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SOLVING BURGER'S EQUATION USING PHYSICS-INFORMED NEURAL NETWORKS (PINNs)

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Declaration

We hereby explicitly state that this dissertation is our own work done under the capable guidance of Dr. Rhydal Esi Eghan toward the award of the Bachelor of Science (BSc.) in Mathematics and that, to the best of our knowledge, it does not contain any material that has been previously published by another person or material that has been accepted for the award of any other degree from the university, with the exception of instances where appropriate acknowledgement has been made in the text.

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DEDICATION

This work is a testament of our deep gratitude to the Almighty God, whose guidance and presence led us through the entire process and brought it to fruition.We dedicate this thesis to our parents, whose unwavering support and hard work enabled us to pursue our education and cover the expenses of our four-year journey.

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ABSTRACT

Polymer flooding is a widely-used enhanced oil recovery technique that increases oil extraction efficiency by improving the viscosity of the displacing fluid, making it a more cost-effective option compared to water flooding. However, accurately tracking the concentration of polymer solutions in heterogeneous and complex reservoir conditions remains a key challenge.Traditional numerical methods, such as Euler, Runge-Kutta, and Finite Difference, often struggle with these complexities and can suffer from numerical instabilities due to the violation of the underlying physical laws or constraints governing the fluid dynamics. This research aims to address these challenges by employing Physics-Informed Neural Networks (PINNs) to solve Burgers' equation, a nonlinear partial differential equation commonly used in modeling fluid flow during polymer flooding. The methodology integrates physical laws directly into the neural network training process, thereby enhancing the model's ability to adhere to the underlying physics of the problem. The research demonstrates the effectiveness of PINNs in achieving accurate predictions of polymer concentrations and reducing numerical errors associated with traditional methods. Hence this shows that the proposed approach not only overcomes the limitations of conventional techniques but also offers a promising alternative for optimizing enhanced oil recovery strategies.

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Chapter 1

INTRODUCTION

1.1 Background of Study

Partial differential equations (PDEs) are fundamental mathematical tools used to describe physical processes in numerous fields, including physics, engineering, and biology. However, solving PDEs analytically is often infeasible for complex systems, requiring the use of numerical methods. Traditional numerical approaches, such as finite difference and finite element methods, have long been employed for this purpose. While these methods are effective in many cases, they do encounter challenges in handling highly nonlinear systems and complex geometries, often leading to inaccuracies and numerical instabilities.**???**.

In the context of oil recovery, specifically Enhanced Oil Recovery (EOR) techniques, PDEs are essential for modeling the dynamics of fluid flow within reservoirs. Among the EOR methods, polymer flooding has gained prominence as a cost-effective and efficient approach compared to traditional water flooding. By improving the mobility of the injected fluids, polymer flooding significantly enhances oil recovery rates, making it a critical component in modern reservoir management Tan et al. (2020).

However, accurately tracking the movement of the concentration of polymers through heterogeneous and complex reservoirs presents significant challenges. These challenges are compounded by the nonlinearity of the systems involved, which often leads to inaccuracies and numerical instabilities when using traditional numerical methods to solve the PDEs governing the process. One key PDE that arises in fluid dynamics and is particularly relevant to modeling the flow of polymers in reservoirs is Burgers' Equation. This equation, known for capturing nonlinear wave phenomena and viscous effects, provides a simplified yet powerful model for understanding fluid flow and polymer behavior in reservoir conditions. Akram et al. (2021).

Recent advancements in machine learning, particularly deep learning, have introduced innovative methods for solving complex PDEs. Among these, Physics-Informed Neural Networks (PINNs) stand out by integrating physical laws directly into neural network architectures. This approach allows for more accurate and reliable solutions to nonlinear PDEs like

Burgers' Equation, which is essential for modeling fluid dynamics in polymer flooding. PINNs offer promising potential for addressing the limitations of traditional numerical methods, particularly when dealing with complex geometries and boundary conditions Raissi (2018); Wang et al. (2021).

1.2 Problem Statement

Traditional numerical methods, such as Runge-Kutta and finite difference methods, are valuable tools widely used for solving nonlinear partial differential equations (PDEs) across various fields. However, these methods often encounter numerical instabilities and inaccuracies, particularly when dealing with complex geometries or nonlinear phenomena (**???**). These issues can lead to inaccurate predictions and unreliable simulations, impacting critical real-life applications in fields like fluid dynamics.

The limitations of these traditional methods, such as Euler, Runge-Kutta, and finite difference, for solving nonlinear PDEs often do occur due to the violation of the physical laws or constraints governing the equation Grimmer and Stewart (2021). These violations occur when the numerical solution deviates from the fundamental principles of the physical system being modeled. For instance, the conservation of mass, energy, or momentum might not be accurately preserved in the numerical solution, leading to unphysical results such as negative concentrations, non-conservative energy transfer, or incorrect wave propagation speeds. These discrepancies arise from the inherent limitations of the numerical methods in handling complex boundary conditions, highly nonlinear equations, and heterogeneous media, which are common in real-world applications.

In the context of enhanced oil recovery (EOR) through polymer flooding, accurately modeling the dynamics of fluid flow and polymer concentration is essential for optimizing the recovery process. However, traditional numerical methods often fall short to capture the intricate interplay between the polymer and the reservoir, particularly under varying conditions. For example, the nonlinearity and variability of reservoir properties can cause the numerical methods to produce results that violate the physical constraints of the system, such as maintaining a consistent mass balance or accurately modeling the diffusion and advection processes. These violations can lead to erroneous predictions of polymer distribution and, consequently, suboptimal recovery strategies, inefficient resource utilization, and reduced oil recovery efficiency

Cuomo et al. (2022). Hence addressing these challenges is crucial for improving the reliability and accuracy of simulations in various scientific, engineering, and real-life applications.

1.3 Objective

- The objective of this study is to employ Physics-Informed neural network (PINN)–based methods to mitigate numerical instabilities in solving nonlinear partial differential equations (PDEs).

1.4 Justification

1.4.1 Method

Physics-Informed Neural Networks (PINNs) offer a novel approach to solving PDEs by integrating physical laws directly into the neural network's loss function. This method allows for the simultaneous satisfaction of data fidelity and adherence to the governing physical equations, which is particularly advantageous in complex systems like polymer flooding Raissi et al. (2019b); Karniadakis et al. (2021).Unlike traditional numerical methods, PINNs can better handle the nonlinearities and irregular geometries typical of real-world reservoirs, leading to more stable and accurate solutions Cuomo et al. (2022). This capability is critical in enhancing the reliability of simulations in scenarios where traditional methods often fail due to instabilities and inaccuracies.

