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University of Southern Queensland
FACULTY OF ENGINEERING AND SURVEYING

Numerical Simulations of Water Surfaces for Improved Evaporation Prediction

A dissertation submitted by

Mr Wesley James Williams

In fulfillment of the requirements of

ENG 4111/1 and ENG 4112/2 Research Project

Towards the degree of

Bachelor of Engineering (Civil)

Submitted: October 2014

Abstract

Water is normally stored in open reservoirs such as dams. A key consideration and challenge that water resource managers are currently facing for improved water management is the evaporation rate in such storage facilities. The impacts that the changing climate has on communities currently and into the future will prove a considerable task for water resource managers to meet the demands for a national population which is growing at a fast pace. Being able to satisfactorily quantify the rate of evaporation from open water storage reservoirs within Australia will enable the correct implementation of measures to mitigate losses that are expected in the coming decades due to a rising climate, estimated changes in precipitation rates and currently experienced changes in wind patterns. Not only is the increased pressure on the distribution of water to maintain public health but agricultural practices and a large number of other varied industries are also suffering.

The consequential effects of evaporation losses are numerous and may prove to be linked to decreased productivity and efficiencies within many sectors of industry. This brings the value of maintaining important and valuable water supplies to the top of the list for many industrial sectors. This has increased the need for further understanding to be gained via research into the effects and prevention of losing so much of a precious resource every year.

Currently, research is being undertaken at the National Centre for Engineering in Agriculture (NCEA) at the University of Southern Queensland that investigates methods of reducing the evaporation rate in a cost-effective fashion. Recent findings suggest that the "aqueous thermal boundary layer" is a key component contributing to the evaporation rate. This is the small region close to the surface of the water where temperature gradients are important.

It the intended purpose of this dissertation to provide insight into current research whilst also adding new research that provides results by performing simulations of the thermal boundary layer. This is in order to characterise the conditions under which the temperature gradient promotes or retards evaporation.

University of Southern Queensland

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ENG4111/1 ***Research Project***

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Wesley James Williams

Student Number: 0061018967

Acknowledgements

I would like to thank Dr Andrew Wandel for he has provided me with some great advice and insight into computational fluid dynamics and evaporation modelling. I thank him for all his patience and efforts during this project.

The support provided by my employer Roads and Maritime Services, New South Wales, has also been greatly appreciated during the development of this research project. Without the understand and ongoing commitment provided to me by management this thesis would not have been completed.

I would also like to thank Emily Smith. The support she had provided me in the toughest times during the development of this thesis has been greatly appreciated and will never be forgotten. Without her support, completion of this thesis would not have been possible.

This dissertation has been completed using the Latex template.

Wesley James Williams

University of Southern Queensland
October 2014

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Chapter 1

Introduction

With excess water wastage and increases in potential evaporation losses, many Australian, and in particular rural communities are facing the undesirable reality of evaporative effects potentially outweighing the received precipitation on a yearly basis. The necessity of forecasting increased evaporation losses presents challenging issues to be resolved in order to reduce economic losses. These economic losses stem from spasmodic regional water restrictions and the purchase of water in the agricultural industry. The loss of water as a valuable resource can be mitigated by the use and application of a monomolecular film to an open water reservoir surface. The variability of the monolayer performance is however, highly variable and is subject to many influencing factors. Biodegradability, ultra-violet radiation, rate of application, bio-organics and predominant wind velocity coupled with wave action are such parameters that affect monolayer performance.

With a direct interest the predominant degrading factor of wind, the performance of a monolayer must be predicted based on the upper and lower wind velocities deemed to be detrimental to its structure. With the aim of complementing existing literature, this study will determine how generated waves will affect the temperature distribution immediately next to water surfaces and will also help characterise conditions which retard or promote evaporation in open water storage reservoirs. A computational fluid dynamics model will be developed and explored within the turbulent flow regime, utilising large eddy simulation to validate research results and conclusions.

Chapter 1 provides an overview of this dissertation. The topics outlined include the project background, specific project objectives, a methodology summary, project contributions and a dissertation outline.

1.1 Consequential Effects of Research

The nature of this project is limited to creating a computational fluid dynamics model that simulates a real world environment in order to quantify evaporation losses from an open water storage reservoir. Pertaining to the consequential effects of this research and the results that are provided furthermore, it has been deemed that no harm will come to the public in an immediate sense.

Realisations of possible mitigation techniques can and may be loosely derived from this dissertation that may enhance the possibility of harmful risks to the community, although these techniques or associated products required to mitigate evaporation losses will not be endorsed as a result of this dissertation. Water resource managers may find it useful to implement such mitigation techniques or products that may be inadvertently supported by this research but it is advised that an independent risk analysis must be undertaken prior to doing so by the relevant authority in control of such infrastructure.

It is the general aim of this research to positively add to the improved sustainability of water resources in order to benefit communities, industries and the general economy. No negative effects to public health and society have been identified or are predicted as a result of the research findings.

Ethically, this research has met the standard of the University of Southern Queensland and has not breached the code of ethics Engineers Australia requires the author of this document to adhere to.

It has been deemed that the only harm to come from the undertaken research is harm to the general health of the author whilst conducting the research and producing the dissertation.

1.2 Identification of Resource Requirements

Resources that have been deemed essential to satisfactorily complete this dissertation have been listed below. In unfortunate cases the availability of such resources will need to worked around if not available. This could be due to outstanding issues that may need to be resolved with computer software at various times throughout the project or possibly due to reviews being undertaken by the supervisor of the research being undertaken. It is therefore proposed that the person conducting the research must at times utilise other resources or means of continuing project work to progress. Essential resources are:

- ANSYS suite of software to allow generation of three dimensional model and subsequent analysis of turbulent flow by utilising large eddy simulations.
  ANSYS will also provide the capability of post analysing the simulation enabling detailed results to be obtained and published. The software will be provided by the University of Southern Queensland.

- Current research sourced from a variety of databases and libraries.
  This includes utilising the University of Southern Queenslands student access portal to online databases that are able to provide published research papers that support or contradict current trends, assumptions, research and practices.

- The National Centre for Engineering in Agriculture (NCEA) will be able to provide project support as staff that are currently employed as well as not currently employed have undertaken exceptional research into water resource related sustainability issues. This research has been primarily supported or done on behalf of the Cooperative Research Centre for Irrigation Futures and will be useful to include in the dissertations literature review.

- University of Southern Queensland engineering faculty staff.
  Engineering faculty staff will provide supervisory support throughout the entire projects life and will also provide the service of reviewing completed work at various stages throughout the projects life. It will also be the University of Southern Queensland who provide certification and support of this research with certain limitations imposed. (Please refer to the Limitations of Use and Certificate of Dissertation provided early in the report).

Chapter 2

Review of Existing Literature

2.1 Evaporation Losses

With the world moving towards a more globalised economy that is becoming more competitive and difficult for countries and continents to market their macro-industrial or macro-agricultural products to the world-wide market, comes the issues of sustaining a national and international economy. Losses pertaining to efficiencies and production rates are therefore being investigated very thoroughly by governments and organisations across the world in order to improve a nation's economy and sustain its' nation's wellbeing far into the future. It is quite obvious that a nation's wellbeing is dependent on its state of agricultural and industrial affairs, however lost production in the specific industries therein cannot be improved upon when environmental factors are at play and cannot be adequately dealt with unless a substantial amount of capital is invested to protect the industry.

Such an environmental factor that contributes to loss and that is specifically being referred to can be attributed to the natural hydrological cycle, specifically evaporation that reduces open water storage reservoir capacity yields that the agricultural industry relies on as an essentiality. In Australia alone 70 percent of the nations fresh water is stored in more than a million open water reservoirs that are used for irrigation purposes (Craig, Mossad and Hancock, 2009). This supports the importance of providing products to the market that enable water resource managers and, on a lesser scale, individual farmers to better equip themselves against evaporative losses which ultimately contribute to loss of recreation, economic gains, water availability for drinking purposes and essential irrigation practices. As stated by Ikweiri, Gabril, Jahawi and Almatrdi (2008), it is water that supports the increasing domestic, agricultural and industrial demands that a nation faces daily. This supports the argument that as storage capacities are reduced, the yields of agricultural production and available drinking water also suffers (Ikweiri et al, 2008).

Because of this large economic impact, an interest has been shown by water supply managers to address the loss of water from open water storage reservoirs in particular. For a large hot and dry continent like Australia, this challenge is of great importance. Recent prolonged periods of drought that were experienced nation-wide have taught many government agencies that are responsible and accountable for the management of water resources, a valuable lesson when it comes to providing adequate measures to mitigate evaporation. To highlight how extreme the losses can be, Ikweiri et al (2008) produced a study which focused on the Omar Muktar open water storage reservoir in Libya and found during their preliminary investigative studies that over 20 percent of the reservoirs water was lost due to evaporation in 2004 (Ikweiri et al, 2008). This accounts for 4.7 million cubic metres of lost water, which for a dry continent is of extreme value.

It was further stated by Considine (2007), in an article developed to promote research being undertaken by the Cooperative Research Centre for Irrigation Futures and National Centre for Engineering in Agriculture, that approximately 40 percent of water is lost to evaporation from farm dams and large water storages in Australia per year (Considine, 2007). A slightly more drastic approximation was provided by Craig, Mossad and Hancock who state that 50 percent of the water stored in open reservoirs across Australia could be lost due to evaporation. This prompted the authors to initiate research into quantifying the evaporation losses based on a more in depth understanding of dam thermodynamics and evaporation physics (Craig et al, 2009).

When taking into account the above information, it is also important to note that a study undertaken by Johnson and Sharma, at the University of New South Wales in 2008 included data obtained from the CSIRO which shows an evaporation rate of 3000mm per year in the North-west of the country. This is in contraction to the

Bureau of Meteorology data that shows a rate of 4000mm per year in the north-west of the country. That part of the country is obviously known to be dry but the variation in estimated rates stands on its own merits to highlight the issues that the nation is currently facing and what Australia will continue to face into the future.

In terms of quantifying evaporation losses on the eastern coast of Australia, a large difference in estimated evaporation losses between the CSIRO data and Bureau of Meteorology data cannot be found. However, a joint report published by both the CSIRO and Bureau of Meteorology named "State of the Climate 2014" has investigated and shown alarming signs of climatic change across the nation. Within this report several key items have been highlighted. The issues that Australia is currently facing and the issues that Australia will continue to face into the future are discussed in detail within the report published by the two organisations. For simplicity and to compliment the problem of increased evaporation, the items included within the report that are directly related to increased temperature and reduced rainfall have been listed below. It is obvious that these two items are parameters that influence the amount of evaporation loss and the amount of water which recharges water storages nation-wide. It can be seen from the below listed items that it is almost inevitable that the continued loss of water due to evaporation will definitely increase.These items are:

- Annual average rainfall projections are uncertain in northern Australia
- Frequency and intensity of extreme daily rainfall are set to increase for most regions across the country
- There is a forecast potential long-term decrease in the number of tropical cyclones but with an overall increase in intensity when cyclones are predicted
- Extreme fire-weather days are also set to increase in southern Australia with the undesirable result of having longer fire seasons
- Annual average rainfall is predicted to decrease in southern Australia resulting in an increase in droughts and the duration of these droughts
- Temperatures are also predicted to rise, with more hot days and fewer cool days across the country

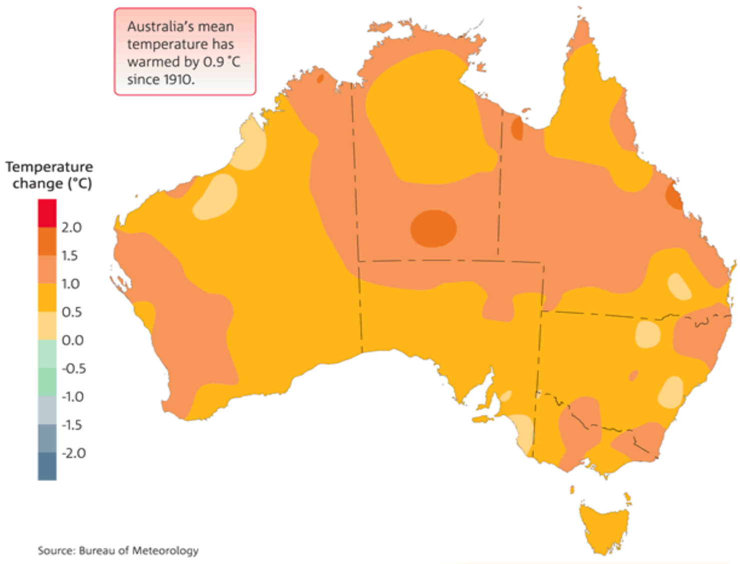


Figure 2.1: Annual mean temperature change across Australia since 1910 (BOM, 2014)

The images provided overleaf form a general informative background into the changing rates of evaporation that Australia is having to deal with. These images demonstrate evaporation rates that are comparative between the years 1990-2005 as published by the CSIRO and also shows the data obtained from Johnson and Sharma (2008).

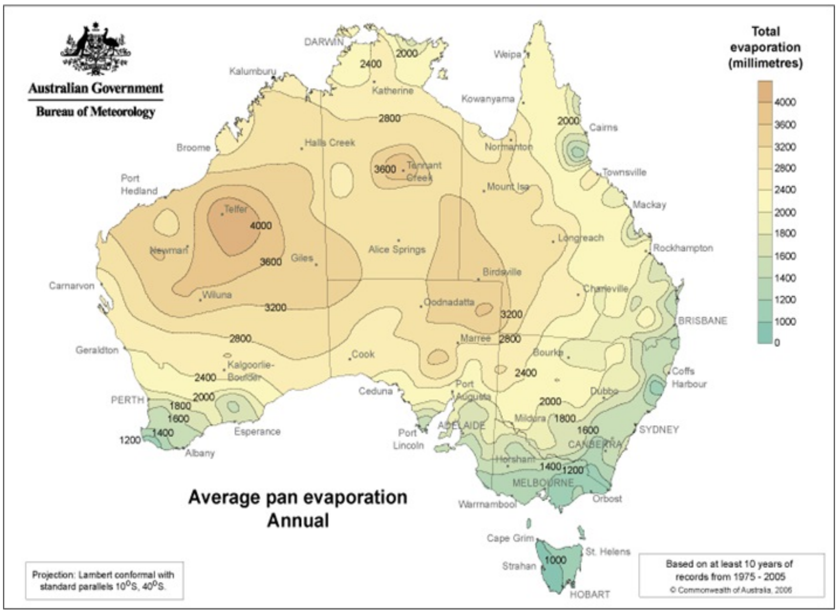
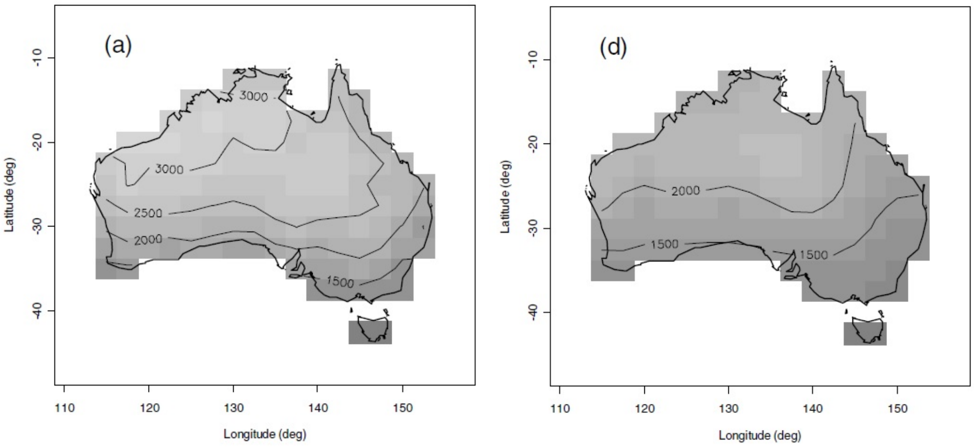


Figure 2.2: Average Pan Evaporation Annual (CSIRO, 2005)



(a) BOM Output

(b) CSIRO Output

Figure 2.3: Comparison of Annual Average Open Water Body Evaporation for 1961 to 1990 (Jonshon and Sharma, 2009)

The challenge is to quantify evaporation using historically developed formulae whilst also taking advantage of computer software packages that enable water resource managers to simulate the real world effect the environment and its variables have on evaporation. This has been a key topic of research that Craig et al are trying to accomplish. The use of computational fluid dynamics (CFD) software has enabled them to initiate the production of a two dimensional computational fluid dynamics model in order to model evaporation from small farm dams. Although at the time of research the model has been stated to be in the very early stages it is hoped that the model will be able to adequately predict evaporation losses in order to mitigate water losses.

Unfortunately, the model intended to be produced by Craig et al also requires the input of real data that is highly variable and extremely important to include to gain a complete and validated output of calculated predicted losses. This can be confirmed by literature that describes current equations that are used to predict evaporation losses from a large variety of media. Evaporation from media as such can include evaporation from soil to the open atmosphere, from plants to the open atmosphere and from a water body to the open atmosphere for example. All of which are influenced by an extremely large and complex variety of parameters that relate to the individual media alone. This is in support of Warnaka and Pochops (1988) research which concluded that, due to the complexity of evaporation modelling, a design model or formula must be ideally chosen to reflect evaporation losses for a particular area only. The creation of a general evaporation model is extremely hard to achieve on the back of research conducted by Warnaka and Pochop (1988) who also found that the various different formulae, used to predict evaporation losses, either over-predicted or under-predicted evaporation losses at two lakes within Wyoming, United States of America. Johnson and Sharma (2004) support this argument by also stating that evaporation modelling is not a straight forward task.

For simplicity and to keep on track with the intended research from this thesis, the case of open water storage to the atmosphere only is only considered.
Ikweiri et al (2008) state that there are 4 cases of variables that influence open water storage evaporation rates.

