Analytic Solutions to a 1D Advection-Diffusion Equation and Comparison to Observations.

By

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THIS THESIS IS SUBMITTED TO THE UNIVERSITY OF GHANA, LEGON IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF MASTER OF PHILOSOPHY MATHEMATICS DEGREE.

DECLARATION

This thesis was carried out in the Department of Mathematics, University of Ghana, Legon from September 2020 to December 2021 in partial fulfilment of the requirements for the award of Master of Philosophy degree in Mathematics under the supervision of Dr. Joseph K. Ansong and Dr. Vincent T. Teyekpiti of the University of Ghana.

I hereby declare that except where due acknowledgement is made, this work has never been presented wholly or in part for the award of a degree at the University of Ghana or any other University.

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ABSTRACT

In this study, we provide two analytic solutions to a one dimensional Advection-Diffusion Equation (ADE). The ADE is solved using a constant and an exponentially decaying inlet boundary condition, together with a Dirichlet and Neumann outlet conditions. The analytic solutions are shown to be simple if a combination of the initial concentration and the transformed boundary condition result in a non-zero singularity pole of inverse Laplace transform. The differences between the two analytic solutions are elucidated. Additionally, to verify the analytic solutions provided, comparisons are done with a solution to a mathematically related problem in Kim (2020a) and an error that appears in the paper is corrected.

Moreover, the analytical solutions are compared to some observational data from the Fena river in the Ashanti region of Ghana and the difference between the two (analytical and observational) are clarified.

DEDICATION

To my lovely friend, Dorcas Agyeiwaa Appiah.

ACKNOWLEDGEMENTS

“The ultimate kind of prayer is appreciation,” observed Alan Cohen, “ because it acknowledges the existence of good wherever you beam the light of your appreciative thought.”

I wish to offer my sincere thanks to my supervisor: Dr. Joseph K. Ansong for his patience, prompt attention and suggestions that has translated this work into reality. Dr. Ansong, I say I am much grateful. It’s been a fantastic learning opportunity. To Dr. Vincent T. Teyekpiti, I say a big thanks for co-supervising this thesis work. His partnership with Dr. Ansong to supervise this work is highly commendable.

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Chapter 1

Introduction and Motivation

1.1 Introduction

It is commonly known that water covers around 71% of the Earth's surface, implying that protecting the Earth's water should be a top concern for everyone. "Thousands have survived without love, but not one without water," wrote British poet W.H. Auden. According to the United Nations, polluted water kills more people each year than all other types of violence combined, including war.

Water pollution occurs when hazardous substances, such as chemicals or microbes, infiltrate an ocean, lake, stream, aquifer, or other river bodies, deteriorating water quality and making it harmful to humans or the environment. According to the Ghana Water Resource Commission, nearly, 60% of water bodies in Ghana are polluted due to illegal mining and other activities. The discharge of waste substances, which contain hazardous compounds such as mercury and other organic chemicals used in mineral ores processing during mining activities, heavily contributes to water pollution in Ghana. In addition, the leaching of heavy metallic compounds such as lead and zinc oxides, which can enter the environment and, more particularly, seep into surface and subterranean water bodies, poses a greater threat to aquatic life and human population that rely on such resources, Duncan (2020). Figure 1.1 and Figure 1.2 are examples of polluted river caused by the activities of illegal mining.

The transport of pollutants in rivers has become a matter of concern for environmental engineers and scientists as well as mathematical modelers. Accurate prediction of the transport of these pollutants is critical for efficient management of these pollutant processes, Zoppou and Knight (1997). The concentration of these pollutants released

Figure 1.1: Polluted River Ankobra in the Western Region of Ghana

Source:https://citinewsroom.com/2020/05/pollution-of-ankobra-river-by-illegal-miners-intensifies/

into the water bodies may be described by the Advection-Diffusion Equation (ADE).

A one-dimensional advection-diffusion equation, with constant coefficients, derived from the principle of mass conservation, is given by

$$\frac{\partial C}{\partial t} + V_0 \frac{\partial C}{\partial x} = D_0 \frac{\partial^2 C}{\partial x^2}, \tag{1.1}$$

where $C(x,t)$ is the concentration at position, x and time t, and V_0 and D_0 are the constant advective velocity and diffusion, respectively. The advection-diffusion equation is sometimes referred to as the convection-diffusion equation, especially from the literature on heat transfer studies. The equation is basically a combination of advection and diffusion equations and it represents a physical phenomenon in which contaminants or other physical quantities are transported inside a physical system by to two processes: advection and diffusion. It's a second-order partial differential equation of the parabolic type, derived from Fick's Law and mass conservation.

Advection refers to the transport of a substance or material by motion of the fluid, that is, with either water or airflow. During advection, a pollutant is transported

Figure 1.2: River Fena in the Ashanti Region of Ghana

along with the fluid. The fluids motion is described mathematically as a vector field, and the transported material as a scalar field, showing its distribution over space and time. The vector field is mostly represented by the velocity of the fluids motion, whereas the scalar field is described by the concentration of the contaminant being transported by the fluid. Diffusion, on the hand, refers to the fact that the transported pollutant tend to spread out and diffuse from a region of higher concentration to a lower concentration as time varies. The ADE is equally important in modeling atmospheric pollutants such as smoke or dust, dispersion of chemicals in reactors, tracer dispersion in a porous medium and the intrusion of salt water into fresh water aquifers. It also has a wide range of applications in many other engineering fields.

Obtaining analytic solutions to the advection-diffusion equation is of great importance to various scientific disciplines. The equation is solved to find the spatial and temporal distribution of concentration of a pollutant using a variety of analytical approaches. The Laplace transform technique is the most widely used method in providing analytical solutions to the one, two and three dimensional advection-diffusion equation. Other methods such as separation of variables, Hankel transform method and methods using Green's functions, have also been used to obtain analytical solutions to the ADE's.

Many analytical solutions along with varying initial and boundary conditions have been developed to quantitatively describe the one dimensional Advection-Diffusion Equation with contant coefficients. Mohsen and Baluch (1983) provided an analytic solution to a one-dimensional convection-diffusion equation for fixed concentration boundary conditions on a finite domain. The transformed equation was decomposed into two components and separation of variables was used to obtain the required result. Mojtabi and Deville (2015) also provided analytical solution to a one-dimensional advection-diffusion equation using separation of variables but with a sinosoidal initial condition and a homogeneous boundary condition. Davis (1985), by means of a Laplace transform technique, provided two different analytic solutions to a single convection-diffusion equation over a finite domain. The differences between the two solutions were clarified.

Kumar et al. (2012) presented analytical solutions to a one dimensional advection-diffusion equation with variable coefficients along with initial and boundary conditions in a semi-infinite domain where the diffusion term is considered to be proportional to the square of the spatially dependent velocity. Using a simple transformation, the governing equation was transformed into an advection-diffusion equation with contant coefficients. The equation was solved for three different solute dispersion problems, which were inhomogeneous steady, temporally dependent homogeneous and inhomogeneous respectively. Laplace transform technique was used to obtain the solutions. Zoppou and Knight (1997) provided analytical solution for a one-dimensional transport of a pollutant in an open channel with steady unpolluted lateral inflow uniformly distributed over its whole length. The problem was described approximately by spatially variable coefficient advection and advection-diffusion equations with the velocity proportional to distance, and the diffusion constant coefficients proportional to the square of the velocity. The equations were transformed into constant coefficient problems and the Laplace transform technique was used to provide the analytical solutions for general initial and boundary conditions.

Most of the works done on the advection-diffusion equation have other variants that include Source, Reaction, and other terms, depending on the application. Van Genuchten (1982) presented analytical solutions to a one-dimensional, single-ion convection-dispersive transport equation; which includes terms accounting for linear equilibrium adsorption, zero-order production and first-order decay. The solutions were derived for a semi-infinite medium and several sets of initial and soil surface boundary conditions. In a recent paper by Kim (2020a), a general 1D analytic solution of a Convection-Diffusion Reaction Source (CDRS) equation was obtained by using a one-sided Laplace transform by assuming a constant diffusivity, velocity and reactivity. A complementary and a particular solution was obtained using the Laplace transform technique and the residue theorem in complex analysis was used to find the general solution.

This study presents analytical solutions to a one-dimensional advection-diffusion equation with constant coefficients together with initial and two boundary conditions. The choice of the initial and boundary conditions is motivated by observational data on a polluted river at Fenaso in the Ashanti Region of Ghana. The Laplace transform technique and residue theorem from complex analysis is used to obtain the solutions.

1.2 Motivation

Illegal small scale mining is known to contaminate river bodies heavily; the chemicals used and the trash heaps are a source of long term pollution in our water bodies. The menace caused by 'Galamsey' (illegal mining) operators to the quality of water resources in Ghana has become a major public concern because it has resulted in the closing down of some water treatment plants in the country, Duncan (2020). The activities of these operators often result in the release of toxic chemicals into rivers with the eventual transport to the sea and other locations in the environment, putting the local populace in danger especially those who rely on such water bodies for drinking and other household purposes. An important question to address is "which of the analytical solutions of the 1D advection-diffusion equation best describes the transport of these pollutants in our waters"? An answer to this question is important because the most appropriate model would enable us to know the temporal and spatial distribution of pollutants in a river. Besides, this could also help in predicting how long an effluent could take to be transported away from a polluted site.

1.3 Goals and Objectives

The overall goal of the study is to adequately explore analytical solutions of the 1D ADE, and to determine which solution best characterize the transport of pollutants in river Fena in the Ashanti region of Ghana based on available data.

To this end, the study seeks to:

1. explore the application of the one-sided Laplace transform to finding analytical solutions to a 1D advection-diffusion equation.
2. find analytical solutions to a 1D advection-diffusion equation of a continuous release of a pollutant in a river.
3. compare these analytical solutions to available observational data for the Fena river.

Chapter 2

Literature Review

Numerous analytical solutions have been developed to quantitatively describe one-dimensional advection-diffusion solute transport. In earlier works, the approach to obtaining analytical solutions to problems involving pollutants transport, is to reduce the advection-diffusion equation to a heat equation which already has known solutions, Mohsen and Baluch (1983), Mojtabi and Deville (2015), Ogata and Banks (1961). This was mostly done by introducing another dependent variable.

Mohsen and Baluch (1983) presented a solution to the one-dimensional convection-diffusion equation which was solved for fixed concentration boundary conditions on a finite domain. The unsteady convection-diffusion equation in one-dimension over the finite domain $0 \leq x \leq L$ was stated as

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{2.1}$$

subject to the boundary conditions, $c(0,t) = c_0$, $c(L,t) = 0$ and initial condition, $c(x,0) = 0$.

The aim of their paper, Mohsen and Baluch (1983), was to develop an analytical solution valid at the end points of the domain of interest. Using a simple transformation, the convection-diffusion equation in Eq.(2.1) was transformed into a heat conduction equation with source term given as

$$\frac{\partial \phi}{\partial T} = \frac{\partial^2 \phi}{\partial \xi^2} - \phi, \;\; 0 < \xi < \lambda, \;\; T > 0 \tag{2.2}$$

with transformed boundary and initial conditions

$$\phi(\xi = 0, T > 0) = 1,$$

$$\phi(\xi = \lambda, T > 0) = 0,$$

$$\phi(\xi, T = 0) = 0.$$

Eq.(2.2) has a known solution quoted from the paper by Carslaw and Jaeger (1959),

$$\frac{c}{c_0} = \frac{2\pi}{\lambda^2} \sum_{n=1}^{\infty} \frac{n}{\left(1 + \frac{n^2\pi^2}{\lambda^2}\right)} \sin(n\pi X) \left[\exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right)T\right\} - 1\right]. \tag{2.3}$$

They found that the solution presented in Eq.(2.3) is not valid at the boundary point $X = 0$. To obtain a solution which is valid at the end point of the domain, separation of variables was used to solve the convection-diffusion equation. A required solution for ϕ was obtained by decomposing the equation into two components. The complete analytic solution which is valid at the endpoint of the finite domain was reported as;

$$\phi(\xi, T) = \frac{\sinh(\lambda - \xi)}{\sinh \lambda} - \frac{2\pi}{\lambda^2} \sum_{n=1}^{\infty} \frac{n}{\left(1 + \frac{n^2\pi^2}{\lambda^2}\right)} \sin\left(\frac{n\pi\xi}{\lambda}\right) \times \exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right)T\right\}. \tag{2.4}$$

In Appendix (A) we present the solution of Mohsen and Baluch (1983) with additional details missing in their paper.

A similar goal, requiring continuity at the extremeties of a finite domain was reported by Davis (1985). The objective of the paper was to use the Laplace transform technique to obtain two different analytical solutions to a single diffusion-convection equation over a finite domain where one analytical solution is continuous at both ends of the domain of interest, while the other solution is discontinuous at the origin. The convection-diffusion equation was transformed into a second order ordinary differential equation using the Laplace transform. The inverse Laplace transform gives the final solution to be

$$c(X,T) = c_0 \exp(\lambda X) \left[\frac{\sinh\left(\frac{P_e}{2}(1-X)\right)}{\sinh\left(\frac{P_e}{2}\right)} \right] - c_0 \exp(\lambda X) \\ \times \left[2\pi \sum_{n=1}^{\infty} \frac{n \sin(n\pi X)}{(\lambda^2 + n^2\pi^2)} \times \exp\left[-(\lambda^2 + n^2\pi^2)T\right] \right] \tag{2.5}$$

which is continous at the end point of the domain. Two typographical errors were identified in the solution given by Mohsen and Baluch (1983) in Eq.(30). First, $2\pi/\lambda$ prior to the summation should have read $2\pi/\lambda^2$, and before the final square bracket a T was ommited. Davis (1985) further provided an analytical solution which is discontinous at $X = 0$, given as

$$\frac{c(X,T')}{c_0} = 2\pi \exp(\lambda X) \sum_{n=1}^{\infty} \frac{n \sin(n\pi X)}{(\lambda^2 + n^2\pi^2)} \left[1 - \exp\left\{-\left(\lambda^2 + n^2\pi^2\right)T'\right\}\right]. \tag{2.6}$$

Comparing Eq.(2.6) with that of Eq.(2.3) provided by Mohsen and Baluch (1983), Davis (1985) stated that the results provided by Mohsen and Baluch (1983) was incorrectly given as the negative of Eq.(2.6). He further asserted that the lack of the exponential term outside the series in Eq.(2.3) indicates that their equation is a solution for ϕ and not c/c_0. He found that the discontinuity in Eq.(2.6) at $X = 0$, is due to the Fourier sine series expansion for the ratio of hyperbolic sines in Eq.(2.6).

In Appendix (B), we present the solutions of Davis (1985) with additional details missing in his paper.

Kumar et al. (2012) presented analytical solutions to a one-dimensional advection-diffusion equation with variable coefficients along with initial and boundary conditions in a semi-infinite domain where the diffusion term is considered to be proportional to the square of the spatially dependent velocity. The equation was given as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_0 f_1(x,t) \frac{\partial C}{\partial x} - u_0 f_2(x,t) C \right) \tag{2.7}$$

where D_0 and u_0 are constants whose dimensions depend upon the expressions for $f_1(x,t) = (1+ax)^2$ and $f_2(x,t) = (1+ax)$ respectively. Using a simple transformation, Eq.(2.7) was transformed into a constant ADE of the form

$$\frac{\partial C}{\partial t} = a^2 D_0 \frac{\partial^2 C}{\partial Z^2} - \omega_0 \frac{\partial C}{\partial Z} - a u_0 C. \tag{2.8}$$

Using Laplace transform technique, Eq.(2.8) was reduced to a second order ordinary differential equation, the solution of which is expressed by the complementary function. They stated that the analytical solution obtained can be used for a variety of variations in dispersion and velocity due to spatial dependence and temporal dependence respectively.

Zoppou and Knight (1997) provided analytical solutions for a one-dimensional transport of a pollutant in an open channel with steady unpolluted lateral inflow uniformly distributed over its whole length using the Laplace transform technique. The problem was described approximately by spatially variable coefficients conservative and nonconservative advection-diffusion equations. They found that the nonconservative form of the advection-diffusion equation can yield exact solutions that are not consistent with physical problems.

Most of the derived analytical solutions for the advection-diffusion equation have other variants that include Source, Reaction, and additional terms, depending on the application. Van Genuchten (1982) presented analytical solutions for the movement of a chemical in a porous medium as influenced by linear equilibrium adsorption, zero-order production and first-order decay, given as;

$$D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - R \frac{\partial c}{\partial t} = \mu c - \gamma \tag{2.9}$$

where R is the Retardation factor, γ is the first-order liquid phase decay constant and μ is the general first-order decay constant. The solutions were derived for a semi infinite-medium and several sets of initial and soil surface boundary conditions by means of a Laplace transform. They stated that the analytical solutions obtained can be used to predict the movement of various chemicals in field soil.

Kim (2020a) provided a general 1D analytic solution of a Convection-Diffusion Reaction Source (CDRS) equation using a one-sided Laplace transform by assuming a constant diffusivity, velocity and reactivity. He further presented a general formalism to derive one-dimensional analytic solution for Dirichlet-Dirichlet and Dirichlet-Neumann boundary conditions. He found that the derivation of the CDRS equation is straightforward if a combination of the source function and the initial condition provides a non-zero singularity pole of inverse Laplace transform. This method is presented in chapter 4.

Chapter 3

Theoretical Background

3.1 Transport, Advection and Diffusion

Water pollution has become a frequent occurrence due to human activities. The transport of pollutants and other chemical compounds in rivers and other surface water bodies are of paramount concern to scientist working in the engineering field and mathematical modelers. Pollutant transport acts to move pollutants away from the location at which they are generated, resulting in impacts that might be far away from the pollution source. The physical process of a pollutant can be divided into two categories; Advection and Diffusion.

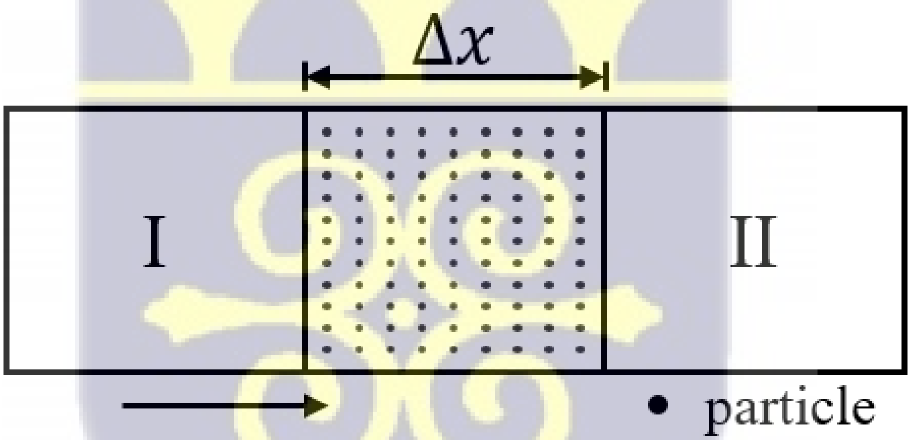
3.1.1 Advection and Diffusion

Advection is the process by which pollutants are transported by motion of the fluid. The fluids motion is described mathematically as a vector field, and the transported material as a scalar field, showing its distribution over space and time. In contrast, diffusion refers to the fact that the transported pollutant tend to spread out and diffuse from a region of higher concentration to a region of lower concentration as time varies. For example, if a spot of a dye is dropped into the center of a river, advection will move the mass of the dye downstream. Diffusion on the other hand, will spread out the spot of dye from a higher region of concentration to less concentrated region. Diffusion arises from two types of random motion. Molecular diffusion which results from the random motion of molecules and turbulent diffusion which arises due to random eddies in the fluid.

Molecular diffusion occurs as a result of random motion of individual molecules in a fluid, Honrath (1995). The molecules only travel in a straight line and may collide with other molecules along the way. The rate of molecular diffusion depends on the temperature and other molecular properties such as the mass and volume of the molecules involved. Turbulent diffusion, on the other hand, is the transport of mass within a system due to the random eddies in the fluid. It occurs much faster than molecular diffusion. Thus, in turbulent diffusion, it is the random motion of the fluid that does the mixing, while in molecular diffusion it is the random motion of the pollutant molecules that is important, Honrath (1995).
The next section considers flux density which arises from the theory of advection and diffusion.

3.1.2 Advective Flux

The flux of any quantity (mass or any dissolved substance) is defined as the amount of that quantity that crosses a boundary or any imaginary surface per unit area and per unit time. We analyze the advection flux, $\overrightarrow{F_A}$ with two control volumes, I and II.



Let Δx be the distance with which a particle passes in a time interval, Δt.
The quantity of mass moving from control volume I to II in time interval Δt is given by

$$Q = C\,\Delta x\,A \tag{3.1}$$

where Q is the quantity of mass, $[M]$, C is the concentration, $[ML^{-3}]$ and A is the cross sectional area, $[L^2]$ between the control volume.

Then, the quantity of mass passing from I to II per time per unit area is given by

$$\frac{Q}{\Delta t A} = \frac{C\Delta x}{\Delta t}. \tag{3.2}$$

The expression $\dfrac{Q}{\Delta t A}$ is known as the advective flux, $\overrightarrow{F_A}$. Thus,

$$\overrightarrow{F_A} = \frac{\Delta x}{\Delta t} C \tag{3.3}$$

Taking the limit as $\Delta x \mapsto 0$ and $\Delta t \mapsto 0$,

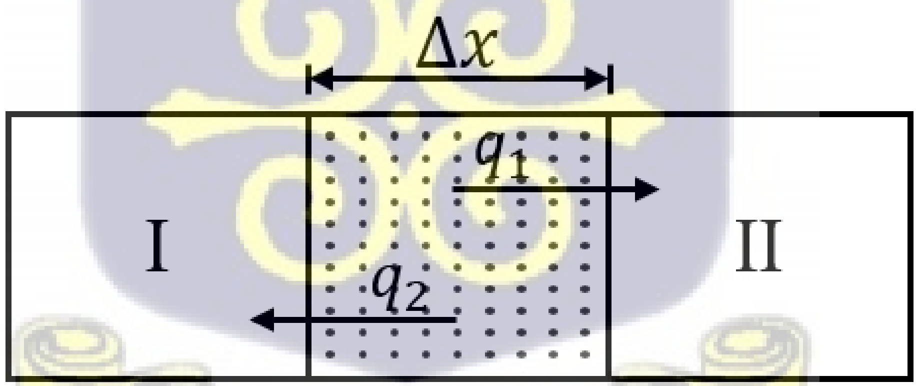
$$\begin{aligned}\overrightarrow{F_A} &= \frac{\partial x}{\partial t} C \\ &= \overrightarrow{u} C\end{aligned}$$

where $\overrightarrow{u} = \dfrac{\overrightarrow{\partial x}}{\partial t}$ is called the advective velocity. Thus, the advective flux is

$$\overrightarrow{F_A} = \overrightarrow{u} C. \tag{3.4}$$

3.1.3 Diffusive Flux

The diffusive flux, $\overrightarrow{F_D}$ would also be analyzed with two control volumes I and II, taking into consideration the assumptions outlined below.



Assumptions

1. Diffusion occurs towards both directions in time interval Δt.

2. The particle does not change direction during the time interval Δt.

3. The probability to move to either positive or negative x directions are equal (50%) for all particles.

Let

$$q_1 = 0.5C_1\,\Delta x\,A, \tag{3.5}$$

$$q_2 = 0.5C_2\,\Delta x\,A \tag{3.6}$$

be the quantities of mass moving from control volume I to II and from II to I respectively. The change in the quantity of mass Q moving from I to II in time interval Δt is given as

$$\frac{Q}{\Delta t} = \frac{0.5\,\Delta x\,A(C_1 - C_2)}{\Delta t}. \tag{3.7}$$

But

$$\lim_{\Delta x \to 0}\left(\frac{C_2 - C_1}{\Delta x}\right) = \frac{\partial C}{\partial x}. \tag{3.8}$$

So,

$$C_1 - C_2 \approx -\frac{\partial C}{\partial x}\,\Delta x. \tag{3.9}$$

Substituting Eq.(3.9) into Eq.(3.7) gives,

$$\frac{Q}{\Delta t} \approx \frac{-0.5\,\Delta x\,A\dfrac{\partial C}{\partial x}\,\Delta x}{\Delta t}. \tag{3.10}$$

The quantity of mass passing from I to II per time per unit area, (Flux, $\overrightarrow{F_D}$) is given as

$$\frac{Q}{\Delta t\,A} \approx \frac{-0.5\,\Delta x\,\dfrac{\partial C}{\partial x}\,\Delta x}{\Delta t}, \tag{3.11}$$

$$\overrightarrow{F_D} = \frac{-0.5\,(\Delta x)^2}{\Delta t}\,\frac{\partial C}{\partial x}. \tag{3.12}$$

Let $D = \dfrac{0.5\,(\Delta x)^2}{\Delta t}$, then

$$\overrightarrow{F_D} = -D\frac{\partial C}{\partial x} \tag{3.13}$$

where D is diffusion coefficient. In 2 or 3 dimensions, the diffusive flux becomes

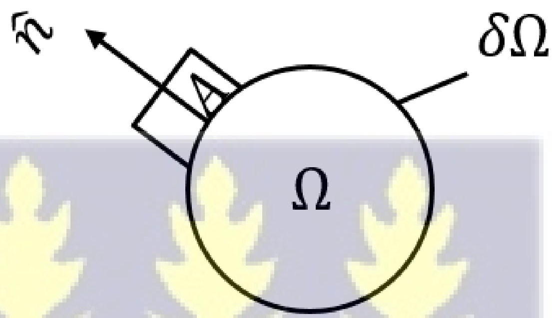
$$\overrightarrow{F_D} = -D\overrightarrow{\nabla} C. \tag{3.14}$$

Combining Equations (3.4) and (3.14), the total advection-diffusion flux is given as

$$\overrightarrow{f} = \overrightarrow{u}C - D\overrightarrow{\nabla}C. \tag{3.15}$$

3.1.4 The Advection-Diffusion Model

Consider an arbitrary control volume with domain Ω and boundary denoted by $\delta\Omega$. To determine the mass flux, $\overrightarrow{f}$ crossing the boundary of the control volume, we shall examine a small part of area, A on the boundary where the flow velocity, $\overrightarrow{u}$ is normal to the area. At every point on the boundary, we have a unit normal vector $\hat{n}$, pointing outwards.



