NUMERICAL MODELING OF THERMAL BEHAVIOR IN LAKE ONTARIO

USING THE EFDC MODEL

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Abstract

by

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This research improves the 3D hydrodynamic model Environmental Fluid Dynamics Code (EFDC), to better capture thermal behaviors in Lake Ontario. Lake Ontario, being in temperate Great Lakes region, exhibits special thermal characteristics including thermal bar evolution in spring and thermal stratification patterns in summer. The thermal bar is a vertical wall of dense sinking water at the temperature of maximum density (4°C), which reduces horizontal mixing, inhibits the exchange of nutrients, and may intensify eutrophication in near-shore areas. During the summer months, the thermal bar disappears, and the lake becomes stratified. Summer temperature differences establish strong vertical density gradients (thermocline) between the epilimnion and hypolimnion, which serve as an energy barrier to vertical mixing.

Evolution of the spring thermal bar and summer stratification patterns through Lake Ontario is simulated using EFDC. The model is forced with the hourly meteorological data from weather stations around the lake and flow data for the Niagara and St. Lawrence Rivers. The lake bathymetry is interpolated on a curvilinear grid (cells
are ~ 2 km$^2$) with 20 vertical sigma layers. The simulation is performed from early April to mid-October 2011.

The model is improved by (a) updating the evaporation algorithm following Quinn (1979) and Croley (1989) to ensure accurate simulation of evaporation rates and latent heat fluxes (b) specifying appropriate solar radiation attenuation coefficients to ensure sufficient absorption of incoming solar radiation by the water column (c) updating the vertical mixing scheme following eddy diffusivity parameterization by Vinçon-Leite et al. (2014) and eddy viscosity parameterization by Pacanowski and Philander (1981) to better capture thermal stratification. In addition, values for horizontal mixing coefficients, bed heat flux parameters are specified through the model calibration process, and convective velocity mixing is implemented to thoroughly mix the water column from late August.

The improved EFDC model simulates overall surface temperature profiles with RMSEs between 1.5-2.5°C. The vertical temperature profiles during the lake mixed phase (early April to late May) are captured with RMSEs < 0.5°C, and the evolution of the thermal bar is replicated. With the newly implemented vertical mixing parameterization, the model captures the summer thermal stratification and thermocline formation from late May to mid-October. The simulated temperature profiles match the observed profiles for a deep (180 m) location, with RMSEs between 0.6-1.6°C. The model captures the thermocline formation at a shallow (19 m) location, with RMSEs of 1.25-3.7°C.

The model is further augmented with meteorological data from the North American Regional Reanalysis (NARR) climate model. Simulated vertical profiles at the
deep location, and surface temperature profiles using NARR over-lake data match observed data better than the simulations forced by land station based data. This comparative study establishes a baseline for the future coupling of EFDC Lake Ontario model with a regional climate model.
The person who made my life more meaningful, my beloved son

RAFAYET SM ARIFIN
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CHAPTER 1:
INTRODUCTION

1.1 Overview

This research investigates the thermal behavior of Lake Ontario, specifically spring warming, thermal bar formation, and summer stratification using the three-dimensional hydrodynamic model, Environmental Fluid Dynamics Code (EFDC). Integrated climate, hydrology, and lake hydrodynamics play a pivotal role in this lake's thermal transformation process. Meteorological parameters like air temperature, solar radiation, cloud cover, wind speed, and hydrologic parameters like precipitation, evaporation, and inflow/outflow, directly influence the lake heat budget and hence affect its thermal evolution. Thermal bar phenomena (during late spring to early summer) and summer stratification patterns are investigated, under the influence of these hydro-meteorological parameters.

Lake Ontario is one of the five Great Lakes located in northeastern North America, on the Canada–United States border. The lake has a surface area of 19,000 km², with a maximum length of 311 km, a maximum width of 85 km; average depth is 86 m, with a maximum depth of 244 m. It is the smallest of the five lakes but has an average depth greater than all except Lake Superior. Because the lake is located at a higher latitude and has a fairly high depth to surface area ratio, the lake displays interesting thermal characteristics including thermal bar phenomena. Figure 1.1 shows Lake Ontario
with bathymetry data and local weather stations. Inflow is from the Niagara River and outflow to the St. Lawrence River.

![Lake Ontario with bathymetry, rivers, and seven weather stations around the lake.](image)

Figure 1.1: Lake Ontario with bathymetry, rivers, and seven weather stations around the lake.

The lakes thermal behavior varies under the influence of the seasonal cycle. During winter the lake stratifies with ice on top and dense water at 3-4°C at the bottom. In temperate regions, aquatic plant, plankton, and fish survive during freezing winter months because of this natural stratification mechanism. With spring heating, the ice cover melts and temperatures at the lake surface rise above 0°C. Below 4°C, as the surface warms, the density of water increases and shallow mixing occurs. As the shallow mixed layer approaches 3 or 4°C, the entire water column has about the same density; helped by wind the lake is deeply mixed and the entire water column becomes essentially isothermal. When the temperature of the surface layer eventually exceeds 4°C, the lake begins to stratify. The lake also demonstrates another phenomenon known as a “thermal bar,” which results from inhomogeneous thermal heating between shallow nearshore areas (which warm and stratify more quickly) and deep offshore regions (which remain
colder and partially or fully mixed for a longer time). The thermal bar acts as a vertical column of deeply mixed water with a temperature near 4°C. It inhibits horizontal transport of heat and solutes and effectively traps nutrients delivered by river flow near the edges of the lake, compounding eutrophication problems in the near-shore environment (Holland and Kay, 2003). As the lake continues to warm and the surface temperature eventually rises above 4°C in the deepest areas of the lake, the thermal bar disappears, and the lake enters the summer stratification phase. Warm water stays on top, cold dense water remains below, and an intermediate zone with strong vertical density gradient (thermocline) develops between these two regions. The thermocline is a strong physical barrier to mixing, and the depth of mixing (and the resulting depth of the thermocline) during the stratified period is primarily influenced by the history of wind forcing.