- Barometric pressure where evaporation increases with decreasing pressure.
- The concentration and specific type of dissolved matter that is present in the water at the time of evaporation. This is important to quantify as the vapour pressure of water is decreased which in turn decreases the rate of evaporation. This effect may be thought to be tied to the dissolved matters capability to retard temperature changes at certain points or within aqueous layers that can be within the water body. This is a highly important variable to quantify but also a very complicated one. This suggests that the limnological layers

of the water body can have an influence on retarding evaporation. To aid in this understanding Craig et als development of an evaporation model via computational fluid dynamics also aims to provide insight into the advective accumulation of warmer water at shallower areas downstream of the winds initial influence.

- The shape and situation of the water body under examination also is said to influence or retard evaporation due to a number of factors which can include the wind speed from multiple directions under certain barometrical conditions and the age and state of the vegetation that surrounds the water body. A very basic example of which is provided by Ikweiri et al (2008) that states the near surface velocity of wind travelling over the waters surface is affected by the length of the fetch the wind blows over and the vegetation surrounding the water body. In this case the vegetation, if large and dense enough can act to slow the winds velocity and reduce evaporation.

- The fourth case to be considered as a result of Ikweiri et al (2008) research states that the relative depth of the water body can affect the latent heat that is stored within the water. Expansion of this statement provides background as shallower lakes can have a larger evaporation potential due to a greater amount of energy being stored near the liquid's interface with the atmosphere.

The shape, situation and relative depth variables are also supported by Considine (2007) who suggests that deep narrow dams retain water more effectively than wide shallower dams. This statement from Considine (2007) partly attributes itself to providing a smaller area for wind to influence in the case of cross-winds but along the largest fetch the wind is thought to be influencing a water body with a low amount of energy stored at the atmospheric boundary layer. Evaporation losses are thus assumed to be lower in cases where the water body is narrow and deep.

For the four cases above confirmation is again provided by Craig et al who expand upon the four cases to include the specific influence of air. This refers to air's temperature, velocity and its humidity. To further the support provided by Craig et al, the complex analysis of taking into account the surface roughness of a water body which is consequently influenced by wind or air velocity flowing over the waters surface must also be accounted for. Further suggestions made by Craig et al also state that after consideration of the parameters included in modelling evaporation, it is clear the process becomes very involved which is in support of Warnaka and Pochop (1988).

It has been found by Craig et al that the main driver for evaporation in countries is solar radiation during the day. Considine (2007) supports this by stating that the impact of many environmental factors includes the effect of UV light that accelerates the movement of water molecules from a water body to air. This has been described as being the general definition of evaporation by Craig et al.

It is important to note that the above described variables also play a large part in the rate of evaporation losses and the argument of which is most important is not easy to decide on. This is due to the variables being completely independent of location but also being dependent on each other. This complexity means that in some locations or, situations more generally, most parameters may or may not be present and hence evaporation prediction will constantly vary.

2.2 Evaporation Equations

More than a few methods are available for measuring the potential evaporation from many varieties of media. These varieties of media can range from being soil to the atmosphere, water to the atmosphere and plants to the atmosphere to name the general and basic cases that are most commonly encountered in estimating evaporation losses. Computational fluid dynamics has been at the forefront of the prediction of potential evaporation losses and will continue to develop the industry that at the moment operates in a rapidly changing environment. The major cause of the rapidly changing environment is the advancement of technology. Technology advances now allow extremely accurate measurement of evaporative losses in real world environments. However the challenge that presently exists is to measure and estimate potential evaporation before field studies are conducted to validate results within a controlled and simulated environment. This encompasses using computer generated models that utilise equations developed over time that can represent, as close as possible, what will actually happen and what can be expected in terms of evaporation losses.

Presently there are various papers that aim to provide good correlations between potential evaporation losses that are predicted and actual measured evaporation losses. Research conducted by Warnaka and Pochop (1988) demonstrates comparisons between six equations that are used to estimate to the evaporation losses from open water storage reservoirs in Wyoming, United States of America. They concluded that due to the variability in climatic data used during their analysis and research that the equations vary greatly in their ability to predict the magnitude and variability of free water evaporation (Warnaka and Pochop, 1988). This supports the argument made by themselves that an evaporation model, if needed to estimate losses within certain tolerances, needs to be developed on an independent basis, representative of that particular location only.

The three most common equations that exist and that are used to predict potential evaporation losses are shown below and overleaf:

Daltons Formula:(Craig, 2005)

$E_a = f(u)(e_x - e_a)$

Penmans Formula:(Craig, 2005)

$ET_o = (1/\lambda)[(\Delta/(\Delta + \gamma))(R_n - G) + (\gamma/(\Delta + \gamma))f(u)(e_s - e_a)]$

where:

ET_o is the evaporative flux (mm/day)

λ is latent heat of vapourisation (MJ kg^{-1}) $= 2.501 - 0.002361T(C) \approx 2.45$

R_n is net radiation (MJm-2 day^{-1})

G is the soil or water heat flux (MJm-2 day^{-1})

Δ is the slope of the saturated vapour pressure curve at mean air temperature (kPaC^{-1}) $= 0.2(0.00738T + 0.8072)^7 - 0.00016$

γ is the psychrometric constant (kPaC^{-1}) $= c_pP/0.622\lambda \approx 0.067$

$f(u)$ is a function of windspeed $= 6.43(1 + 0.0536u_2)$

e_s is the saturated vapour pressure (kPa)

e_a is the actual vapour pressure (kPa)

Penman-Monteith Formula:(Craig, 2005)

$\lambda E = [\Delta(R_n - G) + \Delta\rho_a c_p(e_s - e)/r_a]/(\Delta + \gamma)$

where:

ρ_a is the mean air density at constant pressure

c_p is the specific heat of air

γ* is a modified psychrometer constant as follows

$\gamma * = \gamma((1 + r_s)/r_a)$

where:

r_s is the surface (or canopy, leaf, stomatal) resistance (s/m) term controlling release of water vapour to the surface

r_a is the aerodynamic (or ventilative) resistance (s/m) controlling the removal of water vapour away from the surface

$r_a = (ln[(z_m - d)/z_{om}]ln[(z_h - d)/z_{oh}])/k^2u_2$

where:

z_m is the height of wind measurements (m)

z_h is the height of humidity measurements (m)

d is the zero plane displacement height (m)

$z_o m$ is the roughness length governing momentum transfer (m)

$z_o h$ is the roughness length governing transfer of heat and vapour (m)

k is the von Karmon constant = 0.41

u_2 is the windspeed at height 2m above surface (ms^{-1})

$r_s = r_{stom}/LAI_{active} = 0$ for open water storage evaporation

DeBruins Formula:(Winter and Rosenbery, 1995)

$PET = (\alpha/(\alpha - 1))1.141(\gamma/(s + \gamma))((3.6 + 2.5(u_3))(e_s - e_a))$

where:

PET = Potential Evaporation (mm/day)

γ is the psychrometric constant (kPaC^{-1}) $= c_p P/0.622\lambda \approx 0.067$

$(\gamma/(s + \gamma))$ = parameter derived from slope of saturated vapour pressure curve at mean ar temperature

α = Priestley-Taylor coefficient = 1.26

u_3 is the windspeed at height 3m above surface (ms^{-1})

e_s is the saturated vapour pressure (kPa)

e_a is the actual vapour pressure (kPa)

Mass Transfer Formula:(Winter and Rosenberry, 1995)

$E = Nu_2(e_s - e_a)$

where:

E = evaporation dependent on calibration of N (mm/day)

N = mass transfer coefficient (dimensionless) u_2 is the windspeed at height 2m above surface (ms^{-1})

e_s is the saturated vapour pressure (kPa)

e_a is the actual vapour pressure (kPa)

It can be seen that the data input requirements for the various equations shown can vary and range in complexity. However, the equations that utilise the inputs of temperature, wind, humidity and solar radiation are considered to be the most accurate and responsive to climatic variations (Warnaka and Pochop). A report undertaken by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) for estimating evaporation across the Murray-Darling Basin utilises the Penman-Monteith equation. This equation is able to adequately predict evaporation from the basin by using inputs of water surface temperature, are temperature, wind speed and vapour pressure (CSIRO,2008). The above input variables also attributed to uncertainty in the estimates of evaporation and further to this water body depth and size also contributed to the uncertainty of the results. This directly supports findings made by Ikweiri et al (2008), Craig et al and statements made by Considine (2007) whilst also clearly highlighting the sensitivity involved in evaporation modelling.

2.3 Evaporation Trends

On another front of adequate evaporation prediction, many trends have been observed. The trends considered by Johnson and Sharma (2008) actually suggest that decreased pan evaporation rates during the past 40 years act to reduce confidence in the assumption that evaporation actually increases with temperature alone. Johnson and Sharma further suggest that current research into evaporation needs to be reassessed with the effects of wind speed and vapour pressure being considered as the primary variables. This contradicts the statement made by Craig (2005) who suggests that solar radiation is the main driver of evaporation further highlighting the issue that evaporation is a complex issue. The reason for Johnson and Sharma's (2008) suggestion to consider wind and vapour pressure as priorities is due to data obtained by them that shows decreasing pan evaporation on a national level. This is paradoxical to the commonly held belief that evaporation should increase with increasing temperature, which is what the world is currently experiencing as a result of climate change.

In order to support this, wind run changes have been observed by Roderick and Farquhar (2002) who found that decreasing wind speed and solar irradiance were responsible for decreasing trends in pan evaporation. As the influence of wind over a fetch is considered to be an important factor in evaporation the reasons for wind run changes have to be investigated and quantified, if not proved. The above suggestion is again provided in research undertaken by Rayner (2007) who states that the change in wind patterns is not clear and must be investigated.

In direct opposition to the statements made by Johnson and Sharma (2008) and also Roderick (2002) the CSIRO (2007) has found that evaporation is actually predicted to increase Australia wide from the decades of the 2030's to the 2070's. This shows the most dramatic increase in evaporation to be located in the centre of the country. Predictions also made by the CSIRO (2007) also predict a 50 percent reduction in rainfall by the year 2070 while temperature is also expected to increase by up to 5 degrees by 2070. Consequently, this also contradicts the statement made by Johnson and Sharma (2008) where the common assumption of evaporation increasing with temperature needs to be reassessed.

The common underlying factor that unifies all research however is the effect of wind on the trend of evaporation. The aerodynamically effected component is important to model in order to adequately validate an evaporation model. For this wind patterns may need to be assessed for the impacts it may have on evaporation losses from open water storage reservoirs.

2.4 Project Initiation

The consequence of evaporation as explained above is highly undesirable and methods of determining and predicting losses with high precision and accuracy are highly sort after. It was also explained and shown in images contained within chapter 2.1, Evaporation Losses, that as much as we rely on highly reputable organisations to provide adequate predictions and forecasts, they too cannot agree on specific rates of evaporation. The difference in evaporation rates is fundamentally what has driven the need to undertake further research into what is causing evaporation losses and what natural mechanisms are mitigating evaporation. From this the project has been initiated in order to develop a 3-dimensional computational fluid dynamics model to focus specifically on the aqueous thermal boundary layer. Recent research that has been undertaken at the University of Southern Queensland has highlighted that the characteristics of this boundary layer, which is essentially known to be the 1mm thick surface skin of a water body open to the atmosphere, plays an important role in actually mitigating evaporation. This is considered true under certain environmental conditions and influences. The methodology of this report along with the following literature review will further explain the necessary inputs required for the development of a computational fluid dynamics model. It was deemed necessary at this point of the dissertation to explain the reasoning of why the project is being undertaken exactly and to also make sense of why the remainder of chapter 2 past this point has been included and deemed important.

2.5 Aqueous Thermal Boundary Layer

As research has suggested the aqueous thermal boundary layer, near to the waters surface, plays a particularly important role in controlling and maintaining a balance of temperature below the interface of both air and water (Wells et al, 2009). It is understood that whilst the air remains responsible for the governing of the transfer of heat, the aqueous thermal boundary layer is solely responsible for the transfer of C02, O2, CH4, halo-carbons and many other organic compounds.

With this exchanging responsibility identified, the mechanisms controlling the transfer processes of such components, or gases, across the aqueous thermal boundary layer at wavy air to water interfaces continues to remain poorly understood. What are of particular interest are the predictions of temperature gradients and their influences in non-linear, turbulent situations. Jahne (1988) outlined a phenomenon that identified and suggested potentially large enhancements of gas exchange processes that occurred as a result of wave generation. What has been and continues to be essentially difficult is the measurement of and sophisticated techniques that are associated with quantifying and measuring these temperature gradient changes. Earlier research by Katsaros in 1979 stated that, because of these measurement difficulties, much of the research at that specific time was based primarily on hypothesis and inference and thus was largely reliant on laboratory experiments. Interest is also directed toward finding out if whether or not the results and conclusions drawn from lab experiments are generalizable to real life situations and open water reservoirs.

It is known that the aqueous thermal boundary layer has a thickness of 1mm (Wells et al, 2009). It is through research that, the thermal boundary layer has been identified to be relatively cooler when compared with the bulk water below. Wells et al (2009) suggested that this thermal boundary layer of 1mm thickness can have a temperature difference of anywhere between 0.2 degrees Celsius and 0.5 degrees Celsius under conditions of strong cooling. This is the result of sensible, latent and long wave radiation heat fluxes (Wells et al, 2009). Earlier research conducted by Jahne (1988) suggested that a change in surface temperature is approximately 0.5 degrees Celsius at low wind speeds, and approximately 0.2 degrees Celsius at high wind speeds. It is understood that this earlier research highly correlates with later studies as reflected in the conclusions drawn from more research literature conducted by Wells et al (2009). Upon review, it was evident that other research findings suggested slightly more drastic temperature ranges, which was clear in a study by Katsaros (1979) who concluded that there may be temperature differences between a few tenths to 1 degree Celsius.

Although this temperature range proves greater than the temperature ranges suggested in more modern literature, it is still understood that many processes and surface active materials influence the temperature within this very thin layer. This supports additional statements made by Katsaros (1979) who assumed that the thermal boundary layer is manifestation of numerous complex physical processes of exchanges between two diverse media, being air and water (Katsaros, 1979). Prior to understanding completely how the surface temperature considerably varies in the uppermost millimetres of water body surface, researchers generally assumed that the surface and subsurface temperature was in fact identical (Saunders, 1967). This was further supported in subsequent research conducted by Katsaros (1979). However, it was through literature completed by Katsaros in 1979, whereby laboratory experiments concluded and confirmed non-linear temperature gradients as existent within the boundary layer (Katsaros, 1979). A non-linear temperature gradient has been outlined and further described by the Osborne theory. This theory is underpinned by the knowledge of which the thermal boundary layer is represented by two layers, one of which is dominated by advection, where the temperature gradient is linear. The opposing layer, which is situated superior to the advection layer, is balanced by both advection and diffusion (Wells et al, 2009). As a result of this knowledge, particular interest in the temperature divergence at the air-water interface has reawakened activity that seeks to describe the macro-physics of this thin skin, known as the aqueous thermal boundary layer. This does certainly not exclude how certain environmental conditions impact the physical characteristics that underpin the boundary layers make-up. If one physical parameter alters, any parameterisation of the boundary layer becomes increasingly questionable. This statement has been made by Jahne et al (1988) in which the researchers concluded that realistic description at any one instance is nearly impossible since natural changes of any parameter is very fast.

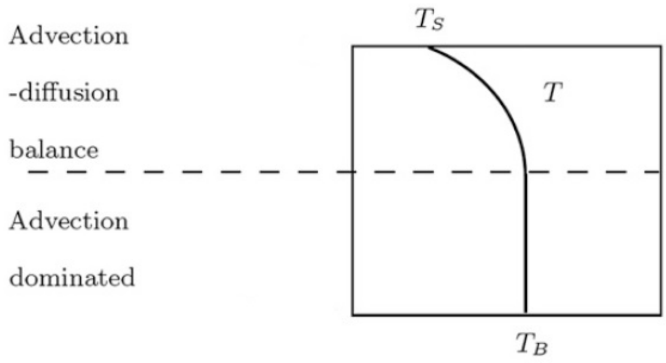


Figure 2.4: Schematic illustration of the temperature gradient profile through the aqueous thermal boudary layer. T_s represents surface temperature, T_b represents temperature of underlying bulk water below the boundary layer (Wells et al, 2009)

It is essential that a sound understanding of how the thermal boundary layers temperature gradient not only exists but alters with wave propagation. For low wind speeds a free convective boundary layer develops, and it is understood that this boundary layer thins in the presence of strong winds as a result of additional shear generated turbulence (Wells et al, 2009). This boundary layer thickness and temperature gradient deviation within can also be modified by the swell of waves, microbreaking, waves and or surfactant and pollutants (Wells et al, 2009). This further highlights the dynamic nature of the aqueous thermal boundary layer.

Katsaros (1979) suggested that the stretching of the waters surface which increases surface area would subsequently affect surface tension. This is a result of a turbulent wind acting to generate waves. The generation of waves of which is an important parameterisation as Katsaros states that at the trough of a generate wave set, the thermal boundary layer proves to thin. In contrast to this the boundary layer is also suggested to thicken at the crest of a wave (Katsaros, 1979).

From the above it can be concluded that the temperature difference is reduced at the trough of a wave and heightened at the crest of a wave. It is the difference between these temperature gradients where evaporative losses are considered important. This is also confirmed by Wells et al (2009) within their published work in which the authors state that the temperature of the aqueous thermal boundary layer can significantly influence the transfer of heat, moisture and gases between the ocean and atmosphere. Its obvious that in these cases, evaporation is most likely to occur where the boundary layer is thinnest and the temperature is closer to that of the bulk water which is considered to be warmer (Wells et al, 2009).

