A Computational Fluid Dynamics Approach for Dissolved Oxygen Modelling

With Application to Wind-Powered Aeration Systems

by

Kamran Mahmudov

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for the degree of Master of Applied Science
Department of Mechanical and Industrial Engineering
University of Toronto

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Abstract

Dissolved oxygen is one of the most critical parameters of water quality in aquaculture. Aeration systems are generally used to improve oxygen levels and yields. However, these systems have high capital and operating cost, require electricity and, thus, are out of reach for farmers in developing countries. There is a need for affordable and sustainable aeration technologies. This thesis presents the development of a computational dissolved oxygen model which evaluates the spatial and temporal distribution of dissolved oxygen to enable evaluation and optimization of new aeration approaches. The three-dimensional model was developed based on Finite Volume Method and validated by bench-scale and field experiments. Results showed that the model was capable of predicting the dissolved oxygen concentration with an average prediction error of 7.2%.

Thesis Supervisor: Amy Bilton

Title: Assistant Professor, Mechanical Engineering, and Director, Center for Global Engineering
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<thead>
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<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Surface area of control volume</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion conductance</td>
</tr>
<tr>
<td>$DO(t)$</td>
<td>Dissolved oxygen concentration</td>
</tr>
<tr>
<td>$DO_{air}$</td>
<td>Change in oxygen content due to re-aeration (mg/Lh)</td>
</tr>
<tr>
<td>$DO_{conv}$</td>
<td>Convective oxygen transport between control volumes (mg/Lh)</td>
</tr>
<tr>
<td>$DO_d$</td>
<td>Oxygen diffusion between control volumes (mg/Lh)</td>
</tr>
<tr>
<td>$DO_{fr}$</td>
<td>Cumulative animal respiration rate of the cultured livestock (mg/Lh)</td>
</tr>
<tr>
<td>$DO_{ph}$</td>
<td>Photosynthetic oxygen generation by phytoplankton (mg/Lh)</td>
</tr>
<tr>
<td>$DO_{pr}$</td>
<td>Respiration rate of phytoplankton, also known as photorespiration (mg/Lh)</td>
</tr>
<tr>
<td>$DO_{sed}$</td>
<td>Sediment (benthic) oxygen demand (mg/Lh)</td>
</tr>
<tr>
<td>$F$</td>
<td>Convective mass flux per unit area</td>
</tr>
<tr>
<td>FAO</td>
<td>Food and Agriculture Organization of the United Nations</td>
</tr>
<tr>
<td>FDM</td>
<td>Finite Difference Method</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite Element Method</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite Volume Method</td>
</tr>
<tr>
<td>$k_l$</td>
<td>Gas transfer velocity</td>
</tr>
<tr>
<td>MAPE</td>
<td>Mean absolute percentage error</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equations</td>
</tr>
<tr>
<td>$Q$</td>
<td>Mass flux of oxygen</td>
</tr>
<tr>
<td>$Q_{tur}$</td>
<td>Mass flux of oxygen at the air-water interface, turbulent water body</td>
</tr>
<tr>
<td>$Q_y$</td>
<td>Mass flux of oxygen at the air-water interface, stagnant water body</td>
</tr>
<tr>
<td>$r$</td>
<td>Renewal frequency (1/s)</td>
</tr>
<tr>
<td>RNG</td>
<td>Renormalization Group</td>
</tr>
<tr>
<td>rpm</td>
<td>Revolution per minute</td>
</tr>
<tr>
<td>RSME</td>
<td>Root-mean-squared-error</td>
</tr>
<tr>
<td>$t$</td>
<td>Time (s)</td>
</tr>
<tr>
<td>$t_k$</td>
<td>Kolmogorov time scale (s)</td>
</tr>
<tr>
<td>$t_r$</td>
<td>Renewal time (s)</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$S_{\varphi}$</td>
<td>Source of dissolved oxygen</td>
</tr>
<tr>
<td>USD</td>
<td>United States Dollar</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume of a control volume</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Velocity field</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Turbulent dissipation rate</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinematic viscosity of water</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of Water</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>Dissolved oxygen concentration (mg/L)</td>
</tr>
<tr>
<td>$\varphi_{sat}$</td>
<td>Saturated dissolved oxygen concentration (mg/L)</td>
</tr>
<tr>
<td>$\varphi_0$</td>
<td>Initial dissolved oxygen concentration (mg/L)</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Diffusion coefficient of oxygen in water (m^2/s)</td>
</tr>
<tr>
<td>$Pe$</td>
<td>Peclet Number</td>
</tr>
</tbody>
</table>
Chapter 1

1. Introduction

1.1. Motivation

Fisheries and aquaculture are important sources of food, protein and income for hundreds of millions of people around the world. According to the Food and Agriculture Organization of the United Nations (FAO), global fish production reached about 171 million tonnes in 2016 with a total first sale value of 362 billion USD. Studies by the FAO also show that the world’s fish supply reached 20.5 kg per capita in 2017 with aquaculture providing 53% (total worth of USD 232 billion) [1]. More than 30% of the world’s wild fish capture is considered unsustainable due to overfishing, resulting in a great interest in aquaculture. Figure 1-1 shows the world’s total wild fish capture and aquaculture production by volume from 1950 to 2016. In fact, aquaculture is also the fastest growing food production sector with an average annual growth rate of 8-10% [2].

In the Asia Pacific region alone, there are more than 20 million people engaged in fish farming. According to FAO, 85% of the total employment in the fisheries and aquaculture sectors is in Asia (10% in Africa, 5% in Latin America and the Caribbean). Additionally, 96% of the global population engaged in aquaculture primarily live in Asia [1].
Aquaculture systems can be categorized into three main groups based on the level of intensification: extensive (small-scale or traditional farming), semi-intensive (medium-scale farming) and intensive (large-scale farming). There are multiple differentiating factors among these categories, however, the main ones are the quantity (biomass) of livestock cultured within a specified water area. This quantity is commonly known as stocking density and yield within a specified water area per year. Table 1-1 highlights levels of intensifications based on the aforementioned factors.

<table>
<thead>
<tr>
<th>Group</th>
<th>Stocking Density (kg/ha)</th>
<th>Yield (t/ha/yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extensive</td>
<td>&lt; 1000</td>
<td>0 – 1</td>
</tr>
<tr>
<td>Semi-Intensive</td>
<td>1000 – 5000</td>
<td>1 – 15</td>
</tr>
<tr>
<td>Intensive</td>
<td>&gt; 5000</td>
<td>15 – 50</td>
</tr>
</tbody>
</table>

The majority of small-scale farmers are individual entrepreneurs or households who are engaged in extensive farming. For many farmers, their yield is the only source of food and income. Their farms solely
rely on natural nutrients available in fish ponds which is similar to natural water bodies hosting multiple fish species. These smallholders usually live in rural areas and in most cases, they do not have secure access to electricity. They are typically resource-poor and not able to apply any advanced aquaculture practices in their systems due to lack of capital. These are homestead ponds, generally not managed and maintained for optimal fish production and often suffer from poor water quality. As a result, yields from extensive farms are substantially lower than semi-intensive and intensive farms, as given in Table 1-1. It should be noted that over 90% of fish farmers (more than 18 million) are classified as small-scale farmers in South-East Asia [2].

There are multiple parameters affecting the productivity of aquaculture systems. One of the major aspects which influences production for smallholder farmers is the lack of water quality management, which has direct impact on survival, growth and reproduction of cultured species. In aquaculture systems, the main parameters which affect water quality are levels of stocking density, nutrients, organic matter, pH, salinity, plankton population and dissolved oxygen (DO). In fact, the most critical component of the healthy aquaculture ponds is the amount of DO present water as all fish require a constant supply of DO. In addition, DO is the most important factor affecting the growth of fish after feed [5].

The amount of oxygen consumed by fish is heavily dependent on the fish species. Cultured fish species in aquaculture systems usually require higher levels of dissolved oxygen, which varies from 4 mg/L to 5mg/L [6]. Experimental studies show that whichever species are cultured, having higher DO levels is always beneficial for farmers. There is a positive correlation between fish growth & health and DO levels [7], [8], [9].

Dissolved oxygen is a crucial component for all organisms in fish ponds as it supports fish, zooplankton, phytoplankton and benthic bacteria on the water bed. There are two main natural sources of oxygen in fish ponds as in other water bodies: oxygen transfer from atmosphere to the surface of the pond and oxygen generation in the pond from the photosynthesis by surface dwelling phytoplankton. Oxygen transfer from atmosphere to the water surface occurs when the oxygen concentration is less than the oxygen saturation
level at the surface of the water. This transfer rate is often limited due to the slow rate of molecular diffusion in the water body, resulting high oxygen concentration at the water surface. Oxygen generation from photosynthesis also tends to occur at the water surface. During the daytime, the sunlight cannot penetrate deeply through water column, resulting in oxygen generation at the surface. However, the opposite happens at night, due to respiration of fish and phytoplankton, oxygen is consumed, and the overall DO content of the pond is lowered. This daily fluctuation in dissolved oxygen level is called a diurnal oxygen cycle which is shown in Figure 1-2.

![Figure 1-2: Daily DO fluctuation at the pond surface](10)

According to Lambert’s law, the amount of thermal energy received by the water column from solar radiation decreases with distance from the surface of the pond. Furthermore, due to continuous solar heating during daytime, the surface water becomes warmer and less dense while water at the bottom of the pond receives less sunlight and remains cool. This creates a negative temperature gradient through the pond depth, which is commonly referred to as thermal stratification as illustrated in Figure 1-3 [11]. The thermal stratification prevents natural pond mixing unless there is heavy rainfall or strong winds during most of the warm months. Thus, since both oxygen transfer and generation happen at the surface, the warm top layer (epilimnion) of the fish pond becomes supersaturated with oxygen while the bottom layer (hypolimnion) lacks oxygen and stays cold. Furthermore, due to supersaturation within the epilimnion, oxygen is being
lost to the atmosphere. This non-uniform oxygen distribution can create anoxic conditions, causing high rates of fish mortality and poor growth if the pond is overstocked [12]. In addition, supersaturated water in the top layers may also lead to fish buoyancy problems, commonly known as Swim Bladder disease [13], [14]. In addition, since the larger portion of pond water is oxygen depleted, it creates uneven stocking distribution, leaving more than half of the pond volume uninhabited, limiting the stocking density and overall yield.

![Figure 1-3: Daytime stratification in a typical 2.5 m deep fish pond [11]](image)

There are several strategies used to solve the problems mentioned in Section 1.3. and improve overall DO content in aquaculture ponds. For example, aeration systems are commonly used by large industrial companies for semi-intensive and intensive farming. Aeration is a process of adding and distributing oxygen throughout the water column in fish ponds by either circulating pond water or injecting oxygen into the
pond. The recent studies show that with aeration systems, fish become more active, grow faster and 47% higher yields can be achieved compared to ponds without aeration systems [15], [16].

There are different types of pond aerators and the common ones used in intensive aquaculture are surface aerators. These systems move oxygen depleted water from the bottom to the surface of the pond and increases the amount of water droplets in contact with air by splashing surface water while bringing oxygen-enriched water to the bottom of the pond. The most common surface aerators are paddle wheel aerators (Figure 1-4), propeller-aspirator pumps, and vertical pump aerators [17]. In addition to an increased oxygen transfer, these systems also introduce mixing and destratification by circulating oxygen enriched water from the surface to different regions of the water. They create uniform oxygen distribution within fish ponds, limit oxygen losses from the surface water to atmosphere and create a healthy environment for fish and all other organisms in the pond.