Because the thermal behavior of Lake Ontario affects nearshore lake health, aquatic species habitat, etc.; the evolution of the spring thermal bar and summer stratification have been an area of interest. For example, high plankton productivity and locally abundant fish populations are associated with the thermal bar overturning circulation (Moll et al., 1993). Transient wind-driven upwelling or downwelling of the thermocline in coastal waters is one of the physical processes that affects the mixing and transport of contaminated waters in the nearshore zone and brings nutrient-rich sub-surface waters to the surface (Rao and Schwab, 2007). Thermal bar formation and its characteristics (propagation, flow circulation, and mixing coefficients associated with thermal bar) have been investigated using observed temperature profiles (Moll et al., 1993; Rao and Schwab, 2007; Rao et al., 2004; Rodgers, 1968; Rodgers, 1987),
laboratory-scale models (Elliott and Elliott, 1969, 1970), theoretical analyses, and numerical models (Csanady, 1971; de Alwis, 1999; Gbah and Murthy, 1998; Malm, 1995; Scavia and Bennett, 1980; Zilitinkevich et al., 1992). Temperature profiles and thermal stratification patterns in Lake Ontario have been simulated using hydrodynamic models forced with observed meteorological parameters, inflow/outflow (Hall, 2008; Huang et al., 2010a; Huang et al., 2010b) and using forecast from climate models (Huang et al., 2010b). Meteorological conditions like wind speed, air temperature, solar radiation, and hydrologic parameters like precipitation, evaporation, etc. affect the lake surface heat flux and overall heat budget within the lake. In large lakes, thermal structures are driven by atmospheric conditions including air temperature, heat transfer at the air-lake interface, precipitation, evaporation, and winds (Gibson et al., 2006; Huang et al., 2010b).

In this study, temperature profiles were simulated during late spring to early summer to explore the lake's transition from the fully mixed phase in early spring to the density-stratified phase in summer. I investigate the suitability of EFDC for thermal-hydrodynamic modeling of large, deep, temperate lakes (e.g., Lake Ontario). Based on the comparisons with observations, improvements were made to the model so that the heat flux and resulting lake temperatures at different depths were replicated by the model.

EFDC was improved to better capture the thermal characteristics of Lake Ontario:

- To explore spring thermal bar evolution (formation and retreat) during spring to early summer in Lake Ontario for 2011.

- To explore thermal stratification patterns in Lake Ontario during summer months for 2011.

To achieve these goals, a specific set of adjustments to the model were required including:
- Updating the evaporation algorithm in EFDC, to accurately compute the net surface heat flux and evaporation rate

- Calibrating solar radiation attenuation coefficients, specifically applicable for Lake Ontario, so that the correct amount of solar radiation is absorbed in the water column.

- Updating the vertical mixing parameterization (eddy diffusivity and eddy viscosity) to capture the transition from lake-mixed phase (spring) to lake-stratified phase (summer). Calibrating the model's parameters (vertical and horizontal mixing coefficients, bed heat flux parameters) to yield a good match between observed and simulated temperature profiles.

The study is organized as follows: Chapter 2 describes the mechanisms of thermal bar formation and thermal stratification patterns in the Great Lakes. A brief overview of historical numerical studies on thermal simulation in lakes/reservoirs is also provided. Chapter 3 provides the overview of EFDC with governing hydrodynamic equations and the heat balance model for the lake. Chapter 4 describes the EFDC Lake Ontario model set-up, input meteorological and flow data, and forcing parameters/coefficients. Chapter 5 describes the improvements made to the EFDC Lake Ontario model to capture the lake's mixed (homogenous temperature) phase and thermal bar formation. The model was improved by (1) updating and refining the evaporation algorithm (Quinn, 1979; Croley, 1989) and (2) calibrating the appropriate solar radiation attenuation coefficients and horizontal mixing coefficients. Chapter 6 describes implementing the new vertical mixing parameterization to EFDC Lake Ontario model, required to better capture the summer thermal stratification pattern better. In Chapter 7, I compare meteorological data from land stations with simulated data from the NARR regional climate model. Finally, the simulated temperature profiles using NARR meteorological forcing data are presented and discussed.
2.1 Lake Physics and Thermal Regimes.

The thermal bar is a plume of dense sinking water at the temperature of maximum density (4°C), and is formed in temperate lakes (lakes located in higher latitudes) in spring and/or fall when waters on either side of the 4°C isotherm mix (Rao and Schwab, 2007). The thermal bar phenomenon regularly occurs in the Great Lakes, and the incident was first reported by Rodgers (1968) in Lake Ontario.

As spring heating proceeds in Lake Ontario, water warms by convective heating, temperatures increase at the surface. With the melting of ice, wind-mixing comes into play, and warm surface water sinks causing upwelling of deep cold water. The heat flux passing into the water is determined mainly by meteorological factors. It varies comparatively weakly in the horizontal direction. Therefore the shallow near-shore zone of a water body is heated quicker than the offshore deep-water zone. As a result, surface temperature becomes inhomogeneous in the horizontal direction (Zilitinkevich et al., 1992). When the surface temperature first exceeds 4°C in nearshore areas, stable thermal stratification develops, but the adjacent deeper parts of the lake still experience deep convection because temperatures are ~ 4°C. As a result, double-cell convection develops with a relatively narrow, dense, descending current at ~4°C between the convection cells. This narrow downwelling zone is the thermal bar (Rao et al., 2004). As warming
continues, the thermal bar progresses from the shallowest to the deepest parts of the lake, until it finally disappears as summer stratification sets in over the deepest part of the lake (de Alwis, 1999; Rao et al., 2004). Figure 2.1 below shows spring turnover and summer stratification events in a typical lake.

![Figure 2.1: Spring turnover and summer stratification.](image)

Thermal stratification usually occurs in late May or early June and lasts through early October in Lake Ontario (Beletsky et al., 1999). Stratification is a function of temperature, which in turn is a function of the overall energy balance and the internal mixing processes of a lake. While wind mixing influences the surface layers of the lakes, its ability to mix the entire water column in summer-stratified lakes is greatly reduced. This is because the warm surface layers (epilimnion) is separated from deep cold layers (hypolimnion) by a transition zone (metalimnion), with a strong density gradient between top and bottom layers. In metalimnion transition zone (in Figure 2.1) temperatures changes rapidly and density gradient varies accordingly. A thermocline is a horizontal plane within this metalimnion zone through the point of maximum density gradient; it acts as a physical barrier between the epilimnion (warm surface layer) and hypolimnion.
(cold deep layer). Although not an absolute barrier, it takes strong winds to disrupt it (Seker-Elci, 2004). During summer, surface water is heated rapidly absorbing direct solar radiation and by wind mixing; cold dense water remains at the bottom of the lake and a thermocline forms between these two temperature-density zones. With strong wind or storm events, turbulent mixing within the water column sometimes disrupts the thermocline; and wind momentum and heat flux penetrate deeper through the water column. The transport of heat by turbulence decreases as the stability of stratification increases during summer months and the variation of heat flux in the hypolimnion reduce with increasing depth (Wetzel, 2001).

Figure 2.2: Layers of thermal stratification in a typical lake; Source: (Seker-Elci, 2004).