2.6 Wave Generation

For a long time it has been widely accepted that when a turbulent wind comes into direct contact with a resting body of water, a wave system is provoked and this wave formation continues to develop under the action of the wind (Phillips, 1958). It has been acknowledged that waves are in fact generated through a number of mechanisms, however, research suggests that it is certainly the wind that contributes, for the most part, to wave generation on the waters surface. The problems associated with as well as the theories behind wind-wave generation remain under developed and poorly understood. It has been this wind-wave generation that has sparked important discussion and research direction for many mariners and oceanographic researchers.

One of the main complications associated with understanding wind wave generation has been the result of difficulties surrounding the use of instrumentation devices. These devices aim to quantify wind and pressure at the waters surface as well as the propagation of the generated wave itself. If this has or can be resolved, empirically historic theories and hind casting techniques that are, or were used to predict wave height and wave length can be validated or invalidated accordingly. It has been made apparent that attempts to investigate and quantify wave generation remain formidable engineering problems as a result of this difficulty.

In a general sense it is obvious and likely that wind indeed does generate waves at the waters surface. Subsequently, it could be expected that a wind blowing over waters surface would first generate waves when the wind velocity is great enough to make one particular type of wave grow. This has been an underpinning philosophy in which Jeffreys developed his sheltering theory around in 1925 (Jeffreys, 1925). From this it can also be proposed, that when a winds velocity exceeds, or increases beyond the wave generating velocity, energy will be imparted onto the waters ruffled and deformed surface, and thus increasing wave height (Jeffreys, 1925) However, it is not been made clear how the wind is initially able to impart energy directly onto the water surface in order to create these waves. As previously stated, this continues to be an important part of oceanographic research.

In contrast to the theory of sheltering developed by Jeffreys, another theory which has since been modified since publication was developed by Phillips in 1958. The theory developed by Phillips suggested that when a turbulent wind blows over a large sheet of water that is initially at rest, a wave system is initiated and developed under continued wind action (Phillips, 1958). It is important to note here, early on, that Phillips does not discount sheltering theory but seeks to describe the origin of wave generation in his philosophy. This merely suggests that sheltering theory describes how wave propagation is sustained and increased. This is in contrast to Phillips theory that examines how the wave is actually created from an initially still water surface.

Modern day theory must however take into account the many factors present in a water body prior to wave generation. One important and obvious factor is surface tension at the waters surface along with the average velocity of the wind, duration of the winds pass or run and the winds fetch distance. This is a current issue as Roderick et al (n.d) have observed considerable wind run changes and found that decreasing wind speeds are in fact a reality. As the influence of wind over a fetch is considered to be an important factor, wind run changes have to be investigated and quantified, if not proved. The above suggestion is again supported in research undertaken by Rayner (n.d) who states that the changes in wind patterns are not clear and must be further investigated.

The first attempts at explaining and quantifying the mechanisms behind wind-wave generation were conducted by Sir William Thomson in 1874. It was through the application of a mechanism called the Kelvin-Helmholtz instability that he used to describe wave generation. However, It wasnt until 1925, were the theory described by Jeffreys, was able to identify that this long abandoned theory that was created by Sir William Thomson was limited and inadequate in describing the generation of surface waves. It was through Jeffreys sheltering theory in 1925 that a far more accurate and longer standing idea on wave generation was presented. (Jeffreys, 1925)

The philosophical idea presented by Jeffreys (1925) only required wind velocities of 1 m/s in order to generate waves. Based on the idea that as wind passes over a wave crest, the airflow becomes separated, and thus a sheltered area is created in the trough of the waters surface which is situated between two concurrent wave crests. (Jeffreys, 1925) It was through this mechanism that Jeffreys identified a pressure differential which is formed within this area. This was suggested to promote the upward movement of the leeward side of the wave. Similarly the great pressure that is transferred to the wind-ward side of the proceeding wave would be promoted in a downward sense. It was advocated that this energy transfer and pressure differential provided the cause for the continuation of wave propagation and is what enables the growth of the wave (Jeffreys, 1925).

In order to further understand this theory it must be understood that when air comes into direct contact with the waters surface the air is known to be travelling at the same speed as the water. This is obvious as a boundary layer exists at the interface and friction between the two phases (air and water) dictates this relationship.

This sheltering theory has been further investigated through research conducted by Banner and Melville (1976). This research was initiated on the premise of Barnett and Kenyon (1975) who questioned whether or not air flow separation does in fact occur over wind waves. In further support to this statement, Banner and Melville (1976) alleged that the difficulties with defining air flow separation near a moving surface have not been forthcoming. Banner and Melville (1976) posed the argument that air flow over a water wave would be less prone to separation than air that is actually flowing over a solid boundary. It is suspected that this argument was put forward with the ideology of water being the more flexible surface. This would indicate that the water surface would in fact conform more to the wind, as opposed to the wind breaking away from the water surface as is observed when considering wind flowing over a solid boundary. However, in support of the sheltering theory, Banner and Melville (1976) stated that the onset of wave breaking is actually sufficient to ensure the existence of air flow separation. This seems to be quite an obvious statement, as it is already recognized that the smoother the surface of any objects (solid or fluidic), the less turbulent the flow will be at the interface. This lends itself quite appropriately to research which has investigated the aerodynamic roughness factors concerning the waters surface.

Experimental results concluded by Banner and Melville (1976) offered strong confirmation that airflow separation does indeed occur for wind that is flowing over a waters surface, if and only if, the generated wave that is produced is breaking. This is in support of Jeffreys sheltering theory, which also suggested the occurrence of the separation mechanism at low wind-speeds. This explains the tendency of separation to occur in even the slightest wind breeze. (Banner and Melville, 1976) However, the air will not separate unless wave breaking is occurring. Wave breaking can be seen as the result of a multitude of factors, which are inevitably unforseen, which lends further support to Banner and Melvilles experiments, where the wave was breaking at airflow of 0.9 m/s, with a 0.75 m/s water flow in the opposite direction to the airflow (Banner and Melville, 1976).

Sheltering theory has been supported in a number of subsequent studies that have identified how accurate and reliable the foundations were that formed the basis of this notion. However, Jeffreys (1925) failed to describe and calculate the first origin of wave development that occurs from a body of water at initial rest. This suggested the need to further investigate the production of waves from an initially still and flat surface. This has provided the foundations for further research by Phillips (1957), who developed a theory on the generation of ripples on a flat sea. It was through this research were Phillips suggested that air pressure fluctuations can potentially ruffle the waters surface (Phillips, 1957) It is understood that Phillips research direction was created in order to add to existing research regarding wave generation theories conducted by Jeffreys in early years. With Jefferys describing and quantifying the propagation of waves, Phillips theory, was targeted at unfolding the mechanisms behind the initial generation of waves (Phillips, 1957). The disadvantage behind the theory that Phillip described indicated that the wind is unable to transfer adequate energy to the waves in order to make them grow as quickly as visual observations have indicated. This suggesting that, the Phillip and Jeffreys theories are highly interlinked; however they represent different times of wind-wave generation. Phillips research has targeted the earliest phase of wave generation, which is shortly followed by Jeffreys theories that have quantified mid-late stages of wave formation and growth (Phillips 1957).

It seems more plausible that the initiation and development of waves is a consequence of fluctuations in normal pressures upon the surface. This is due to the random distribution associated with the onset of a turbulent wind (Phillips, 1957). Phillips has been supported in subsequent research that outlined that the deformation of air flow determines the force exerted by the wind on the sea surface (Miles and Phillips). It is said that this creates a low pressure on the leeward face of the wave, and a high pressure of the wind-ward face of the wave. This draws strong comparison to earlier theories of sheltering. (Jeffreys, 1925). However when both theories are utilised as an adjunct, the mechanisms underpinning and explaining wave generation are far more effective than that proposed singularly by Jeffreys in 1925 (Phillips, 1957). When these theories are considered together, it is suggested that results drawn from such experiments will provide a more valid and reliable representation of true wind-wave generation.

It is an assumption that the components of the pressure fluctuations occurring at the surface will generate small force oscillations on the waters surface, to which the response of the water will not be uniform. Furthermore, according to the theory presented by Phillips (1957), it is suggested that the minimum wind velocity capable of raising the water surface is 0.023m/s. However, the turbulent motion of air is thought to generate surface displacement irrespective of wind velocity.

2.7 Turbulent Inlet Boundary Conditions

One of the great challenges facing the computational fluid dynamics industry is the generation and application of appropriate boundary conditions used for particular simulations. The importance of why this is applicable is due to boundary conditions providing a way of anticipating flow behaviour at the limits of the computational domain (Lodato, Domingo and Vervisch, 2008). This anticipation however is contradicted by the fact that turbulent flow requires randomisation specifically correlated to Gaussian distributions (Baba-Ahmadi et al, 2008) or synthesising a velocity field from the summation of Fourier harmonics (ANSYS, 2011).

The flow profile within a computational domain however could be at risk of predetermined results as a direct result of inappropriately defined conditions at inlets, outlets and at side boundaries or structure walls for which flow regime is to be determined. The need to understand the relationship between the adopted boundaries also demands attention as the boundaries influence the result of flow characteristics within the domain due to the inter-relations between different boundaries. Much of this has been identified and described by research conducted by Lodato, Domingo and Vervisch (2008) where the 3 dimensional boundary conditions for large eddy simulations (LES) of compressible viscous flows were investigated. Lodato et al (2008) identified the recurrent issues in computational fluid dynamics were as a result of boundary condition treatments and the reflections that may be caused by inter-relationships between conditions at the corners of a 3 dimensional model. This has been supported by Montorfano, Piscaglia and Onorati (Unknown) who also state that issues of turbulent flow modelling are caused by boundary conditions at the inlet and at walls of the domain. Baba-Ahmadi and Taber (2008) describe inlet conditions specifically as having a large impact on the flow dynamics and state that the correct implementation and appropriate selection of inlet conditions is of high importance for the construction of a turbulent flow regime. The main goal is to determine an appropriate method for the generation of inlet conditions that are accurate in terms of reproduced flow characteristics defined by precursor methods or synthesised methods (Perret, Delville, Manceau and Bonnet, 2008).

In defining turbulent flow characteristics the fluid flow has no definite frequency or observable pattern. Resulting is the creation of irregular motion by a large number of particles within a short time step or interval. This is concurrent with fluctuating velocity within the flow field accompanied by pressure changes within the computational domain (Finnemore and Franzini, 2002). Fluctuations arise due to the fluid moving in small discrete packets called eddies, jostling each other around in a random manner that are mostly caused by rotation, especially near boundaries (Finnemore and Franzini, 2002). No two individual particles within fluid flow, that has been characterised as turbulent, can follow the same path as it is completely random and follows only an erratic path. It is therefore impossible to adopt a rigid mathematical rule model to describe turbulent flow. Instead only statistical models can be used to appropriately define turbulent flow regimes within a computational fluid dynamics program and computational domain. This is backed by Finnemore et al (2002) who state that statistical methods of evaluation are used to predetermine the random flow variations, velocity and pressure variations characteristic of turbulent flow. Finnemore et al (2002) also state that domain entrance conditions also affect the length of the unestablished turbulent flow / established laminar flow and hence the position of established laminar flow downstream.

Baba-Ahmadi and Tabor (2008) have suggested, in theory, what conditions should generally be met at the inlet boundary for large eddy simulations. These conditions are reproduced below:
The boundary should:

- Be stochastically varying;
- Be on all scales down to the filter scale (spatially and temporally);
- Be compatible with the Navier-Stokes Equations;
- Look like turbulence;
- Allow the easy specification of turbulent properties (turbulence intensities, length scales etc.);
- Be easy to implement and to adjust to new inlet conditions.

Generally, 3 techniques are used to generate inflow conditions particularly for large eddy simulations (LES). These include the precursor method, mapping from an internal field and synthesised turbulence generation. Pertaining to the issues highlighted within the research conducted by Montorfano and others, the issues of turbulence at boundary conditions need to be appropriately dealt with to allow the realistic output of results when undertaking large eddy simulations. Conditions for LES always include a time varying component and at the inlet a method must be formed for generating stochastic (random) fluctuations on the grid scale that shows turbulence is being generated (Baba-Ahmadi and Tabor, 2008).

Pre-cursor methods require a sample simulation to be run first so that turbulent fluid flow is and can be fully developed. A turbulent profile of the fully developed turbulent flow is then saved at a nominal point, either upstream or downstream from an inlet or outlet respectively, within the computational domain and used to define turbulence at the inlet for the actual simulation to be run. This results in genuine turbulence that is computationally correct being developed (Baba-Ahmadi and Tabor, 2008). The efficiency gained in terms of the development of the generated turbulence and quality at the inlet is simpler calculation wise, than the flow that is to be simulated using synthesised methods (Perret et al, 2008). (This is not to be confused by another statement later made in research by Perret et al who claim synthesised methods are the simplest method on a wholistic scale). This method is popular and is prescribed with confidence by Patil and Tafti (2011), Baba-Ahmadi et al (2008) and Perret et al (2008) who support its use in LES modelling.

The pre-cursor method is easily defended by research completed by the respective persons as it is a turbulent flow profile generated under genuine and realistic circumstances. The regime is hence not synthetic and represents realistic conditions. It is further supported by Patil and Tafti (2011) who state that it is the most accurate method for specifying instantaneous velocity fluctuations for LES modelling. This exact statement is reproduced by Jarrin, Benhamadouche, Laurence and Prosser (2006) who also support the accuracy of the pre-cursor method in producing the most realistic and genuine inlet condition for turbulence modelling.

It should be noted that the pre-cursor method is not limited to being run before the real simulation but can also be run concurrently which necessitates the additional need for extra computing power and simulation run time. This method is considered separately from pre-cursor methods and is known as the mapping method. The basis for the creation of this method is founded on the idea that there is no reason why the pre-cursor method could not be integrated into the computational domain whilst running the real simulation. The sampling simply takes place downstream from the inlet with the conditions being mapped back to the inlet (Baba-Ahmadi and Tabor, 2008).

Despite the method meeting all of the requirements for an inlet boundary as published by Baba-Ahmadi and Tabor (2008) the drawback of computational expense is not major. The significant issue with the mapping inlet being used is the ability for perturbations being able to reach the mapping plane from downstream and thus being replicated at the inlet (Payri, Gimeno, Marti-Aldaravi and Bracho, 2013).

Current research also alludes to the fact that synthesised methods can be appropriately used to create random fluctuations in velocity and pressure at the inlet boundary. Synthesised methods used for developing turbulence at the inlet use a randomly perturbated velocity flow field (ANSYS) or randomly distributed eddies to generate instantaneous turbulence spatially and temporally (Patil and Tafti, 2011). A method developed by Jarrin et al.(2006) is able to produce significant results that produce correct spatial statistics and correct spectral context (Perret et al, 2008). This method, known as the vortex method, describes each eddy by a shape function that is localised in space (Davidson, 2007). The method allows eddies to be generated randomly at the inlet.

The overall advantage of the synthesised method is that the process is less computationally expensive, in terms of computer processor use and simulation run time when compared to pre-cursor methods. Baba-Ahmadi and others further suggest that it is not necessary to lengthen the computational domain in order to incorporate turbulent conditions when synthesised methods are to be used. This is thought to be a disadvantage that is necessary for pre-cursor methods using a steady velocity inlet in order to further simplify the pre-cursor simulation.

The disadvantage for pre-cursor methods is supported by Perret et al (2008) who also communicate that unless the domain is large enough for fully turbulent flow to develop from a laminar to turbulent state, from a steady velocity inlet condition, one must be able to prescribe conditions that meet LES conditions. This is where synthesised methods predominate. As it is the simplest method for determining inflow conditions (Perret et al, 2008) wholistically and is also described as being superior to steady inlet flow conditions (Davidson, 2007) that must develop into turbulent flow over large reaches.

2.8 Effect of Roughness on Surface Boundary Conditions for Large Eddy Simulations

For the effect of simulating highly turbulent zones, the effect of surface roughness that a boundary layer may have on turbulence needs to be assessed and understood. The parameterisation of the surface boundary layer or wall boundary layer plays an extremely important role in real world simulations and is a challenge in itself that needs to be met in order to make large eddy simulation environments a more reliable tool.

The specification of local shear stresses that occur instantaneously within the 2-dimensional realm that are temporally varied are based on the resolution of the velocity field. The general and more classical method of resolving this field is by using the Schummann-Grotzbach method. This method is based on the assumption that the locally filtered velocity shear stresses are in complete equilibrium. Although other methods have been created that also resolve the velocity field that are based on similarity theory to compute the average shear stresses.

Similarity theory means that the adopted assumptions or input apply to all flows if certain conditions are met initially. These methods are the shifted Schummann-Grotzbach method, local Schumann-Grotzbach method and the classic Schummann-Grotzbach method where the local and classic methods are used primarily in simulating effects at the atmospheric boundary layer. Disadvantages with simulating the surface shear stresses using the above methods however, are that they under-predict the fluctuations of stresses which vary temporally.

To overcome the above shortfall a model developed by Marusic, Kunkel and Porte-Agel (2001), referred to as the MKP model, was developed and was tested using sub-grid-scale turbulence models. The assumption adopted by Marusic et al (2001) utilises a characteristic constant, α, that does not change with respect to aerodynamic roughness factor. Testing enabled a direct correlation to be made between surface shear stresses and the aerodynamic roughness factor, sometimes referred to as z_o. This forms the rule that as the aerodynamic roughness factor increases along the atmospheric boundary layer of a certain material the surface shear stresses will increase. Conversely as the surface of a material is smoothed out as a result of damping (water waves) or if the materials surface is engineered to produce a smooth surface the shear stresses will also decrease.

MKP modelling does not reflect the above relationship however, as it is formed to be independent of the aerodynamic roughness factor and instead assumes a constant factor of $z_o = 0.10m$ and $/alpha = 0.10$. The aerodynamic roughness factor adopted by the MKP model represents what is normally used for flow over water. Baldocchi (2012) states that values of roughness of water range from 0.10 to 10^{-4}m. This correlates to research undertaken by Marusic et al (2001) who also found that best results are obtained when using α equal to 0.10 as higher values of aerodynamic roughness translate into stronger damping of velocity fluctuations near the surface of the material. A reduced mixing strength due to turbulence thus exists and lower levels of velocity variance also exist. Marusic et al suggest that the MKP model gives a more realistic model for velocity gradients that are independent of surface roughness.