The volume of fluid, dV crossing the boundary with base area, A, during time interval dt is

$$dV = A\,\overrightarrow{u} \cdot \hat{n}\, dt. \tag{3.16}$$

The amount of mass carried by that volume is CdV. Therefore, the rate of change of total mass in the control volume is given by $\dfrac{\partial}{\partial t}\displaystyle\int_{\Omega} CdV$.

Again, the net inflow through the boundary of the control volume is given as $-\displaystyle\int_{\delta\Omega} \overrightarrow{f} \cdot \hat{n}\, dA$.

The law of Conservation of Mass states that matter can neither be created nor destroyed so any increase or decrease in mass must be due to the flux of matter through the surface bounding the volume.

By mass conservation;

$$\frac{\partial}{\partial t}\int_{\Omega} CdV = -\int_{\delta\Omega} \overrightarrow{f} \cdot \hat{n}\, dA. \tag{3.17}$$

We now use the Gauss divergence theorem to convert the surface integral to a volume integral.

Theorem 3.1.5. Stolze (1978) *[Gauss Divergence Theorem]: If Ω is the domain of an enclosed volume and $\delta\Omega$ is its boundary surface, then the flux, $\overrightarrow{f}$ across the boundary surface is equal to the volume integral of the divergence of $\overrightarrow{f}$ over Ω.*

Thus,

$$\int\limits_{\delta\Omega} \overrightarrow{f} \cdot \hat{n}\, dA = \int\limits_{\Omega} \overrightarrow{\nabla} \cdot \overrightarrow{f}\, dV. \tag{3.18}$$

Substituting Eq.(3.18) into Eq.(3.17), we have

$$\frac{\partial}{\partial t}\int\limits_{\Omega} C dV + \int\limits_{\Omega} \overrightarrow{\nabla} \cdot \overrightarrow{f}\, dV = 0. \tag{3.19}$$

We apply Leibniz integral rule to Eq.(3.19).

Theorem 3.1.6. Protter and Morrey (1985) *[Leibniz Integral Rule]: For an integral of the form $\int_a^b f(x,t)dt$, where $-\infty < a, b < \infty$ and a and b are constants and the function $f(x,t)$ and its partial derivative are continuous, then the derivative of the integral can be expressed as*

$$\frac{\partial}{\partial x}\left(\int_a^b f(x,t)dt\right) = \int_a^b \frac{\partial}{\partial x} f(x,t)dt. \tag{3.20}$$

Applying Thoerem 3.1.6 to Eq.(3.19) gives

$$\int\limits_{\Omega} \left[\frac{\partial C}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{f}\right] dV = 0. \tag{3.21}$$

Eq.(3.21) must hold for any control volume no matter the shape and size, therefore, the integrand must be equal to zero. That is,

$$\frac{\partial C}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{f} = 0. \tag{3.22}$$

Notice that the flux, $\overrightarrow{f}$ has components of advection and diffusion. Substituting Eq.(3.15) into Eq.(3.22) gives

$$\frac{\partial C}{\partial t} + \overrightarrow{\nabla} \cdot (\overrightarrow{u} C - D\overrightarrow{\nabla} C) = 0. \tag{3.23}$$

Simplifying further gives

$$\frac{\partial C}{\partial t} + C\overrightarrow{\nabla} \cdot \overrightarrow{u} + \overrightarrow{u} \cdot \overrightarrow{\nabla} C = \overrightarrow{\nabla} D \cdot \overrightarrow{\nabla} C + D\nabla^2 C. \tag{3.24}$$

Eq.(3.24) is the general advection-diffusion model.

For an incompressible flow, the gradient of the fluid density is zero. Therefore, from the continuity equation, $\overrightarrow{\nabla} \cdot \overrightarrow{u} = 0$. Again, if D is constant then $\overrightarrow{\nabla} D = 0$. Eq.(3.24) then reduces to

$$\frac{\partial C}{\partial t} + \overrightarrow{u} \cdot \overrightarrow{\nabla} C = D\nabla^2 C \tag{3.25}$$

which is the three-dimensional Advection-Diffusion Equation (ADE) with constant coefficients. In cartesian form, a three-dimensional ADE with constant coefficients is given as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{3.26}$$

where $\overrightarrow{u} = (u, v, w)$. A one-dimensional ADE is the one given in Eq.(1.1) for a constant $\overrightarrow{u}$ and D.

In the next section we discuss some analytical methods of solving Partial Differential Equations (PDE's). We begin this with some introductory notes on PDE's.

3.2 Partial Differential Equations

A partial Differential Equation (PDE) is an equation which contains an unknown function (the dependent variable) of two or more variables (the independent variables) together with partial derivatives with respect to these variables. If the independent variables are x and t, a PDE in a dependent variable $\phi(x, t)$ will contain **partial derivatives**, as in the ADE below.

$$\frac{\partial \phi}{\partial t} + V_0\frac{\partial \phi}{\partial x} = D_0\frac{\partial^2 \phi}{\partial x^2}. \tag{3.27}$$

The order of a PDE is the order of the highest partial derivative of the dependent variable. Eq.(3.27) is a second order partial differential equation.

A PDE may be linear or nonlinear. It is said to be linear if the differential equation is linear in the unknown function and all its derivatives with coefficients depending only on the independent variables. An example of a linear PDE is the one given in

Eq.(3.27). An equation which is not linear is called a non linear equation.

3.2.1 Second Order Linear PDE

A second order linear partial differential equation in two variables is of the form;

$$a\frac{\partial^2\phi}{\partial x^2} + b\frac{\partial^2\phi}{\partial t\partial x} + c\frac{\partial^2\phi}{\partial t^2} + d\frac{\partial\phi}{\partial x} + e\frac{\partial\phi}{\partial t} + f\phi = g \tag{3.28}$$

where a, b, c, d and e are known constants and where g possibly depends on x, t and ϕ. If g is identically zero, then Eq.(3.28) is homogeneous; otherwise it is nonhomogeneous. The independent variable x is a space coordinate and t is a time coordinate. The solution to Eq.(3.28) describes a surface in space and consists of different space curves called characteristic curves. The discriminant of the slope of the characteristic curve is defined as $b^2 - 4ac$. A PDE is hyperbolic if $b^2 - 4ac > 0$, it is parabolic if $b^2 - 4ac = 0$ and elliptic if $b^2 - 4ac < 0$. The three fundamental types of second order linear partial differential equations in 1D are the Heat/Diffusion Equation,(3.29), the Wave Equation, (3.30) and in 2D the Laplace Equation,(3.31).

$$\frac{\partial u}{\partial t} = \alpha^2\frac{\partial^2 u}{\partial x^2}, \tag{3.29}$$

$$\frac{\partial^2 u}{\partial t^2} = \alpha^2\frac{\partial^2 u}{\partial x^2}, \tag{3.30}$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0. \tag{3.31}$$

The advection-diffusion equation in (3.27) is a second-order linear partial differential equation of parabolic type.

3.2.2 Boundary and Initial Conditions

Physical problems whose solutions are governed by a PDE of second order are formulated in some region D of the (x, t) plane with a boundary Γ of suitable auxiliary conditions, called **boundary conditions**, are imposed that serve to identify a particular problem. A typical boundary condition for a second order PDE defined in a rectangle is that the solution is required to assume specified values on the sides of the rectangle. The most important types of boundary conditions are:

a. the specification of the functional form to be taken by the solution $u(x, t)$ on the boundary Γ, by requiring that

$$u(x, t) = \Phi(x, t) \quad \text{for } (x, t) \text{ on } \Gamma, \tag{3.32}$$

where $\Phi(x, t)$ is a given function. A boundary condition of this type is called **Dirichlet condition**.

b. the specification of the functional form to be taken by the derivative of the solution $u(x, t)$ normal to the boundary Γ, by requiring that

$$\frac{\partial u}{\partial n}(x, t) = \Phi(x, t) \quad \text{for } (x, t) \text{ on } \Gamma, \tag{3.33}$$

where $\Phi(x, t)$ is a given function and $\frac{\partial}{\partial n}$ is the directional derivative normal to the boundary Γ. A boundary condition of this type is called a **Neumann boundary**.

c. the specification of the functional form to be taken by a linear combination of a Dirichlet condition and a Neumann condition by the solution $u(x, t)$ on the boundary Γ, by requiring that

$$a(x, t)u(x, t) + b(x, t)\frac{\partial u}{\partial n}(x, t) = c(x, t) \quad \text{for } (x, t) \text{ on } \Gamma, \tag{3.34}$$

where $a(x, t), b(x, t)$ and $c(x, t)$ are given functions. A boundary condition of this type is called a **mixed condition**, or sometimes referred as **Robin condition**.

Given that the solution u is a function of the space variable x and time t, then it is necessary to specify how the solution starts, that is when $t = 0$, so that Γ becomes the x-axis in 1D such that

$$u(x, 0) = \Phi(x). \tag{3.35}$$

Such a condition is usually called an **initial condition**. Problems requiring initial and boundary conditions are called **initial boundary value problems**(IBVPs). It is important that the initial and boundary conditions be chosen in such a way that the PDE has a unique solution satisfying them. The types of boundary condition that can be imposed on PDE (3.28) depends on its classification and the nature of the region D that is involved.

3.3 Analytical Methods for Solving PDEs

In this section we discuss some analytical methods for solving an Advection-Diffusion Equation subject to some initial and boundary conditions. Specifically, we illustrate how the ADE can be solved by means of separation of variables and Laplace transform.

3.3.1 Separation of Variables

The basis of this method is to attempt to look for a solution $u(x,t)$ of a partial differential equation as a product of functions of single variables by writing

$$u(x,t) = X(x)T(t). \tag{3.36}$$

The advantage of this method is that it is sometimes possible to find X and T as solutions of ordinary differential equations which is much easier to solve than partial differential equations. A simple example below illustrates the general strategy. Consider the one-dimensional heat equation

$$\kappa \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}, \quad \kappa > 0, \tag{3.37}$$

satisfying the conditions

$$u(0,t) = 0 \quad \text{and} \quad u(L,t) = 0. \tag{3.38}$$

We assume a solution of the form Eq.(3.36). Substituting Eq.(3.36) into Eq.(3.37) and dividing through by $u = XT$ we obtain

$$\frac{X''}{X} = \frac{T'}{\kappa T}. \tag{3.39}$$

Since the Left Hand Side of Eq.(3.39) is a function of x only and the right hand side is a function of t only, we conclude that each side must equal some constant, such that

$$\frac{X''}{X} = \frac{T'}{\kappa T} = p \tag{3.40}$$

where p is a constant. We thus have two ordinary differential equations

$$X'' = pX, \tag{3.41}$$
$$T' = p\kappa T.$$

If $p < 0$ such that $p = -\lambda^2$, where λ is a positive real constant, then Eq.(3.41) can be written as

$$X'' + \lambda^2 X = 0, \tag{3.42}$$

$$T' + \lambda^2 \kappa T = 0. \tag{3.43}$$

The transformed boundary conditions are

$$u(0,t) = X(0)T(t) = 0, \quad \Longrightarrow \quad X(0) = 0, \;\; T(t) \neq 0, \tag{3.44}$$

$$u(L,t) = X(L)T(t) = 0, \quad \Longrightarrow \quad X(L) = 0, \;\; T(t) \neq 0. \tag{3.45}$$

The general solutions of Eq.(3.42) and Eq.(3.43) are given as

$$X(x) = A\cos\lambda x + B\sin\lambda x, \tag{3.46}$$

$$T(t) = C\exp(-\lambda^2 \kappa t). \tag{3.47}$$

Applying the conditions in Eq.(3.44) and Eq.(3.45) to Eq.(3.46) gives

$$X(x) = B\sin\left(\frac{n\pi x}{L}\right). \tag{3.48}$$

Combining Eq.(3.47) and Eq.(3.48) to give the assumed solution $u = XT$ yields (absorbing the constant C into B)

$$u(x,t) = B\exp\left[-\left(\frac{n\pi}{L}\right)^2 \kappa t\right]\sin\left(\frac{n\pi x}{L}\right). \tag{3.49}$$

If $p > 0$ such that $p = \lambda^2$, then the temperature increases to infinity which is physically meaningless.

3.3.2 Superposition of Separated Solutions

If a PDE is linear then mathematically acceptable solutions can be formed by superposing solutions corresponding to different allowed values of the separation constants. For example, if

$$u_{\lambda_k}(x,t) = X_{\lambda_k}(x)T_{\lambda_k}(t) \tag{3.50}$$

are solutions of a linear PDE obtained by means of separation of variables, then the superposition

$$u(x,t) = a_1 X_{\lambda_1}(x)T_{\lambda_1}(t) + a_2 X_{\lambda_2}(x)T_{\lambda_2}(t) + ... = \sum_{i=1} a_i X_{\lambda_i}(x)T_{\lambda_i}(t), \tag{3.51}$$

is also a solution for any constants a_i.

Applying Eq.(3.51) to Eq.(3.49) gives

$$u(x,t) = \sum_{n=1}^{\infty} B_n \exp\left[-\left(\frac{n\pi}{L}\right)^2 \kappa t\right] \sin\left(\frac{n\pi x}{L}\right). \tag{3.52}$$

3.3.3 Solving Advection-Diffusion Equation by means of Separation of Variables

Mohsen and Baluch (1983) used separation of variables technique to obtain a solution to a one-dimensional Convection-Diffusion Equation (CDE) which was presented for fixed concentration boundary conditions on a finite domain. The unsteady 1D CDE over the finite domain $0 \leq x \leq L$ was given as

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{3.53}$$

subject to the boundary conditions,

$$c(0,t) = c_0,$$

$$c(L,t) = 0,$$

and initial condition,

$$c(x,0) = 0.$$

The complete analytic solution valid at the endpoints of the finite domain was reported as;

$$\phi(\xi,\tau) = \frac{\sinh(\lambda-\xi)}{\sinh\lambda} - \frac{2\pi}{\lambda^2}\sum_{n=1}^{\infty}\frac{n}{\left(1+\dfrac{n^2\pi^2}{\lambda^2}\right)}\sin\left(\frac{n\pi\xi}{\lambda}\right)$$
$$\times\exp\left\{-\left(1+\frac{n^2\pi^2}{\lambda^2}\right)\tau\right\}. \tag{3.54}$$

See Appendix (A) for a detailed proof.

3.3.4 Laplace Transforms

Definition 3.3.5. Dyke (1999) Let f be a function defined on an interval $[0,\infty)$. The Laplace transform $f(s)$ of a function $F(t)$ is defined by

$$\mathcal{L}[F](s) = f(s) = \int_0^{\infty} e^{-st}F(t)dt \tag{3.55}$$

where s is a complex variable and e^{-st} is called the kernel of the transformation. The improper integral in Eq.(3.55) is defined to be

$$\int_0^{\infty} e^{-st}F(t)dt = \lim_{T\mapsto\infty}\int_0^{T} e^{-st}F(t)dt \tag{3.56}$$

and that this integral converges if and only if the limit exists and is finite.

We next give some examples of Laplace transforms of simple functions.

Example 3.3.6. Let us compute the Laplace transform of the function

$$F(t) = c$$

where c is a constant.

Using Definition 3.3.5,

$$\begin{aligned}\mathcal{L}[c](s) &= \int_0^\infty e^{-st} c dt \\ &= \lim_{T\mapsto\infty} \int_0^T e^{-st} c dt \\ &= \lim_{T\mapsto\infty} \left[-\frac{c}{s}e^{-st}\right]_0^T \\ &= \frac{c}{s}\left(1 - \lim_{T\mapsto\infty} e^{-sT}\right)\end{aligned} \tag{3.57}$$

Taking the complex number $s = \sigma + i\omega$ where σ and ω are real,

$$\lim_{T\mapsto\infty} e^{-sT} = \lim_{T\mapsto\infty} \left[e^{-(\sigma+i\omega)T}\right] = \lim_{T\mapsto\infty} e^{-\sigma T} e^{-i\omega T}.$$

A finite limit exists provided that $\sigma = Re(s) > 0$. Thus,

$$\mathcal{L}[c](s) = \frac{c}{s}. \tag{3.58}$$

Example 3.3.7. Let us determine the Laplace transform of the ramp function

$$F(t) = t.$$

Using Definition 3.3.5,

$$\begin{aligned}\mathcal{L}[F](s) &= \int_0^\infty e^{-st} t dt \\ &= \lim_{T\mapsto\infty} \int_0^T e^{-st} t dt \\ &= \lim_{T\mapsto\infty} \left[-\frac{t}{s}e^{-st} - \frac{e^{-st}}{s^2}\right]_0^T \\ &= \frac{1}{s^2} - \lim_{T\mapsto\infty} \frac{Te^{-sT}}{s} - \lim_{T\mapsto\infty} \frac{e^{-sT}}{s^2}.\end{aligned} \tag{3.59}$$

The limit

$$\lim_{T\mapsto\infty} \frac{Te^{-sT}}{s} = \lim_{T\mapsto\infty} \frac{e^{-sT}}{s^2} = 0$$

provided $\mathrm{Re}(s) > 0$. Thus,

$$\mathcal{L}[F](s) = \frac{1}{s^2}. \tag{3.60}$$

We make a generalization of Eq.(3.60) to deduce the following results.

Corollary 3.3.8. *The Laplace transform*

$$\mathcal{L}[t^n](s) = \frac{n!}{s^{n+1}},$$

where n is a positive integer.

Proof.

$$\begin{aligned} \mathcal{L}[t^n](s) &= \int_0^\infty e^{-st} t^n dt \\ &= \lim_{T \mapsto \infty} \int_0^T e^{-st} t^n dt \\ &= \lim_{T \mapsto \infty} \left[-\frac{t^n}{s} e^{-st} \right]_0^T + \int_0^\infty \frac{nt^{n-1}}{s} e^{-st} dt \\ &= \frac{n}{s} \mathcal{L}(t^{n-1}). \end{aligned} \tag{3.61}$$

□

Suppose that

$$\mathcal{L}\left[t^k\right](s) = \frac{k!}{s^{k+1}}$$

holds for any positive integer k.

Then,

$$\begin{aligned} \mathcal{L}[t^{k+1}](s) &= \frac{k+1}{s} \mathcal{L}(t^k) \\ &= \frac{k+1}{s} \frac{k!}{s^{k+1}} \\ &= \frac{(k+1)!}{s^{k+2}}. \end{aligned} \tag{3.62}$$

Then by induction,

$$\mathcal{L}[t^n](s) = \frac{n!}{s^{n+1}}.$$

Example 3.3.9. Let us determine the Laplace transform of the exponential function

$$F(t) = e^{at}.$$

Using Definition 3.3.5,

$$\begin{aligned}\mathcal{L}[e^{at}](s) &= \int_0^\infty e^{-st}e^{at}dt \\ &= \lim_{T\mapsto\infty}\int_0^T e^{-(s-a)t}dt \\ &= \lim_{T\mapsto\infty} -\frac{1}{s-a}\left[e^{-(s-a)t}\right]_0^T \\ &= \frac{1}{s-a}\left(1-\lim_{T\mapsto\infty} e^{-(s-a)T}\right).\end{aligned} \tag{3.63}$$

Taking the complex number $s = \sigma + i\omega$ where σ and ω are real,

$$\lim_{T\mapsto\infty} e^{-(s-a)T} = \lim_{T\mapsto\infty} e^{-(\sigma-a)T}e^{-i\omega T}.$$

If a is real and provided $\sigma = \mathrm{Re}(s) > a$, the limit exist and is zero. If a is complex, that is $a = x + iy$, then the limit will exist, and be zero, provided $\sigma > x$ (that is $\mathrm{Re}(s)>\mathrm{Re}(a)$). If these conditions are met, then we have

$$\mathcal{L}[e^{at}](s) = \frac{1}{s-a}. \tag{3.64}$$

To determine the Laplace transform of $\sin(t)$ and $\cos(t)$, it is best to determine $\mathcal{L}(e^{it})$, where $i = \sqrt{-1}$. Thus,

$$\begin{aligned}\mathcal{L}[e^{it}](s) &= \int_0^\infty e^{-st}e^{it}dt = \int_0^\infty e^{t(i-s)}dt \\ &= \left[\frac{e^{(i-s)t}}{i-s}\right]_0^\infty = \frac{1}{s-i} \\ &= \frac{s}{s^2+1} + i\frac{1}{s^2+1}.\end{aligned} \tag{3.65}$$

Now,

$$\begin{aligned}\mathcal{L}[e^{it}](s) &= \mathcal{L}\left[\cos(t) + i\sin(t)\right] \\ &= \mathcal{L}[\cos(t)] + i\mathcal{L}[\sin(t)].\end{aligned}$$

Equating real and imaginary parts gives

$$\mathcal{L}[\cos(t)](s) = \frac{s}{s^2+1} \text{ and } \mathcal{L}[\sin(t)](s) = \frac{1}{s^2+1}.$$

3.3.10 Existence of the Laplace Transform

The Laplace transform of a function $F(t)$ defined in Eq.(3.55) exists if and only if the improper integral converges for at least some values of s.

Definition 3.3.11. Dyke (1999) A function $f(t)$ is said to be of exponential order α as $t \mapsto \infty$ if there are constants M and T such that

$$|f(t)| \leq Me^{\alpha t} \tag{3.66}$$

for all $t \geq T$.

Example 3.3.12. The function $f(t) = 3e^{4t}\sin 2t$ is of exponential order, since

$$|f(t)| = 3e^{4t}|\sin 2t| \leq 3e^{4t}.$$

Theorem 3.3.13. *[Linearity of Laplace Transform]: If $F_1(t)$ and $F_2(t)$ are two functions whose Laplace transforms exist and satisfies $|F_1| \leq M_1e^{\alpha_1 t}$ and $|F_2| \leq M_2e^{\alpha_2 t}$ for all $t \geq 0$, then*

$$\mathcal{L}[aF_1 + bF_2](s) = a\mathcal{L}[F_1](s) + b\mathcal{L}[F_2](s) \tag{3.67}$$

where a and b are arbitrary constants.