Depending largely on the season, latitude, and turbulent mixing by the wind, thermoclines may be a semi-permanent feature a water body. Because Lake Ontario is at
a temperate latitude, significant seasonal weather variation is observed, and the summer thermocline is an important feature for this lake.

The development of stratification in lakes and reservoirs is due to three major factors. Lakes and reservoirs have low flow velocities, often laminar in nature. As a result, mixing is controlled by molecular diffusion, which allows stable gradients in temperature. Second, lakes and reservoirs have long residence times. This is important because heating, cooling, and chemical processes in lakes are slow. If the flow through the lake is too fast, there is not adequate time for stratification to develop and turbulent mixing dominates. Third, lakes and reservoirs form in (sometimes deep) depressions that decrease the interaction between surface and bottom waters. Such topography supports stratification. Hence, vertical stratification in lakes and reservoirs becomes increasingly important for low-velocity lakes and those with longer residence times and deeper bottoms (Imboden and Wüest, 1995).

Climatological forcing parameters influence the spring to summer thermal transition process in the Great Lakes. Atmospheric conditions, such as air temperature, heat transfer at the air-lake interface, precipitation, evaporation, and lake surface winds significantly affect the thermal structure, currents, and water level in large lakes (Gibson et al., 2006; Huang et al., 2010a). The air/water interface and the processes occurring at this interface such as wind, waves, heat flux are important phenomena to understand because this is where the exchange of physical quantities such as heat, kinetic energy, momentum, and matter (gases, vapor, aerosols, etc.) occurs (Hall, 2008; Wüest and Lorke, 2003). Another study in the Great Lakes region showed that a 20% increase in precipitation produced a 36% (22 mm) increase in annual surface runoff and a 9%
(2.2 W/m²) decrease in sensible heat flux (Mishra et al., 2010). Bennington et al. (2010) used the MITgcm to simulate the thermal structure and circulation of Lake Superior, and they found that the increase in the modeled lake surface temperature was significantly correlated with increases in wind speed above the lake, increased current speeds, and declining ice coverage. Warmer winter conditions typically lead to more rapid thermal bar formation and disappearance because of the higher heat content in deeper areas of lake, which facilitates lake warming (Rodgers, 1987). Flow circulation in the Great Lakes is driven primarily by wind stress and surface heat fluxes (Beletsky et al., 1999). Rao et al. (2004) studied the spring thermal bar formation in Lake Ontario and concluded that wind-driven circulation seems to be an important feature for thermal bar evolution and progression; hence models must incorporate local wind stresses. Wind-induced transport of heat is often of greater importance than direct solar heating in most lakes, especially where light is rapidly attenuated with depth as it is in Lake Ontario (Wetzel, 2001).

2.1.1 Environmental Impacts of Lake's Thermal Behavior

Physical processes such as a lake's thermal cycle and circulation can have a pronounced influence on water quality in the coastal waters of the Great Lakes (Edsall and Charlton, 1996). The thermal bar is important because of its role in inhibiting the horizontal exchange of water between the nearshore and offshore regions (Gbah and Murthy, 1998; Rao and Schwab, 2007). The thermal bar traps any shore- or river-released nutrients near the edges of the lake compounding eutrophication problems associated with high nutrient loading and limited horizontal mixing (Holland and Kay, 2003). A spring phytoplankton bloom occurred when the formation of the thermal happened in time to entrain spring runoff and did not occur when the formation missed the spring
runoff event in Lake Superior (Auer and Gatzke, 2004). Moll et al. (1993) observed high plankton productivity and locally abundant fish populations that were associated with thermal bar overturning circulation. It is postulated that there may be a significant opportunity for vigorous growth of Cladophora (algae species) during the spring evolution of the thermal bar in Lake Ontario (Rao et al., 2004). Transient wind-driven upwelling or downwelling of the thermocline in coastal waters is another physical process that affects mixing and transport of contaminated waters in the nearshore by bringing nutrient-rich subsurface waters to the surface (Rao and Schwab, 2007). Makarewicz and Howell (2007) noted that despite significant water-quality improvement in the open waters of Lake Ontario, nearshore waters are still suffering from many impairments that severely limit their recreational use and ultimately affect the economic development of the region. Hence, studying the thermal characteristics of Lake Ontario serves as baseline research for further investigating impacts on nearshore lake health.

2.2 Numerical Modeling of Hydrodynamic Processes and Thermal Behavior in Lakes

Numerical thermal simulation studies involve description/investigation of the heat flux balance mechanism within a lake, the temperature transport processes (both horizontally and vertically) and hence, an understanding of the lake hydrodynamic processes as a whole. Hydrodynamic models use lake bathymetry, inflows, outflows, and meteorological data to simulate water levels, flow velocities, temperature, salinity, and sediment transport. Hall (2008) stated that hydrodynamic modeling is the appropriate transport foundation for an accurate lake mass balance model because it offers a basis for simulating transport in response to meteorological forcing functions and the results can be scaled to the desired spatial and temporal resolution. Within a lake domain, wind-
generated surface stresses, buoyancy or density gradient, turbulent momentum, mass balance, and mass transport are the physical processes that must be simulated by the hydrodynamic model.

In hydrodynamic modeling, either a two-dimensional (vertically averaged approach) or a three-dimensional approach is used. A two-dimensional vertically averaged approach is applied when vertical variations of velocity and temperature are not significant, which may be the case for shallow water bodies. In three-dimensional models, the full equations of motion are solved. Lake Ontario is a deep lake, hence capturing the vertical density gradient is important for temperature simulation. Hence, a three-dimensional hydrodynamic approach is required for Lake Ontario.

There are many examples of three-dimensional models for thermal simulation in lakes. Beletsky and Schwab (1998); (Beletsky and Schwab, 2001) applied the Princeton Ocean Model (POM) of Blumberg and Mellor (1987) to Lake Michigan to simulate the thermal structure and circulation. The model was able to reproduce all of the basic features of the thermal structure in Lake Michigan: spring thermal bar, full stratification, deepening of the thermocline during the fall cooling, and finally, an overturn in the late fall. However, they observed that the model could not capture the temperature gradient in the thermocline. They concluded that the model yielded excessive vertical diffusion that resulted in a smaller vertical temperature gradient than was measured.

Ahsan and Blumberg (1999) modeled Lake Onondaga (in New York) using the three-dimensional hydrodynamic model ECOM (Estuarine, Coastal and Ocean Model, ECOM) using a semi-implicit time splitting algorithm and a Z-level vertical coordinate system. They stressed proper assignment of boundary conditions, especially surface heat
fluxes, which are crucial in simulating lake’s hydrothermal dynamics. Significant
differences in the thermal structure of the lake were observed in the simulation year 1985
and 1989 as a result of different meteorological conditions, especially wind forcing. The
mixed layer depth in 1985 was about 3 m deeper (about 9 m) than that in 1989 (about 6 m), consistent with a stronger prevailing wind in 1985.