Chapter 3

Research Methodology

Chapter 4 presents the methodology that underpins numerical simulations of water surfaces. The selected methodology aims to quantify and further establish the conditions in which the aqueous thermal boundary layer is to either promote or retard evaporation losses within an open water reservoir. Emerging research has indicated that the thermal boundary layer is a key contributor to evaporation rates. It is understood that the thermal boundary layer is essentially the surface skin of the water with a depth of around 1mm where the temperature gradients are considered to be important for the purposes of this research project. The physical conditions of the thermal boundary layer are determined by wave propagation of the waters surface which is ultimately influenced by wind velocities and atmospheric pressure differentials above the waters surface. It is suspected that as varying wind velocities interact with the waters surface, the waves generation as a result of frictional resistance between air and water, ultimately affect the physical depth of the thermal boundary layer. It is within these peaks and trophs of the generated waves, where evaporation is considered to be either promoted or mitigated.

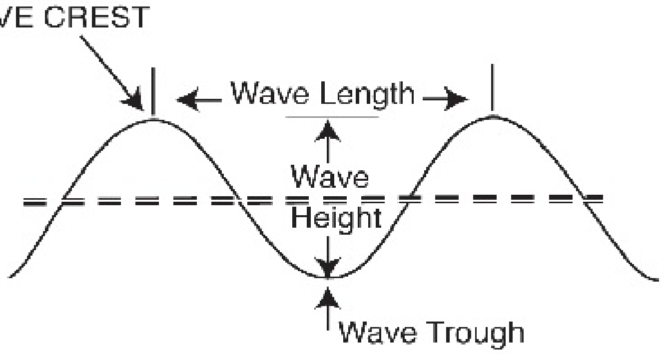


Figure 3.1: Description of wave form (Olsen, 2011)

At the time of publication of this dissertation no research could be found which describes the results of dynamic simulations of the aqueous thermal boundary layer. Contrary to this, some existing literature has indicated the thermal properties and gradient that is thought to exist in the thermal boundary layer. However this research has been limited to mathematical description and has not been able to quantify and describe the effects of the layer using a computational fluid dynamics program.

In order to validate the results of the mathematical research undertaken, less cost-effective methods were utilised to complete simulations of fan injected air flowing over a real body of water. This tank of water was situated within a controlled room or environment. The temperature of the water body was then measured using expensive cameras which were able to also penetrate below the surface by a certain distance. The difference in temperature between both the surface of the water and underlying body of water was then compared and used to validate the temperature change that was predicted to occur through the aqueous thermal boundary layer. It is clear that these methods previously utilised in existing literature are far less cost effective and time efficient. With this being said, computational fluid dynamics simulations have proven to be a far more efficient and cost effective method of simulating the interactions of air flowing over a body of water. These CFD programs are effective in simulating the various wind velocities and the impacts that this may have on the waters surface in generated real-world environments. It is with this knowledge that a CFD simulation model has been thoroughly explored. The choice of simulation is based on an analytical and mathematical approach that utilises the ANSYS suite of analytical software. Within this suite of software the CFD program FLUENT has been selected. The intention of the generated CFD model is to develop an understanding which attempts to resolve the multiple factors that can influence evaporation. This has subsequently involved the characteristics of the aqueous thermal boundary layer.

The establishment or characterisation of the surface layers macro-physics can lead to positive results if utilised by water resource managers. However, it is not the intention of this research to create a dissertation that promotes the use of findings obtained within. This dissertation is created in the hope of adding to current research available which describes the thermal dynamics of water bodies. This is in order to better appreciate the point at which the temperature gradient retards or accelerates evaporation. In order to develop and obtain satisfactory results, a distinct temperature difference was intentionally applied to the phase utilised within the model domain. Simply, the air phase has a temperature of 20 degrees celsius and the water phase has a temperature of 10 degrees celsius.

3.1 Instrument: ANSYS Fluent

This section examines the Computational Fluid Dynamics Software ANSYS Fluent that has been utilised in order to produce simulations concerning the waters surface within an open top storage reservoir.

The ANSYS Fluent model has enabled the simulation and examination of the flow of gaseous products over a liquid (air flowing over water). This capability proved to be an essential component when either proving or disproving the projects original hypothesis. As previously stated it is the intention that the two phase model is able to effectively establish the point at which the thermal boundary layer is able to promote or retard evaporation. The significant advantage that Fluent also offers is made apparent when assigning a realistic turbulent air stream within the model. This program provides the user with the capability of using various turbulence models that can be utilised in order to represent a real-world air flow environment. This is strictly due to the fact that the flow of air is rarely, if not never, actually laminar in an open and uncontrolled environment.

Use of the resource has been made possible by the University of Southern Queensland extending the programs academic license through a virtual private network. The University of Southern Queensland also supplied the program which has enabled the researcher to work remotely and externally when access to the virtual private network was available. This program had preference over other CFD models due to its easy to use and understand graphical user interface (GUI).

The basic incremental steps that determined the success of this project were constantly varying. The methodology adopted to meet the particular requirements of this project are briefly summarised below with more detailed descriptions following on further within this chapter.
The project methodology steps are:

- Create a three dimensional rectangular prism which is to contain the water surface using the software contained within the ANSYS suite of programs. Design Modeller, a computer aided design and drafting program (CADD), in this case will be utilised as the primary software.

An identical rectangular prism was also created to sit directly above the water body prism in order to contain the turbulent air stream that is to flow over the waters surface.

- Create a mesh of high quality that enables the resolution of various parameters used to resolve the model during turbulent simulations.

- Adopt a turbulence model.
  It is of paramount importance that the turbulent inflow conditions are satisfactorily specified at this stage of the models creation. Synthesised turbulence which utilises Fourier Harmonics is the default case to be specified for this research project.

- The sampling region to be utilised when resolving calculated data has been chosen to be away from the walls or boundaries of the three dimensional model to ensure adverse effects from boundaries do not influence the results.

- Post processing will be via Fluent as it also provides post-processing capabilities. MatLab has also been to post process results created from running the simulations.

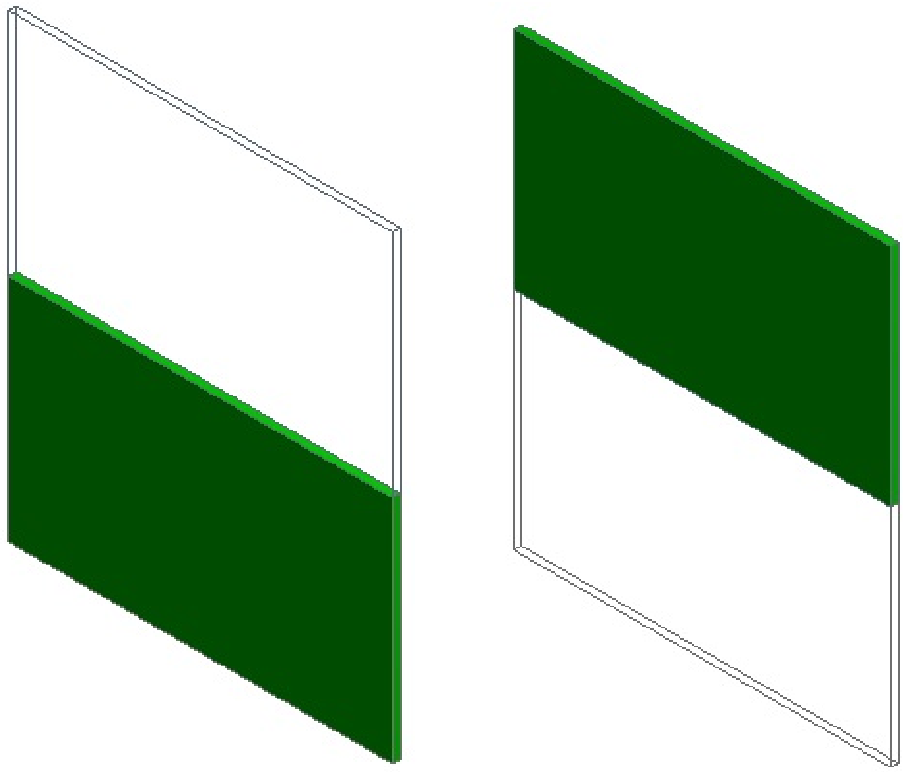
3.2 Size of Computational domain

A three dimensional rectangular prism was created to contain both phases of air and water. In order to do this a CADD program called Design Modeller, which comes a part of the ANSYS suite was used. An initial estimate concluded that a large enough model was to be created in order to ensure that the boundary conditions did not adversely influence the sampling region that was to be derived from the model. This was based on the findings from previous research, which suggested that the boundary conditions often interact and reflect into near boundary regions. These interactions and reflections were considered to potentially influence the resolution of data within the near boundary regions. This initially provided justification behind creating a sufficiently large enough model in which a sampling region could be selected far enough away from near boundary regions without negative influence.
As sampling regions were to be derived away from near boundary regions, it was essential that the model was large enough in order to exclude the extraction of data from where these negative impacts where suggested to occur.

The creation of a water phase (water body) was to be undertaken within the CADD software to represent an open top water storage reservoir. It was also expected that an identical rectangular prism was also to sit above the water phase. This was created in order to contain the turbulent air stream that is to flow over the waters surface. These prisms together represented both the air and water phases.

The initial measurements used provided a model that was 20.0 metres long, 10.0 metres wide and 10.0 metres deep for both air and water phases. This sizing provided a computational domain that was 4000 cubic metres. This sufficiently large model also provided the advantage of allowing wave propagation to be contained within the computational domain under the influence of varying wind velocities that were to be tested. However, the disadvantage of this model size becomes apparent when creating the mesh. A very fine and small element size is required to effectively model and simulate the dynamic nature of the thermal boundary layer. For a model of this amplitude it can be extremely expensive, in terms of computer processer use and time, in order to create a mesh of small element size within a large computational domain. This will be further discussed in section 3.3 of this chapter.

With trial and error, the model size was constantly adapted to a more refined size in order to accommodate an appropriate MESH size that was relatively inexpensive and time efficient when considering computer processor use. With this being said, the refined model provided a computational domain which was 0.5 metres in length, 0.01 metres in width and 0.6 metres in depth. These model dimensions incorporated both the air and water phases. It was predicted that this model size would be sufficient enough for drawing appropriate results and conclusions as a more refined mesh size was easier to produce. This disadvantage for this reduced model size implied that a smaller range of wind velocities could only be examined as an indirect result of the wave propagation height.



(a) Water phase within computational domain. (0.300m x 0.500m x 0.010m)

(b) Air Phase within computational domain. (0.300m x 0.500m x 0.010m)

Figure 3.2: Adopted computational domain showing location of air and water phases within the complete 3-dimensional model used for simulations (0.500m x 0.600 x 0.010m)

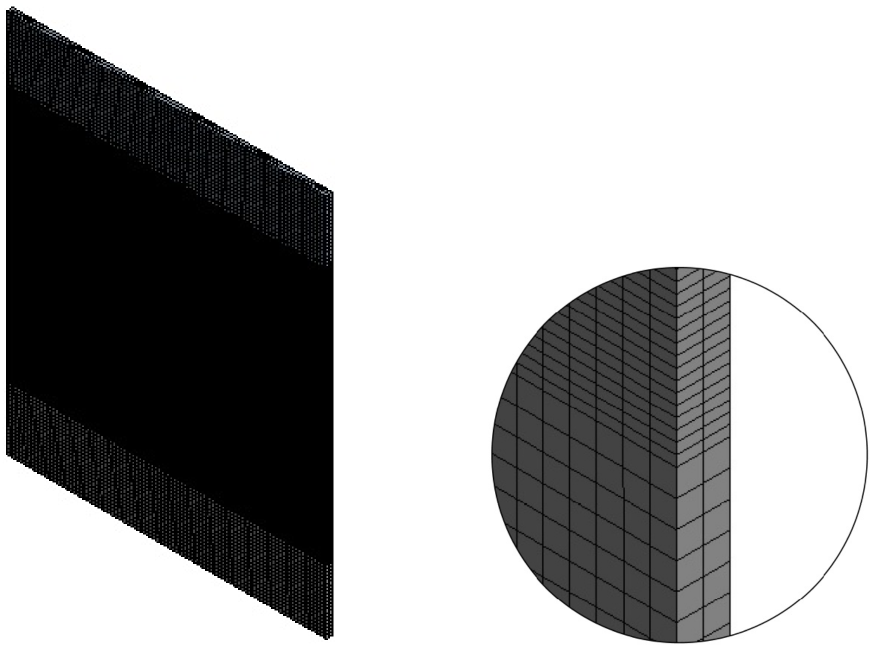
3.3 Mesh

The Mesh generation has been one of the more critical aspects involved in the simulation of air interaction with the waters surface. From previous research and user guide information, developing an appropriate sized mesh was essential to establishing and generating accurate results. As previously stated above, a mesh that is significantly large requires a prolonged run time in order to produce results for the environment to be tested. It was also made clear, that the mesh would ultimately influence the accuracy, convergence and speed of a given solution (ANSYS). In order to produce accurate and precise results, simulations required a mesh of extremely high quality in regards to both the element size and the element shape. Dynamically modelling fluid and gas in turbulent environments has been made especially easy by utilising the graphical user interface that the program named Meshing provides. By utilising the tools available within this program a mesh consisting of 2 distinct regions has been created away from the air-water interface.

The first region was created by taking advantage of an inflation mesh option that the program has available. This region is created both above and below the water surface within the air phase and water phase. The element size selected is sufficiently small enough to be able to resolve the dynamic conditions of the aqueous thermal boundary layer. This meshing region is referred to as fine as it simulates and resolves the specific region that we are trying to obtain results for. The size of elements within the second region located further away and outside of the first region of fine meshing, has been selected to be larger than what is necessary to simulate the thermal boundary layer. This mesh is referred to as coarse as it does not resolve or model the specific region we are intending on obtaining results for. It is simply included to provide model completeness and to provide an indication of wave propagation height outside the fine mesh where the aqueous thermal boundary layer resides. Through trial and error again it was established that once the wave propagation exceeded the layer of fine mesh, the fine mesh layer had to be further increased in order to resolve and characterise the conditions of the thermal boundary layer. This becomes an independent and variable process as different wind velocities are known to produce altering wave propagations. This indicates that as larger wind speeds are simulated within the model larger areas of fine mesh are required both above and below the waters surface.

As a benchmark the element size for the fine, inflation mesh, has been adopted as 2.0mm that is both 0.2m below the water surface within the water phase and 0.2m above the water surface within the air phase. This formed a foundation of which mesh size could be expanded upon under conditions of high wind velocity and wave propagation.

The final mesh adopted was considered to be of an appropriate magnitude for deriving accurate and precise results during the preliminary phase of simulations. However, the complexities of resolving the physical characteristics of the thermal boundary layer as a result of utilising this mesh are further explained in chapter 4 Results and Discussions and chapter 5 Conclusions and Recommendations of this dissertation. Findings suggest that a smooth or fine mesh improves the validity of specific fluid dynamic simulations. For the developed mesh this has been achieved.



(a) Mesh developed for computational domain

(b) Close look showing difference between fine (inflation) layer of mesh and coarse mesh

Figure 3.3: Constructed mesh that was developed for the computational domain

3.4 Turbulence Model

To produce a close to realistic environment careful consideration had to be placed on the choice of turbulence model that would be used to model the multiphase system. Choice of the turbulence model would ultimately determine the quality of results obtained and also affect the wholistic quality of the simulation. It is from the above that adequate and in depth model choice had to be ensured in order to validate the model as being reliable for a realistic environment simulation.

The most appropriate way to model turbulence would be through the use of Direct Numerical Simulation (DNS). This aims to resolve all the turbulent scales in time and space. This is not a realistic outcome, nor has it been considered within the initial stages of project initiation. Computational resources required to undertake Direct Numerical Simulations are far more advanced that what is actually available in todays world. The current, most popular, way of resolving turbulence is by using the Reynolds Averaging Navier Stokes (RANS) equations. RANS simulations actually eliminate all turbulent structures from the flow field and provide a smoother averaged velocity and pressure field (ANSYS).

From this, an original focus was placed on utilising large eddy simulations as the prioritised turbulence model. Large Eddy simulations are described as being a mathematical model that is used to simulate atmospheric air currents within a defined environment. This mathematical model is a part of the family of Scale-Resolving Simulations (SRS). By using SRS not all, but a small part of the model is resolved for turbulence. It was assumed that by using the large eddy simulation model, potential results would represent more realistic conditions under the above premise. The problem being with large eddy simulations is that in wall bounded flows the results that are produced may be incorrect and inadequately represent what is expected within a realistic environment. This is apparent in the regions close to the wall boundaries.

What was found to be more appropriate for the small domain that was to be analysed was the use of a hybrid turbulence model. This rectifies the large resolution requirements and computational expense required to fully utilise large eddy simulations on a standalone basis. Hybrid turbulence models provide the advantage of using both the large eddy simulation model and Reynolds Averaged Navier Stokes simulation to model the computational domain. Within wall boundary layers RANS methods typically model turbulence while larger and more separated regions are modelled using large eddy simulations (ANSYS). The model of choice that considers all of the above is the Detached Eddy Simulation (DES) turbulence model. Detached eddy simulations however do require more computer resources than RANS which is a disadvantage. An easily made decision in order to compromise for the lost computer performance is that, as stated above, 2 turbulence models are used. It is from this that the results obtained are believed to be as close as possible to a realistic scale. ANSYS Fluent, being the fluid dynamics program adopted for the numerical simulations, provides great ease in selecting Detached Eddy Simulations as the model of choice through its graphical user interface.

