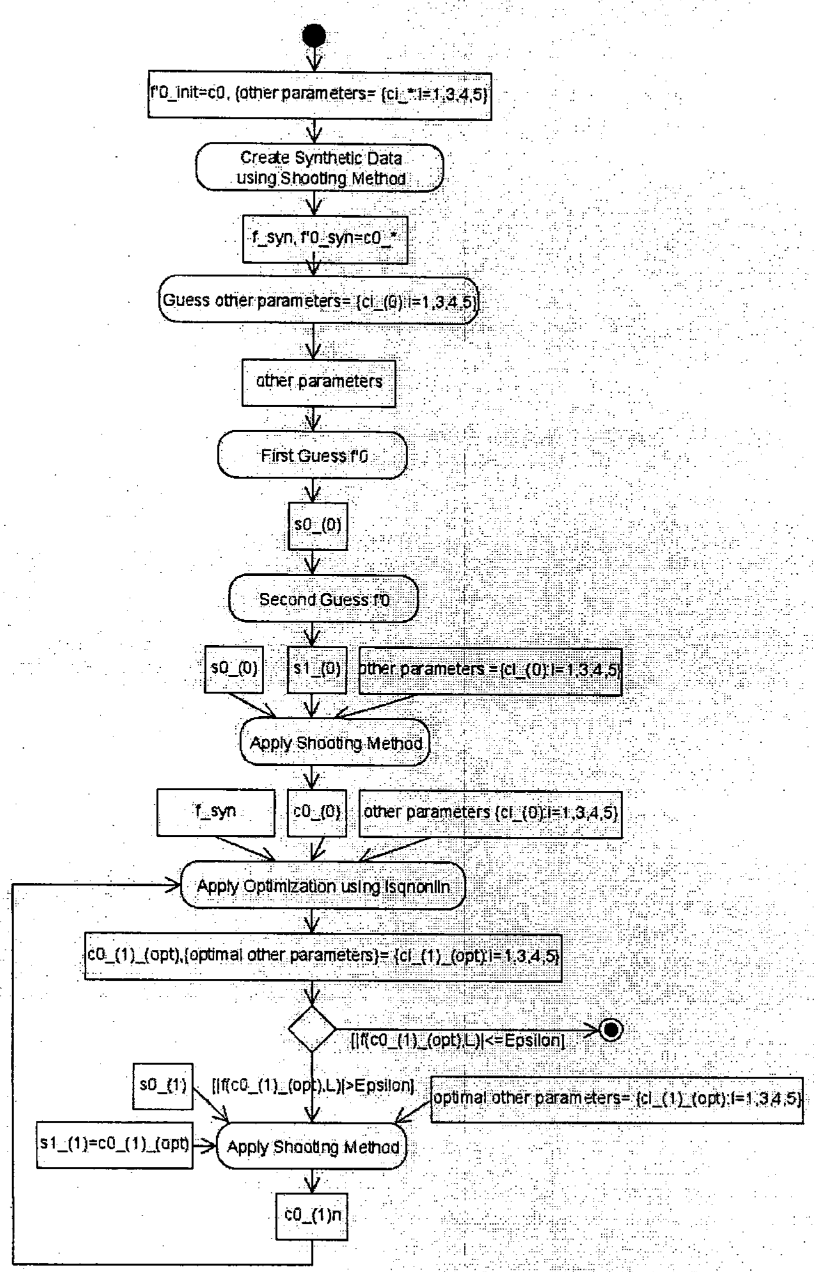
This will result in a new vector $p_{(opt)}^{(1)} = [c_{0(opt)}^{(1)}, c_{1(opt)}^{(1)}, c_{3(opt)}^{(1)}, c_{4(opt)}^{(1)}, c_{5(opt)}^{(1)}]$ of optimal values.

*Step 4*:

Test if $\left|f(c_0^{(1)}, L)\right| < \varepsilon$, where $\varepsilon$ is the specified tolerance. If not, consider the IVP with $c_i = c_i^{(1)}$, $i = 1, 3, 4, 5$. Set $s_0^{(1)} = c_0^{(1)}$ and guess a new value $s_1^{(1)}$ of $f_0'$. Use these new values to apply the shooting method to the new IVP. Get a new value $c_0^{(1)n}$ of $f_0'$, such that $f(c_0^{(1)n}, L) = 0$.