Proof.

$$\begin{aligned}
\mathcal{L}[aF_1 + bF_2](s) &= \int_{t_0}^{\infty} (aF_1 + bF_2)e^{-st}dt \\
&= \int_{t_0}^{\infty} (aF_1e^{-st} + bF_2e^{-st})dt \\
&= a\int_{t_0}^{\infty} F_1e^{-st}dt + b\int_{t_0}^{\infty} F_2e^{-st}dt \\
&= a\mathcal{L}[F_1](s) + b\mathcal{L}[F_2](s)
\end{aligned}$$

where we have assumed that

$$|F_1| \leq M_1e^{\alpha_1 t} \text{ and } |F_2| \leq M_2e^{\alpha_2 t}$$

so that

$$\begin{aligned}|aF_1 + bF_2| &\le |a||F_1| + |b||F_2| \\ &\le |a|M_1 e^{\alpha_1 t} + |b|M_2 e^{\alpha_2 t} \\ &\le (|a|M_1 + |b|M_2)e^{\alpha_3 t}\end{aligned}$$

where $\alpha_3 = max\{\alpha_1, \alpha_2\}$. This proves the theorem. □

Example 3.3.14. Let us determine the Laplace transform of

$$\mathcal{L}[2t + 4e^{3t}].$$

Using the results in Eq.(3.60) and Eq.(3.64),

$$\mathcal{L}[t](s) = \frac{1}{s^2}, \ \ \text{Re(s)} > 0.$$

$$\mathcal{L}[e^{3t}](s) = \frac{1}{s-3}, \ \ \text{Re(s)} > 3.$$

By the linearity principle,

$$\begin{aligned}\mathcal{L}[2t + 4e^{3t}](s) &= 2\mathcal{L}[t](s) + 4\mathcal{L}[e^{3t}](s) \\ &= 2\left(\frac{1}{s^2}\right) + 4\left(\frac{1}{s-3}\right) \\ &= \frac{2}{s^2} + \frac{4}{s-3}.\end{aligned}$$

3.3.15 Inverse Laplace Transform

Definition 3.3.16. If $F(t)$ has the Laplace transform $f(s)$, that is

$$\mathcal{L}[F](s) = f(s)$$

then the inverse Laplace transform is defined by

$$\mathcal{L}^{-1}[f(s)](t) = F(t). \tag{3.68}$$

For example, given that

$$\mathcal{L}[e^{at}](s) = \frac{1}{s-a} \tag{3.69}$$

then it follows from Eq.(3.68) that

$$\mathcal{L}^{-1}\left[\frac{1}{s-a}\right](t) = e^{at}. \tag{3.70}$$

Theorem 3.3.17. ***Linearity of the Inverse Laplace Transform***

$$\mathcal{L}^{-1}[af_1 + bf_2] = a\mathcal{L}^{-1}[f_1] + b\mathcal{L}^{-1}[f_2]. \tag{3.71}$$

Proof. Since the Laplace transform is linear Eq.(3.67), we have appropriately well behaved functions $F_1(t)$ and $F_2(t)$:

$$\begin{aligned} \mathcal{L}[aF_1(t) + bF_2(t)] &= a\mathcal{L}[F_1(t)] + b\mathcal{L}[F_2(t)] \\ &= af_1 + bf_2. \end{aligned} \tag{3.72}$$

Taking the inverse Laplace transform of Eq.(3.72), we have

$$aF_1(t) + bF_2(t) = \mathcal{L}^{-1}\left[af_1 + bf_2\right]. \tag{3.73}$$

Eq.(3.73) is the same as;

$$\mathcal{L}^{-1}[af_1 + bf_2] = a\mathcal{L}^{-1}[f_1] + b\mathcal{L}^{-1}[f_2]$$

and this establishes the Linearity of $\mathcal{L}^{-1}[f]$. □

Example 3.3.18. Let us find

$$\mathcal{L}^{-1}\left[\frac{1}{(s+3)(s-2)}\right]. \tag{3.74}$$

Resolving Eq.(3.74) into partial fractions,

$$\frac{1}{(s+3)(s-2)} = \frac{-\frac{1}{5}}{s+3} + \frac{\frac{1}{5}}{s-2}.$$

Given that $\mathcal{L}^{-1}\left[\dfrac{1}{s-a}\right](t) = e^{at}$ and by the linearity principle Eq.(3.71),

$$\begin{aligned}
\mathcal{L}^{-1}\left[\frac{1}{(s+3)(s-2)}\right](t) &= \mathcal{L}^{-1}\left[\frac{-\frac{1}{5}}{s+3} + \frac{\frac{1}{5}}{s-2}\right] \\
&= -\frac{1}{5}\mathcal{L}^{-1}\left[\frac{1}{(s+3)}\right] + \frac{1}{5}\mathcal{L}^{-1}\left[\frac{1}{(s-2)}\right] \\
&= -\frac{1}{5}e^{-3t} + \frac{1}{5}e^{2t}.
\end{aligned}$$

3.3.19 Derivative Property of the Laplace Transform

This section discusses the Laplace transforms of derivatives such as $F'(t), F''(t)$ and in general $F^n(t)$.

If a differentiable function $F(t)$ has Laplace transform $f(s)$, then by definition, the Laplace transform of $F'(t)$,

$$\mathcal{L}[F'](s) = \int_0^\infty e^{-st}F'(t)dt$$

can be found through the following theorem.

Theorem 3.3.20. *If $F(t)$ is a differentiable function of t, then*

$$\mathcal{L}[F'](s) = \int_0^\infty e^{-st}F'(t)dt = -F(0) + sf(s). \tag{3.75}$$

Proof. Integrating by parts gives,

$$\begin{aligned}
\mathcal{L}[F'](s) &= \left[F(t)e^{-st}\right]_0^\infty + \int_0^\infty se^{-st}F(t)dt \\
&= -F(0) + sf(s).
\end{aligned} \tag{3.76}$$

where $F(0)$ is the value of $F(t)$ at $t = 0$. □

Theorem 3.3.21. *If $F(t)$ is a twice differentiable function of t, then*

$$\mathcal{L}[F'](s) = s^2f(s) - sF(0) - F'(0). \tag{3.77}$$

Proof.

$$\begin{aligned}
\mathcal{L}[F''](s) &= \int_0^\infty e^{-st}F''(t)dt \\
&= \left[F'(t)e^{-st}\right]_0^\infty + \int_0^\infty se^{-st}F'(t)dt \\
&= -F'(0) + \left[sF(t)e^{-st}\right]_0^\infty + \int_0^\infty s^2e^{-st}F(t)dt \\
&= -F'(0) - sF(0) + s^2f(s) \\
&= s^2f(s) - sF(0) - F'(0).
\end{aligned} \tag{3.78}$$

□

Example 3.3.22. Let us find the solution to the differential equation

$$y'' - y' - 2y = 0, \quad y(0) = 1, \quad y'(0) = 0.$$

Applying the Laplace transform to the differential equation,

$$\mathcal{L}[y'' - y' - 2y] = \mathcal{L}[0] = 0.$$

Theorem 3.3.13 says that the Laplace transform is a linear operator,

$$\mathcal{L}[y''] - \mathcal{L}[y'] - 2\mathcal{L}[y] = 0. \tag{3.79}$$

Applying Theorems 3.3.20 and 3.3.21 to Eq.(3.79) yields,

$$\left[s^2\mathcal{L}[y] - sy(0) - y'(0)\right] - \left[s\mathcal{L}[y] - y(0)\right] - 2\mathcal{L}[y] = 0$$

which is equivalent to the equation,

$$\begin{aligned}
(s^2 - s - 2)\mathcal{L}[y] &= s - 1 \\
\mathcal{L}[y] &= \frac{s-1}{s^2 - s - 2} \\
\mathcal{L}[y] &= \left[\frac{1}{3(s-2)} + \frac{2}{3(s+1)}\right].
\end{aligned}$$

From Definition 3.3.16,

$$y = \mathcal{L}^{-1}\left[\frac{1}{3(s-2)} + \frac{2}{3(s+1)}\right].$$

Given that $\mathcal{L}^{-1}\left[\frac{1}{s-a}\right](t) = e^{at}$ and by the linearity principle in Eq.(3.71),

$$\begin{aligned} y &= \mathcal{L}^{-1}\left[\frac{1}{3(s-2)} + \frac{2}{3(s+1)}\right] \\ &= \frac{1}{3}\mathcal{L}^{-1}\left[\frac{1}{(s-2)}\right] + \frac{2}{3}\mathcal{L}^{-1}\left[\frac{1}{(s+1)}\right] \\ &= \frac{1}{3}e^{2t} + \frac{2}{3}e^{-t}. \end{aligned}$$

3.3.23 Solving Convection-Diffusion equation by means of Laplace Transform

The Laplace transform provides a potent technique for solving linear differential equations with constant coefficients. When the transform is applied in time t to a PDE in $\phi(x,t)$ with two independent varibales x and t, the result is an ODE for the equation in $\phi(x,s)$. The ODE is then solved for $\phi(x,s)$ and the inverse transform yields $\phi(x,t)$.

Davis (1985), presented an analytic solution to a convection-diffusion equation over a finite domain using the Laplace transform. The dimensionless CDE to be solved is

$$\frac{d^2\hat{c}}{dX^2} - P_e\frac{d\hat{c}}{dX} - p\hat{c} = 0 \tag{3.80}$$

subject to the boundary conditions,

$$\hat{c}(0,p) = \frac{c_0}{p},$$

$$\hat{c}(1,p) = 0$$

and initial condition;

$$\hat{c}(X,0) = 0$$

where p is the transform variable. The solution was reported to be

$$\begin{aligned} c(X,T) = c_0\exp(\lambda X)&\left[\frac{\sinh\left(\frac{P_e}{2}(1-X)\right)}{\sinh\left(\frac{P_e}{2}\right)}\right] - c_0\exp(\lambda X) \\ &\times\left[2\pi\sum_{n=1}^{\infty}\frac{n\sin(n\pi X)}{(\lambda^2+n^2\pi^2)}\times\exp\left[-(\lambda^2+n^2\pi^2)T\right]\right]. \end{aligned} \tag{3.81}$$

See Appendix (B) for a detailed derivation.

3.4 Laurent Series, Singularities and Residues

In this section we start discussions on the main method that will be used in our study. We begin the section with some introductory notes on Laurent series and singularities.

3.4.1 Laurent Series

Definition 3.4.2. A Laurent series is a series of the form

$$\sum_{n=-\infty}^{\infty} a_n(z-z_0)^n$$

where

$$\sum_{n=-\infty}^{\infty} a_n(z-z_0)^n = \sum_{n=1}^{\infty} a_{-n}(z-z_0)^{-n} + \sum_{n=0}^{\infty} a_n(z-z_0)^n.$$

We call

$$\sum_{n=1}^{\infty} a_{-n}(z-z_0)^{-n} \tag{3.82}$$

the principal part of the Laurent series. Thus, the principal part of a Laurent series is the part that contains all the negative powers of $(z-z_0)$.

3.4.3 Singularities

Definition 3.4.4. A singularity of a function $f(z)$ is a complex number z_0 at which $f(z)$ is not differentiable.

Example 3.4.5. If $f(z) = \dfrac{1}{z}$, then f has a singularity at $z = 0$, since f is not defined at the origin.

Definition 3.4.6. A function f is said to have an isolated singularity at z_0 if f is analytic in a deleted neighbourhood D of z_0 but is not analytic at z_0.

Example 3.4.7. For the function $f(z) = \dfrac{1}{z}$, $z = 0$ is an isolated singular point, since $f(z)$ is analytic in the open disc $0 < |z| < R,\ R > 0$.

3.4.8 Poles

Suppose that a function f has an isolated singularity at z_0 and that the principal part of the Laurent series Eq.(3.82) has finitely many terms in it. That is

$$f(z) = \frac{b_m}{(z-z_0)^m} + ... + \frac{b_1}{(z-z_0)} + \sum_{n=0}^{\infty} a_n(z-z_0)^n \tag{3.83}$$

where $b_m \neq 0$, then we say that f has a pole of order m at z_0. A pole of order 1 is called a simple pole.

Example 3.4.9. Let

$$f(z) = \frac{1}{z}, z \neq 0.$$

Then $f(z)$ has a simple pole at $z = 0$.

Example 3.4.10. Let

$$g(z) = \left(\frac{z+1}{z-1}\right)^3$$

then $g(z)$ has a pole of order 3 at $z = 1$.

3.4.11 Residues

Suppose that f is analytic in a domain D except for an isolated singularity at $z_0 \in D$. Suppose f has Laurent expansion

$$f(z) = \sum_{n=0}^{\infty} a_n(z-z_0)^n + \sum_{n=1}^{\infty} b_n(z-z_0)^{-n}.$$

The residue of f at z_0 is defined to be

$$Res(f, z_0) = b_1.$$

That is, the residue of f at the isolated singularity z_0 is the coefficient of $(z-z_0)^{-1}$ in the Laurent expansion.

Remark 3.4.12. If we can write $f(z) = \dfrac{g(z)}{h(z)}$ where g and h are differentiable and $g(z) \neq 0$ when $h(z) = 0$ then the poles of $f(z)$ occurs at the zeros of h.

Lemma 3.4.13. *If f has a simple pole at z_0 then*

$$Res(f, z_0) = \lim_{z \mapsto z_0} (z - z_0) f(z). \tag{3.84}$$

Proof. If f has a simple pole at z_0, then it has a Laurent series

$$f(z) = \frac{b_1}{z - z_0} + \sum_{n=0}^{\infty} a_n (z - z_0)^n.$$

Thus,

$$(z - z_0) f(z) = b_1 + \sum_{n=0}^{\infty} a_n (z - z_0)^{n+1}$$

so that

$$\lim_{z \mapsto z_0} (z - z_0) f(z) = b_1.$$

□

Example 3.4.14. Let

$$f(z) = \frac{\cos \pi z}{z - 1}.$$

This has a simple pole at $z = 1$ and satisfies the hypothesis of Lemma 3.4.13. Hence,

$$\begin{aligned} Res(f, 1) &= \lim_{z \mapsto 1} (z - 1) \frac{\cos \pi z}{(z - 1)} \\ &= \cos \pi = -1. \end{aligned}$$

Chapter 4

Main Results

In this chapter we present solutions to the Advection-Diffusion Equation (ADE) subject to various initial and boundary conditions. Without using an inverse Laplace transform, analytic solutions to the ADE are obtained using the Laplace transform technique and the residue theorem in complex analysis.

4.1 The Residue Theorem Approach

We next discuss a method expounded by Kim (2020a) who obtained a general analytic solution of a Convection-Diffusion-Reaction-Source equation (CDRS) by using Laplace transform and residue theorem approach. The solution to the CDRS equation was decomposed into two components, the steady state solution and transient state solution. The steady state solution was obtained by using the residue theorem approach at the primary singular pole. The unsteady part of the solution was found as a product of the spatial and transient weighting factor, using the initial condition. This approach is quite useful if the inverse Laplace transform (iLT) of some functions in the transformed equation are often challenging to evaluate or cannot be found in the iLT tables.

4.1.1 The Main Method

The 1D unsteady CDRS equation is given by

$$\frac{\partial C}{\partial t} = D_0 \frac{\partial^2 C}{\partial x^2} - V_0 \frac{\partial C}{\partial x} - K_0 C + S(x) \tag{4.1}$$

with initial condition

$$C(x,0) = C_1(x)$$

and two boundary conditions,

$$C(x_0,t) = C_0(t),$$

$$C(x_1,t) = C_1(t),$$

where K_0 is a first-order reaction constant and $S(x)$ is a source function.

Using the dimensionless quantities

$$\phi(\xi,\tau) = C(x,t)/C_\infty, \quad \tau = tD_0/L^2, \quad \xi = x/L,$$

$$P_e = 2\lambda = LV_0/D_0, \quad \kappa = K_0L^2/D_0 \quad \sigma = SL^2/D_0C_\infty,$$

where C_∞ is a reference (often bulk or initial) concentration, L is the length scale of the spatial domain, P_e is the Peclet number and the factor 2 of λ is for mathematical convenience. Note that the dimensionless quantity for κ in Kim (2020a) has a typographical error.

Eq.(4.1) can be rewritten as

$$\frac{\partial[\phi(\xi,\tau)C_\infty]}{\partial\left[\dfrac{\tau L^2}{D_0}\right]} = \frac{D_0\,\partial^2\left[\phi(\xi,\tau)C_\infty\right]}{\partial[\xi L]^2} - \frac{2\lambda D_0\,\partial[\phi(\xi,\tau)]C_\infty}{L\partial[\xi L]} - \frac{\kappa D_0}{L^2}\,\phi(\xi,\tau)C_\infty + \frac{\sigma D_0 C_\infty}{L^2},$$

$$\Longrightarrow \quad \frac{D_0C_\infty}{L^2}\frac{\partial\phi(\xi,\tau)}{\partial\tau} = \frac{D_0C_\infty}{L^2}\frac{\partial^2\phi(\xi,\tau)}{\partial\xi^2} - \frac{2\lambda D_0C_\infty}{L^2}\frac{\partial\phi(\xi,\tau)}{\partial\xi} - \frac{\kappa D_0C_\infty\ \phi(\xi,\tau)}{L^2} + \frac{\sigma D_0C_\infty}{L^2}.$$

Multiplying through by $\dfrac{L^2}{D_0C_\infty}$, the dimensionless form of Eq.(4.1) becomes

$$\frac{\partial\phi}{\partial\tau} = \frac{\partial^2\phi}{\partial\xi^2} - 2\lambda\frac{\partial\phi}{\partial\xi} - \kappa\phi + \sigma(\xi), \quad 0 < \xi < 1, \quad \tau > 0 \tag{4.2}$$

with initial condition,

$$\phi(\xi,0) = \mu_1(\xi), \quad 0 < \xi < 1$$

and two boundary conditions,

$$\phi_0(\xi_0,\tau) = \phi_0(\tau), \quad \tau > 0,$$

$$\phi_1(\xi_1,\tau) = \phi_1(\tau), \quad \tau > 0. \tag{4.3}$$

The Laplace transform of the dimensionless concentration $\phi(\xi,\tau)$ is defined as

$$\Phi(\xi,p) := \mathcal{L}[\phi(\xi,\cdot)](p) = \int_0^\infty e^{-p\tau}\,\phi(\xi,\tau)\,d\tau. \tag{4.4}$$

Applying Eq.(4.4) to Eq.(4.2), we have

$$\mathcal{L}\left[\frac{\partial\phi}{\partial\tau}\right] = p\Phi - \phi(\xi,0) = p\Phi - \mu_1(\xi)$$

$$\mathcal{L}\left[\frac{\partial^2\phi}{\partial\xi^2}\right] = \frac{\partial^2\Phi}{\partial\xi^2}; \qquad \mathcal{L}\left[2\lambda\frac{\partial\phi}{\partial\xi}\right] = 2\lambda\frac{\partial\Phi}{\partial\xi},$$

$$\mathcal{L}[\kappa\phi] = \kappa\Phi; \qquad \mathcal{L}[\sigma(\xi)] = \frac{\sigma(\xi)}{p}.$$

The dimensionless Eq.(4.2) after applying the Laplace transform is

$$p\Phi - \mu_1(\xi) = \frac{\partial^2\Phi}{\partial\xi^2} - 2\lambda\frac{\partial\Phi}{\partial\xi} - \kappa\Phi + \frac{\sigma(\xi)}{p}$$

or equivalently

$$\frac{d^2\Phi}{d\xi^2} - 2\lambda\frac{d\Phi}{d\xi} - (\kappa+p)\Phi = -\left[\mu_1(\xi) + p^{-1}\sigma(\xi)\right]. \tag{4.5}$$

Let $\mathscr{D}_\xi = \dfrac{d}{d\xi}$ and $\Omega(\xi) = \mu_1(\xi) + p^{-1}\sigma(\xi)$, then Eq.(4.5) becomes

$$\mathscr{D}_\xi^2\Phi - 2\lambda\mathscr{D}_\xi\Phi - (\kappa+p)\Phi = -\Omega(\xi),$$

$$\implies \quad \left[\mathscr{D}_\xi^2 - 2\lambda\mathscr{D}_\xi - (\kappa+p)\right]\Phi = -\Omega(\xi), \tag{4.6}$$

$$\implies \quad [\mathscr{D}_\xi - \lambda_m]\,[\mathscr{D}_\xi - \lambda_p]\Phi = -\Omega(\xi)$$

where $\lambda_m = \lambda - \beta$, $\lambda_p = \lambda + \beta$, and $\beta = \sqrt{\alpha^2 + p}$, $\alpha^2 = \lambda^2 + \kappa$.

A new function is defined for simplicity as follows:

$$\begin{aligned}
\Phi^{\dagger} &\equiv [\mathscr{D}_{\xi} - \lambda_p]\Phi \\
&= \frac{e^{\lambda_p \xi}}{e^{\lambda_p \xi}} \left[\mathscr{D}_{\xi} - \lambda_p\right] \Phi \\
&= e^{\lambda_p \xi} \left[e^{-\lambda_p \xi} \mathscr{D}_{\xi} \Phi - \lambda_p e^{-\lambda_p \xi} \Phi\right] \\
&= e^{\lambda_p \xi} \mathscr{D}_{\xi} \left(\Phi e^{-\lambda_p \xi}\right).
\end{aligned} \tag{4.7}$$

We now write Eq.(4.6) as

$$\left[\mathscr{D}_{\xi} - \lambda_m\right] \Phi^{\dagger} = \frac{e^{\lambda_m \xi}}{e^{\lambda_m \xi}} [\mathscr{D}_{\xi} - \lambda_m] \Phi^{\dagger} = -\Omega(\xi),$$

$$e^{\lambda_m \xi} \left[e^{-\lambda_m \xi} \mathscr{D}_{\xi} \Phi^{\dagger} - \lambda_m e^{-\lambda_m \xi} \Phi^{\dagger}\right] = -\Omega(\xi),$$

$$e^{\lambda_m \xi} \mathscr{D}_{\xi} (\Phi^{\dagger} e^{-\lambda_m \xi}) = -\Omega(\xi),$$

$$\mathscr{D}_{\xi} (\Phi^{\dagger} e^{-\lambda_m \xi}) = -\Omega(\xi) e^{-\lambda_m \xi}. \tag{4.8}$$

The general solution for $\Phi^{\dagger}$ is given as

$$\int \mathscr{D}_{\xi} \left(\Phi^{\dagger} e^{-\lambda_m \xi}\right) d\xi = \int -\Omega(\xi) e^{-\lambda_m \xi} d\xi + B_1,$$

$$\Phi^{\dagger} e^{-\lambda_m \xi} = B_1 - \int_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta,$$

$$\implies \quad \Phi^{\dagger} = e^{\lambda_m \xi} \left[B_1 - \int_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta\right], \tag{4.9}$$

where B_1 is an integration constant which is a function of β as will be seen in Eq.(4.34). Substituting Eq.(4.9) into Eq.(4.7), one obtains

$$e^{\lambda_p \xi} \mathscr{D}_{\xi} (\Phi e^{-\lambda_p \xi}) = e^{\lambda_m \xi} \left[B_1 - \int_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta\right],$$

$$\mathscr{D}_{\xi} (\Phi e^{-\lambda_p \xi}) = e^{-\lambda_p \xi} e^{\lambda_m \xi} \left[B_1 - \int_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta\right],$$

$$\mathscr{D}_\xi(\Phi e^{-\lambda_p \xi}) = B_1 e^{-\lambda_p \xi} e^{\lambda_m \xi} - e^{-\lambda_p \xi} e^{\lambda_m \xi} \int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta. \tag{4.10}$$

Taking the Integral of Eq.(4.10) with respect to ξ, we have

$$\begin{aligned}
\Phi e^{-\lambda_p \xi} &= B_1 \int e^{(\lambda_m - \lambda_p)\xi} d\xi - \int e^{(\lambda_m - \lambda_p)\xi} \left[\int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta \right] d\xi + B_2 \\
&= B_1 \frac{e^{(\lambda_m - \lambda_p)\xi}}{\lambda_m - \lambda_p} + B_2 - \int e^{(\lambda_m - \lambda_p)\xi} \left[\int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta \right] d\xi \\
&= B_1 \frac{e^{(\lambda_m - \lambda_p)\xi}}{-2\beta} + B_2 - \int e^{(\lambda_m - \lambda_p)\xi} \left[\int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta \right] d\xi \\
&= B_1 e^{\lambda_m \xi} \cdot e^{-\lambda_p \xi} + B_2 - \int e^{(\lambda_m - \lambda_p)\xi} \left[\int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta \right] d\xi,
\end{aligned} \tag{4.11}$$

where -2β is absorbed in B_1. The general solution for $\Phi(\xi, p)$ is given as

$$\Phi(\xi, p) = B_1 e^{\lambda_m \xi} + B_2 e^{\lambda_p \xi} - e^{\lambda_p \xi} \int e^{(\lambda_m - \lambda_p)\xi} \left[\int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta \right] d\xi, \tag{4.12}$$

where

$$\Phi_c(\xi, p) = B_1 e^{\lambda_m \xi} + B_2 e^{\lambda_p \xi} \tag{4.13}$$

and

$$\Phi_p(\xi, p) = -e^{\lambda_p \xi} \int e^{(\lambda_m - \lambda_p)\xi} \left[\int\limits_{\xi} \Omega(\eta) e^{-\lambda_m \eta} d\eta \right] d\xi \tag{4.14}$$

are the complementary and particular solution respectively.

Now, having two boundary conditions, one can use the inverse Laplace transform to obtain the transient solution $\phi(\xi, \tau)$ in real space:

$$\phi(\xi, \tau) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\tau z} \Phi(\xi, z) dz = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\tau z} \frac{\Lambda(\xi, z)}{z} dz \tag{4.15}$$

where the integration parameter p is replaced by a complex variable z and c is a constant.