![Figure 1-4: Paddle-wheel aerator](image)

Surface aerators have high capital and maintenance cost and require uninterrupted access to electricity [18]. Thus, these systems are only used in medium- and large-scale aquaculture farms and are economically out of reach for extensive farmers residing in rural communities of developing countries, such as in rural
Bangladesh or Vietnam [19]. Thus, smallholder farmers across the rural Southeast-Asia region suffer from poor pond productivity, which is the result of low stocking density and frequent fish kills. Furthermore, paddle-wheel aerators have an average market cost of ~$800 and require 1.5kW of continuous power consumption annually. Power consumption of these aerators comprises up to 15% of operating costs for semi-intensive and intensive farmers, which significantly lengthens pay-back periods for these technologies to reach a break-even point for adoption.

Based on a survey conducted among smallholders during field visits and in-person interviews in rural Bangladesh, less than a third of 2,388 sampled households have access to grid electricity. Moreover, those who have access to electricity experience multiple power outages each month. In another survey conducted among 120 fish farmers in Mymensingh, Bangladesh, it was found that only 5 farmers used paddle-wheel aerators, while a number of them relied on the use of oxygen tablets to maintain dissolved oxygen levels. A specific example of the oxygen tablets used in Bangladesh is ACI’s ‘Aci-Ox’ oxygen tablets as shown in Figure 1-5.

![Aci-Ox oxygen tablets](image)

*Figure 1-5: ACI animal health oxygen tablets used by extensive farmers in Mymensingh, Bangladesh*

Oxygen tablets rapidly release oxygen into the pond, help control the growth rate of phytoplankton, and limit the spread of parasites in the water. Farmers add these tablets to their ponds when low DO conditions
are suspected. Farmers in the survey would typically apply these tablets every two weeks to help boost dissolved oxygen content in the water. However, oxygen tablets have several limitations. First, they are used primarily when low DO conditions arise, meaning the farmer must constantly monitor the pond status and determine when the tablets are needed. In the developing world, this is often determined based on fish behavior and by the time DO level increases the fish are already stressed resulting in low productivity. Secondly, it has a large ongoing cost. Finally, these tablets have been shown to affect other water properties, such as pH parameters, which have adverse effects on fish growth and health.

Thus, there is a need for (a) affordable, sustainable aeration technologies which will reliably improve dissolved oxygen concentration and require no secure electricity access for extensive farmers in rural areas and (b) precision aquaculture systems that will decrease operating costs of aeration devices in semi-intensive and intensive aquaculture systems. Current practices show that in order to design such technologies, experimental studies are carried out, which are time consuming and very expensive. Therefore, there is a demand for mathematical models to develop aquaculture technologies, especially aeration devices. However, to date, there are limited models to design and optimize aeration systems to have higher dissolved oxygen concentration throughout the ponds. Such models would enable designers to estimate spatial and temporal distribution of DO in aquaculture ponds and determine aeration system configurations that achieve the highest efficiency.

1.2. Thesis Objective and Contributions

The objective of this thesis was to develop a computational fluid dynamics (CFD) based dissolved oxygen model to evaluate the spatial and temporal distribution of DO concentration in an aquaculture pond. The proposed model uses a custom CFD code to determine the influence of factors on DO levels, such as circulation due to aeration devices and oxygen transfer from the atmosphere. Various discretization schemes were analyzed, and the most suitable techniques were selected for the given application. The model
was developed based on the Finite Volume Method (FVM), coded in Python and validated through multiple experiments conducted in laboratory and in field. During these experiments a newly developed concept, a wind powered aeration system – hereafter referred as WERLWind – was tested. It was found that WERLWind has a huge potential to improve the livelihood of over 18 million extensive fish farmers.

1.3. Thesis Outline

The outline of this thesis begins with Chapter 2 which presents a review of the existing model from literature that aided in the development of the proposed DO model. Chapter 2 also reviews some of the CFD techniques used to create this model. Following this, Chapter 3 introduces the development of the three-dimensional dissolved oxygen model. Next, Chapter 4 presents the bench-scale validation and calibration of the model. Next, Chapter 5 reviews the field experiments conducted in the aquaculture research facility in Australia. Lastly, Chapter 6 summarizes the thesis and discusses future work.
Chapter 2

2. Literature Review and Background

This chapter presents a literature review conducted to understand the strengths and limitations of current dissolved oxygen models. Furthermore, additional studies were carried out to compare different tools that can be used to develop the proposed numerical dissolved oxygen model, especially various finite volume computational fluid dynamics techniques. The last section of this chapter describes the design and working principle of a wind powered aeration system, WERLWind, which is used for multiple lab-scale experiments and field trials conducted by the author to validate the computational dissolved oxygen model.

2.1. Existing and Proposed Dissolved Oxygen Models

There have been many attempts to develop a dissolved oxygen model capable of predicting the DO concentration based on the environmental conditions and cultured livestock species in aquaculture ponds. The most recent dissolved oxygen model was developed by Ahmed Mahmoud [20]. In this work, Mahmoud developed a one-dimensional DO model capable of modelling the upper and bottom layers of the pond. In the simplest form, the DO of a volume of water can be modelled using Equation 2.1.

\[
\frac{dC}{dt} = \frac{P - R + k(C_s - C)}{z} \quad (2.1)
\]

where \( P \) is the instantaneous rate of oxygen production in the pond (mg/Lh), \( R \) is the instantaneous rate of oxygen respiration in the pond (mg/Lh), \( k \) is the molecular diffusivity of oxygen between air and water (m/h), \( C_s \) is dissolved oxygen concentration at atmospheric equilibrium (mg/m\(^3\)), \( C \) is dissolved oxygen
concentration (mg/m³) and z is the layer depth (m). To account for the vertical variation, Mahmoud derived a one-dimensional DO model which splits water body into two control volumes, the top and bottom layers as shown in Figure 2-1.

\[
\frac{dDO}{dt}_{CV} = (DO_{ph} - DO_{pr}) - DO_{fr} \pm DO_{air} - DO_{sed} \pm DO_d \pm DO_{conv} \quad (2.2)
\]

where:
\(\frac{d DO}{dt}_{CV}\) is the net dissolved oxygen change in the control volume (mg/Lh)

\(DO_{ph}\) is the photosynthetic oxygen generation by phytoplankton (mg/Lh) [21]

\(DO_{pr}\) is the respiration rate of phytoplankton, also known as photorespiration (mg/Lh) [23]

\(DO_{fr}\) is the cumulative animal respiration rate of the cultured livestock (mg/Lh) [23]

\(DO_{air}\) is the change in oxygen content due to re-aeration (mg/Lh) [22]

\(DO_{sed}\) is the sediment (benthic) oxygen demand (mg/Lh) [21]

\(DO_{d}\) is the rate of oxygen diffusion between control volumes (mg/Lh)

\(DO_{conv}\) is the rate of convective oxygen transport between control volumes (mg/Lh)

After calculating net change of dissolved oxygen concentration in each control volume, a time-series model was used to predict dissolved oxygen levels over a specified time period for each control volume. The following equation was used to find the DO profile:

\[
DO(t)|_{CV} = DO(t - 1)|_{CV} + \left(\frac{d DO}{dt}\right) \Delta t \quad (2.3)
\]

where \(DO(t)|_{CV}\) and \(DO(t - 1)|_{CV}\) are the DO concentrations (mg/L) at time \(t\) and \((t - 1)\), respectively, for a given control volume, and \(\Delta t\) is the time step (h) in the time-series model.

There is a limitation with this model, in that it does not consider the spatial variation of dissolved oxygen concentration. According to this model, DO levels are uniform within each control volume. Therefore, it is impossible to assess the impact of aeration technologies in three-dimensions.

The proposed DO model in thesis is a 3-D, transient, custom computational fluid dynamics based model which simulates DO dynamics to predict spatial and temporal variations of DO concentration due to any aeration technologies. As shown in Figure 2-2, the proposed model splits the water bodies into multiple,
uniform control volumes and calculates dissolved oxygen concentration at the center of each control volume.

The proposed model is developed based on the Finite Volume Method (FVM) and programmed in Python. The following sections review the Finite Volume Method and some of the techniques used to develop the DO model. The last section describes the working principle of the WERLWind device.

2.2. Numerical Method – Finite Volume Method

The Finite Volume Method (FVM) is a numerical technique which converts transport equations or conservation equations (described in the following section) from the partial differential equation (PDE) form into a system of linear algebraic equations. These linear equations are applied to the finite control volumes which are also called cells or elements. There are two main steps involved in this process like in
other numerical techniques such as the Finite Element Method (FEM) or the Finite Difference Method (FDM): integration and transformation of the PDE’S into a balance equation over each cell and transformations of algebraic relations into a system of algebraic linear equations by using interpolation techniques. The system of linear equations is then solved to find the values of the unknown variables for each control volume, where each equation corresponds to a control volume.

There are several advantages of using the Finite Volume Method. Firstly, this method is strictly conservative which makes it the preferred method for energy and mass transfer problems. This is because in the FVM, some terms in the conservation equations are converted into face fluxes which are then calculated at the finite volume faces. The face fluxes entering and leaving the adjacent volumes are equal to each other which makes the method conservative. In addition, although in this thesis uniform mesh structures were used, in the FVM, the unstructured polygonal meshes can be easily generated. Finally, different types of boundary conditions can be implemented in a non-invasive manner using the Finite Volume Method. This is because the dependent variables are calculated at the center of each cell and not at faces.

Overall, due to aforementioned advantages of the FVM, it is the most suitable method for the computational analysis of fluid flow, mass and heat transfer problems.

2.3. The General Transport Equation: Differential and Integral Forms

By denoting a dependent variable \( \varphi \), the general differential form of the transport equation can be written as:

\[
\frac{\partial (\rho \varphi)}{\partial t} + \text{div} (\rho \varphi \mathbf{v}) = \text{div} (\Gamma \text{grad} \varphi) + S_\varphi \tag{2.4a}
\]

or

\[
\frac{\partial (\rho \varphi)}{\partial t} + \nabla \cdot (\rho \varphi \mathbf{v}) = \nabla \cdot (\Gamma \nabla \varphi) + S_\varphi \tag{2.4b}
\]
where

\[ \frac{\partial (\rho \phi)}{\partial t} \]

is the transient or temporal term representing rate of change of \( \phi \)

\[ \text{div}(\rho \phi \mathbf{v}) \text{ or } \nabla \cdot (\rho \phi \mathbf{v}) \]

is the convective term

\[ \text{div}(\Gamma \text{grad} \phi) \text{ or } \nabla \cdot (\Gamma \nabla \phi) \]

is the diffusion term

\( S_{\phi} \)

is the source or sink term

In addition, \( \rho \) is the density of fluid, \( \mathbf{v} \) is the velocity vector, and \( \Gamma \) is the molecular diffusion coefficient. The general representation of the transport equation consists of the unsteady term, the convection term, the diffusion term and source term. The unknown or dependent variable \( \phi \) may represent a concentration of a species, a velocity component or enthalpy depending on the problem. In this thesis, \( \phi \) represents concentration of dissolved oxygen in mg/L.