Let $p^{(1)n} = [c_0^{(1)n}, c_1^{(1)}, c_3^{(1)}, c_4^{(1)}, c_5^{(1)}]$. Go back to Step 3, and apply the optimization algorithm to the IVP but now with $p = p^{(1)n}$. Repeat until the condition in Step 4 is satisfied.

This algorithm is illustrated in Fig.(3.41) below



Fig(3.41): Flowchart illustrating the algorithm used for parameter estimation. The algorithm couples the shooting algorithm with an optimization routine to give optimal parameters.

Note that the Levenberg-Marquardt method tends to be quite fast and efficient but may lead to local minima. To improve the chance of finding the global minima, prior information about the parameters is needed. As mentioned previously, this information will be taken from the moments of the PBE derived earlier.

### 3.4.2. Numerical Experiments

Our algorithm is tested first on the following example, before applying it to the actual problem.

Example 1:

$$
\begin{aligned}
& f(x) = e^{-c_5 x} g(x), \\
& g''(x) = -(x - c_3) g(x) + c_4 \int_0^x g(x-t) g(t)\, dt + (x-4)\sin x + 2x\cos x, \\
& f(0) = c_1, f'(0) = c_0, \\
& g(0) = f(0) = c_1, g'(0) = c_2 = c_5 c_1 + c_0, \qquad 0 \le x \le 4
\end{aligned}
\tag{3.60}
$$

*1/ Generation of a synthetic data set.*

Guess$f_0' = 0.4$, and set $c_1 = 0.0, c_3 = 1.0, c_4 = 4.0$, and $c_5 = 1.0$. Apply the shooting method with tolerance $\varepsilon = 10^{-3}$, to get a new value for $f_0' = 0.0175$. Solve the resulting IVP to generate a synthetic data.

*2/ Shooting method and optimization.*

*Step 1*:

Guess values: $s_0^{(0)} = 0.04$, $s_1^{(0)} = 0.05$, $c_1^{(0)} = 0.3$, $c_3^{(0)} = 0.5$, $c_4^{(0)} = 3.0$, and $c_5^{(0)} = 0.5$.

*Step 2*:

Apply the shooting method to the IVP (3.60) with the above guesses.

Get a new value of $f_0' : c_0^{(0)} = -0.5483$.

This Step is illustrated in Fig.(3.42) below

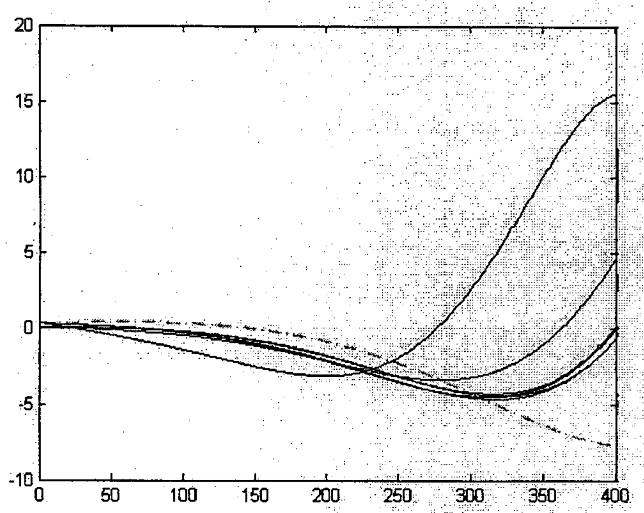



Fig.(3.42): Illustration of the shooting method applied to (3.6) with $s_0^{(0)} = 0.04, s_1^{(0)} = 0.05, c_1^{(0)} = 0.3, c_3^{(0)} = 0.5, c_4^{(0)} = 3.0$, and $c_5^{(0)} = 0.5$.

*Step 3*:

Consider (3.60) with $p = p^{(0)} = [-0.5483, 0.3, 0.5, 3.0]$ and the synthetic data set generated earlier.

Apply the optimization routine *lsqnonlin* which uses 23 iterations to give the following optimal values:

$f'_{0(opt)} = 0.175, c_{1(opt)} = 0.0, c_{3(opt)} = 1.0, c_{4(opt)} = 4.0, c_{5(opt)} = 1.0.$
Notice that these results perfectly match the actual values.

Remark.