The evolution of thermal bar in lakes has been previously investigated because of
its environmental significance. Thermal bar formation and its characteristics
(propagation, flow circulation, and mixing coefficients associated with thermal bar) have
been investigated with laboratory-scale models (Elliott and Elliott, 1969, 1970),
theoretical analyses, and numerical models (Csanady, 1971; Gbah and Murthy, 1998;
Malm, 1995; Scavia and Bennett, 1980; Zilitinkevich et al., 1992). Propagation of the
thermal bar has been characterized by Elliott and Elliott (1970), Zilitinkevich et al.
(1992), Malm et al. (1993).

The formation of the thermal bar in Lake Ontario was simulated for 1997-1999
using the time-dependent, 3D hydrodynamic model ALGE by de Alwis (1999).
Simulated lake surface temperatures were compared and validated with Advanced Very
High-Resolution Radiometer (AVHRR) satellite images. The study incorporated spatially
varying (non-uniform) meteorological conditions, high-resolution bathymetry data,
varying horizontal and vertical resolutions to improve thermal modeling of Lake Ontario.

Rao et al. (2004) used observations from thermistors and current meters in Lake
Ontario to study spring thermal bar circulation and its effects on horizontal and vertical
mixing processes. Their study described that the thermal bar decreased the magnitude of
both alongshore and cross-shore horizontal exchange coefficients thereby inhibiting the
horizontal exchange of water. The vertical exchange coefficients were high in the water column because of convective mixing during the thermal bar period and decreased considerably in the nearshore regions under stable stratification. Hence, horizontal and vertical mixing coefficients play a major role in transport and stratification of temperature. This study also mentioned that models that incorporated the effect of horizontal heat flux in the thermal bar region were able to predict the increase in thermal bar progression.

EFDC was applied to simulate density-driven circulation in Lake Billy Chinook, Oregon Yang et al. (2000). Their analysis revealed that the existing hydrothermal behavior in Lake Billy Chinook is primarily a result of four different types of forcings: (1) temperature/density stratification, (2) wind stresses, (3) river inflows, and (4) power plant intake withdrawal. Temperature-related density stratification is the dominant forcing mechanism, with secondary influences from wind stresses.

Hodges et al. (2000a) summarized the sources of energy for transport, turbulence, internal waves, and mixing in stratified reservoirs/lakes. They described the challenges of numerically modeling transport processes in stratified lakes. Because wind over a lake is directly influenced by the surrounding topography, use of a uniform wind from one measurement station may not lead to correct simulation of circulation gyres. Instead, multiple wind stations around the lake must be monitored, and data from these stations should be used in modeling the hydrodynamic circulation. Hodges et al. (2000a), also discussed the tendency of numerical models to artificially diffuse sharp temperature gradients faster than physical processes.
Hall (2008) depicted summer thermal stratification in Lake Ontario using the three-dimensional Estuary and Lake Computer Model (ELCOM). ELCOM slightly underestimated lake temperatures when compared to observed data. The thermocline was also more diffused in ELCOM simulations, probably due to numerical diffusion and failure to capture basin-scale internal waves that provide the driving forces for vertical and horizontal fluxes in a stratified lake.

Huang et al. (2010a) described thermal modeling in Lake Ontario and simulated variations of lake surface temperatures and vertical stratification at seasonal and synoptic time scales. The hydrodynamic model is based on the Princeton Ocean Model (POM). Model sensitivity experiments revealed that errors in simulating surface net heat flux (SNHF) have a significant impact on simulations of water temperature in the surface and near-surface layers, whereas errors in simulating wind stress cause significant changes of water temperature in the thermocline.

The solutions of three lake hydrodynamic models, namely, Princeton Ocean Model (POM), Canadian Version of Diecast Model (CANDIE), and Estuary, Lake, and Coastal Ocean Model (ELCOM), are compared with each other and with observations in Lake Ontario to simulate lake's thermal behavior and circulation pattern (Huang et al., 2010b). All models produced large errors in simulating the temperatures in the thermocline, associated with errors in simulating the depth of the mixed layer, but performed better near the coast. Using s or z levels, the models all showed diffused thermoclines. This indicates that differences in the simulated temperature distribution may be more related to differences in the parameterization of vertical mixing, instead of that in the vertical discretization. Most of the hydrodynamic thermal models discussed
above determined that spatially varying meteorological forcing around the lake (especially a non-uniform wind profile) and heat flux exchange at the air-water interface are important for modeling the thermal characteristics of lakes. Simulating density driven temperature gradient at the thermocline proved challenging for these hydrodynamic models. Surface wind stresses and wind-mixing along with vertical and horizontal mixing coefficients should be accurately captured by the models. The basic equations used in the simulation process expressed time-dependent temperatures as a function of horizontal/vertical mixing coefficients, advective flow, and surface heat flux exchange. Detailed governing equations and approaches for Lake Ontario hydrothermal modeling using EFDC are discussed in next two chapters.
CHAPTER 3:
ENVIRONMENTAL FLUID DYNAMICS CODE (EFDC) MODEL

3.1 Overview of the EFDC Hydrodynamic Model

EFDC is a public-domain multifunctional surface-water modeling system incorporating fully integrated hydrodynamics, sediment-contaminant, and water-quality components. EFDC is extremely versatile, and can be used for 1D, 2DV, 2DH, or 3D simulations of flow and transport processes in surface water systems including rivers, lakes, reservoirs, wetlands, estuaries, and coastal ocean regions. EFDC has been applied to over 100 water body modeling studies in support of environmental assessment, management, and regulatory requirements. The model is presently being used by universities, research organizations, governmental agencies, and consulting firms. The physical processes represented in the EFDC model and many aspects of the computational scheme are similar to those in the ECOMSed model (Blumberg and Mellor, 1987) and the U. S. Army Corps of Engineers' (USACE) Chesapeake Bay model (Johnson et al., 1993).

EFDC was developed by John Hamrick (Hamrick, 1992) at Virginia Institute of Marine Science (VIMS) in the early 1990s with primary support from the Commonwealth of Virginia and subsequent support from U.S. Environmental Protection Agency (EPA) and National Oceanic and Atmospheric Administration's (NOAA) Sea Grant Program. EFDC is still being developed and maintained by John Hamrick at Tetra
Tech, Inc. with primary external support from the EPA. US EPA's EFDC version is open source and can be upgraded/augmented as per user requirement. Parallelized version of EFDC is developed by IBM Research at Ireland (O'Donncha et al., 2015; O'Donncha et al., 2014).