1.4.2 Research

Oil remains a critical source of revenue for many countries, driving the need for innovative methods to enhance recovery rates from reservoirs. Polymer flooding, an advanced technique in enhanced oil recovery (EOR), offers a way to increase extraction efficiency by improving the sweep of oil through the reservoir. By enabling precise tracking of polymer concentration, this method ensures that the injected fluid effectively displaces oil, leading to a higher recovery rate. The ability to monitor and control this concentration is vital for maximizing output and reducing operational costs. Given the importance of maintaining high recovery rates to sustain economic growth, this research focuses on optimizing polymer flooding as a reliable and efficient EOR strategy (Smith et al., 2023).

1.5 Structure of Thesis

The thesis is structured as follows:

1. **Introduction**: Provides an overview of the research topic, objectives, and methodology.
2. **Literature Review**: Surveys existing literature on PDEs, numerical methods, and machine learning techniques, with a focus on the application of PINNs in enhanced oil recovery.
3. **Methodology**: Describes the implementation of PINN-based methods and the rationale behind their selection.
4. **Results and Analysis**: Presents the results of experiments and analyses, comparing the performance of PINNs with traditional methods.
5. **Discussion and Conclusion**: Provides a comprehensive discussion of the findings, implications in the field of oil recovery, and limitations of the research, followed by the conclusion and suggestions for future work.

Chapter 2

LITERATURE REVIEW

2.1 Background of Partial Differential Equations (PDEs)

Partial Differential Equations (PDEs) form a fundamental part of mathematical modeling, finding extensive application across various fields of science and engineering. They describe how quantities such as temperature, pressure, and concentration change continuously in space and time Evans (2010). PDEs are essential tools for understanding and predicting complex phenomena in nature, ranging from fluid dynamics and electromagnetism to heat transfer and quantum mechanics Strang (2007).

Classification of PDEs is based on various factors, including their order, linearity, and the number of independent variables Logan (2014). PDEs can be classified as elliptic, hyperbolic, or parabolic based on their characteristics and the types of solutions they possess. Elliptic equations arise in problems involving steady-state phenomena, such as electrostatics and steady-state heat conduction Haberman (2012). Hyperbolic equations describe wave-like behavior and are prevalent in problems involving wave propagation, such as acoustic waves and electromagnetic waves Strang (2007). Parabolic equations are commonly encountered in problems involving diffusion and heat conduction, where the evolution of the system depends on both time and space Logan (2014).

In fluid dynamics, PDEs serve as the foundation for modeling the behavior of fluids, capturing the complex interactions between velocity, pressure, and density under varying conditionsLogan (2014); Chanson (2011); Zienkiewicz et al. (2000); Griffiths (2005). Among these, Burgers' Equation stands out as a simplified yet powerful model that illustrates essential nonlinear dynamics, such as turbulence and shock wave formation. Despite its relatively simple form, Burgers' Equation effectively represents the interplay between advection and diffusion in viscous fluid flow. This makes it a valuable tool not only for theoretical studies but also for practical applications in engineering, such as in the analysis of polymer flooding in enhanced oil recovery (EOR). By understanding the solutions to Burgers' Equation, engineers can gain insights into more complex systems, improving the efficiency of processes like oil recovery and advancing the field of fluid mechanics Akram et al. (2021); Chanson (2011).

2.2 Traditional Numerical Methods for Solving PDEs

Traditional numerical methods have been the cornerstone of solving Partial Differential Equations (PDEs) for decades, providing engineers and scientists with practical tools to simulate and analyze complex physical phenomena. These methods typically involve discretizing the spatial and temporal domains of PDEs and solving the resulting algebraic equations iteratively. Finite difference methods (FDMs) are among the most widely used techniques, where derivatives in the PDEs are approximated by finite differences, leading to a system of algebraic equations that can be solved numerically LeVeque (2007). Another popular approach is the finite element method (FEM), which discretizes the domain into smaller elements and represents the solution as a combination of basis functions over these elements Zienkiewicz et al. (2000). Additionally, finite volume methods (FVMs) are commonly used, where the domain is divided into control volumes, and the fluxes across the control volume boundaries are computed based on the PDEs Ferziger and Peric (2002).

Despite their widespread use, traditional numerical methods face several challenges and limitations. Nonlinearity in PDEs can lead to difficulties in achieving convergence and accuracy, as linear methods may not directly apply or may require extensive modificationsLi and Wang (2021). Handling complex geometries and boundary conditions can also be cumbersome, especially with the Finite Difference Method, which struggles with irregular domains Zhu and Zhang (2019). Numerical instabilities are a common issue, particularly in time-stepping schemes, where small errors can amplify over time, leading to unreliable results. Additionally, traditional methods can sometimes violate physical laws, such as conservation principles, boundary conditions, due to discretization errors or inadequate numerical schemes. These limitations highlight the need for more advanced techniques to address these challenges by offering a more robust approach to solving PDEs in complex scenarios Raissi et al. (2020).

2.3 Enhanced Oil Recovery and Polymer Flooding

Enhanced Oil Recovery (EOR) techniques have evolved significantly over the decades, playing a crucial role in extending the life of mature oil fields. Among the various EOR methods, polymer flooding stands out as a particularly effective approach due to its ability to improve the sweep efficiency of waterflooding. The concept of polymer flooding dates back to the 1960s, when early laboratory experiments demonstrated the potential of adding polymers to water to increase its viscosity, thereby enhancing the displacement of oil trapped in porous reservoir rocks. Over the years, extensive field trials and research have refined the process, leading to the development of high-molecular-weight polymers specifically tailored for use in diverse reservoir conditions. Polymer flooding involves injecting these water-soluble polymers into the reservoir to increase the viscosity of the displacing fluid, reducing the mobility ratio between the oil and the injected water. This improved viscosity contrast between the injected fluid and the oil enhances the displacement efficiency, making polymer flooding an essential method in modern reservoir management. Today, it is considered one of the most promising EOR techniques, particularly in reservoirs with unfavorable mobility ratios, where traditional waterflooding alone would be insufficient Seright (2017); Green and Willhite (2018); Speight (2017).

Modeling fluid flow during polymer flooding is inherently complex due to the nonlinear behavior of the polymer solutions and the heterogeneous nature of reservoirs. Traditional numerical methods, such as finite difference and finite element methods, often struggle with these complexities, leading to inaccuracies and numerical instabilities. The use of Partial Differential Equations (PDEs) is essential for simulating the interactions between the polymer, oil, and reservoir rock. To overcome these challenges, there is a need for more advanced computational models that can handle the complexities of real-world reservoirs. Improving these models will help optimize polymer flooding techniques, leading to more effective oil recovery and better management of reservoir resources.Liu and Sharma (2020); Tan et al. (2020).