The first step in obtaining the integral form of transport equation is the integration of equation (2.4a) over a three-dimensional control volume denoted as (CV). This process results in equation (2.5) shown below:

\[ \int_{CV} \frac{\partial (\rho \phi)}{\partial t} dV + \int_{CV} \text{div}(\rho \phi \mathbf{v}) dV = \int_{CV} \text{div}(\Gamma \text{grad} \phi) dV + \int_{CV} S_{\phi} dV \quad (2.5) \]

According to Gauss’s divergence theorem, for a given vector \( \mathbf{a} \) the following relationship can be obtained.

\[ \int_{CV} \text{div}(\mathbf{a}) dV = \int_{A} \mathbf{n} \cdot a dA \quad (2.6) \]

where \( \mathbf{n} \) represents a normal vector to a surface element \( dA \). In other words, \( \mathbf{n} \cdot a \) is the component of vector \( a \) in the direction of normal vector \( \mathbf{n} \). Applying the Gauss’s divergence theorem, equation (2.5) can be transformed into the following equation:

\[ \frac{\partial}{\partial t} (\int_{CV} \rho \phi dV) + \int_{A} \mathbf{n} \cdot (\rho \phi \mathbf{v}) dA = \int_{A} \mathbf{n} \cdot (\Gamma \text{grad} \phi) dA + \int_{CV} S_{\phi} dV \quad (2.7) \]
In steady-state problems, the first term on the left side of equation (2.7) is dropped. However, for unsteady problems, this equation is integrated with respect to time \( t \) over a time step or interval \( \Delta t \). This results in the general integral form of transport equation as shown below.

\[
\int_{\Delta t} \frac{\partial}{\partial t} \left( \int_{CV} \rho \varphi dV \right) dt + \int_{\Delta t} \int_{A} \mathbf{n} \cdot (\rho \varphi \mathbf{v}) dA dt = \int_{\Delta t} \int_{CV} \mathbf{n} \cdot (\Gamma \nabla \varphi) dV dt + \int_{\Delta t} \int_{CV} S_{\varphi} dV dt
\] (2.8)

The following section describes different types of discretization techniques applied to each term in the integral form of the transport equation. In order to show the discretization methods for each term separately, the one-dimensional steady-state version of each term was used.

### 2.4. Discretization of Diffusion and Source Terms

A one-dimensional steady-state diffusion equation with a source term is shown below.

\[
\frac{\partial}{\partial x} \left( \Gamma \frac{\partial \varphi}{\partial x} \right) + S_{\varphi} = 0
\] (2.9)

where \( \Gamma \) is the diffusion coefficient and \( S_{\varphi} \) is the source term.

The first step in the finite volume method is grid generation. A control volume having a central node \( P \) with two neighboring nodes denoted as east and west (E and W) is shown below.

![Figure 2-3: 1-Dimensional control volume with adjacent nodes [24]](image)
In this configuration, lower case letters (e and w) show the element faces. Distances between the nodes W-P and P-E are denoted as $\delta x_{WP}$ and $\delta x_{PE}$ respectively. Also, distances between face w-P and P-e are identified as $\delta x_{wp}$ and $\delta x_{pe}$ respectively. In this configuration, the width of the control volume is given as $\Delta x = \delta x_{we}$. It is worth mentioning that the numerical model that is developed in this thesis uses uniform grid structures. Thus, distances between the nodes and faces are equal ($\Delta x$).

The second step of the finite volume method involves the discretization process. To do so, the 1D governing equation is integrated over a control volume as shown below.

$$
\int_{\Delta V} \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \psi}{\partial x} \right) dV + \int_{\Delta V} S_{\psi} dV = 0 \tag{2.10}
$$

This can be written as:

$$
\left( \Gamma A \frac{\partial \psi}{\partial x} \right)_e - \left( \Gamma A \frac{\partial \psi}{\partial x} \right)_w + S_{\psi} \Delta V = 0 \tag{2.11}
$$

In equation (2.11) $\Delta V$ is the volume and $A$ is the cross-section of the control volume or area of the faces. The main feature of this discretized equation is that the differences between flux of $\psi$ leaving and entering the control volume equals the generation of $\psi$ inside the control volume.

To calculate the value of the property $\psi$ at nodal points, linear approximation or central differencing method is used. The result is given below.

$$
\left( \Gamma A \frac{\partial \psi}{\partial x} \right)_e = \Gamma_e A_e \left( \frac{\psi_e - \psi_F}{\delta x_{FE}} \right) \tag{2.12a}
$$

$$
\left( \Gamma A \frac{\partial \psi}{\partial x} \right)_w = \Gamma_w A_w \left( \frac{\psi_w - \psi_E}{\delta x_{WP}} \right) \tag{2.12b}
$$

It is practical to approximate the source term $S_{\psi}$ as a function of a dependent variable. This approximation, shown below, is linear and well-suited for the finite volume method.
\[ S_{\varphi} \Delta V = S_u + S_p \varphi \]  \hspace{1cm} (2.13)

Substituting all the equations shown above into equation (2.11) gives:

\[ \Gamma_e A_e \left( \frac{\varphi_E - \varphi_P}{\delta x_{PE}} \right) - \Gamma_w A_w \left( \frac{\varphi_P - \varphi_W}{\delta x_{WP}} \right) + (S_u + S_p \varphi) = 0 \]  \hspace{1cm} (2.14a)

or

\[ \left( \frac{\Gamma_e}{\delta x_{PE}} A_e + \frac{\Gamma_w}{\delta x_{WP}} A_w - S_p \right) \varphi_p = \left( \frac{\Gamma_e}{\delta x_{PE}} A_e \right) \varphi_E + \left( \frac{\Gamma_w}{\delta x_{WP}} A_w \right) \varphi_W + S_u \]  \hspace{1cm} (2.14b)

This equation can be written in a simple form as:

\[ a_p \varphi_p = a_W \varphi_W + a_E \varphi_E + S_u \]  \hspace{1cm} (2.15)

where the coefficients are given in Table 2-1.

<table>
<thead>
<tr>
<th>( a_W )</th>
<th>( a_E )</th>
<th>( a_p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>\frac{\Gamma_w}{\delta x_{WP}} A_w</td>
<td>\frac{\Gamma_e}{\delta x_{PE}} A_e</td>
<td>a_W + a_E - S_p</td>
</tr>
</tbody>
</table>

### 2.5. Discretization of Convection Term

A one-dimensional steady-state convection-diffusion equation without a source term is shown below:

\[ \frac{d}{dx} (\rho u \varphi) = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \varphi}{\partial x} \right) \]  \hspace{1cm} (2.16)

where \( u \) is the one-dimensional flow field and \( \rho \) is the density of the fluid.

In addition, the flow field must meet the continuity requirement as shown below:

\[ \frac{d(\rho u)}{dx} = 0 \]  \hspace{1cm} (2.17)
A one-dimensional control volume having a central node P with two neighboring nodes denoted as east and west (E and W) is shown below.

![Figure 2-4: 1D control volume](image)

The 1D governing equation is integrated over a control volume as shown below.

\[
(ρuAφ)_e - (ρuAφ)_w = \left( ΓA \frac{∂φ}{∂x} \right)_e - \left( ΓA \frac{∂φ}{∂x} \right)_w 
\] (2.18)

\[
(ρu)_e - (ρu)_w = 0 \] (2.18)

Two variables are introduced to conveniently represent convective mass flux per unit area \( F \) and diffusion conductance \( D \) at cell faces, where

\[
F = ρu \] (2.20a)

\[
D = \frac{Γ}{A} \frac{∂A}{∂x} \] (2.20b)

Substituting these equations into equations (2.18) and (2.19) and as gives following two equations:

\[
F_eφ_e - F_wφ_w = D_e(φ_E - φ_P) - D_w(φ_P - φ_W) \] (2.21a)

\[
F_e - F_w = 0 \] (2.21b)

Assuming the flow field is given, to solve the equations above, values of \( φ \) should be calculated at the faces of the control volume. There are different schemes to conduct these calculations. The following paragraphs give brief descriptions on these discretization schemes.
The Central Differencing Scheme

The central differencing scheme uses linear approximation to calculate the face values. For the one-dimensional uniform grids, this approximation is given below:

\[ \varphi_e = \frac{(\varphi_P + \varphi_E)}{2} \]  

(2.22a)

\[ \varphi_w = \frac{(\varphi_W + \varphi_P)}{2} \]  

(2.22a)

Substituting these approximations into equation (2.21a) results in following discretized one-dimensional convection-diffusion equation:

\[ a_P \varphi_P = a_W \varphi_W + a_E \varphi_E + S_u \]  

(2.23)

where the coefficients are given in Table 2-2.

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(a_w)</td>
<td>(a_e)</td>
<td>(a_p)</td>
</tr>
<tr>
<td>(D_w + \frac{F_w}{2})</td>
<td>(D_e - \frac{F_e}{2})</td>
<td>(a_w + a_e - (F_e - F_w))</td>
</tr>
</tbody>
</table>

Table 2-2: Coefficients of 1D discretized convection - diffusion equation with central differencing scheme

The Upwind Differencing Scheme

The upwind differencing scheme uses flow direction information to calculate the value of \(\varphi\) at a cell face. The value of the transported property \(\varphi\) at a cell face is assumed to be equal to the value at the upstream node. Mathematical representation of the one-dimensional upwind differencing scheme is given below.

If the flow is in the positive direction: \(u_w > 0, \ u_e > 0\)

\[ \varphi_w = \varphi_W \text{ and } \varphi_e = \varphi_P \]

If the flow is in the negative direction: \(u_w < 0, \ u_e < 0\)
\[ \varphi_w = \varphi_p \text{ and } \varphi_e = \varphi_E \]

Substituting the above expressions into equation (2.21) results in the following discretized one-dimensional convection-diffusion equation:

\[ a_p \varphi_p = a_W \varphi_W + a_E \varphi_E + S_u \quad (2.24) \]

where the coefficients are given in Table 2-3.

**Table 2-3: Coefficients of 1D discretized convection - diffusion equation with upwind differencing scheme**

<table>
<thead>
<tr>
<th>Condition</th>
<th>( a_W )</th>
<th>( a_E )</th>
<th>( a_p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_w &gt; 0, F_e &gt; 0 )</td>
<td>( D_w + F_w )</td>
<td>( D_e )</td>
<td>( a_W + a_E - (F_e - F_w) )</td>
</tr>
<tr>
<td>( F_w &lt; 0, F_e &lt; 0 )</td>
<td>( D_w )</td>
<td>( D_e - F_e )</td>
<td>( a_W + a_E - (F_e - F_w) )</td>
</tr>
</tbody>
</table>

This can be written as:

**Table 2-4: Coefficients of 1D discretized convection - diffusion equation with upwind differencing scheme (general form)**

<table>
<thead>
<tr>
<th>( a_W )</th>
<th>( a_E )</th>
<th>( a_p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_w + \max(F_w, 0) )</td>
<td>( D_e + \max(0, -F_e) )</td>
<td>( a_W + a_E - (F_e - F_w) )</td>
</tr>
</tbody>
</table>

**The Hybrid Differencing Scheme**

This scheme uses a combination of the central and upwind differencing schemes. The final discretized one-dimensional convection-diffusion equation is written as:

\[ a_p \varphi_p = a_W \varphi_W + a_E \varphi_E + S_u \quad (2.25) \]

where the coefficients are given in Table 2-5.
Table 2.5: Coefficients of 1D discretized convection - diffusion equation with hybrid differencing scheme

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_W$</td>
<td>$a_E$</td>
<td>$a_P$</td>
</tr>
<tr>
<td>$\max \left[ F_w, \left( D_w + \frac{F_w}{2} \right), 0 \right]$</td>
<td>$\max \left[ -F_e, \left( D_e - \frac{F_e}{2} \right), 0 \right]$</td>
<td>$a_W + a_E - (F_e - F_w)$</td>
</tr>
</tbody>
</table>

There are other differencing schemes to calculate the face values of the transported property, $\varphi$ such as higher order differencing schemes and the power-law scheme. However, for the purpose of this work, only the three differencing schemes shown above are assessed. These numerical schemes should hold certain properties in order to be physically realistic. The most important properties are conservativeness, boundedness and transportiveness, describes below.