In this study, I am using an augmented version of US EPA's EFDC, named SNL-EFDC which was developed at Sandia National Laboratories at Livemore, CA (James and Boriah, 2010; James et al., 2013; James and Roberts, 2014; Thanh et al., 2008) SNL-EFDC is an extension of EFDC coupled to both the USACE's water-quality code, CE-QUAL-ICM and the sediment dynamics code, SEDZLJ (James et al., 2011). It also simulates the effects of marine hydrokinetic device energy generation (James and Roberts, 2014).

EFDC has been widely used over the years as a standalone hydrodynamic model and also for coupled systems with water quality, hydrology, and thermal, and sediment dynamics models. Some representative recent applications of EFDC in academic research and industrial modeling include: temperature stratification and circulation modeling of Lake Billy Chinook Reservoir, Oregon (Yang et al., 2000); winter circulation, submerged aquatic vegetation and water quality modeling in Lake Okeechobee, Florida (Jin et al., 2002; Jin et al., 2007); hydrodynamic and water quality modeling of the Neuse River Estuary, North Carolina (Wool et al., 2003); sediment transport and shoreline erosion predictions in Hartwell Lake, South Carolina and Georgia (Seker-Elci, 2004); hydrodynamic eutrophication modeling (HEM-3D) of Kwang-Yang Bay, Korea (Park et al., 2005); desalination brine discharge modeling at Corpus Christi Bay, Texas (Hodges et al., 2006); temperature and salinity transport and runoff modeling in St. Lucie Estuary,
Florida (Jin et al., 2007); coupled hydrology-hydrodynamic (HSPF-EFDC) modeling in St. Louis Bay, Mississippi (Liu et al., 2008); water age and thermal structure modeling in Lake Mead, China (Li et al., 2010); water-quality modeling on Cedar Lake, Indiana (James et al., 2006); verifying marine hydro-kinetic energy generation using SNL-EFDC (James et al., 2011; James and Boriah, 2010) and analyzing pH effects on algal-growth hydrodynamic model (James and Boriah, 2010; James et al., 2013).

EFDC (same as SNL-EFDC) solves the three-dimensional, vertically hydrostatic, free-surface equations, formulated using the turbulence-averaged equation of motion with the Boussinesq approximation and with Mellor and Yamada (1982) turbulence closure. The numerical solution techniques are the same as those of Blumberg and Mellor (1987), except for the solution of the free surface, which is implemented with a preconditioned conjugate gradient (direct) solver rather than an alternating-direction implicit method. EFDC’s time integration uses a second-order-accurate, three or two-time-level (three-time level leap-frog, trapezoidal or two-time level trapezoid), finite-difference scheme, on a staggered or C-grid with an internal-external mode splitting technique (Hamrick, 1992). The formulation of the governing equations for environmental flows is characterized by horizontal length scales, which may be orders of magnitude greater than their vertical length scales and begin with the vertically hydrostatic boundary layer form of the turbulent equations of motion for an incompressible, variable-density fluid. Small scale non-hydrostatic processes like internal waves and mixing are represented with appropriate parameterization through calibration. Hence, use of the hydrostatic assumption is justified.
EFDC, like many ocean models, uses a stretched or sigma vertical coordinate (bathymetry following) and Cartesian or curvilinear-orthogonal horizontal coordinates. Each vertical layer is assigned a constant (often equal) fraction of the local depth throughout the model domain; the absolute height (and thickness) of each layer changes with the topology of the model domain (i.e., with 10 layers at 10 m depth, each equal sigma layer would be 1 m thick; at 150 m depth, each layer would be 15 m thick). However, the user can specify the fraction of local depth for each vertical layer. A schematic of sigma vertical coordinates is shown in Figure 3.1.

![Schematic of vertical sigma coordinates](image)

Figure 3.1: Schematic of vertical sigma coordinates; Source: (Ji, 2008).

EFDC uses standard scalar transport equations in the water column (e.g., temperature, salinity, dye, toxics, and sediments). The solution of the transport equations uses an internal/external mode splitting technique, common in oceanographic surface water models for computational efficiency. The theory treats the slower-moving internal waves (or baroclinic mode calculated across each “sigma” layer) separately from the fast moving external free-surface gravity wave (or barotropic mode calculated on the depth average). Hence, two sets of transport equations are used to obtain the numerical solution:
• External – Vertically integrated momentum equations are solved on a small time step to obtain an average horizontal velocity and the shape of the water surface.

• Internal – Vertically resolved momentum equations are solved at the completion of each external solution to resolve changes in the vertical structure of velocity and other water-column properties.

3.2 Governing Equations in the EFDC Hydrodynamic Module

In EFDC, for a realistic representation of horizontal boundaries, the governing equations are formulated such that the horizontal coordinates, x and y, are curvilinear and orthogonal. To provide uniform resolution in the vertical direction (bounded by bottom topography and the free surface including long-wave motion), a stretching transformation is used (Hamrick, 1992):

\[
z = \frac{z^* + z_b^*}{z_s^* + z_b^*}
\]  

(3.1)

where the * denotes original physical vertical coordinate and \( z_s^* , z_b^* \) are the physical vertical coordinates of the free surface and bottom bed.

The formulation of hydrodynamic governing equations in EFDC starts with some basic approximations that are commonly used in the study of surface-water systems. A widely used approximation in the studies of rivers, lakes, estuaries, and coastal waters is the shallow water approximation, which assumes that the horizontal scale of motion is much larger than the vertical scale of motion. This leads to the hydrostatic approximation, which assumes that pressure at any point in the ocean is due to the weight of the water above it (plus local atmospheric pressure). The vertical inertia is considered much smaller than gravitational acceleration and hence omitted. The vertical pressure gradient is balanced by buoyant forcing:
\[
\frac{\partial P}{\partial z} = -\rho g = -gHb = -gH\left(\rho - \rho_o\right)/\rho_o
\]  
(3.2)

where \(P\) is pressure, \(H\) is local water depth, \(b\) is buoyancy with \(\rho\) and \(\rho_o\) the local actual and reference (density of pure water at 4°C) water densities, respectively.

The Boussinesq approximation assumes incompressibility (water density does not change with pressure). In the Boussinesq approximation, variations in water density are only a function of buoyancy. Typically, densities vary by less than a few percent in the water column. So, density changes due to local pressure gradients in the horizontal momentum equations are negligible (Ji, 2008).