2.4 Introduction to Machine Learning and Neural Networks

Machine learning (ML) is a branch of artificial intelligence (AI) that focuses on the development of algorithms and statistical models that enable computers to learn from and make predictions or decisions based on data. At its core, machine learning involves the study of algorithms that can automatically learn patterns and relationships from data without being explicitly programmed. These algorithms are trained on labeled datasets, where each data point is associated with a label or outcome of interest, allowing the model to learn the underlying patterns in the data.One of the key concepts in machine learning is the ability of algorithms to generalize from the training data to make predictions on new, unseen data, which is essential for their practical application in various domains. Bishop (2006).

Neural networks (NNs) are a class of machine learning models inspired by the structure and function of the human brain. These models consist of interconnected nodes or neurons organized in layers, where each neuron receives input signals, processes them using an activation function, and produces an output signal that is passed to the next layer of neurons Goodfellow et al. (2016). Neural networks have gained popularity in recent years due to their ability to automatically learn complex patterns and representations from data, making them well-suited for a wide range of tasks, including image recognition, natural language processing, and speech recognition.

Supervised and unsupervised learning are two fundamental paradigms in machine learning. Supervised learning uses labeled data to map inputs to outputs, enabling predictions on new data. Unsupervised learning discovers hidden patterns in unlabeled data without explicit guidance. Examples include clustering, dimensionality reduction, and generative models.Raschka and Mirjalili (2019) Neural networks have seen significant advancements, making them highly relevant for solving partial differential equations (PDEs). Their ability to approximate complex, high-dimensional functions allows them to model intricate relationships in PDEs effectively. Recent developments highlight their potential in providing accurate solutions where traditional methods struggle. Neural networks excel at generalizing from data, handling large-scale problems, and requiring minimal prior knowledge, which enhances their utility in scientific computing and PDE solutionsHan et al. (2018); Raissi et al. (2019a).

2.5 Physics-Informed Neural Networks (PINNs)

Physics-Informed Neural Networks (PINNs) are a class of machine learning models that combine the power of neural networks with the underlying physical laws governing a system. Unlike traditional numerical methods, which rely on discretizing the governing equations and solving them iteratively, PINNs directly learn the solution of partial differential equations (PDEs) from data while enforcing the physical constraints of the problem Raissi et al. (2019b). The concept behind PINNs is to embed the physics into the neural network architecture, allowing it to learn the solution while respecting the governing equations. This is achieved by incorporating the PDE constraints as additional loss terms during training, which ensures that the network outputs solutions that satisfy both the observed data and the underlying physics Raissi et al. (2019b).

The principles behind PINNs involve training a neural network to minimize a loss function that consists of two components: a data fidelity term and a physics-informed term. The data fidelity term measures the difference between the predicted and observed data, ensuring that the network accurately captures the training data. The physics-informed term, on the other hand, enforces the underlying physical laws by penalizing deviations from the governing equations Raissi et al. (2019b). PINNs have several advantages over traditional numerical methods, including their ability to handle complex geometries and boundary conditions, their data-driven nature, and their flexibility in incorporating additional physical constraints. They have been successfully applied to a wide range of problems, including fluid dynamics, heat transfer, and structural mechanics, demonstrating their effectiveness in solving real-world engineering problems Wang et al. (2021).

2.6 Application of PINNs in Polymer Flooding

Recent studies have explored the application of Physics-Informed Neural Networks (PINNs) in the context of polymer flooding, an advanced Enhanced Oil Recovery (EOR) technique. These studies demonstrate the potential of PINNs to model the complex fluid dynamics involved in polymer flooding, capturing the intricate interactions between the injected polymer and the reservoir's porous media. The ability of PINNs to incorporate physical laws directly into the learning process allows for more accurate predictions of polymer displacement and saturation profiles, which are critical for optimizing the efficiency of the EOR process Raissi et al. (2019b).

In comparison with traditional methods like finite difference or finite element approaches, PINNs have shown superior performance in handling the nonlinearities and high-dimensional parameter spaces inherent in polymer flooding simulations. However, despite these advancements, there remain gaps in the literature, particularly in the detailed modeling of specific polymer types and their interaction with various reservoir conditions. Your research aims to address these gaps by further refining the PINN framework to enhance its accuracy and applicability in diverse polymer flooding scenarios Green and Willhite (2018).

Chapter 3

METHODOLOGY

3.1 Introduction

This chapter outlines the methodology used to solve the Burger's equation for tracking the concentration of polymers in the enhanced oil recovery (EOR) process within a reservoir. The approach leverages Physics-Informed Neural Networks (PINNs), a cutting-edge computational technique that integrates the governing physical laws directly into the neural network framework. This innovative method offers a powerful and flexible solution for solving the partial differential equations (PDEs) that describe the transport and concentration of polymers during EOR.

This chapter provides a detailed overview of the methodology, beginning with the problem formulation, which defines the Burger's equation in the context of polymer concentration tracking, along with the relevant initial and boundary conditions. The data preparation process is also discussed, focusing on the preprocessing and normalization of data necessary for effective model training. The architecture of the PINN model is described, illustrating how it is designed to seamlessly integrate the governing physical laws. Finally, the chapter covers the training process, including the optimization techniques, hyperparameter tuning, and evaluation metrics used to ensure the accuracy and reliability of the PINN model in solving the Burger's equation for EOR applications.

3.1.1 Significance of PINNs in Solving PDEs

The significance of Physics-Informed Neural Networks (PINNs) in solving partial differential equations (PDEs) lies in their advanced ability to model fundamental physical laws while addressing complex real-world scenarios. By directly integrating the governing physical equations into the neural network training process, PINNs ensure results that are consistent with the underlying physics. This makes them particularly effective in handling problems with irregular boundaries, varying initial conditions, and the non-linearities inherent in equations like the Burger's equation. In the context of enhanced oil recovery (EOR), PINNs excel by embedding the physical principles of polymer transport within the neural network, enabling accurate modeling of complex reservoir dynamics. This approach overcomes many limitations of traditional numerical methods, making PINNs a powerful tool for refining predictions using real-world data and achieving reliable solutions to complex PDEs Raissi et al. (2019b) Zhang et al. (2021)

3.2 Problem Formulation

3.2.1 Problem Definition

Polymer flooding, a well-established Enhanced Oil Recovery (EOR) technique, has been extensively used for over four decades to enhance the extraction of residual oil in reservoirs by improving the mobility ratio and thereby increasing the overall recovery efficiency by 5-30% of the original oil in place (OOIP). This method has demonstrated significant technical success, with an efficiency of 0.7 to 1.75 lb of polymer per barrel of incremental oil produced, and is often more cost-effective compared to conventional water flooding methods, which typically leave 50-70% of oil unrecovered. Despite its advantages, a major challenge in polymer flooding is accurately tracking the concentration of polymers within the reservoir, which is critical for optimizing the process and ensuring the economic feasibility of the operation. Our research aims to address this challenge by developing advanced modeling techniques to predict polymer concentration distribution, thereby improving the efficiency and predictability of polymer flooding projects. Abidin et al. (2012).