3.5 Sample Region

The influence of boundary reflections within a 3 dimensional model can have a negative influence on the results that are to be extracted. A defined region of data extraction, that is located within a sufficiently large model, can help reduce the negative effects that are contained within data that has ultimately been influenced by boundary reflections. Based on this premise, during the initial phases of this project, an appropriate sampling region was specified for discrete data extraction practices. Dimensions of the region are not solely dependent on simply specifying a uniform area that is to be used. Instead it involves much more complex ways of determining exactly where this region is to be located and where data is to be mined from.

The 3 dimensional model boundaries have to be assigned before the influence can be understood. However, in depth technical knowledge is required to know what these reflections are and exactly how they influence the results. This is because of the large number of combination possibilities that are available within many different models that can be created using the ANSYS suite of software. These models are not only limited to a 2 phase system consisting of different fluidic materials and can also be influenced if a single phase fluidic system is to be analysed. For the simple purposes of this project, a region located a reasonable distance away from the model extents was assumed to be free from adverse influencing factors.

Model restrictions that present themselves throughout the course of simulation development also render the need to further refine the size and location of the sampling region. As the model is 3 dimensional and operates on a defined mesh of a relatively small element size, it has been determined that a 4000 cubic metre model (20.0 metres long, 10.0 metres wide and 10.0 metres deep) was not realistically viable. This is due to the restricted computer resources available and also the severe amount of data that would consequently be extracted from, what would be a large sampling region.

Due to the small size of the model used in simulations, as a result of initial trouble shooting, the sampling region is now more easily located on a 2 dimensional plane.

The 0.01m wide computational domain is not considered wide enough to effectively locate a sampling region within this plane. The ultimate need is to extract data from a region located away from the inlet boundary and outlet boundary of the domain. This gives a 2 dimensional plane of dimensions 0.5 metres long and 0.6 metres deep to locate the sampling region. It is imperative to still locate this region as far away as practically possible from the inlet and outlet boundaries used during simulations to reduce the inclusion of reflections.

The simplest and easiest location to specify for the smaller sampling region is centred about the middle of the 2 dimensional plane that is mentioned above. A disadvantage of this however is the possibility of the extracted data neither being at the crest or trough of generated wave. This further presents a challenging issue that needs to be resolved. The issue being that the exact time of a crest or trough of a wave must be known. Data must thus be extracted at this exact time.

Chapter 4

Results and Discussion

The culmination of what was within chapter 3, Research Methodologies, has enabled the subsequent and successful simulation of both a turbulent air stream entering the computational domain and the turbulent airstream interacting with the water body included within the developed model.

Within this chapter, the results of volume of fractions will be presented along with total temperature contours for the computational domain. Furthermore, the greater aim of the temperature gradient profiles that are impacted by the generated waves and temperature differential between the air and water that exists through aqueous thermal boundary layer will also be presented. The temperature gradient profiles have ultimately incorporated the entire water body to also show the linearity of temperature below the boundary layer.

The successful resulting simulations originated from the development of the computational domain, which is of dimensions 0.500m x 0.600m x 0.010m. This has enabled the subsequent computational fluid dynamics simulation which was the great intention of this research project. In order to derive the data sets used in providing results, an air phase of a specific velocity and turbulence, was input into the developed computational domain and allowed to pass over a water phase surface whilst also imparting energy to the water body. The spectral synthesiser method, which was discussed in chapter 2.7, Turbulent Inlet Boundary Conditions, has been used at the velocity inlet boundary in order to provide close to realistic turbulent conditions and air flow through the models domain. The interaction between the turbulent air and water created waves which in turn effected the physical characteristics of the aqueous thermal boundary layer.

In order to model and simulate the aqueous thermal boundary layer, the inbuilt volume of fractions function was specified for use within ANSYS Fluent. This further enabled the determination of where the water surface resides when all data was exported. Collaborative use of Microsoft Excel, which has long been used as an engineering tool, provided a great working platform that allowed the efficient and effective use of the very large data sets calculated by ANSYS Fluent during simulations. By exporting the data created by ANSYS Fluent in ASCII format, the file was able to be easily converted into a CSV format file for use within Microsoft Excel. This was an efficient use of a readily available computer program in order to derive results from the data sets selected for use and which had been output from the simulations. The only manual calculation performed within the CSV file, for every included simulation that will be shown further into this chapter, was the conversion of total temperature from units of Kelvin to degrees Celsius. Microsoft Excel allowed the fast implementation of calculation of such a conversion when comparing use of the code dominated Matlab environment. The temperature gradient profiles relied on the conversion of these values in order to simplify the readability of the resulting plots.

Matlab, a mathematical computer program, was also utilised successfully in the derivation of data use to plot the real location of the water body as a check when creating the temperature gradient profiles. The Matlab code generated has been included within this dissertation as Appendix B.

4.1 Volume of Fraction Phase Plots

Several volume of fraction phase contour plots have been created for observation and derivation of results. The volume of fraction phase plots provide a highly informative way of showing the location of wave crests and wave troughs. Other discernable information that can be derived from the volume of fraction phase plots is the location at which water spray separates from the peak of a crest wave. The velocity of winds that have been injected via the velocity inlet boundary of the developed model are 0.833 m/s (3 km/h), 1.111 m/s (4 km/h), 1.388 m/s (5 km/h) and 1.667 m/s (6 km/h). These velocities form the lower bound of monolayer performance, which may in fact be used as an evaporation mitigation product. This forms the basis for utilising such velocities along with literature which suggests that monolayers are ineffective beyond these values of wind velocity. However, it must be understood that prior effects of surface tension, temperature and surfactant presence, that results from monolayer presence and use, has not been assumed and hence not used during the development of the model and during simulations.

The selected data that has been used to formulate the results of this dissertation are shown within the table below. Data has been extracted at specific times as to include temperature gradient profiles within the trough of waves and also at the crest of waves. Difficulty was encountered however, when determining the point or time that a crest of a wave is occurring within the model domain. This has been due to the fact that the model is not large enough to include one complete wave length as measured from crest to crest (please refer to figure 3.1 Description of wave form). To work around this unfortunate event, which has occurred in all simulations, a base case has been utilised. For the purposes of this dissertation, the base case is defined as a point at which the water surface is impacted by the turbulent air stream and has subsequently created waves of small wave height. The crest of the wave is thus not fully developed due to the small simulation run time necessary to obtain data for a base case. It has been deemed that informative results, from which comparisons can be made for the thermal gradient profiles of crest and trough waves, are still able to be formed.

Table 4.1: Data extraction points for specific durations of simulation

	0.833 m/s	**1.111 m/s**	**1.388 m/s**	**1.667 m/s**
Wave Trough (s)	38.0	29.0	50.0	18.0
Base Case (s)	6.0	4.5	3.6	3.0

Similarity between the 4 cases can be noticed quickly as the longer simulation run times produce wave troughs and shorter simulation run times produce water surfaces with wave heights of small propagation. The development of waves troughs is though obviously just a coincidence which has also made data extraction simpler. The trough and base cases for the water surface of the four cases also happen to, approximately, correspond to the centre of the domain. Attention should also be paid to the adoption of pressure outlets at the downstream side of the developed model. This has worked well with no direct visual sign of wave reflection. The same is true also for the pressure inlet and velocity inlet boundaries at the upstream side of the computational domain. Although this sort of problem is usually only encountered with wall boundaries, it provides a good indication that the model has performed well throughout the simulation.

The above statements eliminate the need to determine a designated sampling region away from the upstream and downstream boundaries. This is also possible due to only providing a thermal gradient profile either for the trough of a wave and base case of the water body which all correspond to the centre of the domain. Thus the temperature gradient profiles shown in chapter 4.3, Temperature Gradient Profiles, all approximately correspond to the centre of the domain.

4.1.1 Volume of Fraction Plots for 0.833 m/s Velocity of Air

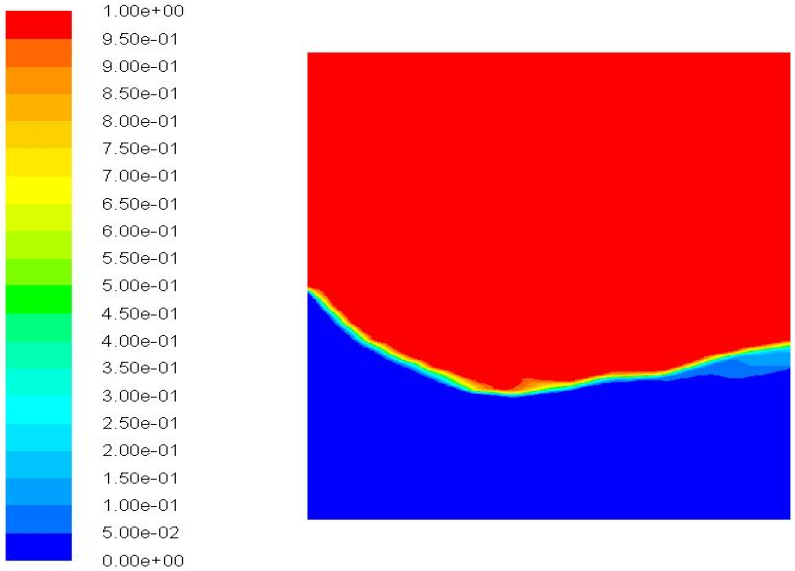


Figure 4.1: Wave Trough. Volume of fraction phase plot for air velocity 0.833 m/s and simulation duration 38.0 s

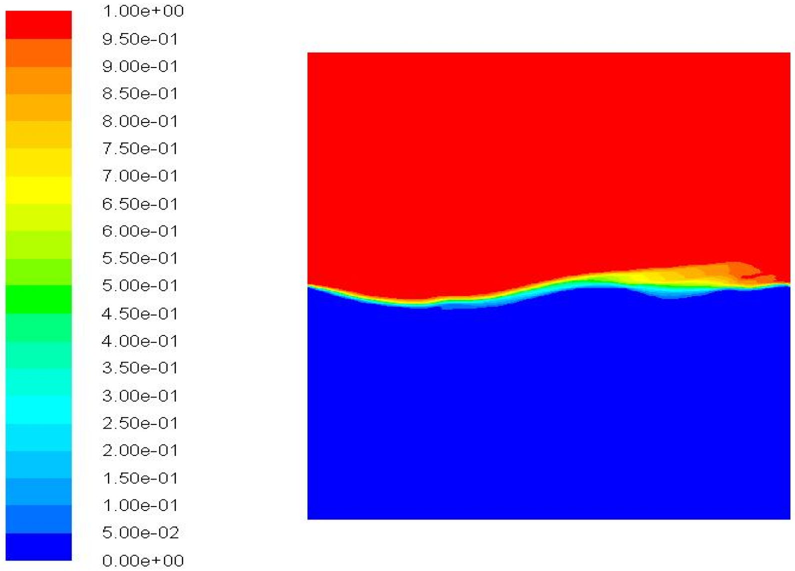


Figure 4.2: Base Case. Volume of fraction phase plot for air velocity 0.833m/s and simulation duration 6.0 s

4.1.2 Volume of Fraction Plots for 1.111 m/s Velocity of Air

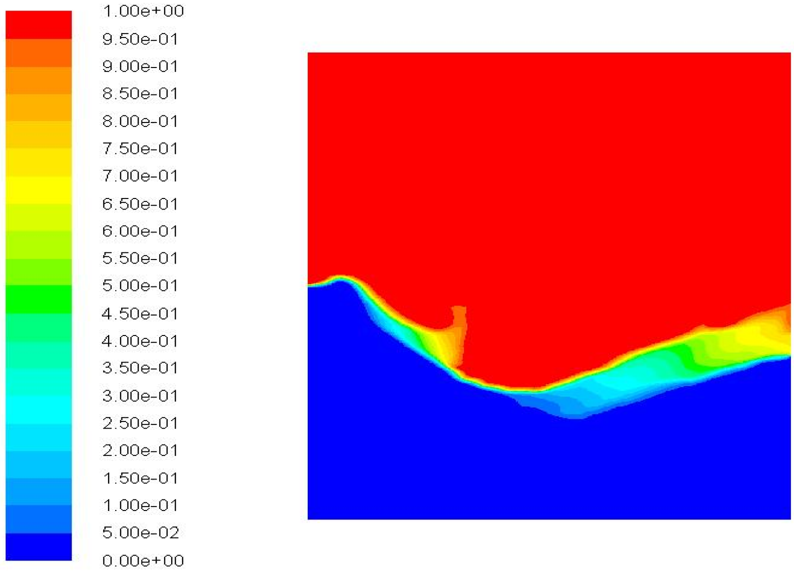


Figure 4.3: Wave Trough. Volume of fraction phase plot for air velocity 1.111 m/s and simulation duration 29.0 s

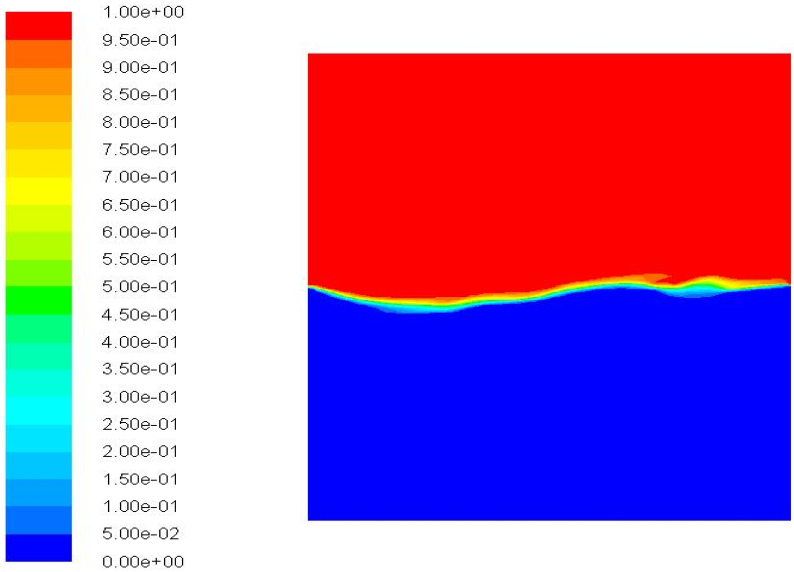


Figure 4.4: Base Case. Volume of fraction phase plot for air velocity 1.111 m/s and simulation duration 4.5 s

4.1.3 Volume of Fraction Plots for 1.388 m/s Velocity of Air

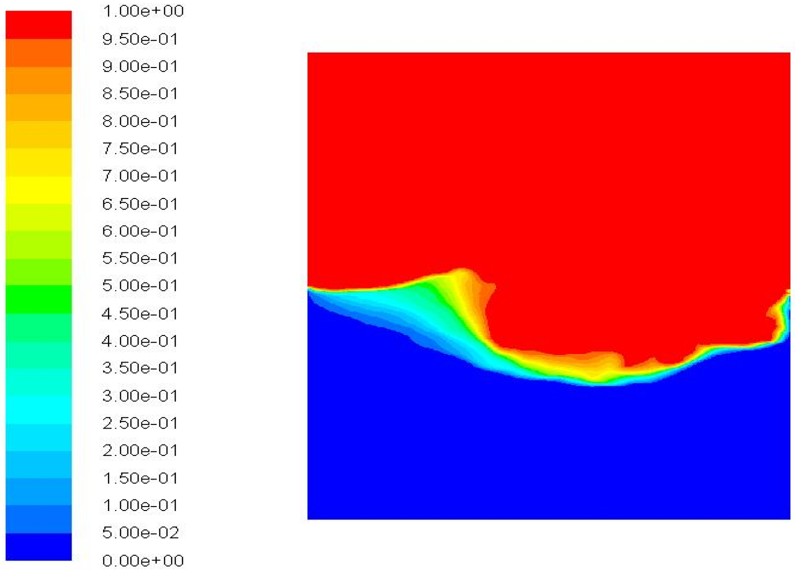


Figure 4.5: Wave Trough. Volume of fraction phase plot for air velocity 1.388 m/s and simulation duration 50.0 s

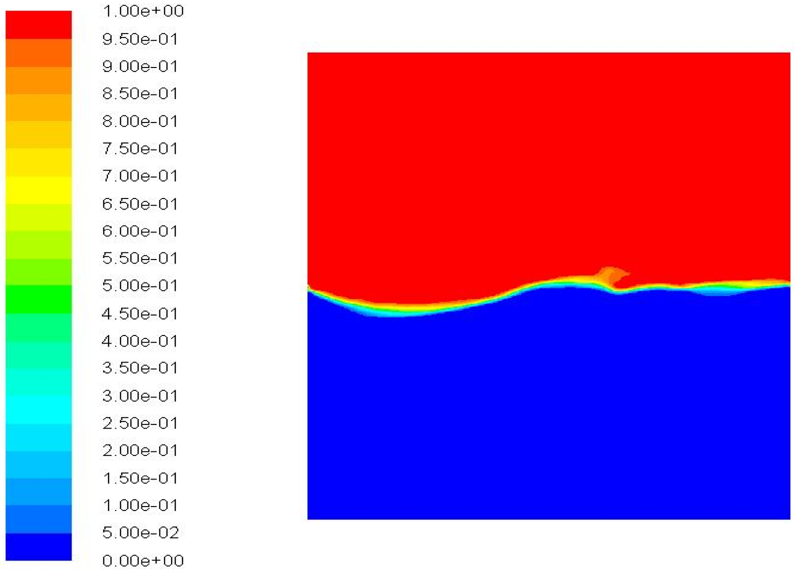


Figure 4.6: Base Case. Volume of fraction phase plot for air velocity 1.388 m/s and simulation duration 3.6 s