In EFDC, the vertical momentum equation is reduced to a hydrostatic equation (Hamrick, 1992; Ji, 2008). Despite its significant depth, Lake Ontario has a low depth to length ratio, the vertical scale of mean properties like turbulence intensity and turbulent length scale are much smaller than the corresponding horizontal properties. Small scale non-hydrostatic processes like internal waves and mixing are represented with appropriate parameterization through calibration. Hence, use of the hydrostatic assumption for simulating vertical flow is justified. Horizontal momentum equations are formulated by transforming the turbulence-averaged Navier-Stoke's equation for vertically hydrostatic flow (pressure at any point is due to the weight of the water and atmosphere above it) with the Boussinesq approximation (variations in density are considered too small to affect inertia, but buoyancy is important) for variable density fluid (Hamrick and Wu, 1997):
\[
\partial_t \left( m_x m_y H \right) + \partial_x \left( m_y H u \right) + \partial_y \left( m_x H v \right) + \partial_z \left( m_x m_y w \right) - f_e m_x m_y H v
\]
\[
= -m_x H \partial_y \left( P + g \eta \right) + m_y \left( -\partial_x h + z \partial_x H \right) \partial_z P
\]
\[
+ \partial_x \left( m_x m_y \frac{A_x}{H} \partial_z u \right) + \partial_y \left( \frac{m_y}{m_x} H A_{H_u} \partial_x u \right) + \partial_y \left( \frac{m_x}{m_y} H A_{H_v} \partial_x v \right)
\]
\[
\partial_t \left( m_x m_y H \right) + \partial_x \left( m_y H u \right) + \partial_y \left( m_x H v \right) + \partial_z \left( m_x m_y w \right) - f_e m_x m_y H u
\]
\[
= -m_x H \partial_y \left( P + P_{um} + g z^* \right) + m_y \left( \partial_y z^* + z \partial_y H \right) \partial_z P
\]
\[
+ \partial_x \left( m_x m_y \frac{A_x}{H} \partial_z v \right) + \partial_y \left( \frac{m_y}{m_x} H A_{H_u} \partial_x v \right) + \partial_y \left( \frac{m_x}{m_y} H A_{H_v} \partial_x v \right)
\]

where \( u \) and \( v \) are horizontal velocity components in the dimensionless curvilinear-orthogonal horizontal coordinates \( x \) and \( y \), respectively, \( m_x \) and \( m_y \) are scale factors of the horizontal coordinates, \( H \) is instantaneous local water depth sum of depth below and free surface displacement (\( \eta = \) free surface displacement), \( h + \eta \).

The vertical velocity in the stretched vertical coordinate \( z \) is \( w \) and is related to physical vertical velocity \( w^* \) by:
\[
w = w^* - z \left( \partial_t \eta + \frac{u}{m_x} \partial_x \eta + \frac{v}{m_y} \partial_y \eta \right) + \left( 1 - z \right) \left( \frac{u}{m_x} \partial_x h + \frac{v}{m_y} \partial_y h \right)
\]
\[
f_e \text{ is the effective Coriolis acceleration that incorporates the curvature acceleration terms with Coriolis parameter, } f, \text{ as:}
\]
\[
f_e m_x m_y = f m_x m_y - u \partial_y m_y + v \partial_x m_y
\]
\[
A_H \text{ is the horizontal eddy viscosity (m}^2\text{/s) when the advective acceleration are represented by central differences. } A_v \text{ is the vertical eddy viscosity (m}^2\text{/s), that relates the shear stresses to vertical shear of the horizontal velocity components as:}
\]
\[ (\tau_{x}, \tau_{y}) = \frac{A}{H} \partial_z (u, v) \]  \hspace{1cm} (3.7)

\( P_{atm} \) is atmospheric pressure referenced to water density.

The density, \( \rho \), is a function of temperature (T) and salinity (S), consistent with incompressible continuity equation under anelastic approximation (Hamrick, 1992).

\[ \rho = (S, T) \]  \hspace{1cm} (3.8)

The three-dimensional continuity equation in the stretched vertical and curvilinear-orthogonal horizontal coordinate system is:

\[ \partial_t \left( m_x m_y H \right) + \partial_x \left( m_y H u \right) + \partial_y \left( m_x H v \right) + \partial_z \left( m_x m_y w \right) = Q_H \]  \hspace{1cm} (3.9)

where \( Q_H \) are volumetric sources and sinks including rainfall, evaporation, groundwater exchange, and lateral inflows/outflows.

The continuity equation has been integrated on \( z \) over the interval (0, 1; where \( z \) is set to 0 at the bed and 1 at the surface) to produce the depth integrated continuity equation:

\[ \partial_t \left( m_x m_y H \right) + \partial_x \left( m_y H \int_0^1 u \, dz \right) + \partial_y \left( m_x H \int_0^1 v \, dz \right) = 0 \]  \hspace{1cm} (3.10)

Hydrodynamic transport includes the following processes: 1. advection, 2. dispersion, 3. vertical mixing (Ji, 2008). Both horizontal and vertical transport should be considered in the system. The generic transport equation for temperature (T), salinity (S) or any dissolved or suspended material (having a mass per unit volume concentration), is:

\[ \partial_t \left( m_x m_y HT \right) + \partial_x \left( m_y HuT \right) + \partial_y \left( m_x HvT \right) + \partial_z \left( m_x m_y wT \right) \]

\[ = \partial_z \left( m_x m_y \frac{K_x}{H} \partial_z T \right) + \partial_x \left( m_y \frac{HK_y}{m_y} \partial_x T \right) + \partial_y \left( m_x \frac{HK_x}{m_x} \partial_y T \right) + Q_T \]  \hspace{1cm} (3.11)
where $K_v$ and $K_H$ are vertical, and horizontal diffusion coefficients. In the preceding transport equation, 1 is accumulation, 2 is advection, 3 is vertical mixing, and 4 is horizontal dispersion while $Q_T$ are external sources and sinks; for temperature transport, 

$$Q_T = \frac{1}{\rho c_p} \partial_z T,$$

where, $I$ is net heat flux and $C_p$ is the specific heat of water.

The set of governing equations (3.2-3.11) provides a closed system for solving flow variables and scalar transport materials. In EFDC, horizontal and vertical flows are solved with boundary conditions:

- Horizontal flows are determined through the horizontal momentum equation with a no-flow boundary condition at later walls ($u, v = 0$).
- Density-dependent vertical flows are established through a solution of the mass balance equation at each cell with a specified flow boundary condition at the bottom due to groundwater exchange (often zero).

The vertical turbulent viscosity, $A_v$, and the diffusivity, $K_v$ must be specified for the solution of the momentum and transport equations. EFDC uses the 2.5 turbulence closure model developed by Mellor and Yamada (1982) and modified by Galperin et al. (1988) to calculate the vertical turbulent viscosity and diffusivity.