3.2.2 Mathematical Representation of the Problem

In polymer flooding, the transport and concentration of polymers within a reservoir can be effectively modeled using the Burgers' equation coupled with an advection-diffusion equation. The governing equation for the polymer concentration $c(x, t)$ is given by:

$$\frac{\partial c}{\partial t} + c\frac{\partial c}{\partial x} = \nu\frac{\partial^2 c}{\partial x^2} \tag{3.1}$$

where:

- $c = c(x, t)$ is the polymer concentration at position x and time t, measured in kg/m^3. A typical initial polymer concentration can be around 1 kg/m^3, depending on the specific application and reservoir conditions.

- ν is the diffusion coefficient for the polymer, which accounts for the spreading of the polymer due to dispersion and molecular diffusion. A realistic value for ν could be in the range of 10^{-3} to 10^{-5} m^2/s, depending on the polymer's properties and the reservoir conditions.

Initial Condition

The initial condition describes the spatial distribution of the polymer concentration in the reservoir at the very beginning of the flooding process (at time $t = 0$). It is given by:

$$c(x,0) = e^{\frac{-(x-0.5)^2}{\nu}} \quad \text{kg/m}^3 \tag{3.2}$$

This expression represents a Gaussian distribution centered at $x = 0.5$ with a variance controlled by the parameter ν. The concentration is highest at the center of the reservoir ($x = 0.5$) and decreases symmetrically towards the edges.

The parameter ν determines the spread of the concentration profile: a smaller value of ν leads to a sharper decline, while a larger value results in a more gradual decrease. This initial condition reflects that the polymer concentration is initially centered around the middle of the reservoir and will disperse over time as the flooding progresses.

Boundary Conditions

The boundary conditions define the behavior of the polymer concentration at the boundaries of the spatial domain. For this problem, the conditions are set as follows:

- **At $x = 0$:**

$$c(0,t) = 0 \quad \text{kg/m}^3 \tag{3.3}$$

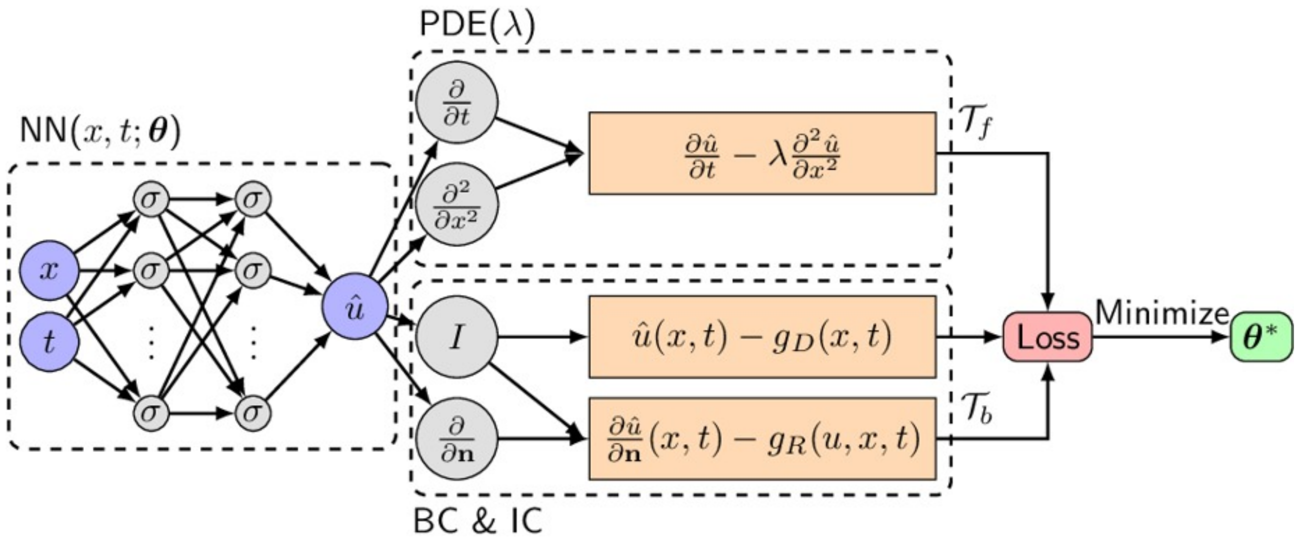
  This condition signifies that there is no flux of polymer concentration across this boundary, potentially due to impermeable barriers or injection strategies that prevent polymer from entering or leaving at this point.

- **At $x = 100$:**

$$c(100,t) = 0 \quad \text{kg/m}^3 \tag{3.4}$$

  Similar to the condition at $x = 0$, this boundary condition indicates no flux of polymer concentration at this boundary, suggesting a closed or controlled boundary at this location.

3.3 Model Architecture



PDE(λ)
NN($x, t; \boldsymbol{\theta}$)
x
t
σ
$\hat{u}$
$\frac{\partial}{\partial t}$
$\frac{\partial^2}{\partial x^2}$
$\frac{\partial \hat{u}}{\partial t} - \lambda \frac{\partial^2 \hat{u}}{\partial x^2}$
$\mathcal{T}_f$
I
$\frac{\partial}{\partial \mathbf{n}}$
$\hat{u}(x,t) - g_D(x,t)$
$\frac{\partial \hat{u}}{\partial \mathbf{n}}(x,t) - g_R(u,x,t)$
$\mathcal{T}_b$
Loss
Minimize
$\boldsymbol{\theta}^*$
BC & IC

Figure 3.1: PINN Architecture

In this study, a Physics-Informed Neural Network (PINN) is employed to model polymer concentration dynamics within a reservoir. The PINN integrates physical laws, represented by partial differential equations (PDEs), directly into the neural network training process. The architecture consists of a neural network with input layers for spatial (x) and temporal (t) coordinates and an output layer for the predicted solution $\hat{u}$.

The network comprises several hidden layers with activation functions designed to capture complex relationships between inputs and outputs. The PINN's loss function is composed of two main components: the PDE residual and the boundary and initial condition (BC & IC) residuals. The PDE residual is calculated by differentiating the network's output with respect to time and space, ensuring that the solution satisfies the governing PDE. The BC & IC residuals measure the discrepancy between the networkâs predictions and the known boundary and initial conditions, ensuring physical consistency.