If we increase the value of $L$, allowing for more oscillations, the shooting algorithm although may find a solution that satisfies the BVP, this solution may not satisfy the condition $\lim_{x\to\infty} f(x) = 0$, as it will keep on oscillating for $x > L$. Note also, that for some initial guesses of $f'_0$, not sufficiently close to the exact value of $f'_0$, the algorithm may find a solution that is different from the exact solution of the BVP as illustrated by the example in Section 3.2 above, and by Fig.(3.43) and Fig.(3.44) below

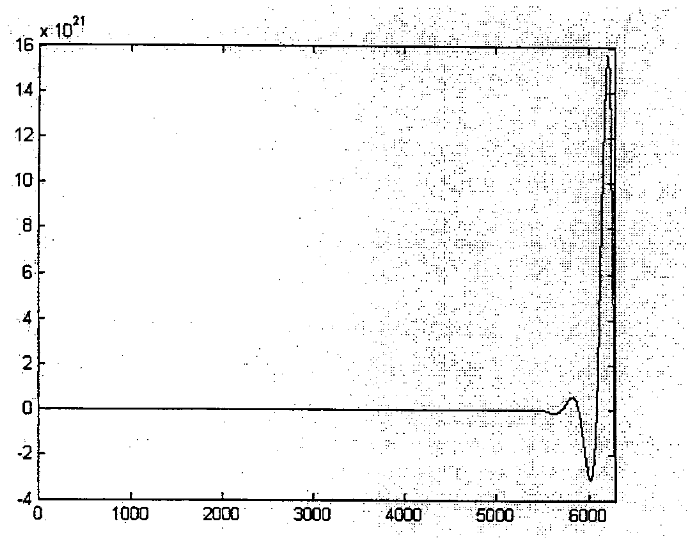



Fig.(3.43): Solution of (3.60) with $L = 4\pi$, and initial guess $f'_0 = -0.6$.

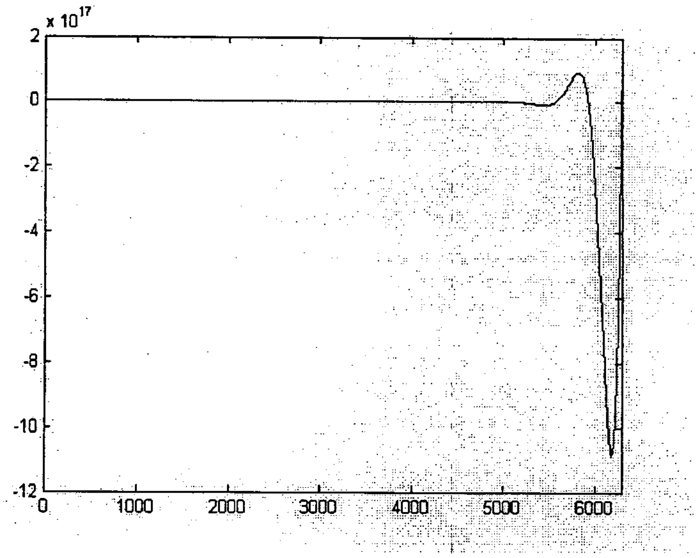



Fig.(3.44): Solution of (3.60) with $L = 4\pi$, and initial guess $f_0' = 0.4$.

Remark.

The solutions given by the shooting algorithm are not positive.

Example 2:

In this example, we consider BVP(3.0)

$$
\begin{aligned}
&f''(x) - Pef'(x) - Pe\sqrt{1 + \frac{4\lambda\,(Pe - f'(0))}{Pe}}f(x) = -\lambda Pe \int_0^x f(x-\varepsilon)f(\varepsilon)d\varepsilon, \\
&f(0) = 1, \qquad (3.70) \\
&f'(0) = f_0'.
\end{aligned}
$$

where $f_0'$, $Pe$, and $\lambda$ are unknown parameters.

**Trial 1:**$Pe = 0.01$, and $\lambda = 0.01$.

This is close to a limiting case where we have high dispersion (small $Pe$) but very low agglomeration rate (small $\lambda$).

*1/ Generation of a synthetic data set.*

Guess $f_0' = -0.1$, and set $Pe = 0.01$, and $\lambda = 0.01$. Apply the shooting method with tolerance $\varepsilon = 10^{-3}$, to get a new value of $f_0' = 0.1062$.