**Conservativeness**

The main idea behind the finite volume method is to integrate the convection-diffusion equation over a certain number of finite control volumes which results in a set of discretized equations. These equations involve surface fluxes of $\varphi$. The conservativeness property states that fluxes of $\varphi$ entering a control volume should equal the fluxes of $\varphi$ leaving the control volume.

The Central, Upwind and Hybrid Differencing Schemes are all conservative.

**Boundedness**

The finite volume method produces a set of algebraic equations that need to be solved by using different techniques. Most common numerical techniques to solve these equations are iterative numerical techniques. The set of equations is represented by a large matrix. To solve it, it is desirable to have a diagonally dominant matrix, which is the characteristic of the boundedness criterion. In addition, this property also states that if there is no source term the internal nodal values of transported property, $\varphi$ should be bounded by the boundary values. Finally, the boundedness property requires all coefficients of the discretized equations should have the same sign, which is usually positive.
The Central Differencing Scheme does not always hold the boundedness property.

The Upwind Differencing Scheme satisfies the boundedness property.

The Hybrid Differencing Scheme satisfies the boundedness property.

**Transportiveness**

Transportiveness can be explained by introducing the Peclet number, which is the ratio of convection to diffusion and can be written as

\[ Pe = \frac{F}{D} = \frac{\rho u}{\Gamma/\partial x} \]  \hspace{1cm} (2.26)

The equation above states that if there is no convection (i.e., pure diffusion) the fluid will be stagnant and the diffusion process will spread the transported property \( \varphi \) equally in all directions \((Pe \to 0)\). In case of pure convection, the transported property \( \varphi \) at a given nodal point will only be affected by the upstream values and the effect of the downstream values will be zero \((Pe \to \infty)\). The transportiveness property holds the influence of the magnitude of the Peclet number and the direction of the flow.

The Central Differencing Scheme does not satisfy the transportiveness property.

The Upwind Differencing Scheme satisfies the transportiveness property.

The Hybrid Differencing Scheme satisfies the transportiveness property.

### 2.6. Discretization of the Temporal Term

There are three main schemes to discretize the temporal term of the transport equation. These are explicit, Crank-Nicolson and implicit schemes. However, for explicit and Crank-Nicolson schemes, there is a maximum limit to the time step size [24]. It is a serious limitation for using these two schemes, since the
The purpose of the dissolved oxygen model is to understand the oxygen dynamics in an aquaculture pond for long period of time. Thus, it is not practical to use these schemes.

However, the implicit scheme does not have any maximum limit to the time step size, making it the preferred method for this application [24]. The final discretized one-dimensional unsteady diffusion equation is given below:

\[
a_p \phi_p = a_W \phi_W + a_E \phi_E + a_p^{\circ} \phi_p^{\circ} + S_u \quad (2.27)
\]

where the coefficients are given in Table 2-6.

<table>
<thead>
<tr>
<th>(a_W)</th>
<th>(a_E)</th>
<th>(a_p)</th>
<th>(a_p^{\circ})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{\Gamma_w}{\delta x_{WP}} A_w)</td>
<td>(\frac{\Gamma_e}{\delta x_{PE}} A_e)</td>
<td>(a_W + a_E + a_p^{\circ} - S_p)</td>
<td>(\frac{\Delta V}{\Delta t}), where (\Delta V = \Delta x)</td>
</tr>
</tbody>
</table>

In these equations, superscript zero \((^{\circ})\) refers to the transported property \(\phi\) at time \(t\) and equations above are designed to find the values at time \(t + \Delta t\).

### 2.7. WERLWind – Wind Powered Aeration System

Small-scale or extensive aquaculture is an important source of income and food in many developing countries, especially in South-East Asia. Farmers in this region do not have access to electricity and they are not in good financial standing. As a result they cannot adopt existing aeration technologies because these systems require continuous power along with high capital and operating costs. Thus, smallholders suffer from low yield due to poor water quality management, caused especially by a lack of dissolved oxygen [20].
In this work, a newly developed wind powered aeration device, WERLWind, is used to validate the DO model through multiple experiments [25]. WERLWind could potentially be used in rural communities to more effectively circulate the pond water and improve DO content without electricity. The system includes a vertical axis wind turbine attached to a subsurface impeller via a shaft. The impeller is inside a draft tube. This system converts wind energy directly to mechanical work to rotate the impeller which introduces circulation in a pond and limits dissolved oxygen losses to the atmosphere. An example of this system is seen in Figure 2-5.

![Figure 2-5: Design of the WERLWind system](image)

There are many advantages of using WERLWind. The system does not require any electricity since it is purely based on wind energy. Furthermore, it can operate with low input torques, meaning the device can be used in the areas with low-to-medium wind speeds. In addition, WERLWind can be easily constructed, operated, and maintained by the farmers. Finally, due to the local construction, the device can be made inexpensively and be easily accessible to low-income fish farmers. Figure 2-6 shows the prototype built in Bangladesh.
In this work a motorized version of WERLWind was used to conduct bench-scale and full-scale experiments to validate the dissolved oxygen model. Using the motorized version of the device, the angular velocity of the impeller can be controlled. This allows one to find the flow field accurately by conducting CFD analysis on ANSYS Fluent. Details of this work are explained in next chapter.

2.8. Chapter Summary

In this chapter, a brief overview of the most recently developed dissolved oxygen model was described. It was found that the existing DO models are not capable of predicting the DO distributions spatially and temporally, which is crucial to the design and optimization of aeration devices. Subsequently, the proposed dissolved oxygen model was introduced, which uses FVM techniques. Moreover, in order to develop the model, the general transport equation was introduced, and a literature review was conducted on different discretization schemes. Finally, the working principles of the newly developed wind powered aeration
system were described. The following chapter aims to use the techniques studied in this chapter and describes the process of developing the DO model.
Chapter 3

3. Dissolved Oxygen Modeling

This chapter presents a newly developed dissolved oxygen model. The chapter starts with the discretization of the three-dimensional, transient transport equation. The following section describes the boundary conditions used to model oxygen transfer in aquaculture ponds. In order to obtain a velocity field and oxygen transfer coefficients generated by the aeration devices, fluid flow simulations were conducted using ANSYS Fluent software. The parameters of these simulations are introduced in this chapter. Detailed experimental validation of the developed CFD model is also described. Finally, the computational solver used to calculate the dissolved oxygen concentration is introduced.

3.1. Discretization of the Transport Equation

Dissolved oxygen dynamics in aquaculture ponds can be represented with a three-dimensional transient convection-diffusion equation with a source term as shown below.

\[
\frac{\partial}{\partial t} (\rho \varphi) + \frac{d}{dx} (\rho u \varphi) + \frac{d}{dy} (\rho v \varphi) + \frac{d}{dz} (\rho w \varphi) = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \Gamma \frac{\partial \varphi}{\partial z} \right) + S_{\varphi} \quad (3.1)
\]

where:

\[\varphi\] is the dissolved oxygen concentration

\[\rho\] is the density of water
\(u, v, w\) are components of the velocity field in \(x, y\) and \(z\) direction respectively

\(\Gamma\) is the diffusion coefficient of oxygen in water

\(S_\varphi\) oxygen generation or consumption in water

Before discretizing the transport equation, a 3D control volume is introduced. A control volume having a central node \(P\) with six neighboring nodes denoted as east, west, north, south, top and bottom (E, W, N, S, T, B) is shown in Figure 3-1.

![Figure 3-1: A 3-Dimensional control volume with adjacent nodes](#)

In order to discretize the diffusion term, the central differencing scheme was used. Since the upwind differencing scheme meets conservativeness, boundedness and transportiveness requirements, and due to easiness of its implementation, this scheme was chosen to discretize the convection term. Finally, as was
stated in Chapter 2, since the implicit scheme does not have any maximum limit to the time-step size, it was chosen to discretize the temporal term in the transport equation.

By following the same discretization steps described in Chapter 2, the final three-dimensional discretized equation with a source term will be as follows:

\[ a_p \varphi_p = a_W \varphi_W + a_E \varphi_E + a_S \varphi_S + a_N \varphi_N + a_B \varphi_B + a_T \varphi_T + a_{p} \varphi_p^{o} + S_u \]  \hspace{1cm} (3.2)

where the coefficients are given in Table 3-1.

**Table 3-1: Coefficients of discretized 3D transport equations**

<table>
<thead>
<tr>
<th>( a_W )</th>
<th>( a_E )</th>
<th>( a_S )</th>
<th>( a_N )</th>
<th>( a_B )</th>
<th>( a_T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_w ) ( + \max(F_w, 0) )</td>
<td>( D_e ) ( + \max(0, -F_e) )</td>
<td>( D_s ) ( + \max(F_s, 0) )</td>
<td>( D_n ) ( + \max(0, -F_n) )</td>
<td>( D_b ) ( + \max(F_b, 0) )</td>
<td>( D_t ) ( + \max(0, -F_t) )</td>
</tr>
<tr>
<td>( a_p )</td>
<td>( \varphi_p^{o} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a_W + a_E + a_S + a_N + a_B + a_T + a_p^{o} - S_p )</td>
<td>( \frac{\Delta V}{\rho \Delta t} ), where ( \Delta V = \Delta x \Delta y \Delta z )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 3.2. Boundary Conditions

In order simulate the oxygen transfer processes in aquaculture ponds, two types of boundary conditions were used: wall boundary conditions and oxygen transfer at the air-water interface. Figure 3-2 shows the boundary conditions on sectional views.
3.2.1. Wall Boundary Condition

The wall-boundary condition implies that there is no oxygen transfer across the sides and bottom of the pond. In other words, except the top surface of the pond, there is no mass transfer across the boundaries, and this can be written mathematically as:

\[ \nabla \phi = 0 \text{ or } \nabla \phi = 0 \quad (3.3) \]
In the case of east and west walls equation (3.3) becomes $\frac{\partial \varphi}{\partial x} = 0$. In case of north and south walls the equation becomes $\frac{\partial \varphi}{\partial z} = 0$. Finally, for the bottom wall it becomes $\frac{\partial \varphi}{\partial y} = 0$.

### 3.2.2 Air-water Interface

At the surface of the pond, there is an oxygen transfer between the atmosphere and the water across the air-water interface. The amount of oxygen transfer can be mathematically written as:

$$-\Gamma \frac{\partial \varphi}{\partial y} = k_l (\varphi_{ext} - \varphi)$$  \hspace{1cm} (3.4)

where $k_l$ is the gas transfer velocity with the units LT^{-1} [26]. The challenge here is to find the gas transfer velocity and the following section introduces a method to calculate it.

### 3.3. Air-water Interface: Gas Transfer Velocity

In order to calculate the gas transfer velocity, boundary fluxes of oxygen at the air-water interface should be understood. The net mass flux of oxygen at the interface is denoted as $Q$ in this work and it completely depends on hydrodynamics at the surface of the water. Thus, in order to make a simple introduction, the following section considers only the stagnant water case. In this situation there are no hydrodynamic effects on mass flux.