Additionally, the architecture leverages automatic differentiation to compute the derivatives necessary for the PDE and BC & IC residuals. These components are combined into a total loss, which is minimized to optimize the network parameters, θ, ensuring that the model predictions align with both the underlying physical laws and the available data.

3.3.1 Mathematical Representation of the Architecture

The architecture of the Physics-Informed Neural Network (PINN) is distinguished by its layered structure, where each layer performs distinct mathematical operations that facilitate the integration of physical laws into the learning process.

Input Layer

The input layer consists of neurons that receive input features representing the state of the reservoir. These features might include spatial coordinates, time, initial polymer concentration, and other relevant parameters.

Let $\mathbf{x}$ represent the input vector with n features:

$$\mathbf{x} = [x_1, x_2, \dots, x_n]^T \tag{3.5}$$

Hidden Layers

The model includes one or more hidden layers, each containing neurons that apply a linear transformation followed by a non-linear activation function. For a hidden layer j, the output $\mathbf{h}^{(j)}$ is given by:

$$\mathbf{h}^{(j)} = \sigma(\mathbf{W}^{(j)}\mathbf{h}^{(j-1)} + \mathbf{b}^{(j)}) \tag{3.6}$$

where:

- $\mathbf{W}^{(j)}$ is the weight matrix of layer j,
- $\mathbf{h}^{(j-1)}$ is the output vector from the previous layer (with $\mathbf{h}^{(0)} = \mathbf{x}$ for the input layer),
- $\mathbf{b}^{(j)}$ is the bias vector of layer j,
- σ is the activation function (tanh).

The weights and biases are learnable parameters that are optimized during training to minimize the prediction error.

Output Layer

The output layer produces the final prediction, which in this case is the polymer concentration $\hat{c}$. The output is a linear combination of the activations from the last hidden layer:

$$\hat{c} = \mathbf{W}^{(out)}\mathbf{h}^{(L)} + \mathbf{b}^{(out)} \tag{3.7}$$

where:

- $\mathbf{W}^{(out)}$ is the weight matrix of the output layer,
- $\mathbf{h}^{(L)}$ is the output vector from the last hidden layer L,
- $\mathbf{b}^{(out)}$ is the bias term for the output layer.

Loss Function and Optimization

The model's parameters, including weights and biases, are optimized by minimizing a loss function $\mathcal{L}$, which measures the discrepancy between the predicted and actual polymer concentrations. A common choice for regression tasks is the Mean Squared Error (MSE) loss:

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N}(c_i - \hat{c}_i)^2 \tag{3.8}$$

where c_i and $\hat{c}_i$ are the actual and predicted concentrations for the i-th sample, respectively, and N is the number of samples.

The optimization of the loss function is typically performed using gradient descent-based methods such as Adam or SGD.

3.4 Model Building

3.4.1 Data Generation and Processing

Data Generation: The data is generated based on the initial and boundary conditions specified for the Burgers' equation. For the initial condition, polymer concentration is defined by

$$u(x, 0) = e^{\frac{-(x-0.5)^2}{\nu}}$$

over a spatial domain x ranging from 0 to 100. Boundary conditions are $u(0, t) = 0$ and $u(100, t) = 0$. This data generation results in initial and boundary condition datasets, which are crucial for training and evaluating the model.

Scaling: Data scaling is performed to normalize the features and target values within a range of [0, 1], improving the performance and stability of the neural network training process. The Min-Max scaling technique is used for this purpose. It transforms the data by subtracting the minimum value of the feature and dividing by the range of the feature values. This is applied separately to the spatial x, temporal t, and polymer concentration u data.

Splitting: The dataset is split into training and testing sets using an 80:20 ratio. This means 80% of the data is used for training the neural network, and 20% is reserved for testing and validating the model. This split ensures that the model is trained on a substantial amount of data while retaining a portion for performance evaluation. The split is done sequentially to maintain the temporal ordering of the data.

3.4.2 Neural Network Model Definition

The neural network model used is a **Physics-Informed Neural Network (PINN)**, designed to solve partial differential equations like the Burgers' equation.

Parameters and Hyperparameters:

- **Number of Layers:** 4
  This denotes the number of hidden layers in the neural network. Each layer helps the model learn different levels of abstraction from the input data.

- **Units per Layer:** 20
  Each hidden layer consists of 20 neurons. The number of units determines the capacity of the network to capture complex patterns in the data.

- **Activation Function:** 'tanh'
  The hyperbolic tangent activation function is used for the hidden layers. It introduces non-linearity into the model, allowing it to learn complex mappings from inputs to outputs.

- **Output Layer:** 1 neuron, no activation
  The output layer has a single neuron to produce a continuous value for the polymer concentration. No activation function is applied to this layer, providing a raw output value.

Model Definition Code:

```
class PINN(tf.keras.Model):
    def __init__(self, num_layers=4, units_per_layer=20, activation='tanh'):
        super(PINN, self).__init__()
        self.dense_layers = []
        for _ in range(num_layers):
            self.dense_layers.append(tf.keras.layers.Dense
            (units_per_layer, activation=activation))
        self.dense_layers.append(tf.keras.layers.Dense(1, activation=None))

    def call(self, inputs):
        x = inputs[:, 0:1]
        t = inputs[:, 1:2]
        u = tf.concat([x, t], axis=1)
        for layer in self.dense_layers:
            u = layer(u)
        return u
```

3.4.3 Loss Function

The loss function used in the training of the model includes several components to ensure that the model adheres to the differential equation and boundary conditions.

Loss Function Equation:

$$\text{Loss} = \text{Loss}_{\text{PDE}} + \text{Loss}_{\text{IC}} + \text{Loss}_{\text{BC}_{\text{left}}} + \text{Loss}_{\text{BC}_{\text{right}}}$$

Where:

- Loss_{PDE} measures the deviation of the model's predictions from the Burgers' equation.

$$\text{Loss}_{\text{PDE}} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - b\frac{\partial^2 u}{\partial x^2}\right)^2$$

- Loss_{IC} ensures that the initial condition $u(x, 0) = e^{\frac{-(x-0.5)^2}{\nu}}$ is satisfied.

$$\text{Loss}_{\text{IC}} = \frac{1}{M} \sum_{j=1}^{M} \left(u(x, t = 0) - e^{\frac{-(x-0.5)^2}{\nu}} \right)^2$$

- $\text{Loss}_{\text{BC}_{\text{left}}}$ enforces the boundary condition at $x = 0$.

$$\text{Loss}_{\text{BC}_{\text{left}}} = \frac{1}{K_1} \sum_{k=1}^{K_1} (u(0, t))^2$$

- $\text{Loss}_{\text{BC}_{\text{right}}}$ enforces the boundary condition at $x = 100$.

$$\text{Loss}_{\text{BC}_{\text{right}}} = \frac{1}{K_2} \sum_{k=1}^{K_2} (u(100, t))^2$$

3.4.4 Training Process

The training process involves optimizing the neural network parameters to minimize the defined loss function.