4.1.4 Volume of Fraction Plots for 1.667 m/s Velocity of Air

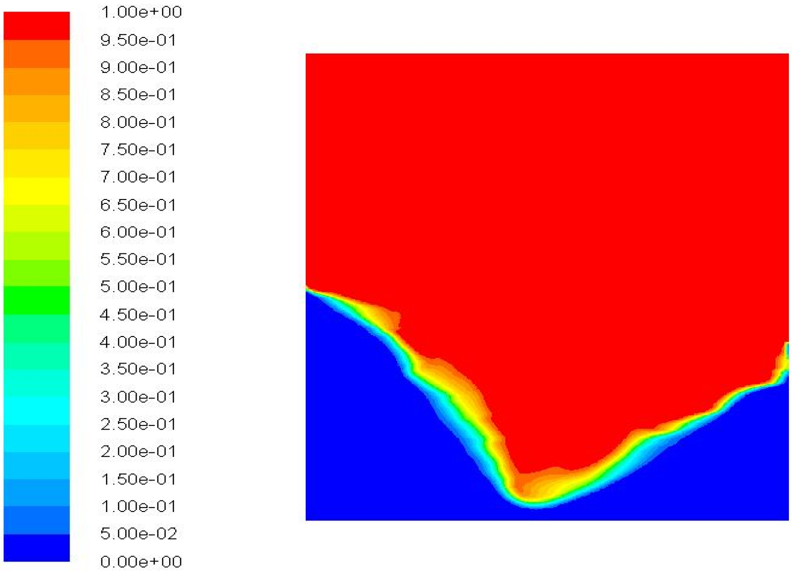


Figure 4.7: Wave Trough. Volume of fraction phase plot for air velocity 1.667 m/s and simulation duration 18.0 s

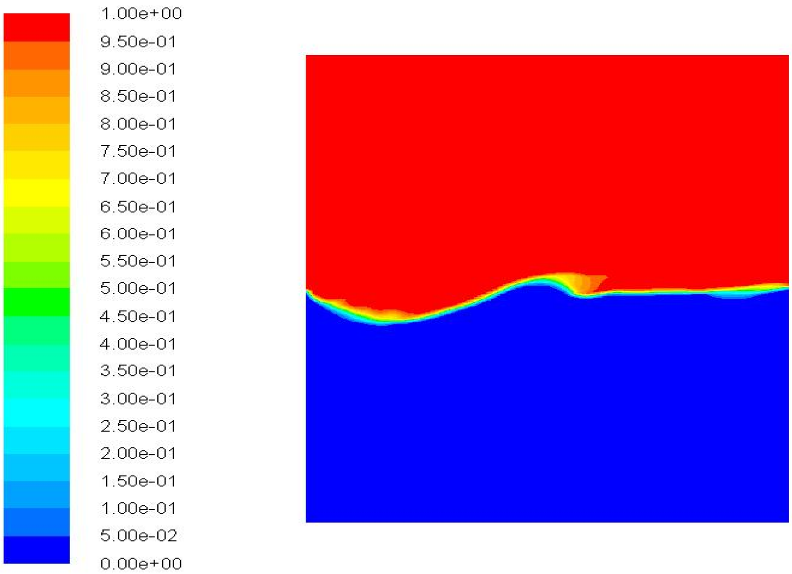


Figure 4.8: Base Case. Volume of fraction phase plot for air velocity 1.667 m/s and simulation duration 3.0 s

4.2 Temperature Plots

To supplement the temperature gradient profiles which resulted from running many simulations, a temperature contour plot has been produced to show the location of a cool skin overlying the water surface. As was the case with the volume of fraction phase plots, temperature plots have been created for the four air velocity cases that have been injected into the computational domain.

As can be observed from visually inspecting the temperature plots the water temperature which lies beneath the surface interface between air and water is and remains cooler than the air flowing above. Although mixing of temperature between the two phases occurs when sufficient turbulence and interaction is available. This can be seen to happen close to the air water interface and especially in situations where the volume of fraction phase plot also shows water spray or mist separating from the bulk water body.

4.2.1 Temperature Plots for 0.833 m/s Velocity of Air

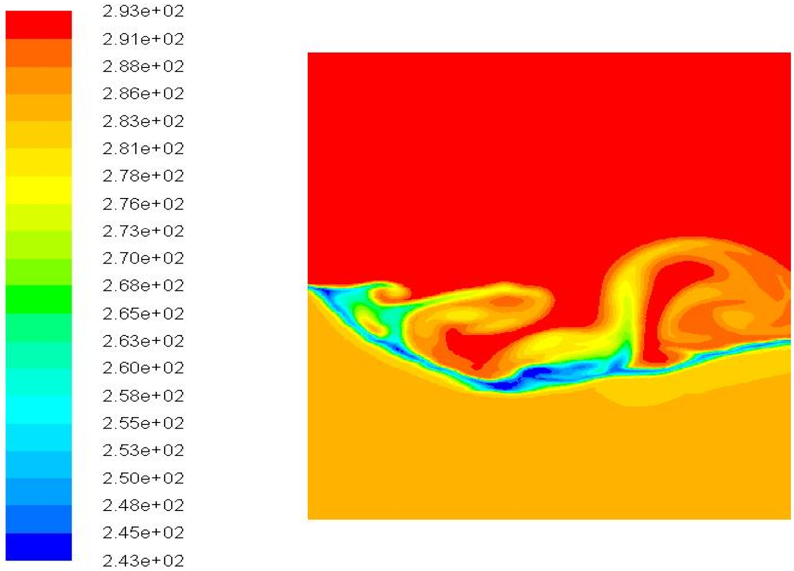


Figure 4.9: Temperature plot for air velocity 0.833 m/s and simulation duration 38.0 s

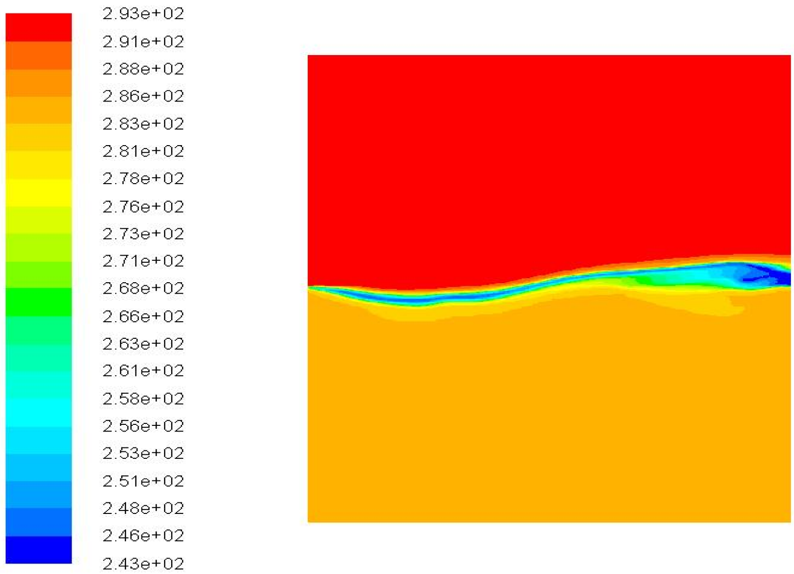


Figure 4.10: Temperature plot for air velocity 0.833m/s and simulation duration 6.0 s

4.2.2 Temperature Plots for 1.111 m/s Velocity of Air

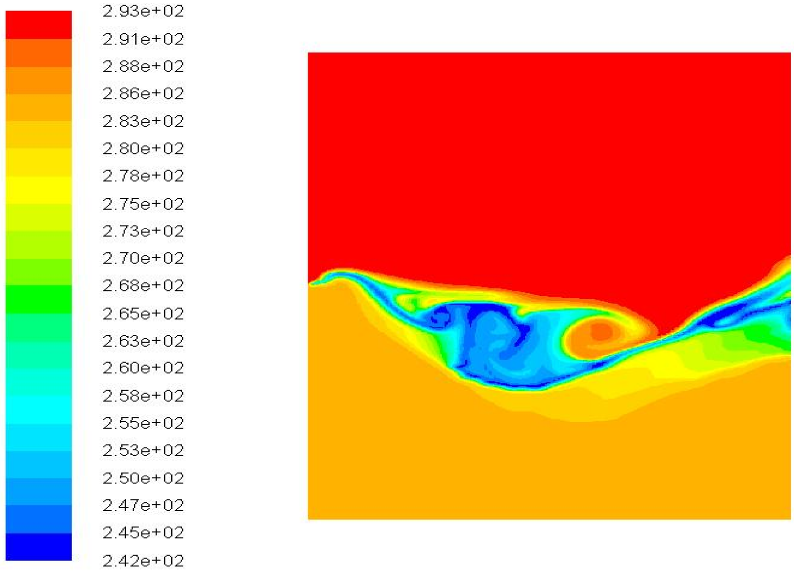


Figure 4.11: Temperature plot for air velocity 1.111 m/s and simulation duration 29.0 s

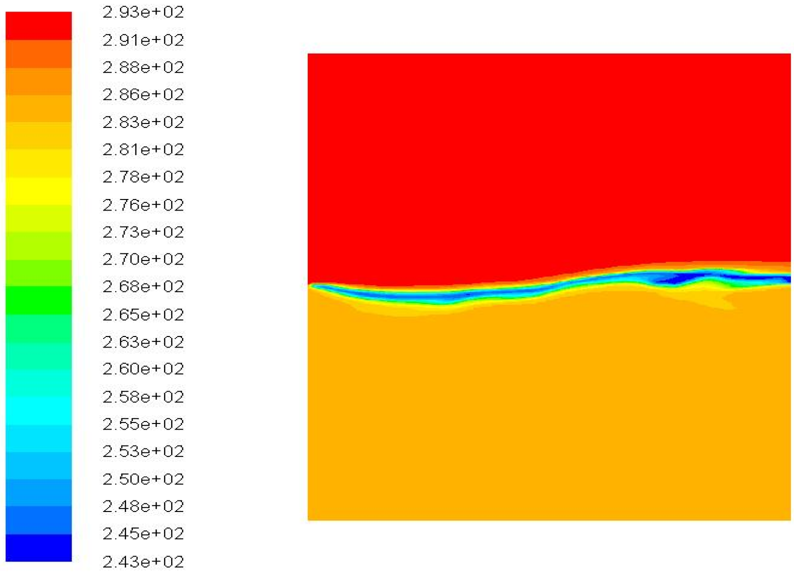


Figure 4.12: Temperature plot for air velocity 1.111 m/s and simulation duration 4.5 s

4.2.3 Temperature Plots for 1.388 m/s Velocity of Air

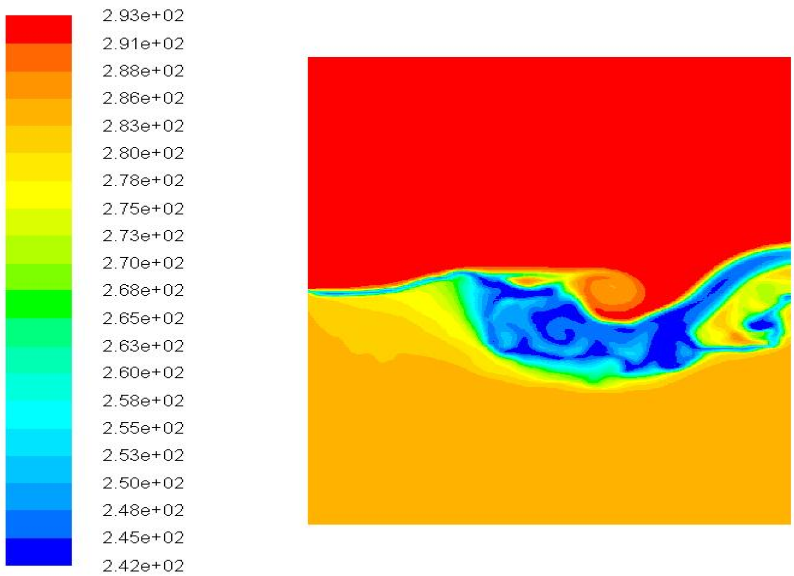


Figure 4.13: Temperature plot for air velocity 1.388 m/s and simulation duration 50.0 s

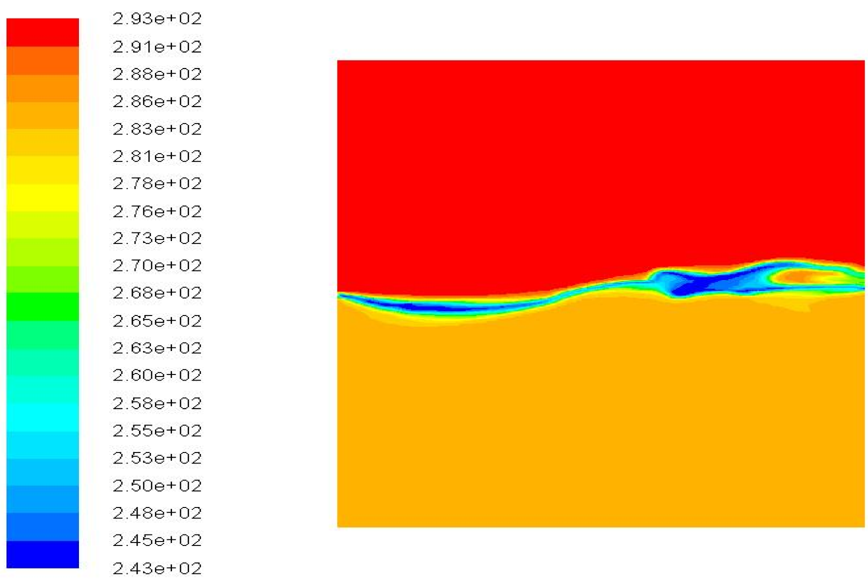


Figure 4.14: Temperature plot for air velocity 1.388 m/s and simulation duration 3.6 s

4.2.4 Temperature Plots for 1.667 m/s Velocity of Air

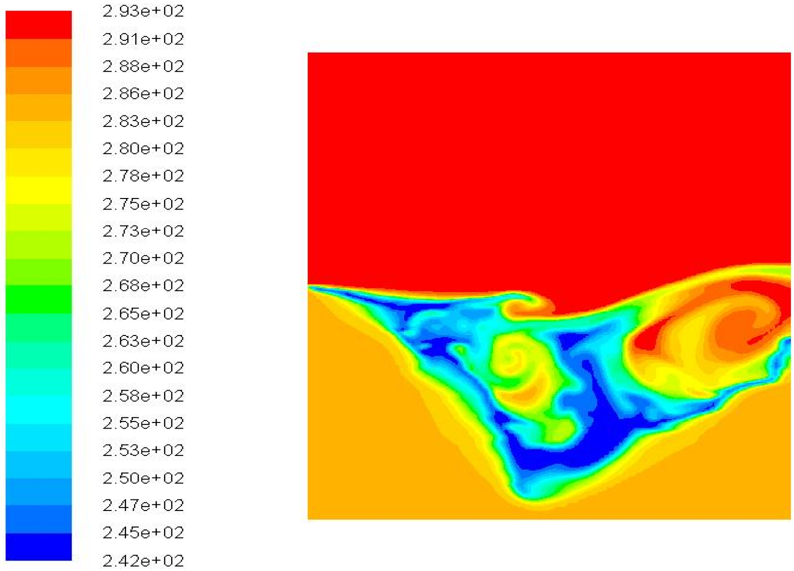


Figure 4.15: Temperature plot for air velocity 1.667 m/s and simulation duration 18.0 s

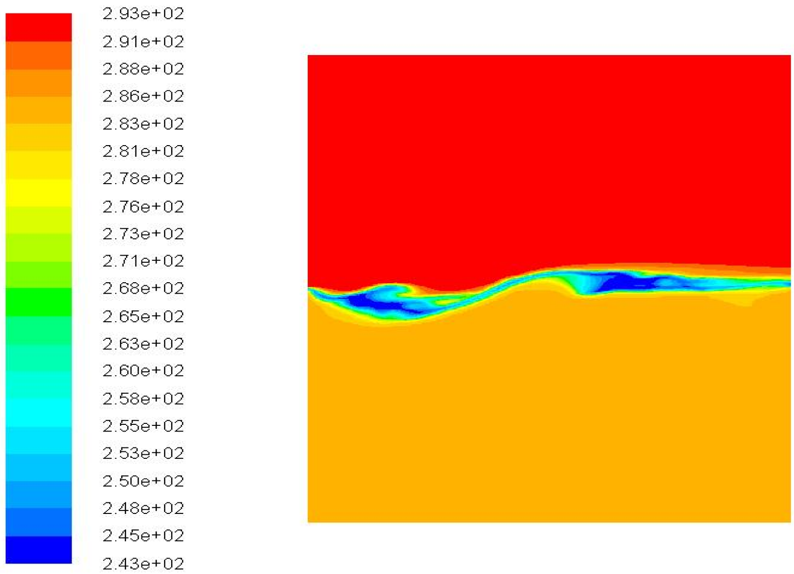


Figure 4.16: Temperature plot for air velocity 1.667 m/s and simulation duration 3.0 s

4.3 Temperature Gradient Profiles

Past research has alluded to the fact that the surface of a water body is in fact actually cooler than the bulk water that lies beneath. As mentioned within the literature review, specifically chapter 2.5 Aqueous Thermal Boundary Layer, Wells et al (2009) provided insight that described the aqueous thermal boundary layer being a union of two distinctly related layers. One of which is dominated by advection, where the temperature gradient is linear and the opposing layer, which is situated superior to the advection layer, is balanced by both advection and diffusion. This is the general description of what Osborne‘s theory of the aqueous thermal boundary layer consists of on a macro-physical scale.