#### 3.3.1 Air-water Interface: Stagnant Water Bodies

Figure 3-3 describes a case where a semi-infinite water body is completely stagnant and thus, the hydrodynamic effects are negligible. In this figure, the initial condition is that a semi-infinite water body has a uniform initial concentration of oxygen, $\varphi_0$, which is less than the saturation level, $\varphi_{sat}$. The surface is instantaneously exposed to an infinite source of oxygen. Oxygen transfer to the water body will continue until the concentration of DO reaches a uniform saturation level, $\varphi_{sat}$.
In order to formulate this case quantitatively, the general transport equation is considered. Since it is assumed that the water body is semi-infinite and there are no hydrodynamics effects, then following assumptions can be made:

$$\frac{\partial \varphi}{\partial x} = 0, \frac{\partial \varphi}{\partial z} = 0$$  one-dimensional diffusion.

$$v = 0$$  no convection, stagnant water.

As a result, the final governing equation for this case will be given as:

$$\frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial y} \left( \Gamma \frac{\partial \varphi}{\partial y} \right)$$  (3.5)

The boundary and initial conditions are given as follows:

$$\varphi(y, 0) = \varphi_0$$  initially, water body has a uniform concentration of $\varphi_0$.

$$\varphi(\infty, t) = \varphi_0$$  representing that the water body is semi-infinite.

$$\varphi(0, t) = \varphi_{sat}$$  surface is exposed to an infinite source of the oxygen, $\varphi_{sat}$.
The solution of the transport equation for stagnant water case with the conditions given above is shown below:

\[
\frac{\varphi(y,t) - \varphi_0}{\varphi_{sat} - \varphi_0} = 1 - erf\left(\frac{-y}{\sqrt{4\Gamma t}}\right) \quad (3.6)
\]

It is worth mentioning that this solution is only valid for negative \(y\) values, since as it is shown in Figure 3-3, the direction of the \(-y\) is down.

In order to find the mass flux, \(Q\), at \(y = 0\), the following expression is used:

\[
Q_y(t) = -\Gamma \frac{\partial \varphi}{\partial y} \bigg|_{y=0} \quad (3.7)
\]

By substituting the solution (3.6) into equation (3.7), mass flux at the air-water interface at a given time period, \(Q_y(t)\), can be found which is shown below.

\[
Q_y(t) = -(\varphi_{sat} - \varphi_0) \sqrt{\frac{\Gamma}{\pi t}} \quad (3.8)
\]

The characteristic thickness or concentration boundary layer, \(\delta\), is shown below.

\[
\delta = \sqrt{2\Gamma t} \quad (3.9)
\]

The expression above shows that the boundary layer thickness for a stagnant water body, over which \(\varphi\) changes from \(\varphi_0\) to \(\varphi_{sat}\), is a function of time. It gradually grows deeper over time as is shown in Figure 3-3.

Finally, the general equation for \(Q_y(t)\) can be written as follows:

\[
Q_y(t) = -k_t(\varphi_{sat} - \varphi_0) \quad (3.10)
\]

where \(k_t = \sqrt{\Gamma/\pi t}\) is the transfer velocity for stagnant water bodies [27, 28].
3.3.2. Air-Water Interface: Turbulent Water Body

When there is motion in the pond water, a large portion of the water body at the air-water interface will interact with air. It is also called turbulent mixing. These hydrodynamic effects limit the growth of the concentration boundary layer thickness and, thus, increases the concentration gradient at the air-water interface as shown in Figure 3-4. This results in enhanced mass flux of oxygen, \( Q \). Furthermore, due to the turbulence at the air-water interface the effective diffusivity close to the surface of water also increases which again results in a higher flux of oxygen.

![Figure 3-4: Turbulent water body [27]](image)

In order to calculate the transfer velocity, \( k_t \), for turbulent water bodies, the film-renewal model is introduced. According to this model, the characteristic thickness or the mixing layer is allowed to grow deeper similar to the stagnant water case for a certain period of time, also called the renewal time, after which due to the presence of turbulence the water in the boundary layer is completely replaced. Thus, the boundary layer or “film” starts growing from the beginning and this process continues periodically. Thus, the model is called the film-renewal model.
In this model, the renewal time is denoted as $t_r$. Thus, the average mass flux, $Q_{tur}$, at the air-water interface for turbulent water bodies over the renewal time period, from $t = 0$ to $t = t_r$, can be written as follow:

$$ Q_{tur} = \frac{1}{t_r} \int_{t}^{t+t_r} Q_y(t) \, dt $$

(3.11)

By substituting equation (3.8) into equation (3.11), the expression above can be written as:

$$ Q_{tur} = \frac{1}{t_r} \int_{t}^{t+t_r} -(\varphi_{sat}-\varphi_0) \sqrt{\frac{\Gamma}{\pi t}} \, dt $$

(3.12)

Denoting the renewal frequency as $r = 1/t_r$, results in a final equation for the average mass flux for turbulent water bodies at air water interface which is shown below.

$$ Q_{tur} = -(\varphi_{sat}-\varphi_0) \sqrt{\frac{4\Gamma r}{\pi}} $$

(3.13)

Thus, the average transfer velocity for turbulent water bodies is given as

$$ k_l = \sqrt{\frac{4\Gamma r}{\pi}} $$

(3.14)

Where $\Gamma$ is diffusion coefficient and $r$ is renewal frequency. It is worth mentioning that the gas transfer velocity for the turbulent water cases is independent of time but only depends on the renewal frequency which needs to be predicted. It is a characteristic of the turbulent flow and can be found by using the Kolmogorov time scale, $t_k$, which is a function of the turbulence dissipation rate, $\varepsilon$, and kinematic viscosity of water, $\nu$ as shown below [27].

$$ t_k = \sqrt{\frac{\nu}{\varepsilon}} $$

(3.15)

By taking renewal frequency $r$ as $1/t_k$, the final equation for the gas transfer velocity for the turbulent water bodies becomes

$$ k_l = 2\Gamma^{1/2}\varepsilon^{1/4}\pi^{-1/2}\nu^{-1/4} $$

(3.16)
It should be noted that in literature there are some models which estimate gas transfer velocity as a function of wind speed. Higher wind speeds create waves which increase the surface area of the water, thus increasing the gas transfer velocity. However, the reason this model has been chosen is that wind speed is not a significant factor for the applications being considered in this work. This is because in South East Asia where most of the small-scale fish farms are located, wind speeds are relatively low. Additionally, a common trend in intensive fish farming shows that multiple, small ponds are favoured over a single large-scale pond. Since ponds with smaller surface areas do not experience large waves due to winds, this model has been chosen.

Finally, it should be mentioned that all values, with the exception of the turbulence dissipation rate, $\epsilon$, can be obtained from the water properties. The turbulence dissipation rate is found from CFD analysis which calculates the velocity field when exposed to an aerator. The following section describes the methods taken to obtain the velocity field to solve the transport equation. In addition, the turbulence dissipation rate is also found from CFD simulation to calculate the gas transfer velocity.

### 3.4. Velocity Field Analysis

In order to solve the transport equation, knowledge of the velocity components is required. Thus, transient CFD simulations were conducted on ANSYS Fluent to find the velocity field due to the effect of aeration devices, specifically due to the wind powered aeration system. Separate research studies were conducted by the author to assess the feasibility of the WERLWind. During these studies, the CFD models were developed and validated by a set of bench-scale experiments. The same settings were also applied for the full-scale simulations. Below is the summary of the work, which was published in the Journal of Energy for Sustainable Development.
3.4.1. CFD Model Setup

The first step in the CFD model setup was setting the geometry. Since the WERLWind system must create vertical circulation, different types of impellers were analyzed, and the Lily impeller (Figure 3-5) was chosen as the most suitable impeller for this study.

![Lily impeller](image)

*Figure 3-5: Lily impeller*

The dimensions and operating conditions for this impeller and the fluid domain were chosen based on available tank sizes and the 3D printer specifications for the bench-scale experiment. The height and the maximum diameter of the impeller were 75mm and 55mm respectively. The size of the fluid domain was 500mm x 250mm x 250mm. The inner diameter and the height of the draft tube were 70mm and 120mm respectively. In order to set up the fluid control volume, the “boolean” operation was used in ANSYS Design Modeller. The dimensions of the complete geometric setup for the bench-scale CFD simulations are shown in Figure 3-6 and Figure 3-7. Wall boundary conditions were applied to both the sides and bottom of the fluid domain. A no-slip boundary condition was applied to both the sides and bottom of the domain except for the top surface where shear stress was set to zero in order to model the air-water interface.
Results of literature review studies on CFD turbulence models showed that the Renormalization Group (RNG) k-\(\varepsilon\) was the most suitable model for the given flow conditions. The RNG k-\(\varepsilon\) model also has a sub-model for swirl dominated flow since the Lily impeller creates a swirling motion in the fluid. Furthermore, since the system circulates the water through the draft tube, using special wall treatment functions and the RNG k-\(\varepsilon\) model produced more accurate results \([29, 30]\).

Due to the turbulent flow properties, transient simulations were used to determine the steady-state mass-flow rate through the draft tube. A series of convergence studies were conducted to determine the settings
for the unsteady flow simulations using the sliding mesh method. The fluid domain was divided into two bodies using a boolean operation. The first domain was a rotating body, which was the part of the fluid domain inside the draft tube. The second body was the rest of the fluid domain and it was considered stationary. For initial simulations, a common angular velocity observed during field evaluation of 20rpm was introduced to the rotating body using the Frame Motion feature in Fluent. A mesh consisting of tetrahedral cells was generated using the functions outlined in Table 3-2.

Table 3-2: Mesh generation parameters

<table>
<thead>
<tr>
<th>Applied Mesh Functions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Advanced size function</strong></td>
<td>Proximity and Curvature</td>
</tr>
<tr>
<td><strong>Relevance Center</strong></td>
<td>Fine</td>
</tr>
<tr>
<td><strong>Face Sizing</strong></td>
<td>3mm at the interference between Rotating and Stationary Bodies</td>
</tr>
<tr>
<td><strong>Inflation Layers on Draft Tube</strong></td>
<td>10 layers with total thickness of 5mm</td>
</tr>
<tr>
<td><strong>Inflation Layer on Impeller</strong></td>
<td>5 Layers with Total Thickness of 1.5mm</td>
</tr>
</tbody>
</table>

The time-step size for the first simulation was chosen as 0.01 seconds and the mass flow rate leaving the draft tube was monitored. In addition, the time step sensitivity was analyzed by running simulations for time-steps of 0.05s and 0.2s for the same amount of flow time. Results for mass flow rates for each simulation are given in Figure 3-8. The average mass flow rate for the last 10 seconds of flow for each simulation are given in Table 3-3. The results showed that the mass flow rate increased 0.8% and 2.7%. Considering time savings for the computational analysis and the limited 2.7% error, a time-step of 0.2s was used for the rest of the simulations.
A mesh refinement study was conducted to increase the accuracy of results from the k-ε model. The two main parameters chosen for the mesh independency analysis were the number of inflation layers on the impeller and the draft tube. The total thickness of inflation layers on the impeller and draft tube was set to 1.4 mm and 5 mm respectively. In order to find the effect of the impeller, boundary layers on mass flow rate, the number of inflation layers was increased from 5 to 40 layers, and mass flow rate was monitored (Figure 3-9). In the next stage, four simulations were carried out to choose the number of boundary layers on the draft tube. The number of layers was changed from 25 to 70 and results are shown in Figure 3-10.
Results from Figure 3-9 showed that the inflation layers on the impeller had a negligible effect on mass flow rate. Thus, in order to reduce simulation run-time, only 5 layers were used for all analyses. For the draft tube, the mass flow rate decreased with increasing number of layers as shown in Figure 3-10. The
steady-state mass flow rate was approximately 0.0146 kg/s with 50 and 60 inflation layers. Therefore, the number of inflation layers was set to 50.