Training Process Overview:

- **Optimizer:** Adam optimizer with a learning rate of 0.001 is used for training the model. The Adam optimizer adapts the learning rate during training and is effective for complex models with many parameters.
- **Number of Epochs:** The model is trained for 3000 epochs. Each epoch represents one complete pass through the training data.
- **Training Step Function:** The train_step function performs a single update of the modelâs weights. It computes the gradients of the loss function with respect to the model parameters and updates the weights accordingly.

Training Process Code:

```
def train_step(model, optimizer, x, t, u0, x_left, t_left,
u_left, x_right, t_right, u_right, b):
    with tf.GradientTape() as tape:
        loss_value = loss(model, x, t, u0, x_left, t_left,
        u_left, x_right, t_right, u_right, b)
    grads = tape.gradient(loss_value, model.trainable_variables)
    optimizer.apply_gradients(zip(grads, model.trainable_variables))
    return loss_value

# Training loop
num_epochs = 1000
train_losses = []
test_losses = []

for epoch in range(num_epochs):
    loss_value = train_step(model, optimizer, x_train, t_train, u_train, x_boundary_val,
    t_boundary_val, u_boundary_val,
     x_boundary_val, t_boundary_val,
     u_boundary_val, b)
    train_losses.append(loss_value.numpy())

    # Calculate test loss
    test_loss_value = loss(model, x_test, t_test, u_test, x_boundary_val, t_boundary_val,
    u_boundary_val, x_boundary_val,
    t_boundary_val, u_boundary_val, b)
    test_losses.append(test_loss_value.numpy())

    if epoch % 100 == 0:
        print(f"Epoch {epoch}, Loss: {loss_value.numpy()},
        Test Loss: {test_loss_value.numpy()}")
```

3.4.5 Evaluation and Prediction

Evaluation: The model is evaluated by comparing its predictions against the test data. Performance metrics include the loss values for both training and testing datasets, which help assess the model's ability to generalize to unseen data.

Prediction: Once trained, the model can predict polymer concentration for new data points. Predictions are compared with actual data to visualize and understand the model's accuracy.

Visualization: Various plots are generated to compare predicted and actual values. These include:

- Training and validation loss curves.
- Plots of actual vs. predicted data for both training and testing sets.
- 2D surface plots of predictions to visualize the distribution of the polymer concentration over space and time.

Chapter 4

Results and Analysis

4.1 Introduction

In this chapter, we present and analyze the results obtained from the PINN model applied to solve the Burgers' equation. We focus on visualizing the predicted and actual solutions, the training and test losses over epochs, and the comparison of actual and predicted data values. The performance metrics are also discussed to evaluate the model's effectiveness.

4.2 Visualizations and Data Analysis

4.2.1 Data Generation

Dataset containing 100 data points of the spatial domain (ranging from 0 to 100 meters) and time (from 0 to 100 hours), with corresponding concentration values ($u(x,t)$) in kg/m^3. The concentration values are determined over these spatial and temporal coordinates.

Table 4.1: 100 Data Points Generated

Point	**Spatial Domain (meters)**	**Time (hours)**	**u(x,t) (kg m^{-3})**
1	0	0	77.880
2	1.124	1	86.048
3	2.247	2	92.702
4	3.370	3	97.380
5	4.494	4	99.744
6	5.505	5	99.618
7	6.629	6	97.012
8	7.752	7	92.118
9	8.876	8	85.290
10	9.887	9	77.000
11	11.236	10	67.782
12	12.359	11	58.179
⋮	⋮	⋮	⋮
13	97.752	97	0.000
14	98.876	98	0.000
15	100.000	100	0.000

Data Splitting

The dataset, covering a spatial domain from 0 to 100 meters over 100 hours, was divided into two subsets: 80% of the data points were used for training, while 20% were reserved for testing. This division ensures that the model learns from a substantial portion of the data while also being thoroughly evaluated on unseen data, enabling an accurate assessment of its predictive capabilities in modeling polymer concentration during flooding. Below is the table displaying the training and testing datasets used.

Table 4.2: 80 Training Data Points

Point	Spacial Domain(x)	Time(t)	Actual Value
1	0.00	0	77.880
2	1.124	1	86.048
3	2.247	2	92.702
4	3.370	4	97.380
5	4.494	5	99.744
6	5.505	6	99.618
⋮	⋮	⋮	⋮
7	77.620	77	0.570
8	78.786	78	0.580
9	79.845	79	0.560

Table 4.3: 20 Testing Data Points

Point	Spacial Domain(x)	Time(t)	Actual Value
1	80.967	80	0.525
2	82.065	82	0.368
3	83.156	83	0.220
4	84.956	84	0.188
5	85.856	85	0.157
6	86.156	86	0.112
⋮	⋮	⋮	⋮
7	97.812	97	0.000
8	98.978	98	0.000
9	100.000	100	0.000

DAta Training / Testing

The model's performance is evaluated by comparing predicted values against actual values from both the training and testing datasets. The model was trained for 3000 epochs using the Adam optimizer with a learning rate of 0.001. The results are presented in tabular form, including absolute error analysis to measure the accuracy of the predictions. This comparison enables the assessment of how well the model generalizes to unseen data and evaluates its overall predictive reliability.

Table 4.4: Error Analysis for Training Data

Point	**Spacial Domain(x)**	**Time(t)**	**Actual Value**	**Predicted Value**	**Absolute Error**
1	0.00	0	77.880	55.800	22.080
2	1.124	1	86.048	69.300	16.748
3	2.247	2	92.702	77.800	14.902
4	3.370	4	97.380	83.200	14.180
5	4.494	5	99.744	85.800	13.944
6	5.505	6	99.618	85.700	13.918
⋮	⋮	⋮	⋮	⋮	⋮
7	77.620	77	0.570	0.450	0.120
8	78.786	78	0.580	0.420	0.160
9	79.845	79	0.560	0.410	0.150

Table 4.5: Error Analysis for Testing Data

Point	**Spacial Domain(x)**	**Time(t)**	**Actual Value**	**Predicted Value**	**Absolute Error**
1	80.967	80	0.525	0.515	0.010
2	82.065	82	0.368	0.366	0.002
3	83.156	83	0.220	0.217	0.003
4	84.956	84	0.188	0.187	0.001
5	85.856	85	0.157	0.158	0.001
6	86.156	86	0.112	0.113	0.001
⋮	⋮	⋮	⋮	⋮	⋮
7	97.812	97	0.000	0.000	0.000
8	98.978	98	0.000	0.000	0.000
9	100.000	100	0.000	0.000	0.000