It has been the overall intention of this dissertation to prove or disprove such theory that has been put forward with regards to the direct impact of the aqueous thermal boundary layer ultimately promoting evaporation losses or mitigating evaporation losses. As stated within the literature review also, the development of waves also impacts on the physical characteristics of the thermal boundary layers depth and temperature. More specifically it has been stated by Katsaros (1979) that as a result of wave generation and propagation the aqueous thermal boundary layer thins within the area of a wave trough and thickens or increases in depth at a wave crest. It is important to note however, that Wells et al (2009) stated that as shear generated turbulence increases as a result of increased wind speeds, so does the aqueous thermal boundary layer. It was thought from consideration of these statements that the difference in temperature would decrease at the trough of a wave, making the water surface temperature more aligned to that of the warmer bulk water below, thus increasing the risk of evaporation. The results presented hereafter for the cases of 0.833 m/s, 1.111 m/s and 1.388 m/s present a different and opposite scenario where the temperature difference is actually reduced at the trough of a wave and is increased at the surface of the simulated base cases used. Thus, when using the results from this dissertation, evaporation is suggested to be promoted at a waves crest and mitigated within the area of a wave trough. This is due to reduced temperature differences measured between the surface of the water body and the bulk water below for all base cases (location of small wave crests) and an increase in the difference in temperature within areas of a wave trough.

The temperature gradient profiles, as measured at the centre of the computational domain are presented overleaf for all cases of air velocity. Both the temperature gradient profiles for the wave trough and wave base case (area of small wave propagation or wave crest) will be presented. Consideration must be given to the different depths of water that occurs at different specific simulation times for all cases. This explains why the temperature gradient profiles are of dissimilar data set sizes.

4.3.1 Temperature Gradient Profile for 0.833 m/s Velocity of Air

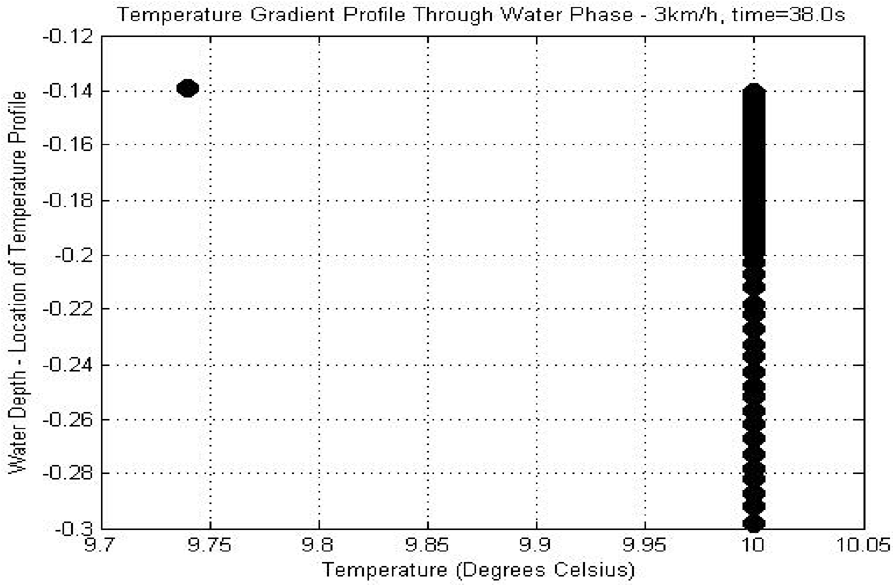


Figure 4.17: Temperature gradient profile for air velocity 0.833 m/s and simulation duration 38.0 s. **Temperature difference = 0.26 degree celsius**

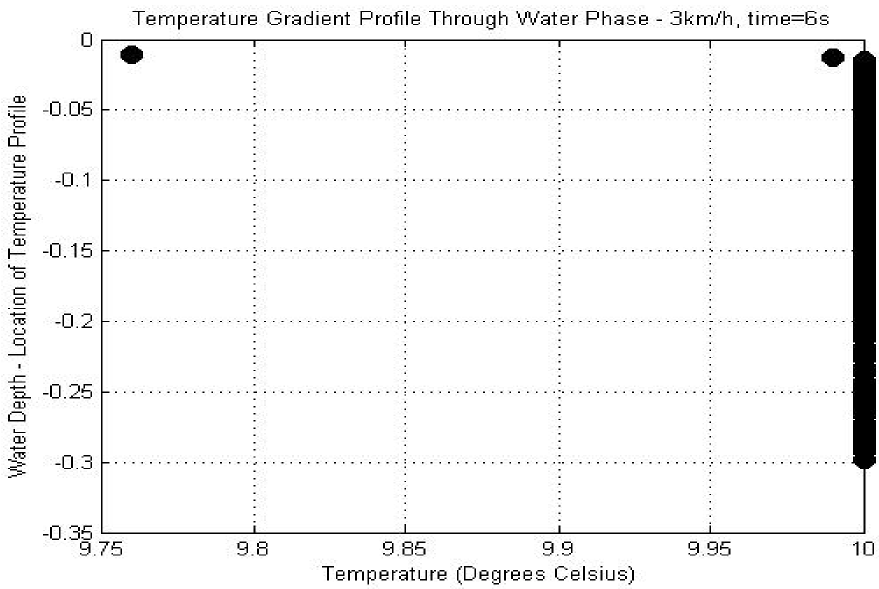


Figure 4.18: Temperature gradient profile for air velocity 0.833m/s and simulation duration 6.0 s. **Temperature difference = 0.24 degree celsius**

4.3.2 Temperature Gradient Profile for 1.111 m/s Velocity of Air

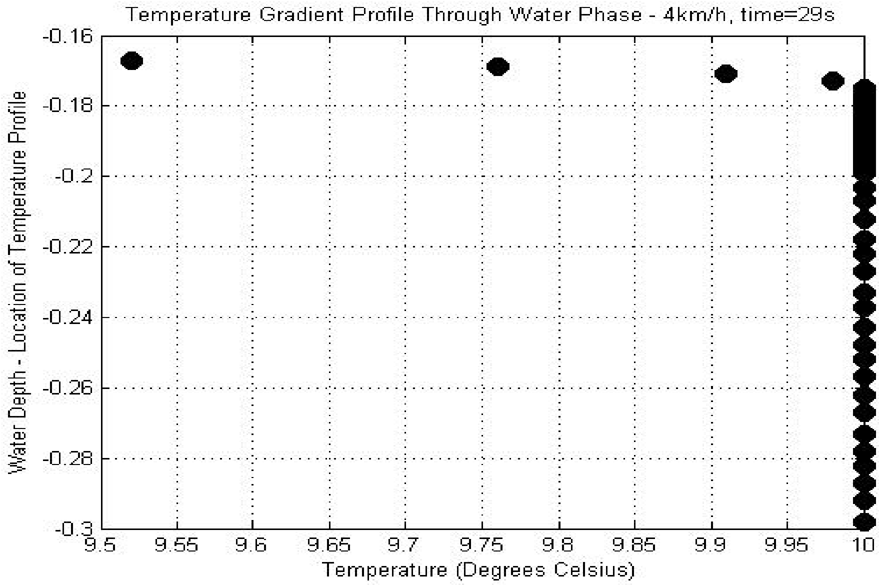


Figure 4.19: Temperature gradient profile for air velocity 1.111 m/s and simulation duration 29.0 s. **Temperature difference = 0.48 degree celsius**

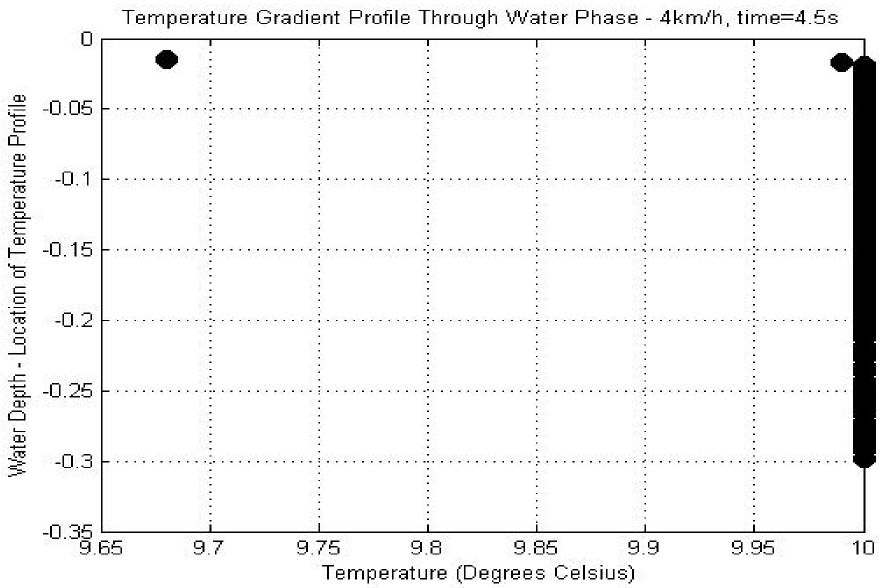


Figure 4.20: Temperature gradient profile for air velocity 1.111 m/s and simulation duration 4.5 s. **Temperature difference = 0.32 degree celsius**

4.3.3 Temperature Gradient Profile for 1.388 m/s Velocity of Air

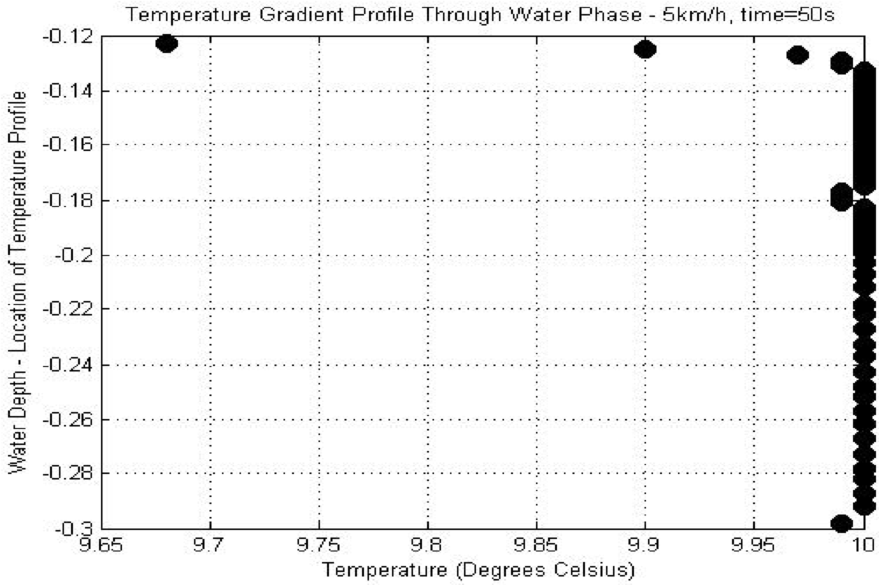


Figure 4.21: Temperature gradient profile for air velocity 1.388 m/s and simulation duration 50.0 s. **Temperature difference = 0.32 degree celsius**

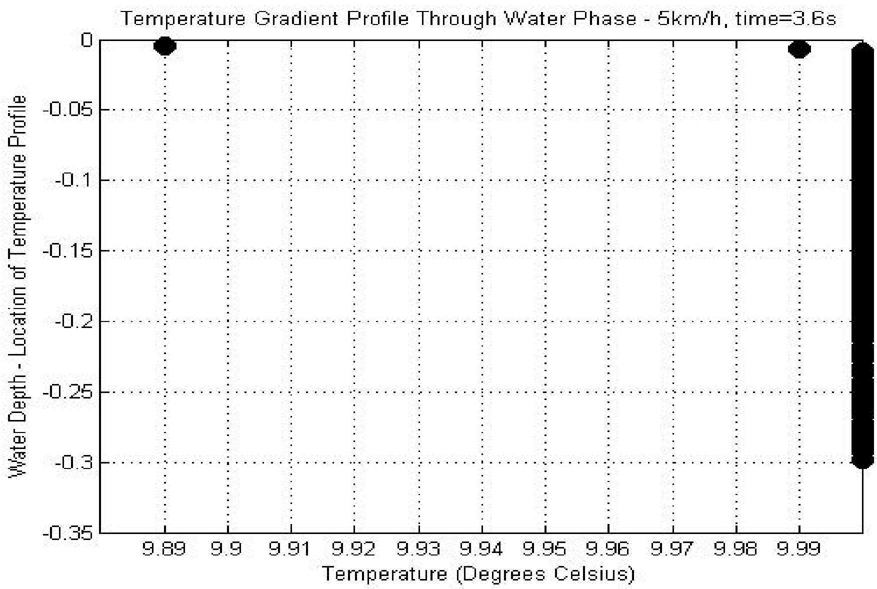


Figure 4.22: Temperature gradient profile for air velocity 1.388 m/s and simulation duration 3.6 s. **Temperature difference = 0.11 degree celsius**

4.3.4 Temperature Gradient Profile for 1.667 m/s Velocity of Air

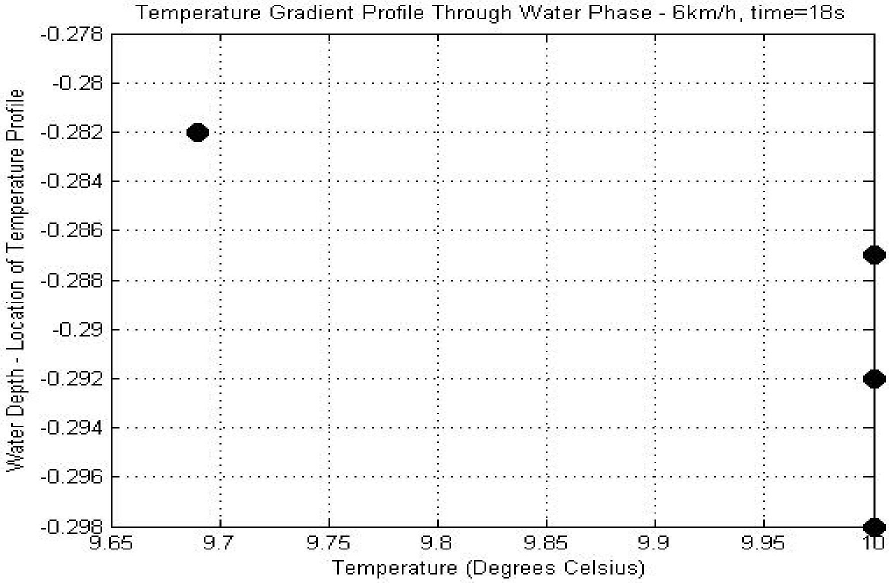


Figure 4.23: Temperature gradient profile for air velocity 1.667 m/s and simulation duration 18.0 s. **Temperature difference = 0.31 degree celsius**

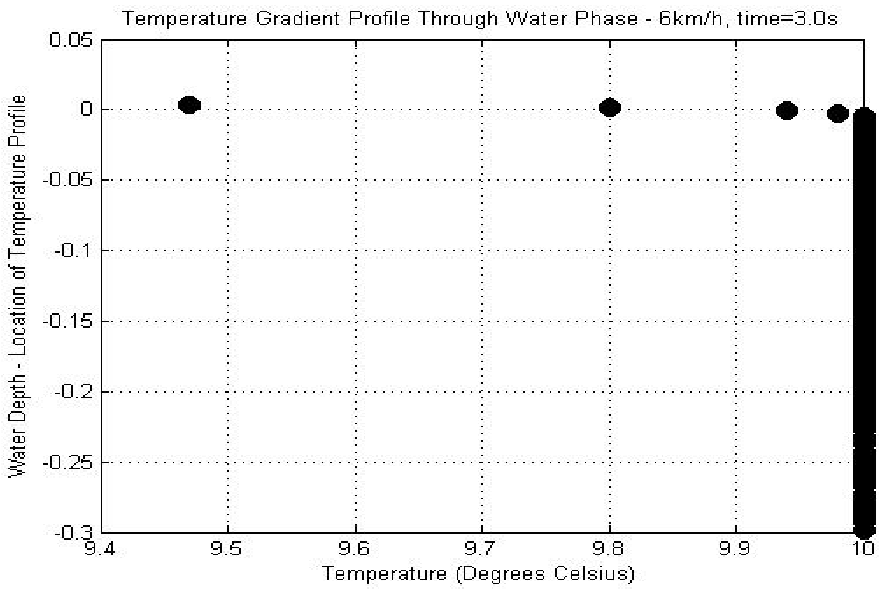


Figure 4.24: Temperature gradient profile for air velocity 1.667 m/s and simulation duration 3.0 s. **Temperature difference = 0.53 degree celsius**

4.4 Summary of Results

The results of fluid dynamics simulations created for the four cases of differing air velocity that were injected into the computational domain and randomly perturbated using the spectral synthesiser method is provided below.

The information provided within the table 4.2 below, is also shown appended to all temperature gradient plots incuded within chapter 4.3, Temperature Gradient Plots.

Table 4.2: Summary of Temperature at Water Surface

	0.833 m/s	**1.111 m/s**	**1.388 m/s**	**1.667 m/s**
Wave Trough (°C)	0.26	0.48	0.32	0.31
Base Case (°C)	0.24	0.32	0.11	0.53

4.5 Discussion of Thermal Gradient Profile Results

The development of the computational fluid dynamics model that has been created in order to validate and obtain data pertaining to non-linear temperature gradients through the thermal boundary layer has been visually presented within chapter 4, Results and Discussion. The temperature gradient profiles that have been developed however, do not prove or adequately fit with what has been suggested by two published works by Katsaros (1979) and Wells et al (2009). Both Katsaros (1979) and Wells et al (2009) suggest that the aqueous thermal boundary layer depth is promoted or increased at the specific location of the crest of a wave. In contrast to the statement included within both works, it has also been suggested that a subsequent thinning of the aqueous thermal boundary layer is apparent in area of a wave trough.

The results provided as a result of this research project do not agree with the statements made by Wells et al (2009) nor do they agree with Katsaros (1979), as stated above. Several thoughts are aroused as to why the results presented could not agree due to the non-inclusion of many important parameters and variables, although logical reasoning still seems to dictate that the theory presented by Katsaros (1979) and Wells et al (2009) should be regarded as correct. The rationale behind this statement in support of their correctness is due to the complex mathematical approach that Katsaros (1979)and Wells et al (2009) employed to prove the theory. But the mathematical approach employed by both parties only justifies that a non-linear temperature gradient does exist throughout the aqueous thermal boundary layer. The parties do not seek to prove or show that this layer actually does increase in size or depth at the crest of a wave, thus mitigating evaporation. The parties also do not seek to prove or show that the layer thins out at the trough of a wave, thus promoting evaporation.