### 3.4.2 Experimental Validation of CFD Model

A set of bench-scale experiments were conducted to validate the CFD results. The setup consisted of a water tank, a 3D-printed impeller, a DC motor to drive the impeller, a stainless-steel shaft to couple the impeller and motor, and an acrylic draft tube as shown in Figure 3-11. Dimensions of each element were identical to the dimensions used for CFD fluid domain.

![Figure 3-11: Bench-scale prototype](image)

The angular velocity of the impeller was set to 20 rpm. To validate the model, the mass flow rate inside the draft tube was measured by injecting 10 fluorescent green polyethylene microspheres into the water. These particles have a density very close to that of water at 25°C (0.999g/cc), thus, by measuring the velocity of each particle, it was possible to find the average mass flow rate. The experiment was recorded using Canon EOS 60D camera at a rate of 29.97 frames per second (fps). The video was divided into individual frames which were then saved as pictures using MATLAB. To calculate the total travel time for each particle, the number of frames between a particle entering and leaving the draft tube was found. Then, the average velocity and mass flow rate values were calculated since the diameter and the height of the draft tube were known. The results showed that the average velocity and mass flow rate inside the draft tube over the 10
samples were 0.0085 m/s and 0.0327 kg/s respectively. There was only a 3.5% difference between CFD simulations (0.0082 m/s and 0.0314 kg/s) and experimental results. The same modeling approach was used for finding the velocity field for the DO model.

3.4.3. Velocity Field Conversion

As it was mentioned before, the dissolved oxygen model was developed using a uniform grid distribution, however, velocity field from ANSYS simulations was obtained by generating unstructured tetrahedral mesh cells. Each cell contains values of velocity components, thus, there is a need for transferring information from unstructured cells to uniform mesh cells. As an example, Figure 3-12 shows the overview of this process for x-velocity.

![Figure 3-12: Calculating x-velocity for uniform mesh](image)

As it can be seen in Figure 3-12, each cell in uniform grid contains multiple smaller sizes tetrahedral cells. x, y, z – velocities and energy dissipation rate for each cell with their volumes and coordinates are extracted from ANSYS Fluent. Since the coordinates of each cell in the uniform grid are also known, it is possible to
find the number of tetrahedral cells within each cell in uniform mesh, which is denoted as $k$. Velocities for the structured mesh is then found by using a volume-averaging method. Below is the example for x-velocity:

$$v_x = \frac{\sum_{n=1}^{k} v_{xn}V_n}{\sum_{n=1}^{k} V_n}$$  \hspace{1cm} (3.17)

where

$v_{xn}$ is the x-velocity

$V$ is the cell volume

$k$ is the number of tetrahedral cells within uniform cell

The same equation is used for finding y- and z- velocities as well as energy dissipation rate, $\epsilon$, to calculate the gas transfer velocity.

### 3.5. Solver

The DO model is developed and coded in Python. In order to solve the system of linear equations, an existing iterative solver, scipy.sparse.linalg.spsolve, is used. In order to solve the matrix expression $Ax = B$, the chosen solver assumes that matrix $A$ is sparse and, thus, computationally inexpensive results are achieved. Furthermore, compressed sparse column format (CSC) is used for matrix $A$ and $B$ to achieve a faster convergence.

### 3.6. Chapter Summary

This chapter presents the fundamentals of the dissolved oxygen model. The three-dimensional transport equation was discretized based on the literature review conducted in Chapter 2. It was found that to
discretize the temporal term, the implicit scheme was the most suitable technique since it did not have any maximum limit to the time step size. The central differencing method was chosen to discretize the diffusion term. Finally, the upwind differencing scheme was used to discretize the convection term because it met all requirements to be physically realistic. It was also easier to implement. Additionally, the boundary conditions were introduced in this chapter. To model an aquaculture pond, the wall-boundary condition was applied to the sides and bottom of the pond while the top surface was treated as the air-water interface. In order to calculate the amount of oxygen transfer from the atmosphere to the water body, an expression for gas transfer velocity was found by using the Kolmogorov time scale for turbulent water bodies. To solve the transport equation one of the unknowns was the velocity field generated by the aeration device. To find the velocity field, a CFD model was developed in ANSYS Fluent and details of this work were presented in this chapter. The next chapter describes validation of the DO model by bench-scale experiments.
Chapter 4

4. Bench-Scale Model Validation

In Chapter 3, a numerical dissolved oxygen model which can resolve the spatial and temporal distribution of DO concentration in aquaculture ponds was presented. The model serves as a tool to assess the performance of aeration technologies and their impact on dissolved oxygen distribution. In this chapter, the developed model is validated by a set of lab-scale experiments under different fluid conditions due to the presence of the WERLWind device.

4.1. Objective of Experimental Work

The objective of the bench-scale experiments was to characterize and validate the dissolved oxygen model developed in Chapter 3. To limit the uncertainty, these experiments were carried out in a controlled environment in which only source of oxygen was the oxygen transfer from the atmosphere. A scaled version of the WERLWind was introduced to the system to achieve forced convection to distribute oxygen and to more quickly achieve a saturated level of oxygen. DO concentration was measured using dissolved oxygen sensors. The DO model was validated by comparing the results with experiment. Upon validation, this model can be used to accurately predict spatial and temporal dissolved oxygen concentration in lab-scale experiments to design and optimize aeration devices.
4.2. Methodology

4.2.1. Experimental Apparatus

In order to validate the numerical dissolved oxygen model, a lab-scale experimental system was constructed. A complete setup including the motorized version of the WERLWind and DO loggers (i.e., sensors) inside the water tank is shown in Figure 4-1.

The dimensions of the plexiglass tank were 91.44 cm (36 in) x 45.72 cm (18 in) x 60.96 cm (24 in). The aerator consisted of a hydrofoil impeller, an acrylic draft tube and an electric mixer. The electric mixer had its own built-in speed controller. Dissolved oxygen and temperature values were measured using optical PME Minidot loggers. During each experiment, four loggers were positioned at different locations inside the tank. Experimental data was retrieved from the loggers for analysis after each experiment.
4.2.2. Experimental Procedure

In total, 6 lab-scale experiments were conducted under different settings. During each experiment the depth and volume of water was 40 cm and 216 L respectively. Prior to each run, water inside the tank was replaced with the required water volume.

In preparation for the aeration tests, the initial dissolved oxygen concentration of the water was measured. The water was deoxygenated using the procedure for aeration tests formed by the American Society of Civil Engineers in 1992. During this process 12 mg/L of sodium sulfite (Na₂SO₃) and 0.1 mg/L of cobalt chloride 6-hydrate (CoCl₂ 6H₂O) was used for every mg/L of dissolved oxygen measured by DO loggers. It was assumed that water was fully deoxygenated until readings from DO loggers ranged from 0 to 0.75 mg/L.

Multiple dissolved oxygen loggers were placed in opposite sides of the tank. These loggers were placed at two different water depths during each experiment which were 2 cm from bottom of the tank and 20 cm from the surface of the water (hereafter locations are referred as bottom and middle of the tank).

The rotational speed of the impeller was adjusted by using the speed controller on the mixer. Experiments were conducted at 50 rpm, 75 rpm and 100 rpm. Each experiment was completed twice to ensure repeatability.

4.3. CFD Simulation

The main objective of the CFD study was to find the velocity field due to the aerator. A set of simulations was conducted at 50 rpm, 75 rpm and 100 rpm using ANSYS Fluent. The simulation setup, physical models, and solver parameters were chosen based on the work presented in Chapter 3. SOLIDWORKS software was used to model a water tank with dimensions of 0.9 m x 0.6 m x 0.4 m. The 3D isometric view of the geometry and the boundary conditions are show in Figure 4-2.
Stationary walls were defined for the tank wall and zero shear stress was set for the top wall. A mesh consisting of tetrahedral cells was generated using the functions outlined in Chapter 3 (Figure 4-3). Angular velocities were introduced to the rotating body using the Frame Motion feature in Fluent.
Figure 4-3: Isometric view of a mesh consisting of tetrahedral cells: bench-scale simulations

Figure 4-4 shows the water velocity magnitude vector field which indicates the flow pattern of water due to the WERLWind under 100rpm. Since molecular diffusion of dissolved oxygen in water is very low, it is mainly distributed throughout the tank due to convective circulation. Thus, it was expected to see DO distribution following the flow patterns illustrated in Figure 4-4. The WERLWind system pushes water with low DO content to the surface through the draft tube while moving oxygen enriched water along the walls and to the bottom of the tank. Therefore, higher DO levels were anticipated at the bottom corners of the tank.
Values of velocity components, energy dissipation rate and cell volumes were exported in ASCII format from ANSYS Fluent. Information from unstructured cells was transferred to uniform mesh cells using the velocity field conversion method described in Chapter 3. Gas transfer velocity was calculated based on the Kolmogorov time scale. The same method was used to find parameters under 50 rpm and 75 rpm. This data was imported into the DO model, which was run to predict dissolved oxygen distribution over time. The results were then compared against experimental results described in next section.

### 4.4. Experimental Results and Bench-Scale Validation of DO model

Figure 4-5, Figure 4-6 and Figure 4-7 show the experimental results at 50 rpm, 75 rpm and 100 rpm respectively. Experimental results show that WERLWind system creates uniform dissolved oxygen distribution throughout the tank. By comparing the results, it can be stated that by increasing the angular velocity of the WERLWind system, the oxygen saturation level can be more quickly achieved. This is because increasing the angular velocity results in a higher turbulence dissipation rate and, thus, higher gas transfer velocity. Furthermore, having higher gas transfer velocity enhances the amount of oxygen transfer into the system. Lastly, higher angular velocity intensifies the mixing in the water column.
Figure 4-5: Bench-scale experiments: 50 rpm

Figure 4-6: Bench-scale experiment: 75 rpm
In order to validate the DO model, results from the bench-scale experiments were compared against the results from the developed DO model as shown in Figure 4-8, Figure 4-9 and Figure 4-10.
Figure 4-9: Bench-scale experiment vs DO model - 75rpm

Figure 4-10: Bench-scale experiment vs DO model - 100rpm
The figures above show that the DO model overestimates oxygen transfer rate. This is because of a higher prediction of the gas transfer velocity. To gauge the accuracy of the model, the mean absolute percentage error (MAPE) and the root-mean-squared-error (RMSE) between the predicted and experimental DO concentrations were calculated. Table 4-1 shows the values of gas transfer velocities, MAPE and RMSE for each experiment.

Additionally, as it can be seen in Figure 4-10, there is an overshoot in the experimental DO concentration compared to the model after ~300 minutes. The experiment started in the evening (t = 0) and the ambient temperature was lower. Since the saturation level of DO in water increases as water becomes colder and decreases as it becomes warmer, there was higher oxygen level at night. In the morning and afternoon the water became warmer which resulted in off-gassing of oxygen to the surroundings. Therefore, DO concentration started to decrease. Since the DO model assumes a constant temperature of water, the results do not capture this phenomenon.

In order to minimize the errors between the model and experiments, the gas transfer velocity values were calibrated. It was found that the Kolmogorov time scale overestimates the transfer velocity by around 15%. Figure 4-11, Figure 4-12, Figure 4-13 show the calibrated results and Table 4-2 shows the new values of the gas transfer velocities as well as MAPE and RMSE between the predicted and experimental DO concentrations.