The Mellor-Yamada 2.5 turbulence closure model, assumes a local balance between production and dissipation of turbulent kinetic energy and uses a set of assumptions that reduce the stress and flux relations to a set of algebraic equations. The model relates the vertical turbulent viscosity and diffusivity to the turbulence intensity, $q$, a turbulent length scale, $l$; and a turbulent intensity and length-scaled-based Richardson number, $Rq$ by:

$$A_v = \mathcal{D}_{A_v} A_0 q l,$$  \hspace{1cm} (3.12)

and
\[ K_r = \varnothing \kappa K_q l, \quad (3.13) \]

where

\[
\varnothing_A = \left( \frac{1 + \frac{Rq}{R_1}}{1 + \frac{Rq}{R_2}} \right) \left( 1 + \frac{Rq}{R_3} \right), \quad (3.12a) \]

\[ A_0 = A_1 \left( 1 - 3C_1 + \frac{6A_1}{B_1} \right), \quad (3.12b) \]

\[
\varnothing_K = \frac{1}{\left( 1 + \frac{Rq}{R_3} \right)}, \quad (3.13a) \]

\[ K_0 = A_2 \left( 1 - \frac{6A_1}{B_1} \right), \quad (3.13b) \]

where the stability functions, \( \phi_A \) and \( \phi_K \), account for reduced and enhanced vertical mixing or transport in stable and unstable vertically density-stratified environments, respectively.

The length scale-based Richardson number \((Rq)\) is:

\[ Rq = \frac{-gH\hat{z}b^2}{q^2H^2}, \quad (3.14) \]

Mellor and Yamada (1982) specify the constants \([A_1, B_1, C_1, A_2, B_2]\) as \([0.92, 16.6, 0.08, 0.74, \text{and } 10.1]\) respectively. Coefficients \(R_1, R_2, R_3\) and \(Rq\) are defined as below:

\[ R_1^{-1} = \frac{3A_2 \left[ (B_2 - 3A_2) \left( 1 - \frac{6A_1}{B_1} \right) - 3C_1(B_2 + 6A_1) \right]}{1 - 3C_1 - \frac{6A_1}{B_1}}, \quad (3.15a) \]

\[ R_2^{-1} = 9A_1A_2, \quad (3.15b) \]
\[ R3^{-1} = 3.42 (6.41 + B2) \]  

(3.15c)

The turbulence intensity, \( q \), and turbulent length scale, \( l \) are determined by the transport equations:

\[
\begin{align*}
\partial_t (m_x m_y Hq^2) + \partial_x (m_y Huq^2) + \partial_y (m_x Hvq^2) + \partial_z (m_m wq^2) \\
= \partial_z \left( m_x m_y \frac{A_q}{H} \partial_z q^2 \right) - 2m_x m_y \frac{Hq^3}{B_1} \\
+ 2m_x m_y \left( \frac{A}{H} \left( (\partial_z u)^2 + (\partial_z v)^2 \right) + \eta \rho c_p D \left( u^2 + v^2 \right)^{3/2} + gK_e \partial_z b \right) + Q_q
\end{align*}
\]

(3.16)

\[
\begin{align*}
\partial_t (m_x m_y Hq^2 l) + \partial_x (m_y Huq^2 l) + \partial_y (m_x Hvq^2 l) + \partial_z (m_x m_y wq^2 l) \\
= \partial_z \left( m_x m_y \frac{A_q}{H} \partial_z (q^2 l) \right) - m_x m_y \frac{Hq^3}{B_1} \left( 1 + E_2 \left( \frac{l}{\kappa H z} \right)^2 + E_3 \left( \frac{l}{\kappa H (1-z)} \right)^2 \right) \\
+ m_x m_y E_1 \left( \frac{A}{H} \left( (\partial_z u)^2 + (\partial_z v)^2 \right) + \eta \rho c_p D \left( u^2 + v^2 \right)^{3/2} + gK_e \partial_z b \right) + Q_l
\end{align*}
\]

(3.17)

where \([E1, E2, E3] = [1.8, 1.33, 0.25]\). The terms \( Q_q \) and \( Q_l \) may represent additional source-sink terms such as subgrid scale horizontal turbulent diffusion. The vertical diffusivity, \( A_q \), is set to \( 0.2ql \) following Mellor and Yamada (1982).

The horizontal turbulent viscosity, \( A_H \) and diffusivity, \( K_H \), in the momentum and transport equations, are determined independently using Smagorinsky's (1963) subgrid scale closure formulation. The horizontal eddy viscosity \( (A_H) \) represents the internal shear forces created by the transfer of momentum between faster and slower regions of flow by means of turbulent mixing. In general, the higher its value, the more uniform is the velocity distribution (Ji, 2008). The horizontal eddy viscosity \( (A_H) \), can be calculated using the Smagorinsky subgrid scale scheme (Smagorinsky, 1963), which is generally written in 2D Cartesian coordinate as:
\[ A_H = C \Delta x \Delta y \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right]^{1/2} \]  

(3.18)

where \( C \) is horizontal mixing constant (typical value between 0.1 to 0.2); \( \Delta x, \Delta y \) are model grid size in x, y direction.

The Smagorinsky formula links numerical model's horizontal mixing to current shear and model grid size. The parameter \( A_H \) is small if velocity gradients are small and if the horizontal grid dimension (\( \Delta x \) and \( \Delta y \)) is of finer spatial resolution.

### 3.2.1 Solid Boundary Condition

Boundary conditions are important in mathematical simulation models to represent hydrodynamics properly in the domain of the model. The solid boundary conditions include no-slip conditions and free-slip conditions. In no-slip boundary conditions, there is no flow along the boundary (\( Velocity_{tangential} = 0 \)) and through the boundary (\( Velocity_{normal} = 0 \)). In free-slip boundary condition, there can be flow along the boundary, but not across it. In the EFDC model, the boundary conditions for horizontal and vertical velocity are defined as no-slip boundary condition:

Horizontal velocities at lateral walls are zeros: \((u, v) = 0\)  

(3.19)

Vertical velocities at surface and bottom are zeros: \(w(0) = w(1) = 0\)  

(3.20)

For the solution of the momentum equations, vertical boundary conditions are related to the specification of the kinematic shear stresses (equation 3.6), at the bed \((z = 0)\) and at the free surface \((z = 1)\). At the free surface, the \(x\) and \(y\) components of the stresses are specified by the wind stress on water surface:

\[ \frac{A_w}{H} \partial_z (u, v)_{z=1} = \left( \tau_{xx}, \tau_{xy} \right) = C_s \sqrt{U_w^2 + V_w^2} \left( U_w, V_w \right) \]  