One can write $\Phi(\xi, z) = \dfrac{\Lambda(\xi, z)}{z}$, where $\Lambda(\xi, z)$ is finite at $z = 0$ and its residue in the inverse Laplace transform provides the steady state solution $\phi_{ss}(\xi)$

$$\phi_{ss}(\xi) = \lim_{z \mapsto 0} z \left[e^{\tau z} \frac{\Lambda(\xi, z)}{z} \right] = \Lambda(\xi, 0). \tag{4.16}$$

By combining Eq.(4.15) and Eq.(4.16), one can write

$$\phi(\xi, \tau) = \Lambda(\xi, 0) + \sum_{k, z_k \neq 0} \text{Res}\left[\exp(\tau \cdot)\Phi(\xi, \cdot) z_k\right] \tag{4.17}$$

where $\Lambda(\xi, 0)$ is at the primary pole of $z_0 = 0$ and z_k is the pole of order $k(\geq 1)$ of the $\Phi(\xi, z)$ function.

If $\Phi(\xi, z)$ has only two poles at $z = z_0 = 0$ and $z = z_1$, then Eq.(4.17) can be simplified as

$$\phi(\xi, \tau) = \Lambda(\xi, 0) + \text{Res}\left[\exp(\tau \cdot)\Phi(\xi, \cdot) z_1\right] \tag{4.18}$$

where the calculation of $\text{Res}[\Phi(\xi, \cdot) z_1]$ requires an inverse Laplace transform, which can be avoided by applying the initial condition to Eq.(4.18): That is

$$\text{Res}\left[\Phi(\xi, \cdot) z_1\right] = \mu_1(\xi) - \phi_{ss}(\xi). \tag{4.19}$$

One can conclude that if a Laplace transform has only one non-zero singularity pole, contributing to the transient behavior, then the solution for $\phi(\xi, \tau)$ is given as

$$\phi(\xi, \tau) = \phi_{ss}(\xi) + [\mu_1(\xi) - \phi_{ss}(\xi)] \times e^{\mathcal{R}(z_1)\tau}, \tag{4.20}$$

where $\mathcal{R}(z_1)$ is the real part of the imaginary pole z_1. If $\Phi(\xi, z)$ contains $N(\geq 2)$ non-zero singularity poles, then the number of required inverse Laplace transform reduces to $N - 1$ by replacing one of the transforms (perhaps the most difficult one) by applying the initial concentration.

Example 4.1.2.

To confirm his method, Kim (2020a) applied it to a specific example from Carslaw and Jaeger (1959) paper. In the absence of reaction, $\kappa = 0$ and source/sink, $\sigma = 0$, the CDRS equation in Eq.(4.2) reduces to the convection-diffusion equation considered by Carslaw and Jaeger (1959) :

$$\frac{\partial \phi}{\partial \tau} = \frac{\partial^2 \phi}{\partial \xi^2} - 2\lambda \frac{\partial \phi}{\partial \xi}.$$

With $\phi_0 = 1, \phi_1 = 0, \mu_1 = 0$ and $\lambda = 1/2$, the general solution after applying the Laplace transform in Eq.(4.5) is given as

$$\Phi(\xi, p) = \frac{e^{\lambda\xi} \sinh[\beta(1-\xi)]}{p \sinh\beta}. \tag{4.21}$$

By replacing the integration parameter p by a complex variable z;

$$\Phi(\xi, z) = \frac{e^{\lambda\xi} \sinh[\beta(1-\xi)]}{z \sinh\beta}, \tag{4.22}$$

where $\beta = \sqrt{\lambda^2 + z}$.
Let

$$\Phi(\xi, z) = \frac{\Lambda(\xi, z)}{z},$$

where

$$\Lambda(\xi, z) = \frac{e^{\lambda\xi} \sinh[\beta(1-\xi)]}{\sinh\beta}.$$

Eq.(4.22) has simple poles at $z = 0$ and $\sinh\beta = 0 \implies z = -\lambda^2$. The residue of the first pole at $z = 0$ is equal to the steady state solution $\phi_{ss}(\xi)$:

$$\phi_{ss}(\xi) = \lim_{z \mapsto 0} z\,[e^{\tau z}\Phi(\xi, z)] = \frac{e^{\lambda\xi} \sinh[\lambda(1-\xi)]}{\sinh\lambda}. \tag{4.23}$$

The second residue gives the transient state solution, $\phi_{tr}(\xi, \tau)$:

$$\phi_{tr}(\xi, \tau) = \lim_{z \mapsto -\lambda^2} [(z + \lambda^2)e^{\tau z}\Phi(\xi, z)] = -\phi_{ss}(\xi)e^{-\lambda^2\tau}. \tag{4.24}$$

The final solution $\phi(\xi, \tau)$ is the sum of Eq.(4.23) and Eq.(4.24);

$$\phi(\xi, \tau) = \frac{e^{\lambda\xi} \sinh[\lambda(1-\xi)]}{\sinh\lambda} \left[1 - e^{-\lambda^2\tau}\right]. \tag{4.25}$$

Eq.(4.25) satisfies the initial condition, $\phi(\xi, 0) = 0$ but does not provide the inlet boundary condition $\phi(0, \tau) = 1$ for arbitrary τ. A proper conditional representation of the full transient solution is

$$\phi_{tr}(\xi, \tau) = \begin{cases} -\phi_{ss}(\xi)e^{-\lambda^2\tau}, & \text{for } 0 < \xi \leq 1 \\ 1, & \text{for } \xi = 0. \end{cases} \tag{4.26}$$

To avoid the above conditional representation in Eq.(4.26), an alternative expression was obtained by using a Fourier series in Mohsen and Baluch (1983). The transient state solution is given as

$$\phi_{tr}(\xi,\tau) = -2\pi\lambda e^{\lambda\xi}\sum_{n=1}^{\infty}\frac{n}{(\lambda^2+n^2\pi^2)}\sin(n\pi\xi) \times \exp\left\{-\left(\lambda^2+n^2\pi^2\right)\tau\right\}$$

which is an improved analytic form from the previous work Carslaw and Jaeger (1959).

4.1.3 Analytical Solution to the CDRS Equation

This section provides general procedure for deriving 1D analytic solutions for the Dirichlet/Dirichlet and Dirichlet/Neumann boundary conditions.

4.1.4 Solution for the Dirichlet-Dirichlet BC:

The boundary conditions considered are

$$\phi(0,\tau) = \phi_0,$$

$$\phi(1,\tau) = \phi_1,$$

with initial condition

$$\mu(\xi) = \mu_0.$$

Given that $\phi(\xi,0) = \mu_0 = \Omega(\xi)$, the particular solution in Eq.(4.14) becomes

$$\begin{aligned}\Phi_p(\xi,p) &= -e^{\lambda_p\xi}\int e^{(\lambda_m-\lambda_p)\xi}\left[\int_{\xi}\Omega(\eta)e^{-\lambda_m\eta}d\eta\right]d\xi \\ &= \frac{\mu_0}{\lambda_m}e^{\lambda_p\xi}\int e^{(\lambda_m-\lambda_p)\xi}\,e^{-\lambda_m\xi}d\xi \\ &= \frac{\mu_0}{\lambda_m}e^{\lambda_p\xi}\int e^{\lambda_p\xi}d\xi = -\frac{\mu_0}{\lambda_m\lambda_p} \\ &= -\frac{\mu_0}{\lambda^2-\beta^2} \\ &= \frac{\mu_0}{\kappa+p}.\end{aligned} \tag{4.27}$$

The general solution for Φ from Eq.(4.12) is

$$\Phi(\xi, p) = B_1 e^{\lambda_m \xi} + B_2 e^{\lambda_p \xi} + \frac{\mu_0}{\kappa + p}. \tag{4.28}$$

Putting $\lambda_m = \lambda - \beta$, $\lambda_p = \lambda + \beta$ into Eq.(4.28);

$$\begin{aligned} \Phi(\xi, p) &= B_1 e^{(\lambda-\beta)\xi} + B_2 e^{(\lambda+\beta)\xi} + \frac{\mu_0}{\kappa + p} \\ &= e^{\lambda\xi}\left[B_1 e^{-\beta\xi} + B_2 e^{\beta\xi}\right] + \frac{\mu_0}{\kappa + p}. \end{aligned} \tag{4.29}$$

Applying the Laplace transform to the boundary conditions gives

$$\Phi(0, p) = \frac{\phi_0}{p}, \tag{4.30}$$

$$\Phi(1, p) = \frac{\phi_1}{p}. \tag{4.31}$$

Applying Eq.(4.30) to Eq.(4.29),

$$B_1 + B_2 + \frac{\mu_0}{\kappa + p} = \frac{\phi_0}{p},$$

$$\implies \quad B_1 = \frac{\phi_0}{p} - \frac{\mu_0}{\kappa + p} - B_2. \tag{4.32}$$

Similarly, applying Eq.(4.31) to Eq.(4.29),

$$e^{\lambda}\left[B_1 e^{-\beta} + B_2 e^{\beta}\right] + \frac{\mu_0}{\kappa + p} = \frac{\phi_1}{p},$$

$$\implies \quad B_1 e^{-\beta} + B_2 e^{\beta} = \left(\frac{\phi_1}{p} - \frac{\mu_0}{\kappa + p}\right) e^{-\lambda}. \tag{4.33}$$

Substituting B_1 into Eq.(4.33) gives

$$\left(\frac{\phi_0}{p} - \frac{\mu_0}{\kappa + p} - B_2\right) e^{-\beta} + B_2 e^{\beta} = \left(\frac{\phi_1}{p} - \frac{\mu_0}{\kappa + p}\right) e^{-\lambda},$$

$$\implies \quad B_2\left(e^{\beta}-e^{-\beta}\right)=\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}-\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\beta},$$

$$\implies \quad B_2=\frac{\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}-\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\beta}}{e^{\beta}-e^{-\beta}}$$

$$=\frac{\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}-\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\beta}}{2\sinh\beta}.$$

Substituting B_2 into Eq.(4.32) gives:

$$\begin{aligned} B_1&=\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)-\frac{\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}-\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\beta}}{e^{\beta}-e^{-\beta}}\\ &=\frac{\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)e^{\beta}-\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}}{2\sinh\beta}. \end{aligned} \tag{4.34}$$

Let

$$C_1=\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p},$$

$$C_2=\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}.$$

Then,

$$B_1=\frac{C_1e^{\beta}-C_2}{2\sinh\beta},$$

$$B_2=-\frac{C_1e^{-\beta}-C_2}{2\sinh\beta}.$$

Substituting B_1 and B_2 into Eq.(4.29) results in

$$\begin{aligned} \Phi(\xi,p)&=e^{\lambda\xi}\left[\left(\frac{C_1e^{\beta-\beta\xi}-C_2e^{-\beta\xi}}{2\sinh\beta}\right)-\left(\frac{C_1e^{-(\beta-\beta\xi)}-C_2e^{\beta\xi}}{2\sinh\beta}\right)\right]+\frac{\mu_0}{\kappa+p}\\ &=e^{\lambda\xi}\left[\frac{C_1\,e^{(\beta-\beta\xi)}-C_1\,e^{(\beta\xi-\beta)}+C_2\,e^{\beta\xi}-C_2\,e^{-\beta\xi}}{2\sinh\beta}\right]+\frac{\mu_0}{\kappa+p}\\ &=e^{\lambda\xi}\left[\frac{C_1\sinh(\beta-\beta\xi)+C_2\sinh(\beta\xi)}{\sinh\beta}\right]+\frac{\mu_0}{\kappa+p}. \end{aligned} \tag{4.35}$$

If we put the expressions for C_1 and C_2 into Eq.(4.35), the solution become

$$\Phi(\xi,p)=\frac{e^{\lambda\xi}}{\sinh\beta}\left[\left(\frac{\phi_0}{p}-\frac{\mu_0}{\kappa+p}\right)\sinh(\beta-\beta\xi)+\left(\frac{\phi_1}{p}-\frac{\mu_0}{\kappa+p}\right)e^{-\lambda}\sinh(\beta\xi)\right]+\frac{\mu_0}{\kappa+p}.$$

$$\Phi(\xi,p)=\frac{e^{\lambda\xi}}{\sinh\beta}\left[\frac{\phi_0}{p}\sinh(\beta-\beta\xi)+\frac{\phi_1}{p}e^{-\lambda}\sinh(\beta\xi)\right]-\frac{e^{\lambda\xi}}{\sinh\beta}\left[\frac{\mu_0}{\kappa+p}\sinh(\beta-\beta\xi)+\frac{\mu_0}{\kappa+p}e^{-\lambda}\sinh(\beta\xi)\right]+\frac{\mu_0}{\kappa+p}.$$

The above equation can be written as:

$$\Phi(\xi,p)=\left[\frac{\phi_0\sinh[\beta(1-\xi)]+\phi_1e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p}-\left[\frac{\sinh[\beta(1-\xi)]+e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{\mu_0e^{\lambda\xi}}{\kappa+p}+\frac{\mu_0}{\kappa+p}. \tag{4.36}$$

This equation is of the form

$$\Phi(\xi,p)=\Phi_{BC}(\xi,p)+\Phi_{IC}(\xi,p)$$

where

$$\Phi_{BC}(\xi,p)=\left[\frac{\phi_0\sinh[\beta(1-\xi)]+\phi_1e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p}$$

and

$$\Phi_{IC}(\xi,p)=-\left[\frac{\sinh[\beta(1-\xi)]+e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{\mu_0e^{\lambda\xi}}{\kappa+p}+\frac{\mu_0}{\kappa+p}$$

are partial solutions of Φ.

Let

$$\Phi_{IC_1}(\xi,p)=-\left[\frac{\mu_0\sinh[\beta(1-\xi)]+\mu_0e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{\kappa+p}$$

and

$$\Phi_{IC_2}(\xi,p)=\frac{\mu_0}{\kappa+p}.$$

The inverse Laplace Transform (iLT) of Eq.(4.36) gives the final analytic solution in the form

$$\phi(\xi,\tau) = \mathcal{L}^{-1}[\Phi(\xi,\cdot)](\tau) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{\tau z}\,\Phi(\xi,z)\,dz$$
$$= \mathrm{Res}\,[\exp(\tau\cdot)\Phi_{BC}(\xi,\cdot)z + \exp(\tau\cdot)\Phi_{IC}(\xi,\cdot)z]$$

where the integration parameter p is replaced by a complex variable z.

The expressions $e^{\tau z}\Phi_{BC}(\xi,z)$ and $e^{\tau z}\Phi_{IC}(\xi,z)$ have simple poles at $z=0$ and $z=-\kappa$ respectively.

The Residue of $e^{\tau z}\Phi_{BC}(\xi,z)$ and $e^{\tau z}\Phi_{IC}(\xi,z)$ at the simple poles are calculated as

$$\mathrm{Res}(\Phi,0) = \lim_{z\mapsto 0}[z\Phi_{BC}(\xi,z)e^{\tau z}] = f(\phi_0,\phi_1,\alpha,\xi)e^{\lambda\xi}$$

where

$$f(\phi_0,\phi_1,\alpha,\xi) = \frac{\phi_0\sinh\alpha(1-\xi) + \phi_1 e^{-\lambda}\sinh(\alpha\xi)}{\sinh\alpha} \tag{4.37}$$

and $\alpha = \beta(z=0) = \sqrt{\lambda^2+\kappa}$.

Also,

$$\mathrm{Res}(\Phi,-\kappa) = \lim_{z\mapsto -\kappa}[(z+k)\Phi_{IC_1}(\xi,z)e^{\tau z}] = -f(\mu_0,\mu_0,\lambda,\xi)e^{\lambda\xi-\kappa\tau}$$

where,

$$f(\mu_0,\mu_0,\lambda,\xi) = \frac{\mu_0\sinh\lambda(1-\xi) + \mu_0 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}. \tag{4.38}$$

Finally,

$$\mathrm{Res}(\Phi,-\kappa) = \lim_{z\mapsto -\kappa}[(z+k)\Phi_{IC_2}(\xi,z)e^{\tau z}] = \mu_0 e^{-\kappa\tau}.$$

Notice that $\Phi_{BC}(\xi,z)$ and $\Phi_{IC}(\xi,z)$ also have the same pole when

$$\sinh\beta = 0 \implies z = -(\lambda^2+\kappa).$$

The Residue of $e^{\tau z}\Phi_{BC}(\xi,z)$ is calculated as

$$\lim_{z\mapsto-(\lambda^2+\kappa)}\left[(z+\lambda^2+\kappa)e^{\tau z}\Phi_{BC}(\xi,z)\right] = \frac{-e^{\lambda\xi-(\lambda^2+\kappa)\tau}}{\lambda^2+\kappa}\mathcal{R}[f(\phi_0,\phi_1,\beta,\xi)]$$

where

$$\mathcal{R}[f(\phi_0,\phi_1,\beta,\xi)] = \lim_{z\mapsto-(\lambda^2+\kappa)}(z+\lambda^2+\kappa)\left(\frac{\phi_0\sinh\beta(1-\xi)+\phi_1 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right)$$

and $\beta = \sqrt{\lambda^2+\kappa+z}$.

Similarly, the residue of $e^{\tau z}\Phi_{IC}(\xi,z)$ is

$$\lim_{z\mapsto-(\lambda^2+\kappa)}\left[(z+\lambda^2+\kappa)e^{\tau z}\Phi_{IC}(\xi,z)\right]=\frac{e^{\lambda\xi-(\lambda^2+\kappa)\tau}}{\lambda^2}\mathcal{R}[f(\mu_0,\mu_0,\beta,\xi)]$$

where

$$\mathcal{R}[f(\mu_0,\mu_0,\beta,\xi)]=\lim_{z\mapsto-(\lambda^2+\kappa)}(z+\lambda^2+\kappa)\left(\frac{\mu_0\sinh\beta(1-\xi)+\mu_0e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right).$$

$\mathcal{R}[f]$ indicates the specific residue to be calculated for $z=-(\lambda^2+\kappa)$.

Summing the residues, the final solution is written as

$$\begin{aligned}\phi(\xi,\tau)=f(\phi_0,\phi_1,\alpha,\xi)e^{\lambda\xi}-f(\mu_0,\mu_0,\lambda,\xi)e^{\lambda\xi-\kappa\tau}-\alpha^{-2}e^{\lambda\xi-\alpha^2\tau}\mathcal{R}[f(\phi_0,\phi_1,\beta,\xi)]\\+\lambda^{-2}e^{\lambda\xi-\alpha^2\tau}\mathcal{R}[f(\mu_0,\mu_0,\beta,\xi)]+\mu_0e^{-\kappa\tau}\end{aligned}\tag{4.39}$$

where the residues are still unknown. A major step in the solution approach is to apply the initial condition $\phi(\xi,0)=\mu_0$ to Eq.(4.39) to calculate the residues. Thus;

$$\begin{aligned}\mu_0=f(\phi_0,\phi_1,\alpha,\xi)e^{\lambda\xi}-f(\mu_0,\mu_0,\lambda,\xi)e^{\lambda\xi}-\alpha^{-2}e^{\lambda\xi}\mathcal{R}[f(\phi_0,\phi_1,\beta,\xi)]\\+\lambda^{-2}e^{\lambda\xi}\mathcal{R}[f(\mu_0,\mu_0,\beta,\xi)]+\mu_0,\end{aligned}$$

$$\implies\alpha^{-2}\mathcal{R}[f(\phi_0,\phi_1,\beta,\xi)]-\lambda^{-2}\mathcal{R}[f(\mu_0,\mu_0,\beta,\xi)]=f(\phi_0,\phi_1,\alpha,\xi)-f(\mu_0,\mu_0,\lambda,\xi).\tag{4.40}$$

Substituting Eq.(4.40) into Eq.(4.39) gives

$$\begin{aligned}\phi(\xi,\tau)=f(\phi_0,\phi_1,\alpha,\xi)e^{\lambda\xi}-f(\mu_0,\mu_0,\lambda,\xi)e^{\lambda\xi-\kappa\tau}-\\(f(\phi_0,\phi_1,\alpha,\xi)-f(\mu_0,\mu_0,\lambda,\xi))e^{\lambda\xi-\alpha^2\tau}+\mu_0e^{-\kappa\tau},\end{aligned}$$

$$\begin{aligned}\implies\quad\phi(\xi,\tau)=f(\phi_0,\phi_1,\alpha,\xi)e^{\lambda\xi}-f(\mu_0,\mu_0,\lambda,\xi)e^{\lambda\xi-\kappa\tau}-f(\phi_0,\phi_1,\alpha,\xi)e^{\lambda\xi-\alpha^2\tau}\\+f(\mu_0,\mu_0,\lambda,\xi)e^{\lambda\xi-\alpha^2\tau}+\mu_0e^{-\kappa\tau},\end{aligned}$$

$$\begin{aligned}\implies\quad\phi(\xi,\tau)=f(\phi_0,\phi_1,\alpha,\xi)\left[1-e^{-\alpha^2\tau}\right]e^{\lambda\xi}-f(\mu_0,\mu_0,\lambda,\xi)\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi-\kappa\tau}\\+\mu_0e^{-\kappa\tau}.\end{aligned}\tag{4.41}$$

Substituting Eq.(4.37) and Eq.(4.38) into Eq.(4.41) gives

$$\phi(\xi,\tau) = \frac{\phi_0 \sinh \alpha(1-\xi) + \phi_1 e^{-\lambda} \sinh(\alpha\xi)}{\sinh \alpha} \left[1 - e^{-\alpha^2\tau}\right] e^{\lambda\xi}$$
$$-\mu_0 \left(\frac{\sinh \lambda(1-\xi) + e^{-\lambda} \sinh(\lambda\xi)}{\sinh \lambda}\right) \left[1 - e^{-\lambda^2\tau}\right] e^{\lambda\xi-\kappa\tau} + \mu_0 e^{-\kappa\tau}. \tag{4.42}$$

Eq.(4.42) is valid for $\xi_0 < \xi < \xi_1$ but excludes the boundaries ξ_0 and ξ_1. The steady-state solution is obtained as

$$\lim_{\tau\mapsto\infty} \phi(\xi,\tau) = \frac{\phi_0 \sinh \alpha(1-\xi) + \phi_1 e^{-\lambda} \sinh(\alpha\xi)}{\sinh \alpha} e^{\lambda\xi}. \tag{4.43}$$

Eq.(4.42) is equivalent to Eq.(8) of Kim (2020a) except that the last term on the right hand side, $\mu_0 e^{-\alpha^2\tau}$, in Eq.(8) of Kim (2020a), should read $\mu_0 e^{-\kappa\tau}$ as shown in the solution for $\phi(\xi,\tau)$. The reason is that Kim (2020a) inadvertently omitted the expression $\dfrac{\mu_0}{\kappa+p}$ prior to the calculation of the residues of the singularity pole Kim (2020b) . Again, the steady-state solution for $\phi(\xi,\tau)$ is wrongly stated in Kim (2020b) supplementary paper. The corrected steady-state solution for $\phi(\xi,\tau)$ is the one given in Eq.(4.43).

The next section provides analytical solution to the CDRS equation for the mixed Dirichlet/Neumann boundary conditions.