<table>
<thead>
<tr>
<th>Gas Transfer Velocity [m/s]</th>
<th>50 rpm</th>
<th>75 rpm</th>
<th>100 rpm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas Transfer Velocity [m/s]</td>
<td>10.4*10⁻⁶</td>
<td>22.3*10⁻⁶</td>
<td>63.4*10⁻⁶</td>
</tr>
<tr>
<td>MAPE (%)</td>
<td>2.3</td>
<td>4.6</td>
<td>5.6</td>
</tr>
<tr>
<td>RMSE (mg/L)</td>
<td>0.16</td>
<td>0.25</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Table 4-1: Gas transfer velocities and error metrics: DO model vs bench-scale experiments
Figure 4-11: Bench-scale experiment vs DO model - 50rpm (calibrated)

Figure 4-12: Bench-scale experiment vs DO model - 75rpm (calibrated)
To illustrate the temporal and spatial dissolved oxygen distribution, contour plots of DO concentration were created at different time steps. These plots show DO concentration at a cross-section through the middle of the domain. Figure 4-14, Figure 4-15 and Figure 4-16 show DO levels at 10, 200 and 900 minutes. These figures show that, as explained in Section 4.3, DO distributions follow the convective flow patterns and consequently there is higher DO concentration at bottom of the tank. Furthermore, due to the continuous
transfer of oxygen from the atmosphere, as time passes overall DO levels increase and reach the saturation level after 900 minutes.

Figure 4.14: Contour plot of DO distribution after 10 mins
Figure 4-15: Contour plot of DO distribution after 200 mins

Figure 4-16: Contour plot of DO distribution after 900 mins
4.5. Chapter Summary

In this chapter, the numerical dissolved oxygen model was experimentally characterized and validated. A bench-scale experimental apparatus was constructed with a motorized version of the WERLWind system. This system consisted of a hydrofoil impeller, an acrylic draft tube and an electric mixer. Water inside the plexiglass tank was deoxygenated with chemicals in the beginning of each experiment and experiments were carried out until DO concentration reached the saturation level. Dissolved oxygen values were measured using optical PME Minidot loggers. Multiple experiments at 50 rpm, 75 rpm and 100 rpm were conducted, and the experimental results were then compared to the predicted values from the DO model. Results showed that the DO model overestimates oxygen levels due to a higher prediction of the gas transfer velocity by the Kolmogorov time scale. The DO model produced results with MAPE of 2.3% at 50 rpm, 4.6% at 75 rpm and 5.6% at 100 rpm while the RSME values were 0.16 mg/L, 0.25 mg/L and 0.34 mg/L respectively for each experiment. The model was then calibrated by decreasing the gas transfer velocity values by 15% and better predictions of DO concentrations were achieved with MAPE of 0.2%, 1.7% and 4.2% and RSME of 0.01 mg/L, 0.05 mg/L and 0.29 mg/L at 50 rpm, 75 rpm and 100 rpm, respectively. The next chapter describes the validation of the DO model by field experiments.
Chapter 5

5. Field Validation Study

The objective of this study was to validate a spatial and temporal 3D DO model to describe the oxygen dynamics of a pond. Field experiments were conducted through the partnership with the Commonwealth Scientific and Industrial Research Organization (CSIRO) at the Bribie Island Research Center (BIRC) on Bribie Island, Australia.

5.1. Test Site Information and Experimental Setup

A set of experiments were conducted to gather the necessary data to validate the DO model in an aquaculture research facility shown in Figure 5-1.

Figure 5-1: Satellite image of BIRC facility
A circular indoor tank with a base area of 125 m² and a height of 4 m was used for these experiments. This tank is mainly used by aeration experts to test the performance of aerators. A full-scale, motorized version of the WERLWind prototype was built to conduct field trials. Diameters of the impeller and the draft tube were 25.4 cm and 31.5 cm respectively. An electric mixer with a built-in speed controller was used to rotate the impeller. Four water containers attached to a surface-painted wood platform were used as a floating structure. Figure 5-2 shows the full-scale prototype of the WERLWind.

![Figure 5-2: Full-scale prototype of WERLWind](image)

### 5.2. Experimental Procedure

The BIRC facility mainly uses filtered ocean water for their aquaculture research projects. Thus, the field experiments also involved sea water instead of freshwater. The tank was filled with sea water to 1m depth.
and salinity was around 35ppt. The motorized version of the WERLWind was placed in the middle of the water tank shown in Figure 5-3.

![Figure 5-3: Complete experimental setup](image)

Four PME Minidot DO loggers were used to measure the DO at the different locations in the tank. Two of the sensors were placed close to the device in the middle and at the bottom of the tank (hereafter locations will be referred as device & middle and device & bottom respectively). Two loggers were placed on the sides of the tank at the surface of the water and at the bottom of the tank (hereafter locations will be referred as tank & top and tank & bottom respectively). Prior to the aeration experiment, artificial oxygen sinks were used to deoxygenate the water in the tank. This was done by using the chemical reaction of cobalt chloride \((\text{CoCl}_2 \cdot 6\text{H}_2\text{O})\) and sodium sulfite \((\text{Na}_2\text{SO}_3)\). Then, the device introduced the circulation into the system and the DO level at various locations was measured. Three sets of experiments were conducted with angular velocities 100rpm, 150rpm and 200rpm. Each experiment continued until oxygen levels reached 80-98% saturation at the bottom of the tank. Results from the loggers were retrieved and compared to the results from the numerical dissolved oxygen model.
5.3. CFD Simulation

A set of simulations was conducted at 100 rpm, 150 rpm and 200 rpm on ANSYS Fluent. The simulation setup, physical models, and solver parameters were chosen based on the work presented in Chapter 3. SOLIDWORKS software was used to model a water tank with dimensions of 8 m x 8 m x 1 m. The 3D isometric view of the geometry and the boundary conditions are show in Figure 5-4. It should be noted that, experiments were conducted in a cylindrical tank, however, the DO model was developed on cartesian coordinate system. Thus, the simulations were conducted in a square tank.

![Isometric view of the full-scale geometric setup used for CFD simulations with boundary conditions](image)

Stationary walls were defined for the tank wall and zero shear stress was set for the top wall. A mesh consisting of tetrahedral cells was generated using the functions outlined in Chapter 3 (Figure 5-5). Angular velocities were introduced to the rotating body using the Frame Motion feature in Fluent.
Figure 5-5: Isometric view of a mesh consisting of tetrahedral cells: full-scale simulations

Figure 5-6 shows the water velocity magnitude vector field which indicates the flow pattern of water due to the WERLWind at an angular velocity of 200rpm. Similar to bench-scale experiments, the WERLWind system pushes water from bottom of the tank to the surface. As the water travels along the surface towards the walls, oxygen is being transferred to the surface water, which then travels down the walls. Therefore, it was expected to see higher DO concentration at the bottom corners of the tank.

Figure 5-6: Water velocity magnitude vector field: full-scale, 200rpm
Values of velocity components, energy dissipation rate and cell volumes were exported in ASCII format from ANSYS Fluent. Information from unstructured cells was transferred to uniform mesh cells using the velocity field conversion method described in Chapter 3. Gas transfer velocity was calculated based on the Kolmogorov time scale. The same method was used to find parameters under 100 rpm and 150 rpm. This data was imported into the DO model, which was run to predict dissolved oxygen distribution over time. The results were then compared against experimental results described in next section.

5.4. Experimental Results and Full-Scale Validation of DO model

Figure 5-7, Figure 5-8 and Figure 5-9 show the experimental results under 100 rpm, 150 rpm and 200 rpm, respectively. Due to limited time available during the field trials, each experiment was conducted until the DO levels reached 80% of saturation.
Figure 5-8: Field experiments - 150rpm

Figure 5-9: Field experiments - 200rpm
Similar to bench-scale experiments, results from field experiments show that the WERLWind system creates a uniform dissolved oxygen distribution throughout the water body and by increasing the angular velocity of the impeller, faster oxygen transfer level can be achieved. Figure 5-10, Figure 5-11 and Figure 5-12 compare the results from the DO model against the field experiments. These figures show that the DO model overestimates oxygen transfer rate with the least amount of error in the case of 200rpm (Figure 5-12) and highest error in the case of 100rpm (Figure 5-10). This result was expected due to following reason: during the field trials, the tank was filled with salty water and for each experiment the water was not exchanged due to large amount of water required. Due to the presence of organic matter from sea water and chemicals used to deoxygenate the water, there was film formation at the surface of the water. The amount of film formed at the surface increased over time which decreased the oxygen transfer at the air-water interface. During the first experiment, the angular velocity was set to 200rpm. Since it was the beginning of the field trials there was little amount film formation at the surface, thus, it did not affect the oxygen transfer coefficient. In addition, due to higher angular velocity, water movement at the surface was also high which prevented film formation. However, as time passed the amount of film formation increased. Furthermore, since during the second and third experiments the velocity of surface water was low due to lower angular velocity of the system, the oxygen transfer coefficient decreased. This resulted in higher error for the prediction of oxygen distribution for 100rpm. Table 5-1 shows the values of gas transfer velocities, MAPE and RMSE for each experiment.
Figure 5-10: Field experiment vs DO model - 100rpm

Figure 5-11: Field experiment vs DO model - 150rpm
To illustrate the temporal and spatial dissolved oxygen distribution, contour plots of DO concentration were created at different time steps. These plots from DO model show DO concentration at a cross-section through the middle of the domain. Figure 5-13 and Figure 5-14 show DO levels at 300 mins and 600 mins. Similar to the results from bench-scale simulations, DO distributions follow the velocity patterns and there is higher DO concentration at bottom of the tank. Moreover, overall DO levels increase as time passes. Lastly, based on the average velocities along the center, surface, wall and bottom of the tank, it was calculated that it took an average of 414 s for an entire circulation cycle under 200 rpm.
Figure 5-13: Contour plot of DO distribution after 300 mins

Figure 5-14: Contour plot of DO distribution after 600 mins
5.5. Chapter Summary

In this chapter, the numerical dissolved oxygen model was characterized and validated by field experiments. A full-scale prototype was constructed with a motorized version of the WERLWind system. The WERLWind device consists of a hydrofoil impeller, a PVC draft tube and an electric mixer. Four water containers attached to a surface-painted wood platform were used as a floating structure. The tank was filled with salty water with an average salinity of 35ppt. Water was deoxygenated with chemicals at the beginning of each experiment and experiments were carried out until DO concentration reached around 80% saturation level. Dissolved oxygen values were measured using optical PME Minidot loggers. Three experiments at 100rpm, 150rpm and 200rpm were conducted, and the experimental results were then compared to the predicted values from the DO model. Results showed that for the first experiment (200rpm), the DO model had a good prediction of dissolved oxygen distribution with MAPE of 5.1% and RSME of 0.19 mg/l. However, these values slightly increased in the case of 150rpm and 100rpm with average MAPE of 8.3% and 0.31 mg/l. It can be explained due to the fact that during last two experiments, there was a film formation at the surface of the water which decreased the actual gas transfer velocity values and the DO model was not able to predict this process. However, overall it can be stated that the DO model produced good results with average MAPE of 7.2% and RSME of 0.27 mg/l.
Chapter 6

6. Ecological Modeling of Aquaculture Ponds

In practice, to test the efficacy of aeration systems, experiments are usually conducted in a controlled environment where the only source of oxygen is the atmosphere. Thus, to validate the DO model oxygen transfer from atmosphere to water bodies, the atmosphere was considered as the only source of oxygen. However, in real fish ponds there are many source and sink terms of dissolved oxygen such as photosynthetic oxygen generation by phytoplankton, respiration by the cultured livestock, water column respiration by other living organisms and sediment respiration. In this chapter, the source and sink terms of oxygen were added to the model and tested.