Actual vs. Predicted Data for Training Dataset

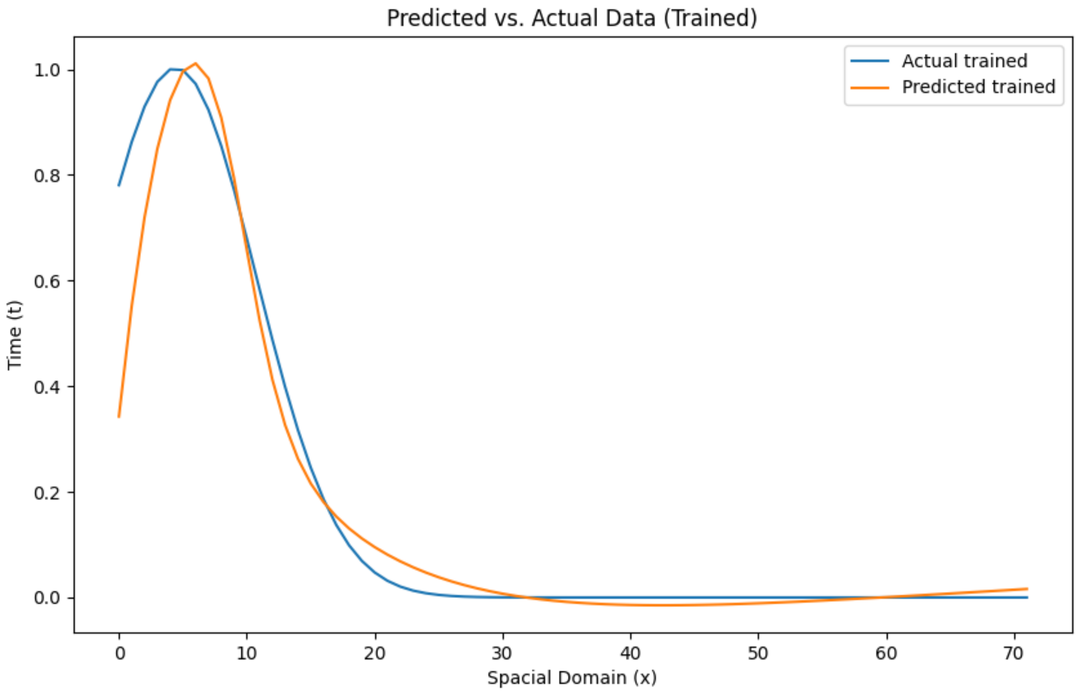


Figure 4.1: Actual vs. Predicted Data for Training Dataset

The plot demonstrates a close alignment between the actual polymer concentration values and those predicted by the PINN model for both training and testing datasets. This suggests that the PINN has effectively captured the spatial and temporal dynamics of polymer concentration in the reservoir. The accurate prediction across different points indicates that the model is well-fitted, reflecting the underlying physical processes described by Burgers' equation without significant deviations.

Actual vs. Predicted Data for Testing Dataset

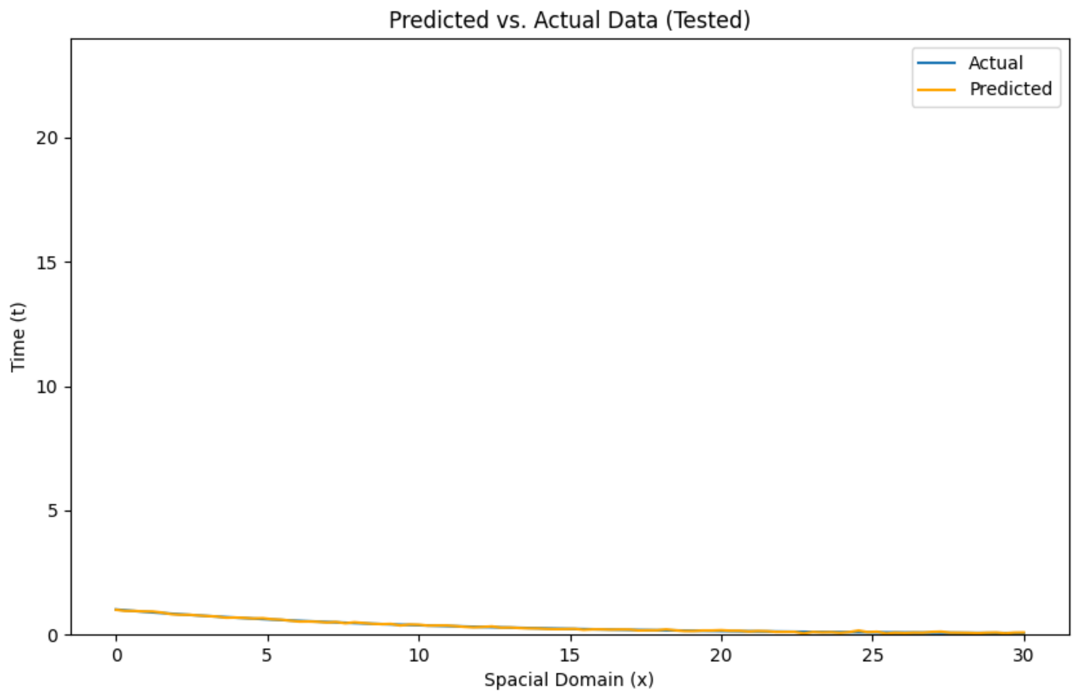


Figure 4.2: Actual vs. Predicted Data for Test Dataset

The plot shows a close alignment between the actual polymer concentration values and those predicted by the PINN model for the test data. The precise tracking of the trend by the predicted test data indicates that the PINN model generalizes well to unseen data. This demonstrates that the model not only captures the underlying dynamics of polymer concentration in the training data but also accurately predicts concentrations for new, unseen conditions, effectively reflecting the spatial and temporal trends.