4.1.5 Solution for Mixed Dirichlet/Neumann BC's

The boundary conditions considered are

$$\phi(0,\tau) = \phi_0,$$

$$\frac{\partial\phi(1,\tau)}{\partial\xi} = J_1,$$

with initial condition

$$\mu(\xi) = \mu_0.$$

Using a new coefficient A_i instead of B_i for $i = 1, 2$, the general solution in Eq.(4.28) for Φ is

$$\Phi(\xi,p) = e^{\lambda\xi} \left[A_1 e^{-\beta\xi} + A_2 e^{\beta\xi}\right] + \frac{\mu_0}{\kappa+p}. \tag{4.44}$$

The Laplace transform of the boundary conditions are;

$$\Phi(0,p) = \frac{\phi_0}{p}, \tag{4.45}$$

$$\frac{\partial \Phi(1,p)}{\partial \xi} = \frac{J_1}{p}. \tag{4.46}$$

Applying Eq.(4.45) to Eq.(4.44);

$$A_1 = \frac{\phi_0}{p} - \frac{\mu_0}{\kappa + p} - A_2.$$

Let

$$C_1 = \frac{\phi_0}{p} - \frac{\mu_0}{\kappa + p}$$

then we have

$$A_1 = C_1 - A_2. \tag{4.47}$$

Now,

$$\frac{\partial \Phi}{\partial \xi} = e^{\lambda\xi}\left[-\beta A_1 e^{-\beta\xi} + \beta A_2 e^{\beta\xi}\right] + \lambda e^{\lambda\xi}\left[A_1 e^{-\beta\xi} + A_2 e^{\beta\xi}\right]. \tag{4.48}$$

Applying Eq.(4.46) to Eq.(4.48) gives

$$A_1\left(-\beta e^{-\beta} + \lambda e^{-\beta}\right) + A_2\beta e^{\beta} + A_2\lambda e^{\beta} = \frac{J_1}{p}e^{-\lambda}. \tag{4.49}$$

Substituting A_1 into Eq.(4.49), one obtains

$$\begin{aligned}
&(C_1 - A_2)\left(-\beta e^{-\beta} + \lambda e^{-\beta}\right) + A_2\beta e^{\beta} + A_2\lambda e^{\beta} = \frac{J_1}{p}e^{-\lambda},\\
\implies\ & A_2\left[(\beta-\lambda)e^{-\beta} + (\beta+\lambda)e^{\beta}\right] = J_1 p^{-1} e^{-\lambda} + C_1(\beta-\lambda)e^{-\beta},\\
\implies\ & A_2\left[2(\lambda\sinh\beta + \beta\cosh\beta)\right] = J_1 p^{-1} e^{-\lambda} - C_1(\lambda-\beta)e^{-\beta},
\end{aligned}$$

$$\implies \quad A_2 = \frac{J_1 p^{-1} e^{-\lambda} - C_1(\lambda-\beta)e^{-\beta}}{2(\lambda\sinh\beta + \beta\cosh\beta)}. \tag{4.50}$$

Substituting A_2 into Eq.(4.47) gives

$$\begin{aligned}
A_1 &= C_1 - \frac{J_1 p^{-1} e^{-\lambda} - C_1(\lambda-\beta)e^{-\beta}}{2(\lambda\sinh\beta + \beta\cosh\beta)}\\
&= \frac{C_1(\lambda+\beta)e^{\beta} - J_1 p^{-1} e^{-\lambda}}{2(\lambda\sinh\beta + \beta\cosh\beta)}.
\end{aligned} \tag{4.51}$$

Substituting Eq.(4.50) and Eq.(4.51) into Eq.(4.44),

$$\begin{aligned}\Phi(\xi,p) &= e^{\lambda\xi}\left[\frac{C_1(\lambda+\beta)e^{\beta}-J_1p^{-1}e^{-\lambda}}{2(\lambda\sinh\beta+\beta\cosh\beta)}e^{-\beta\xi}+\frac{J_1p^{-1}e^{-\lambda}-C_1(\lambda-\beta)e^{-\beta}}{2(\lambda\sinh\beta+\beta\cosh\beta)}e^{\beta\xi}\right]+\frac{\mu_0}{\kappa+p}\\
&= e^{\lambda\xi}\left[\frac{C_1\left[(\lambda+\beta)e^{\beta-\beta\xi}-(\lambda-\beta)e^{-(\beta-\beta\xi)}\right]+J_1p^{-1}e^{-\lambda}\left(e^{\beta\xi}-e^{-\beta\xi}\right)}{2(\lambda\sinh\beta+\beta\cosh\beta)}\right]+\frac{\mu_0}{\kappa+p}\\
&= e^{\lambda\xi}\left[\frac{C_1\left[\lambda\sinh\beta(1-\xi)+\beta\cosh\beta(1-\xi)\right]+J_1p^{-1}e^{-\lambda}\sinh\beta\xi}{\lambda\sinh\beta+\beta\cosh\beta}\right]+\frac{\mu_0}{\kappa+p}.
\end{aligned}\tag{4.52}$$

Substituting the expression, $C_1=\dfrac{\phi_0}{p}-\dfrac{\mu_0}{\kappa+p}$ back into Eq.(4.52);

$$\begin{aligned}\Phi(\xi,p) = e^{\lambda\xi}&\left[\frac{J_1p^{-1}e^{-\lambda}\sinh\beta\xi+\dfrac{\phi_0}{p}\lambda\sinh\beta(1-\xi)+\dfrac{\phi_0}{p}\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\\
&-\left[\frac{\mu_0\lambda\sinh\beta(1-\xi)+\mu_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\frac{e^{\lambda\xi}}{\kappa+p}+\frac{\mu_0}{\kappa+p}.\end{aligned}\tag{4.53}$$

Eq.(4.53) is written as

$$\begin{aligned}\Phi(\xi,p) = &\left[\frac{J_1e^{-\lambda}\sinh\beta\xi+\phi_0\lambda\sinh\beta(1-\xi)+\phi_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\frac{e^{\lambda\xi}}{p}\\
&-\left[\frac{\mu_0\lambda\sinh\beta(1-\xi)+\mu_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\frac{e^{\lambda\xi}}{\kappa+p}+\frac{\mu_0}{\kappa+p}.\end{aligned}\tag{4.54}$$

The equation is of the form

$$\Phi(\xi,p)=\Phi_{BC}(\xi,p)+\Phi_{IC}(\xi,p)$$

where

$$\Phi_{BC}(\xi,p)=\left[\frac{J_1e^{-\lambda}\sinh\beta\xi+\phi_0\lambda\sinh\beta(1-\xi)+\phi_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\frac{e^{\lambda\xi}}{p}$$

and

$$\Phi_{IC}(\xi,p)=-\left[\frac{\mu_0\lambda\sinh\beta(1-\xi)+\mu_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\frac{e^{\lambda\xi}}{\kappa+p}+\frac{\mu_0}{\kappa+p}$$

are partial solutions of Φ. Let

$$\Phi_{IC_1}(\xi,p) = -\left[\frac{\mu_0\lambda\sinh\beta(1-\xi)+\mu_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right]\frac{e^{\lambda\xi}}{\kappa+p},$$

and

$$\Phi_{IC_2}(\xi,p) = \frac{\mu_0}{\kappa+p}.$$

$e^{\tau z}\Phi_{BC}(\xi,z)$ and $e^{\tau z}\Phi_{IC}(\xi,z)$ have simple poles at $z=0$ and $z=-\kappa$ respectively.

$$\text{Res}(\Phi_{BC},0) = \lim_{z\mapsto 0}[z\Phi_{BC}(\xi,z)e^{\tau z}] = f_B e^{\lambda\xi},$$

where

$$f_B = \left[\frac{J_1 e^{-\lambda}\sinh\alpha\xi+\phi_0\lambda\sinh\alpha(1-\xi)+\phi_0\alpha\cosh\alpha(1-\xi)}{\lambda\sinh\alpha+\alpha\cosh\alpha}\right] \tag{4.55}$$

and

$$\text{Res}(\Phi_{IC_1},-\kappa) = \lim_{z\mapsto -\kappa}[(z+\kappa)\Phi_{IC}(\xi,z)e^{\tau z}] = -f_C e^{\lambda\xi-\kappa\tau}$$

where

$$f_C = \left[\frac{\mu_0\lambda\sinh\lambda(1-\xi)+\mu_0\lambda\cosh\lambda(1-\xi)}{\lambda\sinh\lambda+\lambda\cosh\lambda}\right]. \tag{4.56}$$

Also

$$\text{Res}(\Phi_{IC_2},0) = \lim_{z\mapsto -\kappa}[z\Phi_{IC_2}(\xi,z)e^{\tau z}] = \mu_0 e^{-\kappa\tau}.$$

In addition, $\Phi_{BC}(\xi,z)$ and $\Phi_{IC}(\xi,z)$ have the same pole satisfying,

$$\lambda\sinh\beta+\beta\cosh\beta = 0 \implies z=-\alpha^2.$$

The Residue of $e^{\tau z}\Phi_{BC}(\xi,z)$ is calculated to be

$$\lim_{z\mapsto -\alpha^2}\left[(z+\alpha^2)e^{\tau z}\Phi_{BC}(\xi,z)\right] = \frac{-e^{\lambda\xi-\alpha^2\tau}}{\alpha^2}\mathcal{R}[f_B],$$

where

$$\mathcal{R}[f_B] = \lim_{z\mapsto -\alpha^2}(z+\alpha^2)\left(\frac{J_1e^{-\lambda}\sinh\beta\xi+\phi_0\lambda\sinh\beta(1-\xi)+\phi_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right)$$

and $\beta=\sqrt{\lambda^2+\kappa+z}$.

Similarly, the Residue of $e^{\tau z}\Phi_{IC}(\xi, z)$ is calculated to be

$$\lim_{z\mapsto -\alpha^2}\left[(z+\alpha^2)e^{\tau z}\Phi_{IC}(\xi,z)\right] = \frac{e^{\lambda\xi-\alpha^2\tau}}{\lambda^2}\mathcal{R}[f_C]$$

where

$$\mathcal{R}[f_C] = \lim_{z\mapsto -\alpha^2}(z+\alpha^2)\left(\frac{\mu_0\lambda\sinh\beta(1-\xi)+\mu_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right)$$

and $\mathcal{R}[f]$ indicates the specific residue to be calculated for $z = -\alpha^2$.

Summing all the residues, the final solution is given in the form:

$$\phi(\xi,\tau) = f_B e^{\lambda\xi} - f_C e^{\lambda\xi-\kappa\tau} - \alpha^{-2}e^{\lambda\xi-\alpha^2\tau}\mathcal{R}[f_B] + \lambda^{-2}e^{\lambda\xi-\alpha^2\tau}\mathcal{R}[f_C] + \mu_0 e^{-\kappa\tau}. \tag{4.57}$$

We apply the initial condition $\phi(\xi,0) = \mu_0$ to Eq.(4.57) to calculate the unknown residues, $\mathcal{R}[f]$. Thus;

$$\mu_0 = f_B e^{\lambda\xi} - f_C e^{\lambda\xi} - \alpha^{-2}e^{\lambda\xi}\mathcal{R}[f_B] + \lambda^{-2}e^{\lambda\xi}\mathcal{R}[f_C] + \mu_0$$

$$\alpha^{-2}\mathcal{R}[f_B] - \lambda^{-2}\mathcal{R}[f_C] = f_B - f_C. \tag{4.58}$$

Substituting Eq.(4.58) into Eq.(4.57);

$$\begin{aligned}\phi(\xi,\tau) &= f_B e^{\lambda\xi} + f_C e^{\lambda\xi-\kappa\tau} - (f_B - f_C)\,e^{\lambda\xi-\alpha^2\tau} + \mu_0 e^{-\kappa\tau}\\ &= f_B\left[1-e^{-\alpha^2\tau}\right]e^{\lambda\xi} - f_C e^{-\kappa\tau}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \mu_0 e^{-\kappa\tau}.\end{aligned} \tag{4.59}$$

Substituting Eq.(4.55), Eq.(4.56) into Eq.(4.59) gives

$$\begin{aligned}\phi(\xi,\tau) = {}& \frac{J_1 e^{-\lambda}\sinh\alpha\xi + \phi_0\lambda\sinh\alpha(1-\xi) + \phi_0\alpha\cosh\alpha(1-\xi)}{\lambda\sinh\alpha+\alpha\cosh\alpha}e^{\lambda\xi}\left[1-e^{-\alpha^2\tau}\right]\\ &-\frac{\mu_0\lambda\sinh\lambda(1-\xi)+\mu_0\lambda\cosh\lambda(1-\xi)}{\lambda\sinh\lambda+\lambda\cosh\lambda}e^{-\kappa\tau}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \mu_0 e^{-\kappa\tau}.\end{aligned} \tag{4.60}$$

Let

$$h(\xi) = \frac{\sinh\alpha\xi}{\lambda\sinh\alpha+\lambda\cosh\alpha},$$

$$g(\xi) = \frac{\lambda\sinh\alpha(1-\xi)+\alpha\cosh\alpha(1-\xi)}{\lambda\sinh\alpha+\alpha\cosh\alpha},$$

$$q(\xi) = \frac{\lambda\sinh\lambda(1-\xi)+\lambda\cosh\lambda(1-\xi)}{\lambda\sinh\lambda+\lambda\cosh\lambda},$$

then the final solution for $\phi(\xi, \tau)$ is given as

$$\phi(\xi, \tau) = \left[J_1 e^{-\lambda} h(\xi) + \phi_0 g(\xi)\right] e^{\lambda\xi} \left(1 - e^{-\alpha^2\tau}\right) + \mu_0 e^{-\kappa\tau} \left[1 - q(\xi) e^{\lambda\xi}(1 - e^{-\lambda^2\tau})\right]. \tag{4.61}$$

At the constant flux, $J_1 = 0$, the steady-state solution for $\phi(\xi, \tau)$ is given as

$$\phi_{ss}(\xi) = \frac{\phi_0 \lambda \sinh \alpha(1-\xi) + \phi_0 \alpha \cosh \alpha(1-\xi)}{\lambda \sinh \alpha + \alpha \cosh \alpha} e^{\lambda\xi}. \tag{4.62}$$

Eq.(4.61) is equivalent to Eq.(16) in Kim (2020a), except for the second term on the right hand side of Eq.(4.61), where $g(\xi)$ was used instead of $q(\xi)$.

In the next section, we present two solutions for the advection-diffusion equation subject to an inlet exponential BC and a constant exit BC for both Dirichlet and Neumann BC's.

4.2 The Residue Theorem Approach: Dirichlet BCs

Advection-Diffusion Equation with an Inlet Exponential BC

The equation to be solved is

$$\frac{\partial \phi}{\partial \tau} = \frac{\partial^2 \phi}{\partial \xi^2} - 2\lambda \frac{\partial \phi}{\partial \xi} \tag{4.63}$$

with boundary conditions

$$\phi(0, \tau) = \phi_0 e^{-\gamma\tau}, \tag{4.64}$$

$$\phi(1, \tau) = \phi_1 \tag{4.65}$$

and initial condition

$$\phi(\xi, 0) = \omega_0. \tag{4.66}$$

The choice of an exponentially decaying inlet BC is motivated by observational data in Fena river, where the pollutant at the inlet appears to be decaying in time. See Chapter 5, Figure (5.2a).

The general solution for Φ after applying the initial condition, ω_0 to Eq.(4.63) with $\kappa = 0$ and $\sigma = 0$ is

$$\Phi(\xi, p) = e^{\lambda\xi} \left[B_1 e^{-\beta\xi} + B_2 e^{\beta\xi}\right] + \frac{\omega_0}{p}. \tag{4.67}$$

The Laplace transform equations of Eq.(4.64) and Eq.(4.65) are

$$\Phi(0,p) = \frac{\phi_0}{p+\gamma},$$

$$\Phi(1,p) = \frac{\phi_1}{p}.$$

Applying the transformed BC above to Eq.(4.67) one obtains

$$B_1 = \frac{\left(\frac{\phi_0}{p+\gamma} - \frac{\omega_0}{p}\right)e^{\beta} - \left(\frac{\phi_1}{p} - \frac{\omega_0}{p}\right)e^{-\lambda}}{2\sinh\beta}, \tag{4.68}$$

$$B_2 = \frac{\left(\frac{\phi_1}{p} - \frac{\omega_0}{p}\right)e^{-\lambda} - \left(\frac{\phi_0}{p+\gamma} - \frac{\omega_0}{p}\right)e^{-\beta}}{2\sinh\beta}. \tag{4.69}$$

Substituting the values of B_1 and B_2 into Eq.(4.67) gives the general solution in terms of p to be

$$\begin{aligned}\Phi(\xi,p) = &\left[\frac{\phi_0\sinh[\beta(1-\xi)]}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p+\gamma} + \left[\frac{\phi_1 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p}\\ &- \left[\frac{\omega_0\sinh[\beta(1-\xi)] + \omega_0 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p} + \frac{\omega_0}{p}.\end{aligned} \tag{4.70}$$

This is of the form

$$\Phi(\xi,p) = \Phi_{BC}(\xi,p) + \Phi_{IC}(\xi,p)$$

where

$$\Phi_{BC}(\xi,p) = \left[\frac{\phi_0\sinh\beta(1-\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p+\gamma} + \left[\frac{\phi_1 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p}$$

and

$$\Phi_{IC}(\xi,p) = -\left[\frac{\omega_0\sinh[\beta(1-\xi)] + \omega_0 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p} + \frac{\omega_0}{p}$$

are partial solutions of Φ.

Let

$$\Phi_{BC_1}(\xi,p) = \left[\frac{\phi_0\sinh\beta(1-\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p+\gamma},$$

$$\Phi_{BC_2}(\xi,p) = \left[\frac{\phi_1 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right]\frac{e^{\lambda\xi}}{p}.$$

The inverse Laplace Transform (iLT) gives the final analytic solution to Eq.(4.70).

Thus,

$$\begin{aligned}\phi(\xi,\tau) = \mathcal{L}^{-1}[\Phi(\xi,p)] &= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{\tau z}\,\Phi(\xi,z)\,dz \\ &= \operatorname{Res}\left[e^{\tau z}\Phi_{BC}(\xi,z) + e^{\tau z}\Phi_{IC}(\xi,z)\right]\end{aligned} \tag{4.71}$$

where p is replaced by a complex variable z.

The expressions $e^{\tau z}\Phi_{BC}(\xi,z)$ and $e^{\tau z}\Phi_{IC}(\xi,z)$ have simple poles at $z = 0$ and $z = -\gamma$.

The Residue of $e^{\tau z}\Phi_{BC}(\xi,z)$ and $e^{\tau z}\Phi_{IC}(\xi,z)$ at the simple poles are calculated as follows:

$$\operatorname{Res}(\Phi,-\gamma) = \lim_{z\mapsto-\gamma}\left[(z+\gamma)\Phi_{BC_1}(\xi,z)e^{\tau z}\right] = f_{B_1}e^{\lambda\xi-\gamma\tau}$$

where

$$f_{B_1} = \left[\frac{\phi_0\sinh\omega(1-\xi)}{\sinh\omega}\right] \tag{4.72}$$

and $\omega = \sqrt{\lambda^2-\gamma}$. We suppose that $\lambda^2 > \gamma$ and comment on the case where $\gamma > \lambda_2$ later.

Similarly,

$$\operatorname{Res}(\Phi,0) = \lim_{z\mapsto0}\left[z\Phi_{BC_2}(\xi,z)e^{\tau z}\right] = f_{B_2}e^{\lambda\xi}$$

where

$$f_{B_2} = \left[\frac{\phi_1 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\right]. \tag{4.73}$$

Also,

$$\operatorname{Res}(\Phi,0) = \lim_{z\mapsto0}\left[z\Phi_{IC}(\xi,z)e^{\tau z}\right] = -f_C e^{\lambda\xi} + \omega_0$$

where

$$f_C = \frac{\omega_0\sinh\lambda(1-\xi) + \omega_0 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}. \tag{4.74}$$

Besides, $\Phi_{BC}(\xi,z)$ and $\Phi_{IC}(\xi,z)$ have the same pole when

$$\sinh\beta = 0 \implies z = -\lambda^2.$$

The Residues at $z = -\lambda^2$ are calculated below. That of $e^{\tau z}\Phi_{BC_1}(\xi,z)$ is calculated as

$$\lim_{z\mapsto-\lambda^2}\left[(z+\lambda^2)e^{\tau z}\Phi_{BC_1}(\xi,z)\right] = -\frac{e^{\lambda\xi-\lambda^2\tau}}{\lambda^2-\gamma}\mathcal{R}[f_{B_1}]$$

where

$$\mathcal{R}[f_{B_1}] = \lim_{z\mapsto-\lambda^2}(z+\lambda^2)\left(\frac{\phi_0\sinh\beta(1-\xi)}{\sinh\beta}\right)$$

and $\beta = \sqrt{\lambda^2 + z}$.

Similarly, the Residue of $e^{\tau z}\Phi_{BC_2}(\xi, z)$ is calculated as

$$\lim_{z \mapsto -\lambda^2} \left[(z+\lambda^2)e^{\tau z}\Phi_{BC_2}(\xi, z)\right] = -\frac{e^{\lambda\xi - \lambda^2\tau}}{\lambda^2}\mathcal{R}[f_{B_2}]$$

where

$$\mathcal{R}[f_{B_2}] = \lim_{z \mapsto -\lambda^2}(z+\lambda^2)\left(\frac{\phi_1 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right).$$

Lastly, the residue of $e^{\tau z}\Phi_{IC}(\xi, z)$ is

$$\lim_{z \mapsto -\lambda^2} \left[(z+\lambda^2)e^{\tau z}\Phi_{IC}(\xi, z)\right] = \frac{e^{\lambda\xi - \lambda^2\tau}}{\lambda^2}\mathcal{R}[f_C]$$

where

$$\mathcal{R}[f_C] = \lim_{z \mapsto -\lambda^2}(z+\lambda^2)\left(\frac{\omega_0\sinh\beta(1-\xi) + \omega_0 e^{-\lambda}\sinh(\beta\xi)}{\sinh\beta}\right)$$

and $\mathcal{R}[f]$ indicates the specific residue to be calculated for $z = -\lambda^2$.

The final solution is obtained as

$$\begin{aligned}\phi(\xi,\tau) = f_{B_1}e^{\lambda\xi - \gamma\tau} + f_{B_2}e^{\lambda\xi} - f_C e^{\lambda\xi} - (\lambda^2-\gamma)^{-1}e^{\lambda\xi-\lambda^2\tau}\mathcal{R}[f_{B_1}] \\ -\lambda^{-2}e^{\lambda\xi-\lambda^2\tau}\mathcal{R}[f_{B_2}] + \lambda^{-2}e^{\lambda\xi-\lambda^2\tau}\mathcal{R}[f_C] + \omega_0\end{aligned} \tag{4.75}$$

where the residues are still unknown.

We apply the initial condition $\phi(\xi, 0) = \omega_0$ to Eq.(4.75) to calculate for the residues. Thus,

$$(\lambda^2-\gamma)^{-1}\mathcal{R}[f_{B_1}] + \lambda^{-2}\mathcal{R}[f_{B_2}] - \lambda^{-2}\mathcal{R}[f_C] = f_{B_1} + f_{B_2} - f_C. \tag{4.76}$$

Substituting Eq.(4.76) into Eq.(4.75) gives

$$\begin{aligned}\phi(\xi,\tau) &= f_{B_1}e^{\lambda\xi-\gamma\tau} + f_{B_2}e^{\lambda\xi} - f_C e^{\lambda\xi} - (f_{B_1} + f_{B_2} - f_C)\, e^{\lambda\xi-\lambda^2\tau} + \omega_0 \\ &= f_{B_1}\left[e^{-\gamma\tau} - e^{-\lambda^2\tau}\right]e^{\lambda\xi} + f_{B_2}\left[1 - e^{-\lambda^2\tau}\right]e^{\lambda\xi} - f_C\left[1 - e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \omega_0.\end{aligned} \tag{4.77}$$

Substituting Eq.(4.72), Eq.(4.73) and Eq.(4.74) into Eq.(4.77) yields

$$\begin{aligned}\phi(\xi,\tau) = \frac{\phi_0\sinh\omega(1-\xi)}{\sinh\omega}\left[e^{-\gamma\tau} - e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \frac{\phi_1 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\left[1 - e^{-\lambda^2\tau}\right]e^{\lambda\xi} \\ -\omega_0\left(\frac{\sinh\lambda(1-\xi) + e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\right)\left[1 - e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \omega_0.\end{aligned} \tag{4.78}$$

The steady-state solution for $\phi(\xi,\tau)$ is given as

$$\phi_{ss}(\xi) = \frac{\phi_1 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}e^{\lambda\xi} - \omega_0\left(\frac{\sinh\lambda(1-\xi)+e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\right)e^{\lambda\xi} + \omega_0. \qquad (4.79)$$

Interestingly, when $\gamma = 0$ we recover the steady-state solution given in Eq.(4.43), for $\kappa = 0$ and $\sigma = 0$. The solution for $\phi(\xi,\tau)$ holds for $0 < \xi < 1$ but it does not satisfy the conditions at the boundaries in general. However, it can be shown that to satisfy the inlet boundary condition, we must have $\omega_0 = \phi_0$. Similary, to satisfy only the outlet condition one must have $\omega_0 = \phi_1$.

If $\lambda^2 < \gamma$ then the parameter ω becomes complex. Let

$$\omega = i\sqrt{\gamma-\lambda^2} = i\zeta$$

where $\zeta = \sqrt{\gamma-\lambda^2}$ is real. Eq.(4.78) is rewritten as

$$\begin{aligned}\phi(\xi,\tau) = {} & \frac{\phi_0\sinh i\zeta(1-\xi)}{\sinh i\zeta}\left[e^{-\gamma\tau}-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \frac{\phi_1 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} \\ & -\omega_0\left(\frac{\sinh\lambda(1-\xi)+e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\right)\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \omega_0. \qquad (4.80)\end{aligned}$$

Using the relationship between hyperbolic and trigonometric functions, we have

$$\sinh i\zeta(1-\xi) = i\sin\zeta(1-\xi),$$

$$\sinh i\zeta = i\sin\zeta.$$

Eq.(4.80) becomes

$$\begin{aligned}\phi(\xi,\tau) = {} & \frac{\phi_0\sin\zeta(1-\xi)}{\sin\zeta}\left[e^{-\gamma\tau}-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \frac{\phi_1 e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} \\ & -\omega_0\left(\frac{\sinh\lambda(1-\xi)+e^{-\lambda}\sinh(\lambda\xi)}{\sinh\lambda}\right)\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \omega_0. \qquad (4.81)\end{aligned}$$

In this case however, we find that ϕ can take on negative values, which is unrealistic for physical applications.