Measurements of the temperature of the oceans surface that were made from an aeroplane were used to provide support to the theory adopted by Katsaros (1979) and Wells et al (2009) within the work published by Wells et al (2009). These measurements of temperature showed bands of warmer water that developed intermittently on the surface of the ocean. The bands are thought to have coincided with the trough of waves. The theory has not, to the knowledge of this dissertations author, been simulated and proved. The question that could be asked is how accurate is an aerial measurement of the oceans surface, or any water bodys surface, from such a large distance above? Elements such as the constantly moving surface, surfactant presence, salinity and subsurface turbulence or flows could have flawed the results of which the two parties have based their statements on.

Within a mathematical computational environment, the dynamic nature of a water body under the influence of a turbulent airflow was simulated using ANSYS Fluent, a computational fluid dynamics program. What the results of the simulations show is that for the air velocities of 0.833 m/s (3 km/h), 1.111 m/s (4 km/h) and 1.388 m/s (5 km/h), the temperature gradient profile is not constant and no direct relationship is easily formulated. What is constant across the three cases, which were mentioned above, is that for measurements made within the trough of a wave the difference in temperature was actually greater than the temperature difference formulated for the base cases (water surface inclusive of small crest wave height). The case of 1.667 m/s (6 km/h) air velocity, that was injected into the computational domain does, nevertheless support the statements made by Katsaros (1979) and Wells et al (2009). In particular, the slightly higher wind speed could have promoted a larger shear generated stress on the surface of the water body. The result of this according to Wells et al (2009) would be the successive thinning out of the thermal boundary layer. Although when sighting the volume of fractions phase plot for this case, it is hard to understand how in the trough of this wave, shear generated turbulence or stress could interact at the wave trough location. Reasoning is because it is bound between a steep leeward wave face and steep windward wave face. This may seem to be in contradiction to the separation theory developed by Jeffreys (1925) and as discussed in chapter 2.6, Wave Generation. This could act as reasoning to further promote research into the aqueous thermal boundary layer via computational fluid dynamics.

4.6 Dissertation Computational Restrictions and Limitations

4.6.1 Model Development

Constructing the 3-dimensional model within Design Modeller, a computer aided design and drafting program provided within the ANSYS suite of software, was made incredibly easy due to the programs graphical user interface. Extreme problems became apparent, nevertheless, when attempting to generate the model or domain mesh within another program named Meshing, which is also a part of the ANSYS suite of software.

Accurate and precise results were a definite must throughout the course of this projects development. Generating the domain mesh is a key parameter that dictates the validity and exactitude of the data created by and during the computational simulation. For such a small domain, as was used for simulations pertaining to this dissertation, creating a mesh of extremely small and fine element size would generally be handled by a modern day computer with little compromise on processor use and expense. The major problem that came to fruition though was that to simulate the characteristics of the aqueous thermal boundary layer an extremely small mesh size was required. The boundary layer is generally known to be of 1 mm depth or size that sits at the interface between water and air. It can be determined by the extremely small size of the boundary layer that multiple layers of elements of size less than 1mm are needed to simulate the dynamically varying characteristics of the aqueous thermal boundary layer. The dynamic nature of water that is propagating up and down does not lend itself to this situation. Thus, the fine element size must be extended to a depth, both above and below the still waters surface in order to continuously capture the moving water surface wherever it may be, at any point in time, during a specific simulation. In adjusting to meet the demands of the dynamic water surface, the computer resource that was available could not stand up to generating the mesh in a satisfactory amount of time to allow for the increased amount of cells and nodes that were needed to be numerically resolved. This unfortunately calls to question to the validity of the results presented above, although the non-linear temperature trend does seem to fit with what was expected when considering Osbornes theory as discussed by Wells et al (2009) and within chapter 2.5, Aqueous Thermal Boundary Layer.

Leading on from the fact that a mesh of fine element size was not able to be created with the computer that was available as a resource, successive simulation would also not have been possible in a satisfactory amount of time. The large amount of time step iterations required to allow fully developed turbulence to occupy the domain also proved computationally expensive. The fact that the turbulence model specified was detached eddy simulations also added to the fact that computer processor use and computer memory would be allocated to the simulation task. This is because detached eddy simulation turbulence model switches between both Large Eddy Simulations and Reynolds Averaged Navier Stokes turbulence models adding to simulation complexity.

The small domain size has also been shown, via the presented volume of fraction phase plots, to be unable to encompass a complete wave length. The desirable simulation result would be to develop a model sufficiently large enough to show multiple wave fronts and wave lengths occurring within the models domain. This would add further certainty to what is exactly happening as a result of simulations and allow the determination of wave propagation height. A direct velocity, wave, temperature and thermal boundary layer depth or size relationship could be derived if able to successfully incorporated via a larger model.

Savings in term of computer processor use is what ultimately then led to the development of a mesh consisting of both inflation layer meshing and coarse meshing as described within chapter 3.3, Mesh.

4.6.2 Computer Resource

The computer primarily used during the development of this dissertation was a Hewlett Packard (HP) 15-j112TX. The processor the computer had installed was an Intel Core i7-4700MQ central processing unit at 2.40 GHz. The installed memory (random access memory) was 8 gigabytes. Windows 8.1 was the computers operating environment which functioned via a 64-bit operating system.

A resource that was made available during the later stages of this project belonged to the University of Southern Queensland Faculty of Engineering and Surveying. The computer resource enabled more rapidly obtainable simulations. The resource also had a larger central processing unit and larger amount of installed memory. Use of this resource was invaluable during the later stages of this projects completion.

4.6.3 Learning the Ansys Suite of Software

An extremely challenging issue that faced the author of this dissertation was learning a new and foreign computer program within, what could be considered a relatively short amount of time. The ANSYS suite of software provides highly technical analysis program options from which professional training must sort before a person is known to be proficient in any program provided within the ANSYS suite. The University of Southern Queensland had graciously provided access to the licence needed to operate the software and also provided all necessary installation files. Through engagement with the universitys information and communications technology (ICT) team successful installation of the program was able to be achieved.

When it was necessary to create the 3-dimensional model intended for use in fluid dynamics simulations, the task was made easy due to ANSYS incorporating a graphical user interface. The tools and commands that were primarily used in constructing the domain and mesh was also made relatively simple after procuring tutorials used during program training by ANSYS. The tutorials did not fully describe all necessary tools and commands but allowed the successive and satisfactory creation of the model used in simulations that provided the results presented in chapter 4, Results and Discussion, of this dissertation.

The same cannot be said for the program Fluent, the computational fluid dynamics program within the ANSYS suite of software that was used to run simulations. The extreme technical nature of what must be understood before gaining a complete and adequate knowledge of the programs capabilities and options was a difficult task. Comprehension of the sheer amount of modelling techniques that can be used and employed within Fluent is an incredible task in itself. It is understood that if professional training by a person was undertaken, the amount of parameters that the program can include and resolve in a dynamic environment will and could provide an extremely powerful simulation result. From this, a highly precise and accurate result can be obtained. Lack of training within this program has unfortunately restricted the models validity. This can be largely attributed to the technical knowledge that is required to cover all possible scenarios within the simulation. Option upon option can be selected and investigated by referring to the product manual but everything interlinks and has positive and negative effects when resolving the domain. This statement was alluded to by Warnaka and Pochop (1988), Jahne et al (1988), and Craig et al (2009) who have all suggested that evaporation modelling is an extremely large and difficult undertaking. The simulations of the aqueous thermal boundary layer that aim to derive the point at which evaporation is either promoted or mitigated falls into this category as well. The amount of variables that change in a rapid sense can render any simulation useless in the shortest amount of time. In particular Jahne (1988) suggests that as one parameter value changes, any parameterisation of the aqueous thermal boundary layer becomes questionable. This is due to the variables being largely independent of location, the variable being dependent on each other and also the realistic and rapid change of a parameter in a real world environment.

Further to the above computational restrictions and procurement of knowledge of the ANSYS suite of software, a greatly pronounced issue that was encountered during the early phases of this dissertation was the inability of the computer to read the licence for ANSYS from the University of Southern Queenslands server. Access to this licence was provided through a virtual private network (VPN) and as stated by the ICT team, issues had been noted with the Windows 8.1 operating environment when running the ANSYS suite of software. This issue resulted in a large amount of time being wasted on rectification of the problem. Remote access by the ICT team was granted by the author of this dissertation in order to amend and change the computer resources system settings and firewall attributes. Without the help of such skilled staff the dissertation may not have been completed in the time frame provided.

Chapter 5

Conclusions and Recommendations

The aim of this dissertation was to perform computational fluid dynamic simulations of a two phase system. The two phases employed during the simulations were that of water overlain by a body of air. The injection of an air velocity at the upstream velocity inlet boundary was set to produce realistic turbulent conditions using a synthesised method of turbulence generation. The method adopted in order to create this realistic air flow was the spectral synthesiser model that is available for use within the ANSYS Fluent program. Air velocities tested during the simulation phase of this project are listed below. The air velocities simulated were:

- 0.833 m/s (3 km/h)
- 1.111 m/s (4 km/h)
- 1.388 m/s (5 km/h) and
- 1.667 m/s (6 km/h)

Prior to simulations being run background research was obtained for evaporation, thermal boundary layer conditions, turbulence models and computational model boundaries. The research was collated and critically analysed prior to performing simulations of the two system. The modelling of the two phase system was in order to characterise conditions under which the temperature gradient promotes or retards evaporation. The subsequent determination of the point where evaporation is promoted or mitigated by the aqueous thermal boundary layer was enabled via the simulations that had been run. The results contradict historic research which suggests the boundary layer thins out in the area of a trough of a wave, reducing water temperature difference between the boundary layer and bulk water below. Also in addition to this, the suggestion that the boundary layer thickens at a crest of a wave, acting to increase the temperature difference between the boundary layer and bulk water below has not been proven. The opposite has been found as a result of this research. Research results suggest that at the trough of a wave the temperature difference is promoted and at the crest of a wave the temperature difference is decreased.

The aqueous thermal boundary layer is known to be an important parameter that is backed by modern day research, when trying to develop a realistic evaporation prediction model. A conclusion that can be drawn from literature published and included within this report is that evaporation prediction and modelling of the aqueous thermal boundary layer is not a small and simple task. The amount of variables and their constantly varying physical and chemical characteristics must be able to be included within any validated model. Responsibility of creating such a large model requires an extremely long amount of time and real or empirically derived data to calibrate the model against. This also highlights the fact that as realistic environmental data is highly specific to distinct regional areas within a country or continent, evaporation modelling and simulations of any environmentally effected simulation is really only valid for the specific region the data is obtained from.

Computational fluid dynamics is expensive in terms of computer processor use and available resources but in real dollars provides a greater and cheaper alternative to constructing real world experiments in laboratories and in the field. Computational fluid dynamic simulations are still a highly viable technique that can be used to characterise the conditions of the aqueous thermal boundary layer. Although the mesh size adopted in the domain of the model used for this dissertation calls to question the validity of the results. This is because the fine mesh size adopted within an inflation layer in the domain was greater than the known 1mm depth or size of the aqueous thermal boundary layer. This was the result of available computer resource restrictions.

5.1 Recommedations for Further Work

As is the case with any dissertation produced, further improvement upon research can add to the field pertaining to the study of the aqueous thermal boundary layer. The development of this dissertations outcome stemmed around characterising the conditions in which the aqueous thermal boundary layer either promoted or retarded evaporation losses from an open water storage reservoir. As described in chapter 4.6, Dissertation Computational Restrictions and Limitations, the development of the model was severely constrained and regulated by the available computer resources power. Ensuing mesh creation and modelling of the two phase system suffered as a result.

A primary recommendation to be considered, if any further research aims to improve upon this dissertation, is that a computer resource that has sufficiently large installed memory (random access memory) and processor speed by procured. The more powerful the computer used in development of the simulation phase, the more rapid the results will be. An important parameterisation that is instantly improved on by utilising a more powerful computer is also the development of the 3-dimensional domain and the domain mesh. The domain can be increased in size to subsequently allow the formation and visualisation of multiple wave lengths further adding certainty and better understanding of what is occurring within the domain at any instant of time. The mesh element size can also be reduced accordingly in order to effectively, accurately and precisely simulate the dynamic thermal boundary layer within the model domain.

The exclusion of pollutants within the water phase and suspended particles within the air stream can also add to the model being more closely related to a real world situation. It is unclear how suspended particles would be added to the air phase with the ANSYS Fluent environment as it was considered extraneous when considering the simplicity of this models development. It could in fact be a very important parameter than should be included if research can be found that suggests the aerodynamic roughness or shear stress developed and imparted to the water surface, respectively, is effected by suspended particle inclusion within a turbulent air stream. Relationships between pollutant load and the sensitive physical conditions of a water body are also needed to be modelled in further studies. Surfactants that can also lower the surface tension of a water surface will actually also increase the likelihood of water molecule transport from an open storage reservoir to the air. The above statement in regards to surface tension also ignites the need to include a dynamically changing surface tension variable within a developed simulation model. Increases in temperature reduce the surface tension of a water body and hence will also promote water molecule transport to air.

As a result and in summary of this chapter, the recommendations for further work can be corrective or remedial and enhancing to what has been presented within this dissertation. By incorporating the above actions in further work there is a possibility that the theory outlined by both Katsaros (1979) and Wells et al (2009) may be proved. The theory being referenced here is that the aqueous thermal boundary layer is promoted in depth at the crest of a wave and reduced in depth at the trough of a wave.

Chapter 6

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Appendix A

Project Specification

University of Southern Queensland

FACULTY OF ENGINEERING AND SURVEYING

ENG 4111/1 and ENG 4112/2 Research Project

Project Specification

For: **Wesley Williams**

Topic: Numerical Simulations of Water Surfaces for Improved Evaporation Prediction

Supervisor: Dr. Andrew Wandel

Enrolment: ENG 4111 - Semester 1, External, 2014
ENG 4112 - Semester 2, External, 2014

Project Aim: Undertake Computational Fluid Dynamics (CFD) to determine how generated waves affect temperature distribution immediately next to the waters surface and to characterise conditions which retard or promote evaporation in open water storage reservoirs.

Programme: **(Issue A, 04 March 2014)**

1. Research evaporation of water from open water storage reservoirs.
2. Research thermal boundary layer conditions
3. Investigate models / techniques that are used in simulating 2-phase flow
4. Develop models and perform Large Eddy Simulations (LES) on a rectangular prism which contains the water surface.
5. Perform simulations of the thermal boundary layer in order to characterise the conditions under which the temperature gradient promotes or retards evaporation.
6. Recommendations for further studies.

Agreed:	**Wesley Williams** (Student)
Date:	19/03/2014
Agreed:	**Dr. Andrew Wandel** (Supervisor)
Date:	19/03/2014
Agreed:	**Dr. Ian Brodie**
Date:	10/04/2014

Appendix B

Matlab Code

B.1 WSurfTGrad.m

```
% Clear command window and variables from workspace
clc,clear
close all

% Allow Scaled fixed point format with 15 digits for double
% and 7 digits for single.
format long

% Read appropriate data that has been exported from
% ANSYS Fluent
data = csvread('3kmhr_data_complete.csv',1);



% Create a number of matrices to be used in subsequent
% operations
data2 = zeros(24240,1);
watersurf = zeros(24240,2);
temp = zeros(24240,3);

% For loop which determines where the water body and
% water surface resides
for i=1:1:24240;

    data2(i,1) = data(i,6);

    if data2(i,1) <= 0.05;
        watersurf(i,1) = data(i,2);
        watersurf(i,2) = data(i,3);
    end
end

% Delete all valuesoutside of the specified range
```

```
% from the matrix 'watersurf'
watersurf( ~any(watersurf,2), : ) = []; %rows
watersurf( :, ~any(watersurf,1) ) = []; %columns

% Calculate the size of the matrix watersurf to be used as
% a variable in subsequent operations
sizewatersurf1 = size(watersurf);
sizewatersurf  = sizewatersurf1(1,1);

% Plot the location of the entire water body
for l=1:1:sizewatersurf;

    x = watersurf(l,1);
    y = watersurf(l,2);

    plot(x,y,'ro','MarkerFaceColor','b','MarkerEdgeColor','b');
    axis([0,0.500,-0.3,0.3]);
    title('Water Body - 3kmhr, time=38.0s');
    xlabel('Distance (m)');
    ylabel('Depth of Computational Domain (m)')
    grid on
    hold on

end

hold off

% Create data set corresponding tothe centre of the
% computational domain in ANSYS Fluent
for k=50:101:24240;

    if data(k,6) <= 0.05;
```

```
    temp(k,1) = data(k,2);
    temp(k,2) = data(k,3);
    temp(k,3) = data(k,7);

    end

end

% Delete all unnecessary data from the matrix 'temp'
temp( ~any(temp,2), : ) = [];  %rows
temp( :, ~any(temp,1) ) = [];  %columns

% Determine the size of the matrix temp to be used as a variable
% in subsequent operations
sizetemp1 = size(temp);
sizetemp  = sizetemp1(1,1);

% Plot the temperature gradient profile correlating
% to the center of the computational domain within
% ANSYS Fluent
for l=1:1:sizetemp;

    x = temp(l,3);
    y = temp(l,2);

        figure(2)
    plot(x,y,'o','MarkerEdgeColor','k','MarkerFaceColor','k',...
          'MarkerSize',10);
    title('Temperature Gradient Profile Through Water Phase...
           -3km/h, time=38.0s');
    xlabel('Temperature (Degrees Celsius)');
    ylabel('Water Depth - Location of Temperature Profile')
    grid on
```

```
    hold on

end

hold off
```