Training vs. Validation Losses

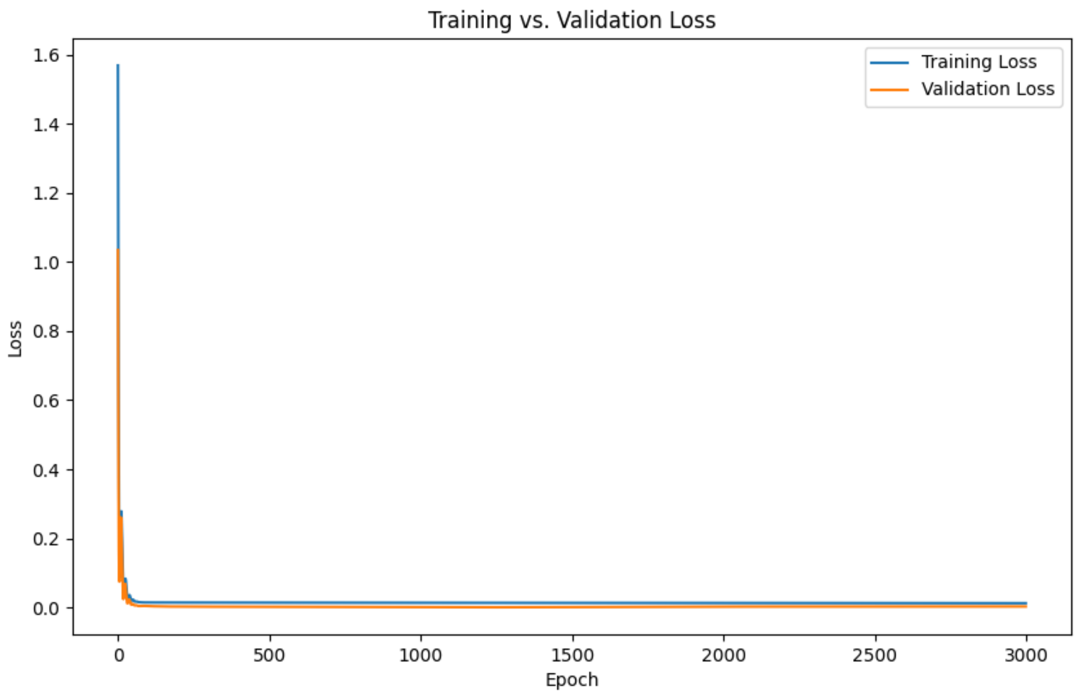


Figure 4.3: Training and Test Losses over Epochs

In Figure 4.3, The plot shows that both training and validation losses decrease quickly during the initial epochs and then stabilize at low values. The alignment of the loss curves suggests that the Physics-Informed Neural Network (PINN) does not overfit and performs well on new, unseen data. The swift convergence to a low loss value indicates that the PINN effectively captures the underlying patterns of polymer concentration in the reservoir simulation with minimal error.

Contour Plot of Predicted Solution

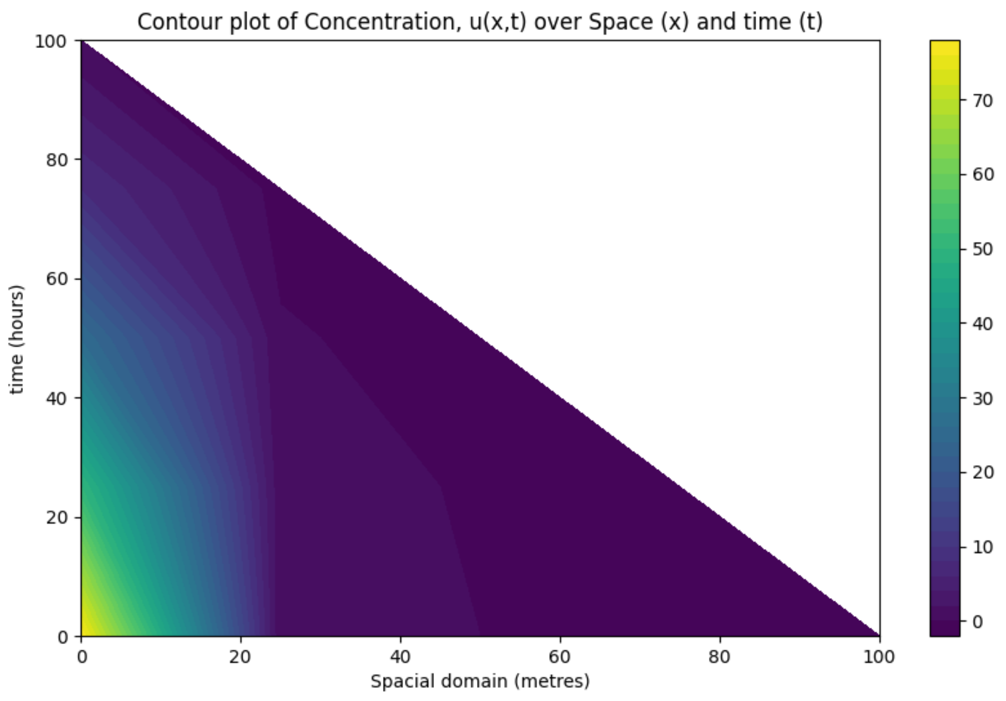


Figure 4.4: Contour Plot of Predicted Solution $u(x, t)$

The contour plot displays the PINN model's prediction of polymer concentration $c(x, t)$ over space and time. The x-axis shows the spatial dimension x, while the y-axis represents time t. The color gradient reflects the concentration magnitude. Smooth color transitions across the spatial and temporal domains indicate that the model effectively captures the variation in polymer concentration over time. The plot reveals how the concentration evolves, including any formation and movement patterns, demonstrating the model's accuracy in simulating polymer dynamics within the reservoir.

Chapter 5

Limitation, Recommendation, and Conclusion

5.1 Limitation

Despite the promising results demonstrated by the PINN model in solving the Burgers' equation, one limitation that needs to be addressed is below:

- **Computational Complexity:** Training PINNs, especially for problems with complex geometries or multi-dimensional spaces, can be quite demanding on computational resources. The use of automatic differentiation, while powerful, leads to significant memory use and longer training times. This means that without ample computational power, PINNs may only be practical for simpler or lower-dimensional problems. Farlow (1993).

5.2 Recommendation

- **Improve Computational Efficiency for Scalability:** Given the strong performance of the current model, itâs essential to focus on making it more efficient for tackling complex problems. This could involve exploring advanced optimization methods like mixed-precision training and model parallelism. Also, utilizing high-performance computing resources such as GPUs and TPUs can help cut down or reduce training times and allow the model to handle more complicated scenarios effectively.

5.3 Conclusion

In this thesis, we explored the use of Physics-Informed Neural Networks (PINNs) to solve Burgers' equation for predicting polymer concentration over space and time in a reservoir. This approach achieved accurate predictions and effectively addressed numerical instabilities by reducing numerical errors. By applying data scaling methods and utilizing the advanced capabilities of PINNs, our model not only achieved accurate predictions of polymer concentration across space and time but also significantly cut down on the cumulative errors that traditional numerical techniques often encounter. The precise scaling of data and thorough training process ensured that the model provided reliable forecasts, proving its effectiveness in predicting polymer concentrations and demonstrating its potential to enhance accuracy in complex reservoir simulations.

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