Solve the resulting IVP to generate synthetic data.

*2/ Shooting method and optimization.*

*Step 1*:

Using the moments equations set $s_0^{(0)} = -0.2230$, $Pe^{(0)} = 0.0358$, $\lambda^{(0)} = 0.0733$ and guess $s_1^{(0)} = 0.1633$,

*Step 2*:

Apply the shooting method to the IVP(3.70) with the above guesses, and with tolerance $\varepsilon = 10^{-3}$.

Get a new value of $f_0' = -0.2230$.

The shooting method is illustrated in Fig.(3.45) below

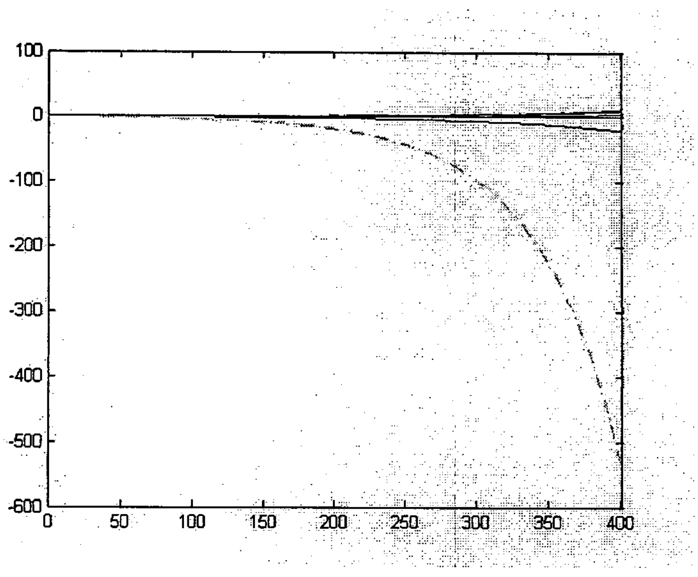



Fig.(3.45): Illustration of the shooting method applied to (3.7) with $s_0^{(0)} = -0.2230$ , $Pe^{(0)} = 0.0358$,and $\lambda^{(0)} = 0.0733$.

*Step 3*:

Consider (3.70) with $f_0' = -0.2230$, $Pe = 0.0358$, $\lambda = 0.0733$, and the synthetic data set generated earlier.

Apply the optimization routine *lsqnonlin* which uses 43 iterations to give the following optimal values:

$f'_{0(opt)} = -0.1095$, $Pe_{(opt)} = 0.0074$, and $\lambda_{(opt)} = 0.0342$

with $|f(-0.1095, L)| = 0.0052 > tolerance$.

*Step 4:*

Since $|f(-0.1095, L)| = 0.0052 > tolerance$, it goes back to Step 2, and apply the shooting method with the optimal parameters obtained, as follows:

$s_0 = f'_{0(opt)} = -0.1095$, $Pe = Pe_{(opt)} = 0.0074$, and $\lambda = \lambda_{(opt)} = 0.0342$. Set $s_1 = -0.2230$.

Get a new $f_0' = -0.1094$.

Apply the optimization routine *lsqnonlin* which uses 31 iterations to give the following new optimal values:

$f'^{(n)}_{0(opt)} = 0.1062, \ Pe^{(n)}_{(opt)} = 0.01$, and $\lambda^{(n)}_{(opt)} = 0.01$

with $|f(-0.1095, L)| = 2.9957 * 10^{-5} < tolerance.$

**Trial 2:**$Pe = 0.5$, and $\lambda = 0.5$.

*1/ Generation of a synthetic data set .*

Guess $f_0' = -0.2541$, and set $Pe = 0.5$, and $\lambda = 0.5$. Apply the shooting method with tolerance $\varepsilon = 10^{-3}$, to get a new value of $f_0' = -0.2944$.

Solve the resulting IVP to generate synthetic data.

*2/ Shooting method and optimization.*

*Step 1*:

Guess values: $s_0^{(0)} = 0.0316, s_1^{(0)} = 0.0370, Pe^{(0)} = 0.5, \lambda^{(0)} = 0.5$.

*Step 2*:

Apply the shooting method to the IVP(3.70) with the above guesses, and with tolerance $\varepsilon = 10^{-3}$.

Get a new value of $f_0' = 0.0376$.