Figure 4.1 shows the plots of Eq.(4.42) and Eq.(4.78) which indicates the time evolution of ϕ along ξ from the initial ($\tau = 0$) to the steady-state. The initial concentration of $\omega_0 = 0$ is represented by the ξ-axis on the horizontal line. It is

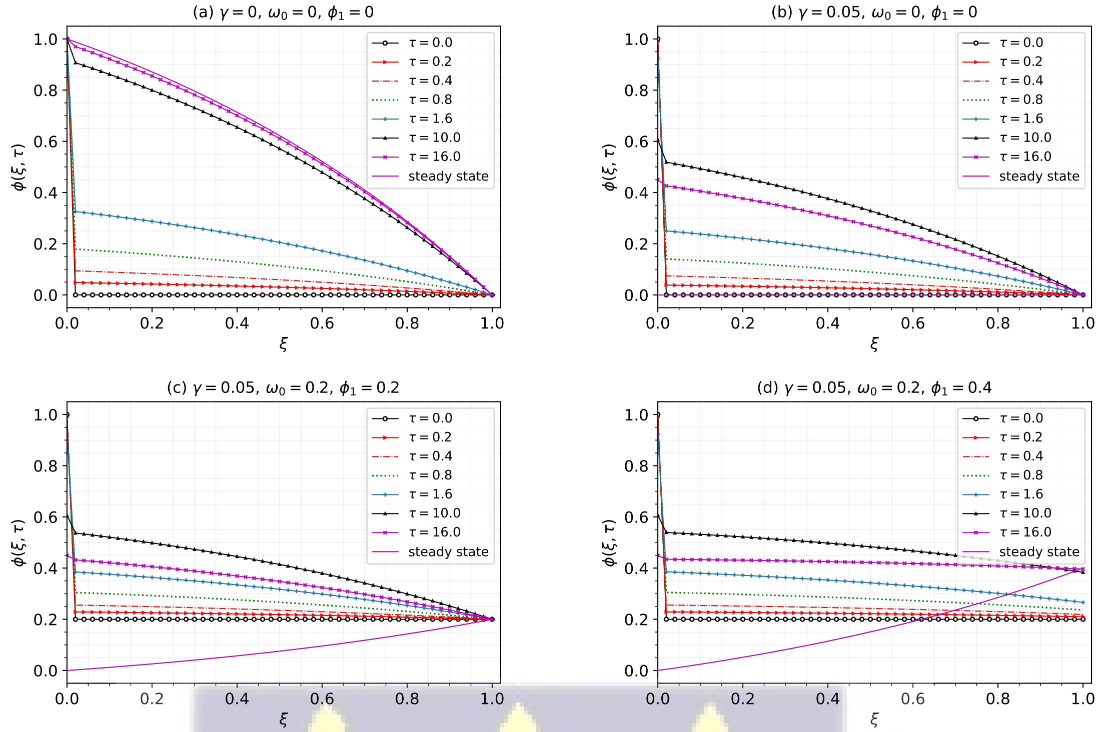


Figure 4.1: Concentrations at different times for $\lambda = 0.5, \phi_0 = 1$ and (a) $\gamma = 0$, $\omega_0 = 0 = \phi_1$ (b) $\gamma = 0.05$, $\omega_0 = 0 = \phi_1$, (c) $\gamma = 0.05$, $\omega_0 = 0, \phi_1 = 0.2$, and (d) $\gamma = 0.05$, $\omega_0 = 0.2, \phi_1 = 0.4$.

interesting to note that if $\gamma = 0$, we recover the solution of Kim (2020a) as displayed in Figure 4.1a. In this case, the concentration everywhere within the domain increases until the system reaches steady state, with concentration decreasing monotonically from the inlet to the outlet. However, in the presence of a decaying inlet condition with a Dirichlet outlet condition, the time evolution of concentration behaves differently from the case for which $\gamma = 0$ as seen in Figure 4.1b. Initially the concentration is zero except at the inlet where it has a maximum value of $\phi(\xi, \tau) = \phi_0 = 1$. As time evolves, the concentration at the inlet begins to decrease while the concentration everywhere within the domain increases, with a monotonically decreasing shape as in Figure 4.1a. The concentration within the domain increases to a maximum point (around $\tau = 10$ in this case) and begins to decrease (see the curve for $\tau = 16$) and eventually goes to zero everywhere at steady-state.

If both the initial concentration and γ are non-zero (e.g., $\omega_0 = \phi_1 = 0.2$, $\gamma = 0.05$), the solution behaves similarly to the case for $\omega_0 = 0$ (Figure 4.1b), but the rate of increase of ϕ within the domain to the maximum point is much faster (Figure 4.1c) since the initial concentration is non-zero. Moreover, the steady state solution is not zero everywhere as in the previous case but increases gradually from zero at the inlet to the value at the outlet. Thus, in this case, the concentration can decrease below the initial concentration due to the exponentially decreasing condition at the inlet. A more general case in which the initial condition and outlet value are non-zero and different from each other is shown in Figure 4.1d. The concentration increases to a maximum value as in Figures 4.1b-c, but tends to converge at the outlet value of $\phi_1 = 0.4$.

4.3 The Residue Theorem Approach: Dirichlet/Neumann BCs

The equation to be solved is

$$\frac{\partial \phi}{\partial \tau} = \frac{\partial^2 \phi}{\partial \xi^2} - 2\lambda \frac{\partial \phi}{\partial \xi},$$

$$\phi(0, \tau) = \phi_0 e^{-\gamma\tau}, \tag{4.82}$$

$$\frac{\partial \phi(1, \tau)}{\partial \xi} = J_1 \tag{4.83}$$

and the initial condition is

$$\phi(\xi, 0) = \omega_0. \tag{4.84}$$

The general solution for Φ is given as

$$\Phi(\xi, p) = e^{\lambda\xi} \left[A_1 e^{-\beta\xi} + A_2 e^{\beta\xi}\right] + \frac{\omega_0}{p}. \tag{4.85}$$

Applying the Laplace transform to Eq.(4.82) and Eq.(4.83), one obtains

$$\Phi(0, p) = \frac{\phi_0}{p + \gamma},$$

$$\frac{\partial \Phi(1, p)}{\partial \xi} = \frac{J_1}{p}.$$

Applying the transformed BC above to Eq.(4.85) yields;

$$A_1 = \frac{C_1(\lambda + \beta)e^{\beta} - J_1 p^{-1} e^{-\lambda}}{2(\lambda \sinh \beta + \beta \cosh \beta)},$$

$$A_2 = \frac{J_1 p^{-1} e^{-\lambda} - C_1(\lambda - \beta)e^{-\beta}}{2(\lambda \sinh \beta + \beta \cosh \beta)}$$

where $C_1 = \dfrac{\phi_0}{p+\gamma} - \dfrac{\omega_0}{p}$.

Substituting the values of A_1 and A_2 into Eq.(4.85) gives the general solution to be

$$\Phi(\xi, p) = \left[\frac{J_1 e^{-\lambda} \sinh \beta\xi}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p} + \left[\frac{\phi_0 \lambda \sinh \beta(1-\xi) + \phi_0 \beta \cosh \beta(1-\xi)}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p+\gamma} - \left[\frac{\omega_0 \lambda \sinh \beta(1-\xi) + \omega_0 \beta \cosh \beta(1-\xi)}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p} + \frac{\omega_0}{p}. \tag{4.86}$$

The equation is of the form

$$\Phi(\xi, p) = \Phi_{BC}(\xi, p) + \Phi_{IC}(\xi, p)$$

where

$$\Phi_{BC}(\xi, p) = \left[\frac{J_1 e^{-\lambda} \sinh \beta\xi}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p} + \left[\frac{\phi_0 \lambda \sinh \beta(1-\xi) + \phi_0 \beta \cosh \beta(1-\xi)}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p+\gamma}$$

and

$$\Phi_{IC}(\xi, p) = -\left[\frac{\omega_0 \lambda \sinh \beta(1-\xi) + \omega_0 \beta \cosh \beta(1-\xi)}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p} + \frac{\omega_0}{p}$$

are partial solutions of Φ.

Let

$$\Phi_{BC_1}(\xi, p) = \left[\frac{J_1 e^{-\lambda} \sinh \beta\xi}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p}$$

and

$$\Phi_{BC_2}(\xi, p) = \left[\frac{\phi_0 \lambda \sinh \beta(1-\xi) + \phi_0 \beta \cosh \beta(1-\xi)}{\lambda \sinh \beta + \beta \cosh \beta}\right] \frac{e^{\lambda\xi}}{p+\gamma}.$$

The expressions $e^{\tau z}\Phi_{BC}(\xi, z)$ and $e^{\tau z}\Phi_{IC}(\xi, z)$ have the simple poles at $z = 0$ and $z = -\gamma$.

The Residue of $e^{\tau z}\Phi_{BC}(\xi, z)$ and $e^{\tau z}\Phi_{IC}(\xi, z)$ at the simple poles are calculated as follows,

$$\mathrm{Res}(\Phi, 0) = \lim_{z \mapsto 0} [z \Phi_{BC_1}(\xi, z) e^{\tau z}] = f_{B_1} e^{\lambda\xi}$$

where

$$f_{B_1} = \left[\frac{J_1 e^{-\lambda} \sinh \lambda\xi}{\lambda \sinh \lambda + \lambda \cosh \lambda}\right]. \tag{4.87}$$

Similarly,

$$\text{Res}(\Phi, -\gamma) = \lim_{z \mapsto -\gamma} [(z+\gamma)\Phi_{BC_2}(\xi, z)e^{\tau z}] = f_{B_2} e^{\lambda\xi - \gamma\tau}$$

where

$$f_{B_2} = \left[\frac{\phi_0 \lambda \sinh \omega(1-\xi) + \phi_0 \omega \cosh \omega(1-\xi)}{\lambda \sinh \omega + \omega \cosh \omega} \right], \tag{4.88}$$

and $\omega = \sqrt{\lambda^2 - \gamma}$. We assume that $\lambda^2 > \gamma$ and later comment on the case for which $\lambda^2 < \gamma$.

Also,

$$\text{Res}(\Phi, 0) = \lim_{z \mapsto 0} [z\Phi_{IC}(\xi, z)e^{\tau z}] = -f_C e^{\lambda\xi} + \omega_0$$

where

$$f_C = \left[\frac{\omega_0 \lambda \sinh \lambda(1-\xi) + \omega_0 \lambda \cosh \lambda(1-\xi)}{\lambda \sinh \lambda + \lambda \cosh \lambda} \right]. \tag{4.89}$$

Again, $\Phi_{BC}(\xi, z)$ and $\Phi_{IC}(\xi, z)$ have the same pole satisfying,

$$\lambda \sinh \beta + \beta \cosh \beta = 0 \implies z = -\lambda^2.$$

The Residue of $e^{\tau z}\Phi_{BC_1}(\xi, z)$ for $z = -\lambda^2$ is calculated as

$$\lim_{z \mapsto -\lambda^2} \left[(z+\lambda^2)e^{\tau z}\Phi_{BC_1}(\xi, z) \right] = \frac{-e^{\lambda\xi - \lambda^2\tau}}{\lambda^2} \mathcal{R}[f_{B_1}]$$

where

$$\mathcal{R}[f_{B_1}] = \lim_{z \mapsto -\lambda^2} (z+\lambda^2) \left(\frac{J_1 e^{-\lambda} \sinh \beta\xi}{\lambda \sinh \beta + \beta \cosh \beta} \right).$$

Similarly, the Residue of $e^{\tau z}\Phi_{BC_2}(\xi, z)$ for $z = -\lambda^2$ is calculated as

$$\lim_{z \mapsto -\lambda^2} \left[(z+\lambda^2)e^{\tau z}\Phi_{BC_2}(\xi, z) \right] = \frac{-e^{\lambda\xi - \lambda^2\tau}}{\lambda^2 - \gamma} \mathcal{R}[f_{B_2}]$$

where

$$\mathcal{R}[f_{B_2}] = \lim_{z \mapsto -\lambda^2} (z+\lambda^2) \left(\frac{\phi_0 \lambda \sinh \beta(1-\xi) + \phi_0 \beta \cosh \beta(1-\xi)}{\lambda \sinh \beta + \beta \cosh \beta} \right).$$

Lastly, the residue of $e^{\tau z}\Phi_{IC}(\xi, z)$ at $z = -\lambda^2$ is

$$\lim_{z \mapsto -\lambda^2} \left[(z+\lambda^2)e^{\tau z}\Phi_{IC}(\xi, z) \right] = \frac{e^{\lambda\xi - \lambda^2\tau}}{\lambda^2} \mathcal{R}[f_C]$$

where

$$\mathcal{R}[f_C] = \lim_{z\mapsto -\lambda^2}(z+\lambda^2)\left(\frac{\omega_0\lambda\sinh\beta(1-\xi)+\omega_0\beta\cosh\beta(1-\xi)}{\lambda\sinh\beta+\beta\cosh\beta}\right).$$

The final solution is obtained as

$$\begin{aligned}\phi(\xi,\tau) = f_{B_1}e^{\lambda\xi} + f_{B_2}e^{\lambda\xi-\gamma\tau} - f_C e^{\lambda\xi} - \lambda^{-2}e^{\lambda\xi-\lambda^2\tau}\mathcal{R}[f_{B_1}] - \\ (\lambda^2-\gamma)^{-1}e^{\lambda\xi-\lambda^2\tau}\mathcal{R}[f_{B_2}] + \lambda^{-2}e^{\lambda\xi-\lambda^2\tau}\mathcal{R}[f_C] + \omega_0.\end{aligned} \tag{4.90}$$

Applying the initial condition $\phi(\xi,0)=\omega_0$ to Eq.(4.90) gives

$$\lambda^{-2}\mathcal{R}[f_{B_1}] + (\lambda^2-\gamma)^{-1}\mathcal{R}[f_{B_2}] - \lambda^{-2}\mathcal{R}[f_C] = f_{B_1} + f_{B_2} - f_C. \tag{4.91}$$

Substituting Eq.(4.91) into Eq.(4.90) then yields

$$\begin{aligned}\phi(\xi,\tau) &= f_{B_1}e^{\lambda\xi} + f_{B_2}e^{\lambda\xi-\gamma\tau} - f_C e^{\lambda\xi} - (f_{B_1}+f_{B_2}-f_C)\,e^{\lambda\xi-\lambda^2\tau} + \omega_0 \\ &= f_{B_1}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + f_{B_2}\left[e^{-\gamma\tau}-e^{-\lambda^2\tau}\right]e^{\lambda\xi} - f_C\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} + \omega_0.\end{aligned} \tag{4.92}$$

Substituting Eq.(4.87), Eq.(4.88) and Eq.(4.89) into Eq.(4.92) gives

$$\begin{aligned}\phi(\xi,\tau) = &\frac{J_1e^{-\lambda}\sinh\lambda\xi}{\lambda\sinh\lambda+\lambda\cosh\lambda}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi} \\ &+\left(\frac{\phi_0\lambda\sinh\omega(1-\xi)+\phi_0\omega\cosh\omega(1-\xi)}{\lambda\sinh\omega+\omega\cosh\omega}\right)\left[e^{-\gamma\tau}-e^{-\lambda^2\tau}\right]e^{\lambda\xi} \\ &-\frac{\omega_0\lambda\sinh\lambda(1-\xi)+\omega_0\lambda\cosh\lambda(1-\xi)}{\lambda\sinh\lambda+\lambda\cosh\lambda}\left[1-e^{-\lambda^2\tau}\right]e^{\lambda\xi}+\omega_0.\end{aligned} \tag{4.93}$$

The steady-state solution is given as

$$\phi_{ss}(\xi) = \left(\frac{J_1e^{-\lambda}\sinh\lambda\xi}{\lambda\sinh\lambda+\lambda\cosh\lambda}\right)e^{\lambda\xi} - \left(\frac{\omega_0\lambda\sinh\lambda(1-\xi)+\omega_0\lambda\cosh\lambda(1-\xi)}{\lambda\sinh\lambda+\lambda\cosh\lambda}\right)e^{\lambda\xi}+\omega_0. \tag{4.94}$$

Notice that we recover the steady-state solution provided by Kim (2020a) in Eq.(4.62) when $\gamma=0$ at the constant flux $J_1=0$.

Let

$$h(\xi) = \frac{\sinh\lambda\xi}{\lambda\sinh\lambda+\lambda\cosh\lambda},$$

$$g(\xi) = \frac{\lambda\sinh\omega(1-\xi)+\omega\cosh\omega(1-\xi)}{\lambda\sinh\omega+\omega\cosh\omega},$$

$$q(\xi) = \frac{\lambda \sinh \lambda(1-\xi) + \lambda \cosh \lambda(1-\xi)}{\lambda \sinh \lambda + \lambda \cosh \lambda},$$

then,

$$\phi(\xi,\tau) = J_1 e^{-\lambda} h(\xi) \left[1 - e^{-\lambda^2 \tau}\right] e^{\lambda\xi} + \phi_0 g(\xi) \left[e^{-\gamma\tau} - e^{-\lambda^2\tau}\right] e^{\lambda\xi} + \omega_0 \left[1 - q(\xi) e^{\lambda\xi}(1 - e^{-\lambda^2\tau})\right] \tag{4.95}$$

and we recover Kim's solution in Eq.(4.61) when $\gamma = 0$.

If $\lambda^2 < \gamma$ then ω becomes complex. Let

$$\omega = i\sqrt{\gamma - \lambda^2} = i\zeta$$

where $\zeta = \sqrt{\gamma - \lambda^2}$ is real. Eq.(4.93) is rewritten as

$$\begin{aligned}\phi(\xi,\tau) = {} & \frac{J_1 e^{-\lambda} \sinh \lambda\xi}{\lambda \sinh \lambda + \lambda \cosh \lambda} \left[1 - e^{-\lambda^2\tau}\right] e^{\lambda\xi} \\ & + \left(\frac{\phi_0 \lambda \sinh i\zeta(1-\xi) + \phi_0 i\zeta \cosh i\zeta(1-\xi)}{\lambda \sinh i\zeta + i\zeta \cosh i\zeta}\right) \left[e^{-\gamma\tau} - e^{-\lambda^2\tau}\right] e^{\lambda\xi} \\ & - \frac{\omega_0 \lambda \sinh \lambda(1-\xi) + \omega_0 \lambda \cosh \lambda(1-\xi)}{\lambda \sinh \lambda + \lambda \cosh \lambda} \left[1 - e^{-\lambda^2\tau}\right] e^{\lambda\xi} + \omega_0. \end{aligned} \tag{4.96}$$

Using the relationships below

$$\sinh ix = i \sin x,$$

$$\cosh ix = \cos x,$$

Eq.(4.96) becomes

$$\begin{aligned}\phi(\xi,\tau) = {} & \frac{J_1 e^{-\lambda} \sinh \lambda\xi}{\lambda \sinh \lambda + \lambda \cosh \lambda} \left[1 - e^{-\lambda^2\tau}\right] e^{\lambda\xi} + \left(\frac{\phi_0 \lambda \sin \zeta(1-\xi) + \phi_0 \zeta \cos \zeta(1-\xi)}{\lambda \sin \zeta + \zeta \cos \zeta}\right) \\ & \times \left[e^{-\gamma\tau} - e^{-\lambda^2\tau}\right] e^{\lambda\xi} - \frac{\omega_0 \lambda \sinh \lambda(1-\xi) + \omega_0 \lambda \cosh \lambda(1-\xi)}{\lambda \sinh \lambda + \lambda \cosh \lambda} \left[1 - e^{-\lambda^2\tau}\right] e^{\lambda\xi} + \omega_0.\end{aligned}$$

Figure 4.2 depicts the plots of the analytical solution given in Eq.(4.60) and Eq.(4.94). It can be observed that the Neumann boundary condition at the outlet has a drastic effect on the behaviour of the solution. In Figure 4.2a, we recover the solution of Kim (2020a) (his Figure 7 with $\kappa = 0$). In this case (with $\gamma = 0, J_1 = 0$), the concentration continues to increase with time; having the same value irrespective of ξ. In other words, apart from the inlet value of $\phi_0 = 1$, the solution is constant $\phi(\xi,\tau) = \phi(\tau)$, and, at steady-state, the solution becomes equal to the inlet value.

If γ is non-zero with $J_1 = 0$, Figure 4.2b-c shows that the concentration begins to increase from the initial value (as in Figure 4.2a) to a maximum value and then starts to decrease until it vanishes everywhere at steady-state, similar to Figure 4.1b. The constant solutions observed in Figures 4.2a-c, are due to the zero flux outlet boundary condition, $J_1 = 0$. If J_1 is non-zero (e.g., $J_1 = 0.1$), Figure 4.2d shows that the solution initially increases with time as before but to satisfy the positive gradient of ϕ at the outlet, the concentration is forced to increase monotonically from the inlet to the outlet point. Thus, at steady-state, the solution is not zero everywhere but increases from zero to a positive value at the outlet.

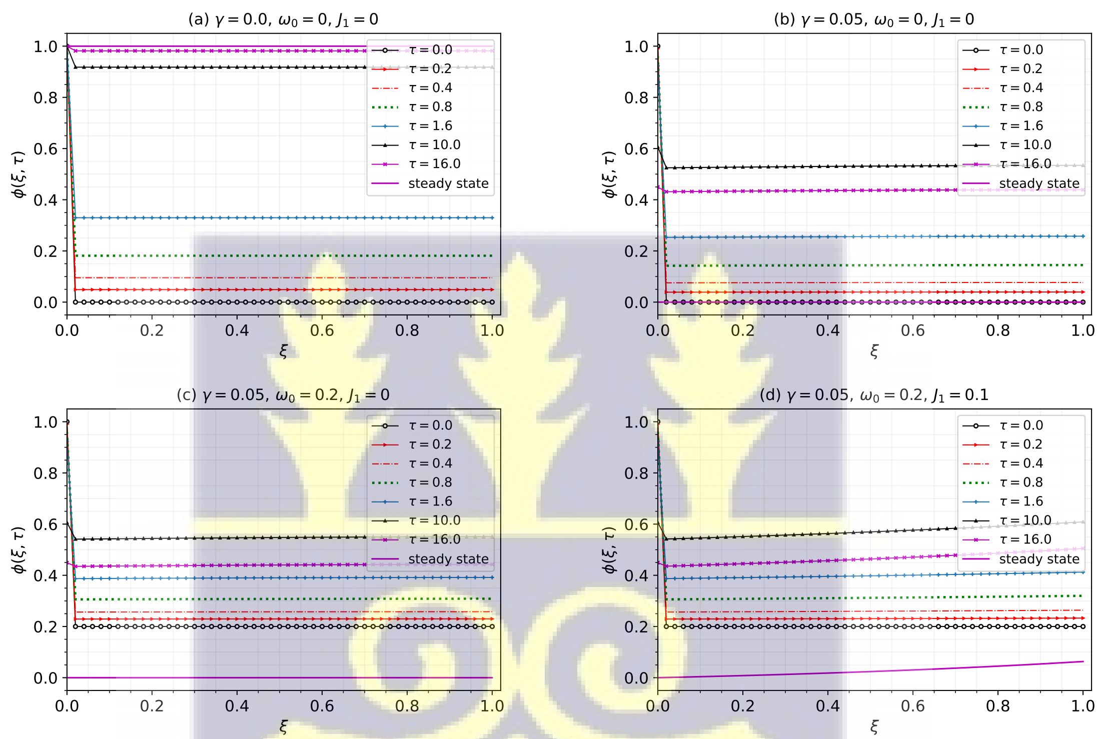


Figure 4.2: Concentrations at different times for $\lambda = 0.5$ and (a) $\gamma = 0$, $\omega_0 = 0$, (b) $\gamma = 0.05$, $\omega_0 = 0$, (c) $\gamma = 0.05$, $\omega_0 = 0.2$ and (d) $\gamma = 0.05$, $\omega_0 = 0.2$ and $J_1 = 0.1$.

Chapter 5

Application to Pollutant Transport

In this section, we attempt to model the transport of a pollutant (Iron) in river Fena in the Ashanti Region of Ghana using the theory in Chapter 4.