6.1. Oxygen Sources and Sinks in Aquaculture Ponds

6.1.1. Photosynthesis

In most aquaculture ponds, phytoplankton provide a major source and sink for dissolved oxygen. During the day and in the presence of sunlight, phytoplankton produce more oxygen by photosynthesis than they consume by photorespiration. The amount of oxygen generation by phytoplankton depends on several factors including the intensity of photosynthetically active radiation (PAR), water column light attenuation, water temperature, and pH. However, due to measurement limitations, only the effects of water temperature and PAR were considered in this work.

To calculate the dissolved oxygen generation by photosynthesis ($DO_{ph}$), following equation was used.
\[ DO_{ph} = P_i \text{ chla} \quad (6.1) \]

where \( P_i \) is the rate of photosynthetic oxygen production within a control volume \((mg_{O_2} mg_{\text{chla}} h)\), and \( \text{chla} \) is the chlorophyll-a content in the aquaculture pond \((mg_{\text{chla}}/L)\) [20], [31].

The rate of photosynthetic oxygen production for a given control volume, \( P_i \), can be found by using an integrated form of Steele’s equation. Steele’s equation has been widely applied to ecological modelling of large water bodies including aquaculture ponds [32]. The equation expresses the oxygen production as a function of three main parameters: \( \text{PAR} \), the saturated \( \text{PAR} \) level, and the maximum production rate. The following equation describes \( P_i \).

\[
P_i = P_{\text{max}} \left( \frac{\exp\left(-\frac{\text{PAR}}{\text{PAR}_{\text{sat}}} \exp(-\eta z_{i+1})\right) - \exp\left(-\frac{\text{PAR}}{\text{PAR}_{\text{sat}}} \exp(-\eta z_i)\right)}{\eta \Delta z} \right) \quad (6.2)
\]

where \( P_{\text{max}} \) is the maximum photosynthetic oxygen production rate \((mg_{O_2} mg_{\text{chla}} h)\), \( \text{PAR}_{\text{sat}} \) is the saturated \( \text{PAR} \) level, \( \eta \) is the light extinction coefficient \((1/m)\), \( z_i \) is the depth of the center of the upper control volume \((m)\), \( z_{i+1} \) is the depth of the center of lower control volume \((m)\), and \( \Delta z \) is the thickness of the control volume \((m)\).

Furthermore, the equation below is widely used to approximate the value of \( P_{\text{max}} \) based on an empirical relationship with a water temperature.

\[
P_{\text{max}} = 9.6 \theta_p(T_{i-20}) \quad (6.3)
\]

where \( \theta_p \) is an empirical photosynthetic production coefficient which is estimated as 1.036, and \( T_{i} \) is the temperature of the control volume.

Finally, there is not any universal method to find the concentration of phytoplankton. Therefore, chlorophyll-a concentration had to be calibrated through trial and error for the DO model. However, the expected \( \text{chla} \) value in aquaculture ponds is in the range of 50 to 1000 mg/L [33], [34].
6.1.2. Photorespiration

There are two main aspects to phytoplankton respiration ($DO_{pr}$) depending on the time of day. During daytime, there is more oxygen generation by photosynthesis in the presence of sunlight than oxygen consumption by respiration [35]. The most widely used approximation of photorespiration rate in literature is 10% of the rate of photosynthesis [36].

During nighttime, there is no oxygen generation by photosynthesis and the respiration rate by phytoplankton and other organic matter is found by the dark bottle experiment. In this experiment, water samples from the pond water are stored in a container at a dark location and the DO level is measured over a period of time. The decline in DO concentration at the end of experiment determines the respiration rate [3], [37]. The empirical formula shown below is used to determine the respiration rate.

$$DO_{pr} = DO_{DB} \theta_r^{(T_w - T_{DB})}$$  \hspace{1cm} (6.4)

where $DO_{DB}$ is the rate of water column respiration from the dark bottle experiment (mg/Lh), $\theta_r$ is an empirical temperature adjustment, estimated as 1.047, $T_w$ is the temperature of the water, and $T_{DB}$ is the temperature of the dark bottle water sample [37].

6.1.3. Sediment Oxygen Demand

Sediment or benthic oxygen demand ($DO_{sed}$) happens due to the presence of organic matter and decomposition of organisms on the pond bed. The rate of $DO_{sed}$ mainly depends on the temperature and the physical, chemical and biological characteristics of the pond bed [38]. The following equation is used to determine benthic oxygen demand:

$$DO_{sed} = \frac{1}{z_{sed}} S_20 \theta_s^{(T_w - 20)}$$  \hspace{1cm} (6.5)
where $S_{20}$ is the sediment oxygen demand at 20 °C, $T_w$ is the temperature of water, $z_{sed}$ is the control volume thickness affected by the sediment oxygen demand (m), $\theta_s$ is an empirical thermal coefficient which is approximated as 1.065 [21]. In literature, sediment oxygen demands vary between 0.024 and 0.125 for inland aquaculture ponds [20], [38]. Finally, it is assumed that $DO_{sed}$ is negligible for ponds utilizing a liner or tarp.

6.1.4. Fish Respiration

Determining respiration rate of cultured species ($DO_{fr}$) is a complex process which depends on many parameters such as the metabolic rate, wet weight, temperature, and the diurnal and nocturnal activities of the cultured species. However, in literature, there is a general empirical equation describing the respiration rate of an average fish per unit weight which was used in this work [36]. This formula, shown below, is valid for all species and water temperature.

$$ R_f = 10^{-\left(1-9.57\times10^{-4}m_f+6\times10^{-7}m_f^2+3.17\times10^{-2}T_w-8.7\times10^{-8}T_w^2+3\times10^{-7}m_fT_w\right)} $$  \hspace{1cm} (6.6)

where $R_f$ is the respiration rate per weight of fish (mg/kg·h), $m_f$ is the average weight of cultured fish species (g), and $T_w$ is the temperature of water.

To find the total oxygen consumption within a control volume, $R_f$ is multiplied by the stocking density of the aquaculture pond as shown below.

$$ DO_{fr} = R_f \frac{N_f m_f}{V_w} $$  \hspace{1cm} (6.7)

where $N_f$ is the number of fish in the pond and $V_w$ is the volume of the pond.

Additionally, it has been observed that the fish usually avoid areas of the pond with low dissolved oxygen concentration. To account for this fact, the critical DO level was set to 2 mg/L which is considered to be
the lowest limit for survivability for most fish species [36]. Thus, the DO model assumes that there is no fish in the areas with DO concentration below this critical DO level and there is a shift in the biomass from the regions with low DO to the regions high DO levels [20].

6.2. Result of Ecological Modeling

The source and sink terms of oxygen were integrated into the dissolved oxygen model using the discretization methods described in Chapter 2. A set of experiments was conducted in one of the ponds in BIRC facility to retrieve the necessary data for source and sink terms for 24 hours. During the experiments PAR and water temperature values were record. It was found that the average water temperature was $T_w = 33^\circ$C. Figure 6-1 shows the PAR value for 24 hours.

![Figure 6-1: PAR values during 24 hrs in BIRC facility, Australia](image)

To test the DO model, the same pond dimensions and aeration configuration used in field experiments were chosen. The test pond with a floor area of 64 m² and a depth of 1 m was used. During the experiments, the pond was covered with a black high-density polyethylene (HDPE) liner. Thus, sediment respiration was neglected in this work. To model animal respiration, 153 fish with average weight of 0.4 kg was used in
these studies. Flow field was obtained from Fluent simulations in which 200 rpm angular velocity was introduced to the WERLWind system.

The model was run to predict the DO distribution for a period of three days. As an initial condition, it was assumed that the pond water had 5 mg/L uniform dissolved oxygen concentration. Figure 6-2 shows the predicted DO levels at the top, middle and bottom of the pond.

![Figure 6-2: Predicted DO concentration with source and sink terms starting from 6am](image)

Lastly, to illustrate the temporal and spatial dissolved oxygen distribution, contour plots of DO concentration were created at different time steps. These plots show DO concertation at a cross-section through the middle of the domain. Figure 6-3, Figure 6-4 and Figure 6-5 show DO levels at 12pm, 6pm and 12am during the second and third day. These plots show that during the daytime, there is oxygen generation by photosynthesis in the presence of sunlight, thus, there is more oxygen close to the surface at 12pm and 6pm. However, during the nighttime, overall DO levels decrease because there is no photosynthesis and a higher respiration rate by phytoplankton, livestock and other organisms. Furthermore, the figures below illustrate that DO distributions follow the convective flow patterns which moves oxygen enriched water to the bottom of the tank.
Figure 6-3: Contour plot of DO distribution at 12pm

Figure 6-4: Contour plot of DO distribution at 6pm
6.3. Chapter Summary

In this chapter, the source and sink terms of oxygen were added to the dissolved oxygen model. These terms include oxygen generation and consumption by phytoplankton, respiration by the cultured livestock, photorespiration by other living organisms and sediment respiration. The input parameters such as photosynthetically active radiation and water temperature were obtained during the field experiments in Australia. Lastly, to model animal respiration 153 fish with average weight of 0.4 kg was used during the simulations. The model was run to illustrate the DO distribution in a pond with dimension of 8 m x 8 m x1 m for 3-days period.
Chapter 7

7. Conclusion

The main contribution of this thesis was the development of a computational model that can predict spatial and temporal distribution of dissolved oxygen concentration in water bodies. The model enables the design and optimize aerations technologies to have higher efficacy.

This model was developed by using FVM techniques and coded in Python. First, the model was validated by a set of lab-scale experiments. During the experiments, a miniature motorized version of the WERLWind device was tested. Results showed that the model overestimated the dissolved oxygen distribution due to a higher prediction of the gas transfer velocity by the Kolmogorov time scale. It was found that decreasing the gas transfer coefficient by 15% gave the best results with a MAPE of 2%. Furthermore, through a partnership with the Commonwealth Scientific and Industrial Research Organization, field experiments were conducted in one aquaculture pond located in the Bribie Island Research Center to test and validate the model in larger scale. Results showed that the current model is capable of predicting the dissolved oxygen concentration with an average prediction error of 7.2%.

To model an aquaculture pond the source and sink terms of dissolved oxygen including photosynthetic oxygen generation by phytoplankton, respiration by the cultured livestock, water column respiration by other living organisms and sediment respiration were added. The DO model was run to predict DO distribution in a test pond with livestock.

The main limitation of the DO model is that it was built on a cartesian coordinate system. Thus, in order to simulate ponds with cylindrical shapes, the model should be integrated into a cylindrical coordinate system.
Furthermore, the model assumes that temperature is uniform throughout the domain. Thus, the energy equation should be solved to find the spatial and temporal temperature distributions. This is especially important for the ecological model of actual fish ponds since the source and sink terms are temperature dependent. In addition, solar radiation can impact pond dynamics by introducing an additional heat source. Finally, field experiments will be conducted to validate a final version of the model with source and sink terms for oxygen. For example, precise measurements and validation of DO contribution by phytoplankton are required.

Upon validation, the model will be used to design and optimize sustainable aeration technologies such as the WERLWind system. This includes finding optimal draft tube diameter and height, impeller rotational speeds, etc. In addition, using the model, the quantity of aeration systems and their respective locations in a given fish pond can be identified to increase fish production for extensive farming. One path for future research is the application of the model to existing aeration technologies, such as paddle-wheel aerators, to optimize them for semi-intensive and intensive farming. This optimization will aim to achieve a reduction in power consumption and thus, operational costs of aeration devices for industrial farming.
References