The shooting method is illustrated in Fig.(3.46) below

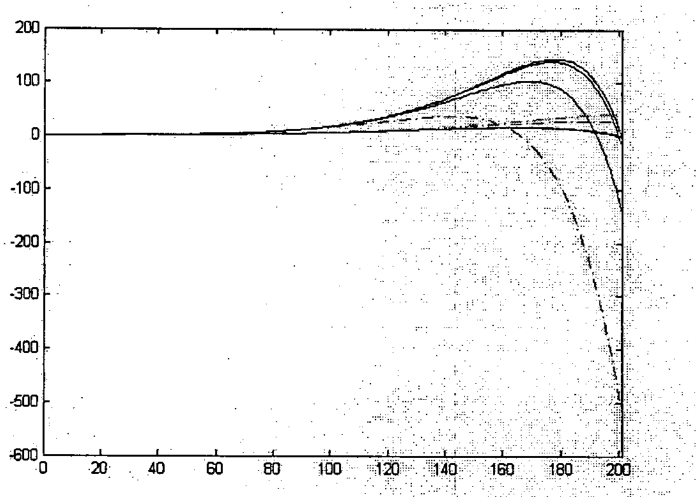



Fig.(3.46): Illustration of the shooting method applied to (3.7) with $s_0^{(0)} = 0.0316, s_1^{(0)} = 0.0370, Pe^{(0)} = 0.5$, and $\lambda^{(0)} = 0.5$.

*Step 3*:

Consider (3.70) with $f_0' = 0.0376$, $Pe = 0.5$, $\lambda = 0.5$, and the synthetic data set generated earlier.

Apply the optimization routine *lsqnonlin* which uses 18 iterations to give the following optimal values:

$f'_{0(opt)} = -0.2944$, $Pe_{(opt)} = 0.5$, and $\lambda_{(opt)} = 0.5$
with $|f(-0.2944, L)| = 3.4701 * 10^{-6} < tolerance$.

Remark.

After running other trials with greater values of $\lambda$ and $Pe$, we have found out the same limitations as in example 1 above. The solution found by the shooting algorithm may be oscillating and not always positive. Such solution is not relevant from a physical point of view — as it may not possess the properties of the number density function that we are seeking.

It would be interesting to attempt to solve this problem — perhaps by implementing some modified version of the shooting method where the shooting is carried out in a more controlled stepwise fashion to maintain the character that is required physically.

# Chapter 4. Conclusion and Future Work

In this research, we have examined the solution of a second order integrodifferential equation arising as a population balance that describes the particle size distribution from suspension crystallizers with random growth dispersion and particle agglomeration, and the associated parameter estimation problem. In particular, we first considered the IVP, established its well-posedness, developed variations on a numerical scheme and evaluated their performance and compared the numerical results with the analytical ones. Numerical experiments showed that our numerical scheme is highly performant. Our tests using Euler-Maclaurin quadrature in place of Hermite quadrature showed that the Hermite quadrature has certain properties that are not captured by the Euler-Maclaurin quadrature of similar order.

For physical considerations, it was necessary to solve an associated BVP. To solve this BVP we employed the shooting method which utilized our numerical method for the IVP. In order to solve the parameter estimation problem, we coupled the shooting method with the Levenberg-Marquardt algorithm. The numerical experiments that we have carried out have demonstrated the feasibility of the solution of this problem with good accuracy for the first example (Example 3.60 above). However, for our physical example, the algorithm performed well for small values of the parameters $Pe$ and $\lambda$. Further investigation in employing a modified version of the shooting method is perhaps necessary to cope with the strong oscillations that may occur in our physical example as the parameters increase in value.

In general, it is possible that the BVP(3.0) does not have a unique solution. This is illustrated in the example in section 3.2 where two different solutions were obtained depending on the values of the initial guesses. Moreover, in our analysis we have obtained in Proposition 3.4 conditions to have a positive monotone decreasing solution. This prompts us to pose the following question:

*Question.* For a given $Pe$ and $\lambda$, does BVP (3.0) has a unique solution when $s$, for the associated IVP (3.3), is chosen to satisfy the conditions given in Proposition 3.4?