5.1 Observational Data

Data are obtained from the published paper by Duncan (2020) who conducted research on the Fena River to determine the level of heavy metal pollution due to illegal mining (locally referred to as "galamsay") activities in and around the river. The location of the river and the sampling points are depicted in Figure 5.1. The river flows southward from Fenaso No. 1 (referred to as Fen-1) through Fenaso No. 3 (referred to as Fen-3) until it enters the Gulf of Guinea in the Atlantic ocean. Fen-1 and Fen-2 are very close to each, less than a kilometer apart. According to Duncan (2020), there were illegal mining activities in and around all the sampling locations except Point A where there was no apparent activity going on. This makes modeling the flow of pollutants using a simple one-dimensional model (with a single source or entry point) much difficult. Nevertheless, we attempt to determine how best our 1D equations can reproduce the level of pollution at Point A, where there was no apparent injection of pollutants. In other words, the concentration of Fe at Point A is likely due to the transport of pollutants from Fen-1 and Fen-2. The three main heavy metal pollutants in the river, exceeding safe drinking water guidelines, were found to be Cadmium (Cd), Lead (Pb) and Iron (Fe) Duncan (2020). Here, we focus on modeling the transport of Iron, because the initial and boundary data are less complex to model than the other two metals. The monthly concentration of Fe at

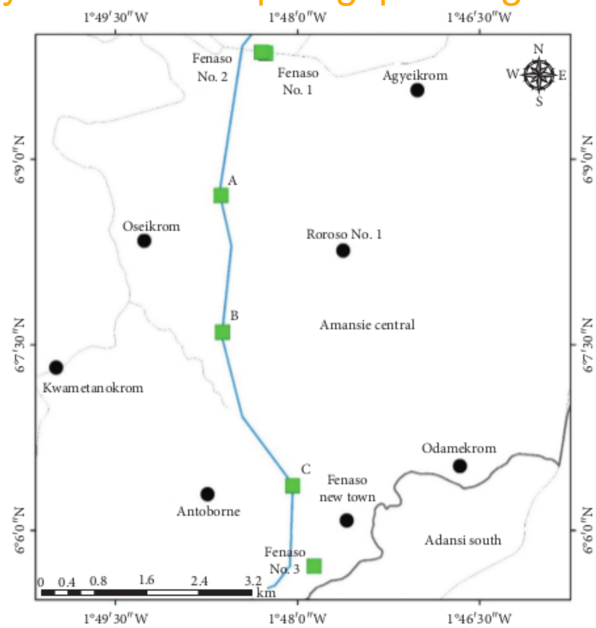


Figure 5.1: Map showing the location of river Fena (blue curve) and the sampling points (green rectangles) Duncan (2020).

each location (obtained from Table 3 of Duncan (2020)) over the one-year period of his study (from January to December in 2020) is shown in Figure 5.2. The highest concentrations occur in Fen-1 and Fen-2 with less concentration of Fe at Point C. The concentration of Fe at Fen-1 is generally decreasing with time over the study period.

5.2 Mathematical Modeling

To apply our mathematical models, we normalized the concentrations by the highest concentration at Fen-1 (see Figure 5.3). The concentration at the inlet is taken to be the concentrations at Fen-1 while the initial concentration is taken to be that of January at all locations. The measured concentration of Fe in January are depicted in Figure 5.4. In Figure 5.4b, the horizontal axis shows the distance (in kilometers) of each location from Fen-1, showing that Fen-1 and Fen-2 are indeed very close to each other. The sample locations are extracted from Figure 5.1.

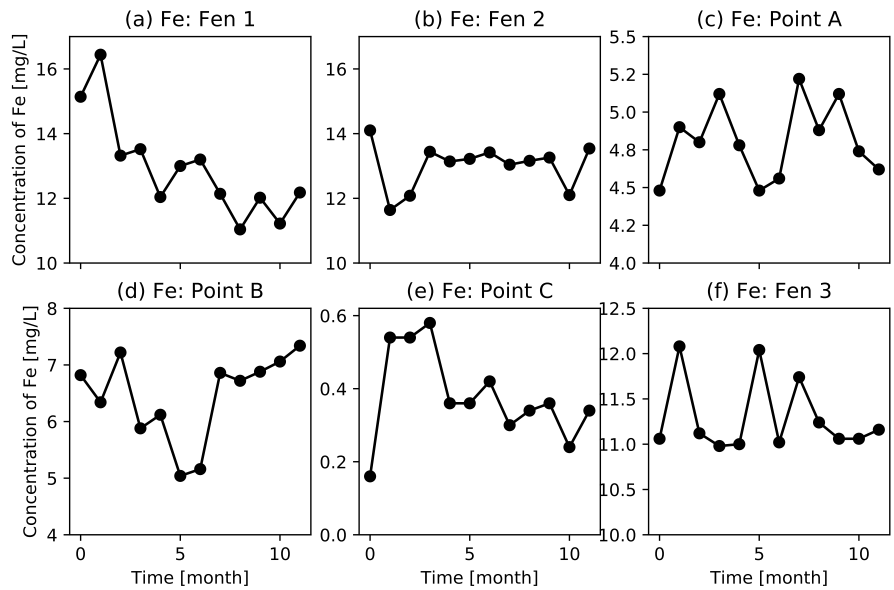


Figure 5.2: Variation of Iron (Fe) concentration over time in river Fena. Note that the vertical axis use different scales to highlight the temporal variations.

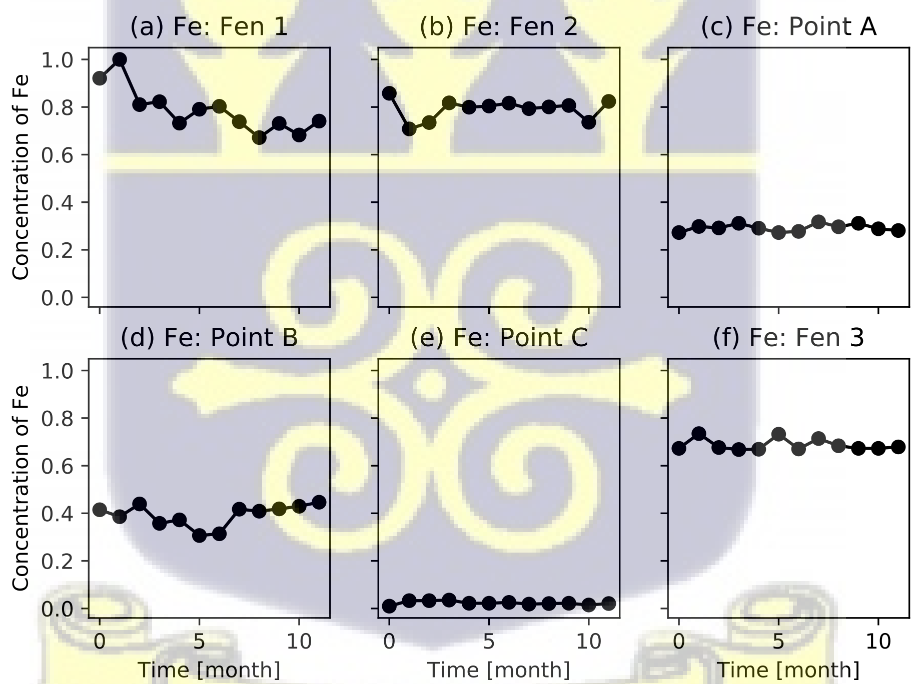


Figure 5.3: Same as Figure 5.2 but concentrations are normalized by the highest concentration at Fen-1.

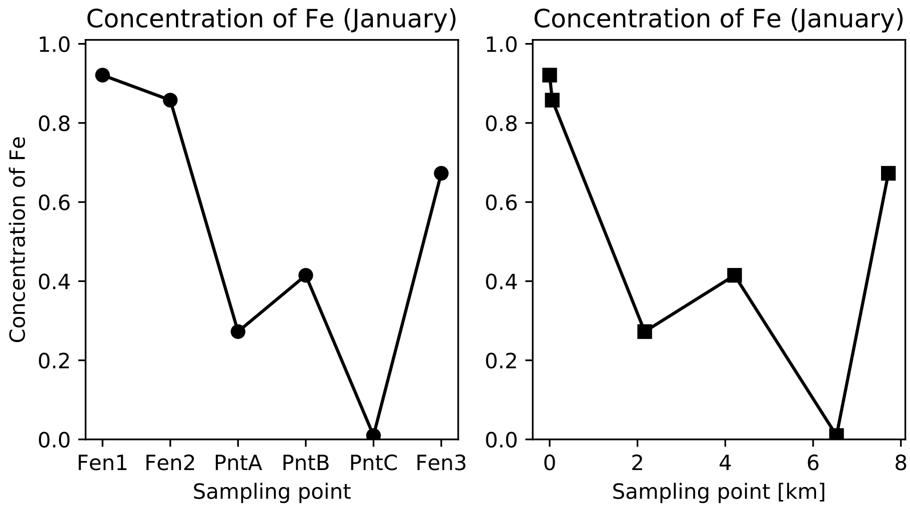


Figure 5.4: Normalized concentration of Fe in January at all sampling points (left panel) and the right panel shows the same sampling locations but as a distance from Fen-1 (right panel).

5.2.1 Diffusion coefficient

The parameter λ in the governing equation is related to the Peclet number $P_e = 2\lambda$ with

$$\lambda = \frac{1}{2}\frac{LV_0}{D_0}$$

where L is the length scale of the domain, V_0 is the averaged velocity of the flow and D_0 is a constant diffusion coefficient. The study by Duncan (2020) did not measure the flow speed or provide any geometric data (e.g., width, depth, sinuosity) of the river because they were mainly concerned with the chemical composition of the water. We estimated the velocity of the river to be $2\,\mathrm{m/s}$, by taking videos of the flow and measuring the speed of the floating objects. We also measured the average width of the river around the same location to be $\sim 5.2\,\mathrm{m}$ and the average depth to be $1.0\,\mathrm{m}$. So the average discharge at the location is about $10.4\,\mathrm{m^3/s}$.

Besides the velocity, the parameter that plays much more critical role in modeling the transport of pollutants in streams and rivers is the longitudinal diffusion coefficient, D_0. Once a pollutant is released into a river or flowing water body, it undergoes various stages of mixing with the ambient water. After the contaminant is mixed in the cross-sectional direction, the most important process is the longitudinal dispersion which is measured by longitudinal dispersion coefficient, Tayfur and Singh (2005). A simple formula for calculating the longitudinal dispersion coefficient was developed by Fischer (1975):

$$D_0 = 0.011 \frac{V_0^2 W^2}{H u_*} \tag{5.1}$$

where H is the average depth of the flow, u_* is shear velocity, and W is the average width of the flow. The shear velocity is given by $u_* = \sqrt{gHs}$, where g is the acceleration due to gravity and s is the stream slope. Fischer (1975) reported that, typically, $(V_0/u_*)^2$ varied between 0.17 and 0.25, with an average value of 0.2. Equation 5.1 is simple to apply if the mean hydraulic parameters are available. Other studies have developed similar empirical formulas for predicting the longitudinal dispersion (e.g., Seo and Cheong (1998), Deng et al. (2001), Kashefipour and Falconer (2002)). Tayfur and Singh (2005) developed a model based on artificial neural network (ANN) for predicting the longitudinal dispersion coefficient. Among other things, they reported that the discharge data alone is sufficient for computing the dispersion coefficient for more frequently occurring low values of the dispersion coefficient ($D_0 < 100\,\mathrm{m}^2/s$). Note that the discharge is given by $Q = HWV_0$. We fitted lines to the data points of Tayfur and Singh (2005) that are closest to the observed data (see their Table 7, case 2) to get the diffusion coefficient, D as a function of discharge to be

$$D = 0.35\,Q + 36 \text{ for } Q \leq 110, \tag{5.2}$$

and

$$D = 0.84\,Q + 18 \text{ for } Q < 1000. \tag{5.3}$$

as depicted in Figure 5.5. Using the formula in Eq.(5.2), we estimate the value of the longitudinal dispersion in Fena river to be $39.6\,\mathrm{m}^2/s$. Thus, the Peclet number is 389 and the parameter $\lambda \approx 194.5$.

5.2.2 Comparison of model results to observational data

We compared the observational data of Iron (Fe) concentration in Fena river to the two analytical solutions of the 1D advection-diffusion equation with Dirichlet boundary conditions (Eq.(4.78); referred to as "Dirichlet model") and Neumann boundary condition at the outlet (Eq.(4.95); referred to as "Neumann model"). The initial concentration $\omega_0 = 0.52$ is taken to be the average concentration at all locations in

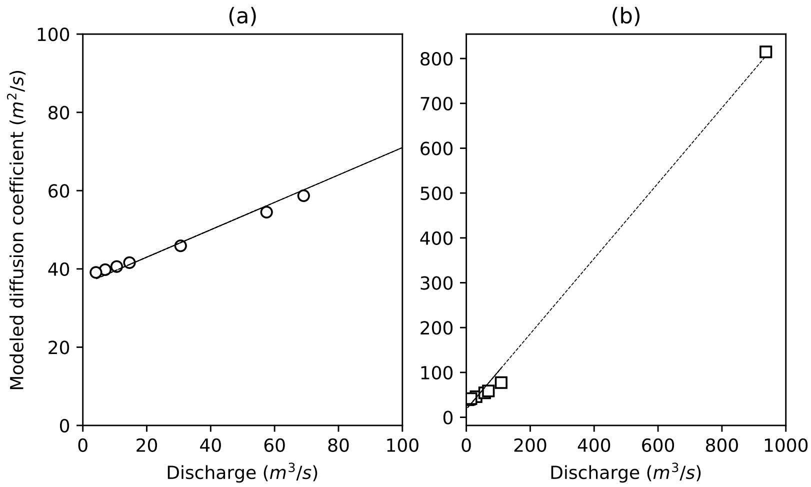


Figure 5.5: Diffusion coefficient as a function of discharge from Table 7 (case 2) of Tayfur and Singh (2005) for (a) $D < 100\,m^2/s$ and (b) $D < 900\,m^2/s$

January (see Figure 5.4). In each case, the inlet boundary is an exponentially decreasing concentration of the form $\phi_0 e^{-\gamma\tau}$ where $\phi_0 = 1$. By fitting an exponentially decreasing function to the data at Fen-1 (see Figure 5.3), we get $\gamma = 0.025$.

The concentration of Iron as a function of time from both the observational data and Dirichlet model is shown in Figure 5.6. Apart from the initial time, the model results at Fen-1, Fen-2 and Point-A are indistinguishable from each other as a results of the relatively high Peclet number. The model captures the concentrations at Fen-1 and Fen-2 relatively well since these locations are closer to each other, and data from Fen-1 is used as the boundary condition. However, the model predicts very large concentrations at Point-A, as also depicted in Figure 5.7. A couple of reasons could account for the high model concentration values at Point-A. One could be the fact that the model is one-dimensional and so does not include lateral dispersion of pollutants which could reduce the amount of Iron at Point-A. Secondly, the fact that the normalized concentration of iron at Point-A appears fixed, with less variation in time, implies that other reactions or factors other than the direct transport of iron from Fen-1 and Fen-2, might be at play and these are not captured in our model.

The results from the Neumann model are not different from that of the Dirichlet model as shown in Figure 5.8. As shown in Chapter 4, differences between the two models are more apparent for smaller Peclet numbers.

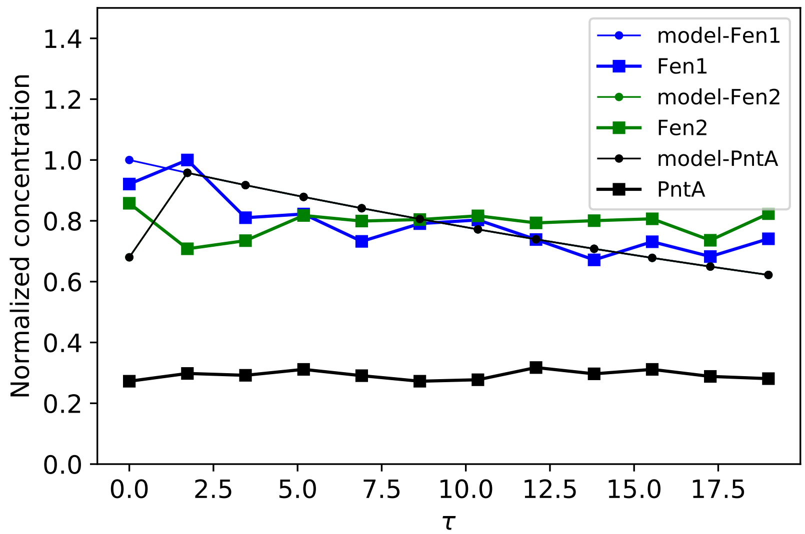


Figure 5.6: Temporal variation of observed and Dirichlet model concentrations at Fen-1, Fen-2 and Point-A.

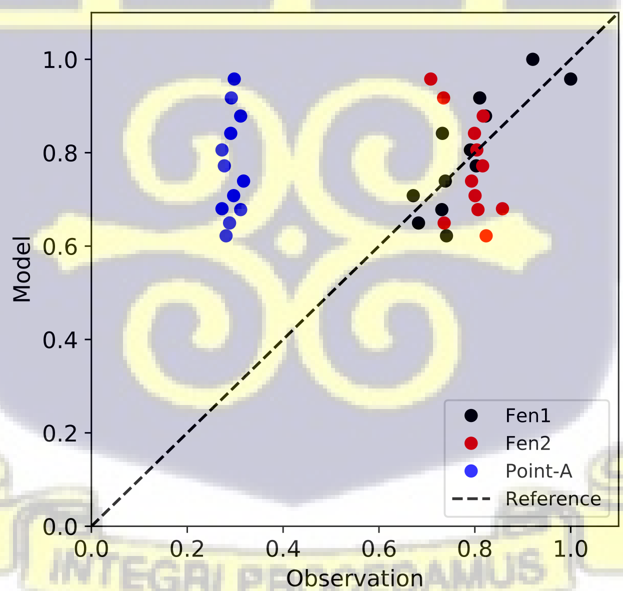


Figure 5.7: Observed and Dirichlet model pollutant concentration at Fen-1, Fen-2 and Point-A.

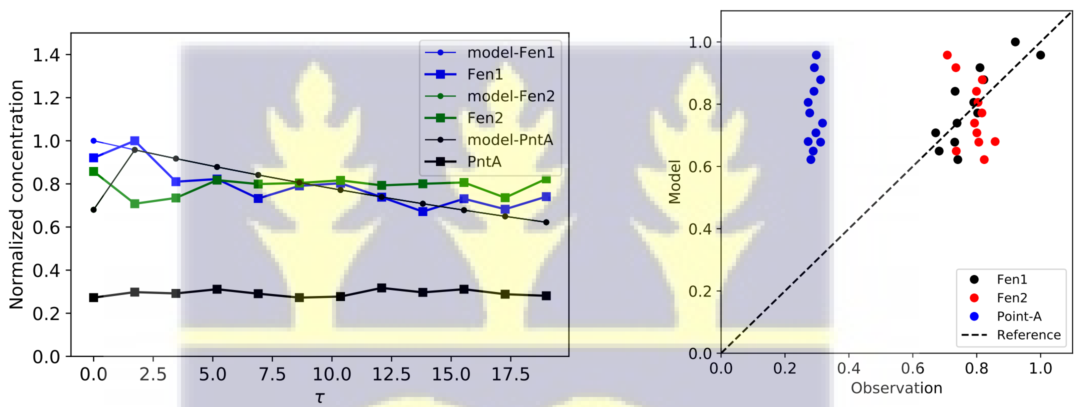


Figure 5.8: Same as in Figures 5.6 and 5.7 but for the Neumann model.

Chapter 6

Summary and Conclusions

Finding the inverse Lapalce Transform (iLT) of certain functions can often be challenging. This study employed the Laplace transform technique and the residue theorem approach to provide two analytic solutions to a 1D advection-diffusion equation without directly computing the inverse Laplace Transform. In addition, the theoretical derivations obtained were compared to some observational data from the Fena river in the Ashanti region of Ghana.

Chapter 1 introduces the advection-diffusion equation often employed in modeling the transport of pollutants in rivers and streams. Chapter 2 reviewed some literature on the model. The Laplace transform technique was found to be the most used method in providing analytical solutions to the 1D advection-diffusion equation. Other methods such as separation of variables was also found to be adopted. In Chapter 3, we derived the advection-diffusion equation. The study also thoroughly discussed the basic theories of some analytical methods of solving the advection-diffusion equation, that is the Laplace transform and separation of variables technique and how these methods are used to provide solution to a 1D advection-diffusion equation. Finally, we ended the chapter with brief discussion on the main method used in the study.

Chapter 4 of the study dealt with providing analytical solution for the 1D advection-diffusion equation with an exponentially decaying inlet boundary condition with Dirichlet outlet BC, (referred to as the Dirichlet model) and Neumann BC, (referred to as Neumann model). Comparisons were made with a mathematically similar problem in Kim (2020a). Interestingly, we recovered the solution in Kim (2020a) for both the Dirichlet and Neumann model in the absense of the exponential term, that is when $\gamma = 0$, as depicted in Figures 4.1a and 4.2a. For the Dirichlet model, it was discovered that the concentration everywhere within the domain increases until the system reaches steady-state with concentration decreasing monotonically from the inlet to the outlet. However, in the presence of a decaying inlet condition, the time evolution of concentration behaved differently. In this case, the concentration was observed to decrease below the initial concentration due to the exponentially decreasing condition at the inlet. In the case of the Neumann model (with $\gamma = 0, J = 0$), the concentration continued to increase with time; having the same value irrespective of ξ and at the steady state, the solution becomes equal to the inlet value. However, in the presence of a decaying inlet condition, ($\gamma \neq 0$ with $J = 0$), it was observed that the concentration increases up to a maximum value and eventually decreases until it vanishes everywhere at the steady-state. With a non-zero outlet flux, it was realized that the concentration is forced to increase monotonically from the inlet to the outlet point.

Chapter 5 of the study involves modeling the transport of a pollutant (iron) in river Fena using the theory in the previous chapter. To apply our mathematical model, we estimated the various parameters in the governing equation. The results obtained were compared to the observational data. It was realized that the model results captured the concentrations at Fen-1 and Fen-2 relatively well as observed in the actual data, as shown in Figure 5.8, for both the Dirichlet model and the Nuemann model. However, the model results predicted very large concentration at point A which was not consistent with the observational data.

6.1 Limitations and Recommendations

The following are some of the study's shortcomings and their corresponding recommendations. Firstly, the model fails to capture the concentration level at point A, where there was no apparant galamsey activity going on. The reason could be that since the model is one dimensional, it failed to capture other factors or reactions that might have contributed to the level of concentration at point A. As an improvement on this work, future studies could consider either two dimensional or three dimensional model and compare it with some data.

Another limitation to the study was the unavailability of data such as the flow speed, depth and the width of the river. An extension of this project would be to provide reliable data on the Fena river to enable accurate comparison of the model to the observed data.

Appendix A

Analytical solution of the 1D convection-diffusion equation over a finite domain by Mohsen and Baluch (1983).

The 1D unsteady convection-diffusion equation is given by

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \tag{A.1}$$

where:

D diffusion coefficient, $[L^2/T]$

c $c(x,t)$ = concentration of diffusing species, $[M/L^3]$

x space coordinate, $[L]$

V convection field, $[L/T]$

t time, $[T]$

with initial condition,

$$C(x,0) = 0 \tag{A.2}$$

and two boundary conditions

$$C(0,t) = C_0 \quad (t > 0), \tag{A.3}$$

$$C(L,t)=0 \quad (t>0). \tag{A.4}$$

Using the dimensionless quantities defined below;

$$P_e=\frac{VL}{D}, \quad T=\frac{Dt}{L^2}, \quad X=\frac{x}{L}, \quad \text{and} \quad \Phi=\frac{C}{C_0}.$$

We rewrite Eq.(A.1) as

$$\frac{\partial(\Phi C_0)}{\partial\left(\dfrac{TL^2}{D}\right)}+\frac{P_eD}{L}\frac{\partial(\Phi C_0)}{\partial(XL)}=D\frac{\partial^2(\Phi C_0)}{\partial(XL)^2},$$

$$\frac{DC_0}{L^2}\frac{\partial\Phi}{\partial T}+\frac{DC_0}{L^2}P_e\frac{\partial\Phi}{\partial X}=\frac{DC_0}{L^2}\frac{\partial\Phi}{\partial X^2}.$$

Multiplying through by L^2/DC_0, we have

$$\frac{\partial\Phi}{\partial T}+P_e\frac{\partial\Phi}{\partial X}=\frac{\partial^2\Phi}{\partial X^2} \tag{A.5}$$

with initial condition

$$\Phi(X,0)=0 \tag{A.6}$$

and the two boundary conditions;

$$\Phi(0,T)=1, \tag{A.7}$$

$$\Phi(1,T)=0. \tag{A.8}$$

We now transform the PDE into one that looks like the heat equation.

We employ the transformation

$$\Phi(X,T)=e^{\left(\frac{P_e}{2}X\right)}\phi. \tag{A.9}$$

Now,

$$\frac{\partial\Phi}{\partial X}=\frac{P_e}{2}e^{\left(\frac{P_e}{2}X\right)}\phi+\phi_X\,e^{\left(\frac{P_e}{2}X\right)}, \tag{A.10}$$

$$\frac{\partial\Phi}{\partial T}=\phi_T\,e^{\left(\frac{P_e}{2}X\right)}, \tag{A.11}$$

$$\frac{\partial^2 \Phi}{\partial X^2} = \frac{P_e^2}{4} e^{\left(\frac{P_e}{2}X\right)} \phi + \frac{P_e}{2} e^{\left(\frac{P_e}{2}X\right)} \phi_X + \frac{P_e}{2} e^{\left(\frac{P_e}{2}X\right)} \phi_X + e^{\left(\frac{P_e}{2}X\right)} \phi_{XX}. \tag{A.12}$$

Substituting Equations Eq.(A.10), Eq.(A.11) and Eq.(A.12) back into Eq.(A.5) gives,

$$\begin{aligned} \phi_T \, e^{\left(\frac{P_e}{2}X\right)} + P_e \left(\frac{P_e}{2} e^{\left(\frac{P_e}{2}X\right)} \phi + \phi_X \, e^{\left(\frac{P_e}{2}X\right)} \right) &= \frac{P_e^2}{4} e^{\left(\frac{P_e}{2}X\right)} \phi + \frac{P_e}{2} e^{\left(\frac{P_e}{2}X\right)} \phi_X \\ &+ \frac{P_e}{2} e^{\left(\frac{P_e}{2}X\right)} \phi_X + e^{\left(\frac{P_e}{2}X\right)} \phi_{XX}, \end{aligned}$$

$$\begin{aligned} \implies \phi_T \, e^{\left(\frac{P_e}{2}X\right)} + \frac{P_e^2}{2} e^{\left(\frac{P_e}{2}X\right)} \phi + P_e \, e^{\left(\frac{P_e}{2}X\right)} \phi_X &= \frac{P_e^2}{4} e^{\left(\frac{P_e}{2}X\right)} \phi + P_e \, e^{\left(\frac{P_e}{2}X\right)} \phi_X \\ &+ e^{\left(\frac{P_e}{2}X\right)} \phi_{XX}, \end{aligned}$$

$$\implies \phi_T + \frac{P_e^2}{4}\phi = \phi_{XX} \quad \implies \quad \frac{\partial \phi}{\partial T} = \frac{\partial^2 \phi}{\partial X^2} - \frac{P_e^2}{4}\phi. \tag{A.13}$$

Setting:

$$\lambda = \frac{Pe}{2}, \quad \xi = \lambda X, \quad \tau = \lambda^2 T$$

into Eq.(A.13) yields,

$$\frac{\partial \phi}{\partial \left(\frac{\tau}{\lambda^2}\right)} = \frac{\partial^2 \phi}{\partial \left(\frac{\xi}{\lambda}\right)^2} - \frac{(2\lambda)^2}{4}\phi,$$

$$\lambda^2 \frac{\partial \phi}{\partial \tau} = \lambda^2 \frac{\partial^2 \phi}{\partial \xi^2} - \lambda^2 \phi. \tag{A.14}$$

Dividing Equation (A.14) through by λ^2,

$$\frac{\partial \phi}{\partial \tau} = \frac{\partial^2 \phi}{\partial \xi^2} - \phi. \tag{A.15}$$

The corresponding boundary conditions of the transformed Eq.(A.15) are:

$$\Phi(0,T) = 1 \quad \implies \quad e^{\left(\frac{P_e}{2}X\right)} \phi(0,\tau) = 1 \quad \implies \quad \phi(\xi = 0, \tau > 0) = 1,$$

$$\Phi(1,T)=0 \implies e^{\left(\frac{P_e}{2}X\right)}\phi(\lambda,\tau)=0 \implies \phi(\xi=\lambda,\tau>0)=0$$

and the initial condition:

$$\Phi(X,0)=0 \implies e^{\left(\frac{P_e}{2}X\right)}\phi(\xi,0)=0 \implies \phi(\xi,\tau=0)=1.$$

A solution to Eq.(A.15) is decomposed into two components;

1. the steady state solution; $\phi_{ss}(\xi)$, and
2. the transient solution, $\phi_{tr}(\xi,\tau)$,

$$\phi(\xi,\tau)=\phi_{ss}(\xi)+\phi_{tr}(\xi,\tau). \tag{A.16}$$

At the steady state, $\dfrac{\partial\phi}{\partial\tau}=0$. The steady state component of Eq.(A.15) is

$$\frac{\partial^2\phi_{ss}}{\partial\xi^2}-\phi_{ss}=0 \tag{A.17}$$

subject to the boundary conditions:

$$\phi_{ss}(0)=1, \tag{A.18}$$

$$\phi_{ss}(\lambda)=0. \tag{A.19}$$

We now look for solutions of the form $\phi_{ss}(\xi)=e^{r\xi}$.

The characteristic equation is

$$r^2-1=0 \implies r=\pm1.$$

The steady state solution is given as

$$\phi_{ss}(\xi)=C_1\,e^{\xi}+C_2\,e^{-\xi}.$$

Using the exponential properties defined below;

$$e^{\xi}=\cosh\xi+\sinh\xi,$$

$$e^{-\xi}=\cosh\xi-\sinh\xi.$$

The steady state solution is given as

$$\phi_{ss}(\xi) = A\cosh\xi + B\sinh\xi \tag{A.20}$$

where $A = (C_1 + C_2)$ and $B = C_1 - C_2$.

Using the boundary conditions in Eq.(A.18) and Eq.(A.19)

$$\phi_{ss}(0) = 1 \quad \Longrightarrow \quad A = 1.$$

Substituting $A = 1$ into Eq.(A.20),

$$\phi_{ss}(\xi) = \cosh\xi + B\sinh\xi. \tag{A.21}$$

Also,

$$\phi_{ss}(\lambda) = 0 \implies \cosh\lambda + B\sinh\lambda = 0 \implies B = -\frac{\cosh\lambda}{\sinh\lambda}.$$

Substituting $B = -\dfrac{\cosh\lambda}{\sinh\lambda}$ into Eq.(A.21);

$$\begin{aligned}\phi_{ss}(\xi) &= \cosh\xi - \frac{\cosh\lambda}{\sinh\lambda}\sinh\xi \\ &= \frac{\sinh\lambda\cosh\xi - \cosh\lambda\sinh\xi}{\sinh\lambda} \\ &= \frac{\sinh(\lambda-\xi)}{\sinh\lambda}.\end{aligned} \tag{A.22}$$

Substituting Eq.(A.16) into Eq.(A.15)

$$\frac{\partial^2(\phi_{ss}+\phi_{tr})}{\partial\xi^2} - (\phi_{ss}+\phi_{tr}) = \frac{\partial}{\partial\tau}(\phi_{ss}+\phi_{tr}),$$

$$\frac{\partial^2\phi_{ss}}{\partial\xi^2} + \frac{\partial^2\phi_{tr}}{\partial\xi^2} - \phi_{ss} - \phi_{tr} = \frac{\partial\phi_{ss}}{\partial\tau} + \frac{\partial\phi_{tr}}{\partial\tau}. \tag{A.23}$$

But $\dfrac{\partial\phi_{ss}}{\partial\tau} = 0$ and $\dfrac{\partial^2\phi_{ss}}{\partial\xi^2} - \phi_{ss} = 0$.

Eq.(A.23) is reduced to

$$\frac{\partial\phi_{tr}}{\partial\tau} = \frac{\partial^2\phi_{tr}}{\partial\xi^2} - \phi_{tr} \tag{A.24}$$

subject to the boundary condition

$$\phi_{ss}(0) + \phi_{tr}(0,\tau) = 1 \implies \phi_{tr}(0,\tau) = 0, \tag{A.25}$$

$$\phi_{ss}(\lambda) + \phi_{tr}(\lambda,\tau) = 0 \implies \phi_{tr}(\lambda,\tau) = 0 \tag{A.26}$$

with initial condition:

$$\phi_{ss}(\xi) + \phi_{tr}(\xi,0) = 0 \implies \phi_{tr}(\xi,0) = -\phi_{ss}(\xi). \tag{A.27}$$

The expression $\phi_{tr}(\xi,\tau)$ has a solution of the form

$$\phi_{tr}(\xi,T) = X(\xi)\,T(\tau). \tag{A.28}$$

Substituting Eq.(A.28) into Eq.(A.24):

$$XT' = X'' - XT,$$

$$\frac{T'}{T} = \frac{(X'' - X)}{X} = -\mu^2,$$

$$\frac{T'}{T} = -\mu^2 \implies \ln T = -\mu^2\tau + c,$$

$$T = e^{-\mu^2\tau + c}.$$

The general solution for $T(\tau)$ is

$$T(\tau) = e^{-\mu^2\tau}. \tag{A.29}$$

Also,

$$\frac{(X'' - X)}{X} = -\mu^2 \implies X'' - X = -\mu^2 X,$$

$$X'' + X(\mu^2 - 1) = 0.$$

We look for solutions of the form $X(\xi) = e^{r\xi}$.

The characteristic equation:

$$r^2 + (\mu^2 - 1) = 0 \implies r = \pm\sqrt{-(\mu^2 - 1)}.$$

Let $\gamma^2 = (\mu^2 - 1)$. If $(\mu^2 - 1) > 0$, then

$$r = \pm\sqrt{-\gamma^2} \implies r = \pm\gamma i.$$

The solution for $X(\xi)$ is

$$X(\xi) = C_1\,e^{\gamma\xi i} + C_2\,e^{-\gamma\xi i}.$$

We employ the exponential properties below,

$$e^{\gamma\xi i} = \cos\gamma\xi + i\sin\gamma\xi,$$

$$e^{-\gamma\xi i} = \cos\gamma\xi - i\sin\gamma\xi.$$

Thus, the solution is

$$X(\xi) = A\,\cos\gamma\xi + B\,\sin\gamma\xi. \tag{A.30}$$

Applying Eqs.(A.25) and Eq.(A.26) to Eq.(A.30)

$$X(0) = 0 \quad \Longrightarrow \quad A = 0.$$

Substituting $A = 0$ into Eq.(A.30)

$$X(\xi) = B\sin\gamma\xi,$$

$$X(\lambda) = 0 \quad \Longrightarrow \quad B\sin\gamma\lambda = 0.$$

For nontrivial solution, $B \neq 0$. Thus,

$$\sin\gamma\lambda = 0 \;\Longrightarrow\; \gamma\lambda = n\pi \;\Longrightarrow\; \gamma = \frac{n\pi}{\lambda}. \tag{A.31}$$

The general solution for $X(\xi)$ is given as

$$X_n(\xi) = B_n \sin\left(\frac{n\pi\xi}{\lambda}\right). \tag{A.32}$$

But

$$\gamma^2 = (\mu^2 - 1) \;\Longrightarrow\; (\mu^2 - 1) = \frac{(n\pi)^2}{\lambda^2} \;\Longrightarrow\; \mu^2 = \frac{n^2\pi^2}{\lambda^2} + 1. \tag{A.33}$$

Substituting Eq.(A.33) into Eq.(A.29) gives

$$T(\tau) = \exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right)T\right\}.$$

By the superposition principle

$$\phi(\xi,\tau) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi\xi}{\lambda}\right)\,\exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right)T\right\}. \tag{A.34}$$

Again, if $(\mu^2 - 1) < 0$, then the characteristic equation

$$r = \pm\sqrt{\gamma^2} \quad \Longrightarrow \quad r = \pm\gamma.$$

The solution for $X(\xi)$ is

$$X(\xi) = A\,\cosh\gamma\xi + B\,\sinh\gamma\xi. \tag{A.35}$$

Applying Eq.(A.25) to Eq.(A.35)

$$X(\xi) = B\sinh\gamma\xi. \tag{A.36}$$

Again, putting Eq.(A.26) into Eq.(A.35)

$$X(\lambda) = 0 \quad \Longrightarrow \quad B\sinh\gamma\lambda = 0.$$

Either $B = 0$ or $\sinh\gamma\lambda = 0$.

If

$$\sinh\gamma\lambda = 0 \quad \Longrightarrow \quad \gamma\lambda = 0.$$

But $\gamma \neq 0$ and $\lambda \neq 0$. Thus, $\sinh\gamma\lambda$ cannot be zero. Therefore, only $B = 0$.

Hence, the general solution is given as

$$X(\xi) = 0 \quad \Longrightarrow \quad \phi(\xi, \tau) = 0. \tag{A.37}$$

Also; if $(\mu^2 - 1) = 0$, then the characteristic equation is

$$r = \pm\sqrt{0} = 0.$$

The solution for $X(\xi)$ is

$$X(\xi) = C_1. \tag{A.38}$$

Applying Eq.(A.25) to Eq.(A.38)

$$X(0) = 0 \quad \Longrightarrow \quad C_1 = 0,$$

$$X(\xi) = 0 \quad \Longrightarrow \quad \phi(\xi, \tau) = 0.$$

Applying Eq.(A.27) to Eq.(A.34);

$$\phi_{tr}(\xi, 0) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi\xi}{\lambda}\right) \tag{A.39}$$

which is a Fourier sine series where the coefficient

$$B_n = -\frac{2}{\lambda}\int_0^{\lambda} \phi_{ss} \sin\left(\frac{n\pi\xi}{\lambda}\right) d\xi.$$

The required solution for $\phi(\xi, \tau)$ is

$$\phi(\xi, \tau) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi\xi}{\lambda}\right) \exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right) T\right\} + \frac{\sinh(\lambda - \xi)}{\sinh\lambda} \tag{A.40}$$

where the coefficients B_n are given as,

$$\begin{aligned} B_n &= -\frac{2}{\lambda}\int_0^{\lambda} \frac{\sinh(\lambda - \xi)}{\sinh\lambda} \sin\left(\frac{n\pi\xi}{\lambda}\right) d\xi \\ &= -2\pi \cdot \frac{n}{\lambda^2\left(1 + \dfrac{n^2\pi^2}{\lambda^2}\right)}. \end{aligned}$$

Eq.(A.40) may now be written as

$$\phi(\xi, \tau) = \frac{\sinh(\lambda - \xi)}{\sinh\lambda} - \frac{2\pi}{\lambda^2}\sum_{n=1}^{\infty} \frac{n}{\left(1 + \dfrac{n^2\pi^2}{\lambda^2}\right)} \sin\left(\frac{n\pi\xi}{\lambda}\right) \exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right) T\right\}. \tag{A.41}$$

In terms of the Peclet number, Pe, the solution may be written as:

$$\begin{aligned} \Phi\, e^{-\left(\frac{P_e}{2}X\right)} &= \frac{\sinh\left[\dfrac{P_e}{2}(1 - X)\right]}{\sinh\left(\dfrac{P_e}{2}\right)} - \frac{8\pi}{P_e^2}\sum_{n=1}^{\infty} \frac{n}{\left(1 + \dfrac{4n^2\pi^2}{P_e^2}\right)} \\ &\quad \times \sin(n\pi X) \exp\left\{-\left(1 + \frac{n^2\pi^2}{\lambda^2}\right) T\right\}. \end{aligned} \tag{A.42}$$

Repalcing Φ with $\dfrac{C}{C_0}$

$$\frac{C}{C_0}\,e^{-\left(\frac{P_e}{2}X\right)} = \frac{\sinh\left[\frac{P_e}{2}(1-X)\right]}{\sinh\left(\frac{P_e}{2}\right)} - \frac{8\pi}{P_e^2}\sum_{n=1}^{\infty}\frac{n}{\left(1+\frac{4n^2\pi^2}{P_e^2}\right)} \times \sin(n\pi X)\,\exp\left\{-\left(1+\frac{n^2\pi^2}{\lambda^2}\right)T\right\}. \tag{A.43}$$

Appendix B

An analytical Solution of the 1D Advection-Diffusion Equation by Davis (1985).

The equation to be solved is:

$$\frac{\partial c}{\partial t} + V\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{B.1}$$

with two boundary conditions

$$c(0,t) = c_0 \ \ (t > 0),$$

$$c(L,t) = 0 \ \ (t > 0)$$

and initial condition,

$$c(x,0) = 0$$

where:

D diffusion coefficient, $[L^2/T]$

c $c(x,t) =$ concentration of diffusing species, $[M/L^3]$

x space coordinate, $[L]$

V convection field, $[L/T]$

t time, $[T]$.

Using the dimensionless quantities defined below,

$$P_e = \frac{VL}{D}, \;\; T = \frac{Dt}{L^2}, \;\; X = \frac{x}{L}.$$

We rewrite Eq.(B.1) as

$$\frac{\partial c}{\partial\left(\frac{TL^2}{D}\right)} + \frac{P_e D}{L}\,\frac{\partial c}{\partial(XL)} = D\,\frac{\partial^2 c}{\partial(XL)^2},$$

$$\frac{D}{L^2}\,\frac{\partial c}{\partial T} + \frac{D}{L^2}\,P_e\,\frac{\partial c}{\partial X} = \frac{D}{L^2}\,\frac{\partial c}{\partial X^2}.$$

Multiplying through by L^2/D we get

$$\frac{\partial c}{\partial T} + P_e\,\frac{\partial c}{\partial X} = \frac{\partial^2 c}{\partial X^2}. \tag{B.2}$$

The corresponding boundary conditions of the transformed Equation (B.2) are:

$$c(0,T) = c_0,$$

$$c(1,T) = 0$$

and the initial condition:

$$c(X,0) = 0.$$

The Laplace transform, $\mathcal{L}$ is defined as

$$\mathcal{L}[c(X,T)] = \hat{c}(X,s) = \int_0^\infty e^{-sT} c(X,T)dT. \tag{B.3}$$

Applying Eq.(B.3) to Eq.(B.2) yields

$$\mathcal{L}\left(\frac{\partial c}{\partial T}\right) = s\hat{c} - \hat{c}(X,0) = s\hat{c},$$

$$\mathcal{L}\left(\frac{\partial c}{\partial X}\right) = \frac{\partial}{\partial X}\mathcal{L}(c) = \frac{\partial \hat{c}}{\partial X},$$

$$\mathcal{L}\left(\frac{\partial^2 c}{\partial X^2}\right) = \frac{\partial^2}{\partial X^2}\mathcal{L}(c) = \frac{\partial^2 \hat{c}}{\partial X^2}.$$

The boundary conditions are:

$$\mathcal{L}[c(1,T)] = \mathcal{L}(0) \quad \Longrightarrow \quad \hat{c}(1,s) = 0, \tag{B.4}$$

$$\mathcal{L}[c(X,0)] = \mathcal{L}(0) \quad \Longrightarrow \quad \hat{c}(X,0) = 0. \tag{B.5}$$

The transformed equation of (B.2) is

$$\frac{d^2\hat{c}}{dX^2} - P_e\frac{d\hat{c}}{dX} - s\hat{c} = 0 \tag{B.6}$$

which is a second order ordinary differential equation.

The characteristic equation is

$$r^2 - P_e\, r - s = 0 \quad \Longrightarrow \quad r = \frac{P_e \pm \sqrt{P_e^2 + 4s}}{2},$$

$$r = \frac{P_e}{2} \pm \sqrt{\frac{P_e^2}{4} + s} \quad \Longrightarrow \quad r = \frac{P_e}{2} \pm a,$$

where $a = \sqrt{\dfrac{P_e^2}{4} + s}$.

The general solution is

$$\begin{aligned} c(X,s) &= A\ \exp\left(\frac{P_e}{2} + a\right)X + B\ \exp\left(\frac{P_e}{2} - a\right)X \\ &= A\ \exp\left(\frac{P_e}{2}X\right)\exp\left(aX\right) + B\ \exp\left(\frac{P_e}{2}X\right)\exp\left(-aX\right) \end{aligned} \tag{B.7}$$

.

Using the exponential properties defined below

$$\exp(aX) = \cosh aX + \sinh aX,$$

$$\exp(-aX) = \cosh aX - \sinh aX.$$

Eq.(B.7) is rewritten as

$$\begin{aligned} c(X,s) &= \exp\left(\frac{P_e}{2}X\right)\left[A(\cosh aX + \sinh aX) + B(\cosh aX - \sinh aX)\right] \\ &= \exp\left(\frac{P_e}{2}X\right)(A\cosh aX + B\sinh aX) \\ &= A\cosh aX\ \exp\left(\frac{P_e}{2}X\right) + B\sinh aX\ \exp\left(\frac{P_e}{2}X\right). \end{aligned} \tag{B.8}$$

Applying Eq.(B.4) to Eq.(B.8)

$$c(0,s) = \frac{c_0}{s} \quad \Longrightarrow \quad A = \frac{c_0}{s}. \tag{B.9}$$

Substituting $A = \dfrac{c_0}{s}$ into Eq.(B.8);

$$c(X,s) = \frac{c_0}{s}\cosh aX\ \exp\left(\frac{P_e}{2}X\right) + B\sinh aX\left(\frac{P_e}{2}X\right). \tag{B.10}$$

Again, applying Eq.(B.5) to Eq.(B.8)

$$c(1,s) = 0 \quad \Longrightarrow \quad \frac{c_0}{s}\cosh a\ \exp\left(\frac{P_e}{2}\right) + B\sinh a\ \exp\left(\frac{P_e}{2}\right) = 0, \tag{B.11}$$

$$\Longrightarrow \ \exp\left(\frac{P_e}{2}\right)\left[\frac{c_0}{s}\cosh a\ + B\sinh a\right] = 0. \tag{B.12}$$

But $\exp\left(\dfrac{P_e}{2}\right) \neq 0$. Thus

$$\frac{c_0}{s}\cosh a\ + B\sinh a = 0 \quad \Longrightarrow \quad B = -\frac{c_0}{s}\frac{\cosh a}{\sinh a}. \tag{B.13}$$

Substituting $B = -\dfrac{c_0}{s}\dfrac{\cosh a}{\sinh a}$ back into Eq.(B.10) yields

$$\begin{aligned} c(X,s) &= \frac{c_0}{s}\exp\left(\frac{P_e}{2}X\right)\left[\cosh aX - \frac{\cosh a}{\sinh a}\sinh aX\right] \\ &= \frac{c_0}{s}\exp\left(\frac{P_e}{2}X\right)\left[\frac{\sinh a\,\cosh aX - \cosh a\,\sinh aX}{\sinh a}\right] \\ &= \frac{c_0}{s}\exp\left(\frac{P_e}{2}X\right)\frac{\sinh(a - aX)}{\sinh a} \\ &= \frac{c_0}{s}\exp\left(\frac{P_e}{2}X\right)\frac{\sinh\left[a(1-X)\right]}{\sinh a}. \end{aligned} \tag{B.14}$$

We now put $a = \left(\dfrac{P_e^2}{4} + s\right)^{1/2}$ into Eq.(B.14) to obtain

$$c(X,s) = \frac{c_0}{s}\exp\left(\frac{P_e}{2}X\right)\frac{\sinh\left[\left(\frac{P_e^2}{4}+s\right)^{1/2}(1-X)\right]}{\sinh\left(\frac{P_e^2}{4}+s\right)^{1/2}}. \tag{B.15}$$

To obtain the solution for $c(X,T)$,we apply the inverse Laplace transform:

$$\mathcal{L}^{-1}[\hat{c}(X,s)] = c(X,T). \tag{B.16}$$

Let $b = \dfrac{P_e^2}{4}$, then

$$c(X,s) = \frac{c_0}{s}\exp\left(\frac{P_e}{2}X\right)\frac{\sinh\left[(b+s)^{1/2}(1-X)\right]}{\sinh(b+s)^{1/2}}. \tag{B.17}$$

From the first translation theorem, we have

$$\mathcal{L}\left[\exp(bT)\,c(X,T)\right] = \left[c(X,s^*)|s \mapsto s^* - b\right], \tag{B.18}$$

$$\exp(bT)\,c(X,T) = \mathcal{L}^{-1}\left[c(X,s^*)|s \mapsto s^* - b\right]. \tag{B.19}$$

Applying Eq.(B.19) to Eq.(B.15), one obtains

$$\exp(bT)\, c(X,T) = \mathcal{L}^{-1}\left[\frac{c_0 \exp\left(\frac{P_e}{2}X\right)\sinh\left[(s)^{1/2}(1-X)\right]}{(s-b)\sinh(s)^{1/2}}\right], \tag{B.20}$$

$$c(X,T) = c_0 \exp\left(\frac{P_e}{2}X - bT\right)\mathcal{L}^{-1}\left[\frac{\sinh\left[(s)^{1/2}(1-X)\right]}{(s-b)\sinh(s)^{1/2}}\right]. \tag{B.21}$$

The inverse Laplace transform can be solved by adopting a complex integral approach. The poles occurs at

$$s-b=0 \quad \Longrightarrow \quad s=b, \tag{B.22}$$

$$\sinh(s)^{1/2}=0 \quad \Longrightarrow \quad s=0. \tag{B.23}$$

By referring to Erdélyi et al. (1954) the solution is given as;

$$\begin{aligned} c(X,T) = c_0 \exp(\lambda X)&\left[\frac{\sinh\left(\frac{P_e}{2}(1-X)\right)}{\sinh\left(\frac{P_e}{2}\right)}\right] - c_0\exp(\lambda X) \\ &\times\left[2\pi\sum_{n=1}^{\infty}\frac{n\sin(n\pi X)}{(\lambda^2+n^2\pi^2)}\times\exp\left[-(\lambda^2+n^2\pi^2)T\right]\right]. \end{aligned} \tag{B.24}$$

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