Note that, by analogy with nonlinear BVPs for ordinary differential equations, to solve this question, one perhaps has to show that when (3.0) has an isolated solution, then $f(L, s) = 0$ has a simple isolated root. Showing that (3.0) has an isolated solution demand that we consider the solution of a certain linearized problem, which in our case involves computing the derivative of the convolution functional with respect to the solution. This will entail the use of further techniques from functional analysis which might also help us solve at the same time the problem of deriving the sensitivity equations that are typically considered in parameter estimation problems to compute standard errors.

Another extension of this work, would be to carry out similar analysis for type (1) boundary conditions given is section 1.2. Although most of the steps in the analysis would essentially be identical, nevertheless, as shown in [SL], there could be some advantages now due to the explicit nature of some of the conditions and constraints derived there for this case — this is in contrast to what we have for type (2) boundary conditions considered herein.

Further investigation to examine the performance of our algorithm on real experimental data, which tend to be more sparse and perhaps more noisy than the synthetic data considered above, would be essential. There are a number of data sets available in the literature for agglomerating particles. However, analysis that take growth rate dispersion into account has not been considered in detail for such systems. This is primarily due to the difficulties which this study has brought up and addressed. It would be interesting to apply our model and algorithm to these existing data sets after adding some noise source that would simulate the growth rate dispersion phenomenon. We note that for no growth dispersion ($Pe \to \infty$), our model reduces to a first order integrodifferential equation. Such equations have markedly different qualitative behavior than the model we have considered in this research. Thus, it would be of interest to examine the effects of considering other sources of randomness, for either the first order or the second order models, and to compare the performance of these models. This would be valuable from the point of view of model selection.

## References


[B] Baker, C. T. H.(1997). *The numerical treatment of integral equations. Monographs on numerical analysis.* Oxford: Clarendon Press.

[BF] Burden, R. L. & Faires, J. D.(2000). *Numerical analysis* (7th ed.). California: Brooks/Cole Publishing.

[C] Conway, J. B., (1990). A Course in Functional Analysis. New York: Springer-Verlag.

[DM] Delves, L. M. & Mohamed, J. L., (1988). Computational methods for integral equations. Cambridge: Cambridge University Press.

[ES] El-Khaldi, K. & Saleeby, E. G., (2009). On a Numerical Solution of an Integrodifferential Population Balance Equation. Proc. Conf.on Analysis & Comp. Math. Singapore:Research Publishing,61-74.

[GLS] Gripenberg G., Londen, S.O. & Staffans, O.(1990). *Volterra Integral and Functional Equations.* Cambridge: Cambridge University Press.

[HK] Hulburt, H. M. & Katz, S., (1964). Some problems in particle technology: A statistical mechanical formulation. *Chem. Engng. Sci. 19*, 555-574.

[K] Khanh, B. D., (1994). Hermite predictor-corrector scheme for regular Volterra integral equations and for some integro-differential equations for turbulent diffusion, J. Comp. & Appl. Math. 51, 305-316.

[M] Melikhov, I. V., Mikhin, E. V. & Pekler, A. M., (1973). Regularities in crystal growth. *Th. Found. Chem.Engng. 7*, 671-621.

[NSMN] Naito, T., Shin, J.S., Murakami, S., & Ngoc, P.H.A.(2007). Characterization of Linear Integral Equations with Nonnegative Kernels. *J. Math. Anal. Appl. 335*, 298-313.

[P] Press, W. H., Flannery, B. P., Teukolsky, S. A. & Vetterling, W. T.,(1991). *Numerical Recipes.* Cambridge: Cambridge University Press.

[SL] Saleeby, E. G. & Lee, H. W., (1995). On the solution of the PBE with agglomeration and random growth dispersion, *Chem. Engng. Sci. 50*, 1971-1981.

[RL] Randolph, A. D. and M.A. Larson, (1988). *Theory of Particulate Processes* (2nd ed.). New York: Academic press.

[RW] Randolph, A. D. & White, E. T., (1977). Modeling size dispersion in the prediction of crystalsize distribution. *Chem. Engng. Sci. 32*, 1067-1076.

[WW] White, E. T. & Wright, P. G., (1971). Magnitude of size dispersion effects in crystallization. *CEP Symp. Ser. 67* (110), 81-87.

[Y] Young,E. C., (1985).On Integral Inequalities of Gronwall-Bellman Type. *Proc. Amer. Math. Soc. 94*(4), 636-640.