(3.21)
where, \( U_w \) and \( V_w \) are the \( x \) and \( y \) components of the wind velocity (m/s) at 10 meters above the water surface. The wind stress coefficient is given by:

\[
C_s = 1.2 \times 10^{-6} \left( 0.8 + 0.065 \sqrt{(U_w^2 + V_w^2)} \right)
\]  

(3.21a)

At the bed, the \( x \) and \( y \) components of the stresses are related to the near bed or bottom layer velocity components by the quadratic resistance formulation:

\[
\left( \tau_{xz}, \tau_{yz} \right) = \left( \tau_{x_0}, \tau_{y_0} \right) = C_b \sqrt{U_1^2 + V_1^2} \left( U_1, V_1 \right)
\]  

(3.22)

where, the \( I \) subscript denotes bottom layer values for horizontal water velocity components \((u, v)\). In a sigma coordinate model, the bottom drag coefficient \((C_b)\) is usually calculated using (Mellor, 1998), under the assumption that the near bottom velocity profile is logarithmic at any instant of time:

\[
C_b = \left( \frac{\kappa}{\ln \left( \frac{\Delta_1}{2z_0} \right)} \right)^2
\]  

(3.22a)

where,

\( \kappa = \) von Karman constant;

\( \Delta_1 = \) dimensionless thickness of the bottom layer;

\( z_0 = \frac{z_0^*}{H}, \) dimensionless roughness height.

Vertical boundary conditions for the turbulent kinetic energy and length scale equations are (absolute values indicate the magnitude of the enclosed vector quantity):

\[
q^2 = B1^{2/3} |\tau_s| : z = 1
\]  

(3.23a)

\[
q^2 = B1^{2/3} |\tau_b| : z = 0
\]  

(3.23b)

\[
l = 0 : z = 0 , 1
\]  

(3.23c)
For scalar transport material (temperature, salinity), the solid boundary condition states that no heatflux across the solid boundary, at lateral walls and bottom (free-slip boundary condition) (Ji, 2008):

\[
\frac{\partial T}{\partial n} = \text{temperature flux across solid boundary} = 0
\]  

(3.24)

where, \( n \) = the unit vector normal to boundary.

The heat fluxes at the surface are maintained by turbulent and/or radiative processes in the atmosphere-ocean boundary layer.

3.3 Equations for Temperature Simulation Module: Full Heat Balance Mechanism

Water temperature is a function of both surface heat flux and the transport of water into and out of the system. The total heat budget for a water body includes the effects of heat exchange with the atmosphere and with bed, inflows/outflows and heat generated by internal reactions. The dominant process affecting the total heat balance is atmospheric heat exchange. The horizontal distributions of the near-surface temperature in Lake Ontario are linked to changes in air-lake heat flux and the redistribution of heat by currents (Huang et al., 2010a). In an analytical study, Elliott and Elliott (1970) showed that the main factors controlling the progression of the thermal bar are surface heat flux and bottom topography. The model assumes that horizontal heat fluxes are of secondary importance and that complete vertical mixing results from convection in the unstably stratified region. However, in addition to air-lake heat flux, it is also important to include the proper boundary conditions for advective exchange (e.g., rivers, thermal discharges). The heat module mechanism within EFDC, which takes into account all the heat exchange fluxes in the air-lake interface, is called the Full Heat Balance mechanism.
The heat exchange between the atmosphere and water columns are dominated by two primary processes:

- Radiative Processes include incoming shortwave and longwave radiation from the sun and outgoing longwave radiation emitted by atmosphere and water surface.

- Turbulent Heat Transfer Processes include latent heat transfer due to evaporation (or condensation) from water surface (or overlying air) and sensible heat transfer between the water surface and atmosphere.

The net surface heat flux balance can be described by:

\[ H_{NSHF} = H_S + H_L - H_B - H_E - H_C + H_T \]  \hspace{1cm} (3.25)

where,

- \( H_S \) = Incoming Shortwave Radiation Heatflux
- \( H_L \) = Incoming Longwave Radiation Heatflux
- \( H_B \) = Outgoing Longwave Radiation Heatflux
- \( H_E \) = Latent Heatflux due to Evaporation
- \( H_C \) = Sensible Heatflux due to Conduction
- \( H_T \) = Advective Heatflux addition/removal from Inflows/Outflows

**Incoming shortwave solar radiation** is the direct radiation coming from the sun.

While other heat fluxes work on the surface, the shortwave radiation is the only heat flux that gets absorbed in water surface and also penetrates through the water column transporting heat within the lake. A part of the radiation is reflected from the water surface (which is the albedo effect). So the net incoming shortwave radiation that gets absorbed into the water body is,

\[ ISR_{net} = (1 - \alpha)ISR_{raw} \]  \hspace{1cm} (3.26)
where, $\alpha = \text{albedo (usually 10\% for water)}$.

The distribution of incoming solar radiation through the water column is in exponential relation to water depth, following Beer-Lambert law (Ji, 2008):

$$H_S = \text{ISR}_{net} \left[ \left( f_r e^{-\beta_f H(1-Z)} \right) + \left( 1 - f_r \right) e^{-\beta_s H(1-Z)} \right] \quad (3.27)$$

where,

- $H_S = \text{shortwave incoming solar radiation heat flux (W/m}^2\text{)}$;
- $\text{ISR}_{net} = \text{incoming net shortwave solar radiation (W/m}^2\text{)}$;
- $\beta_f = \text{fast scale light attenuation coefficient (1/m)}$;
- $\beta_s = \text{slow scale light attenuation coefficient (1/m)}$;
- $f_r = \text{distribution fraction (0-1)}$;
- $Z = \text{normalized vertical layer}$.

The light attenuation coefficient (also called light extinction coefficient) is the measure for the decrease in light intensity with depth within a water column (Leetmaa, 1977). The larger the light attenuation coefficient, the greater the loss of light intensity with depth. Typical values of a light attenuation coefficient range from less than 0.1 m$^{-1}$ in very clear oligotrophic lakes, to greater than 3 m$^{-1}$ in turbid, deeply colored lakes (Davies-Colley et al., 2003).

**Atmospheric radiation** is characterized by much longer wavelengths than solar radiation (hence called longwave radiation) and is related to variables like atmospheric temperature, cloud cover, etc. During the night and cloudy condition, the atmospheric radiation can be a significant component of heat balance and water temperature calculation. Several formulations are available for incoming longwave radiation (Brunt,
1932; Brutsaert, 1975; Idso and Jackson, 1969), however, the formula by Swinbank (1963) it typically used in modeling studies:

\[
H_L = \varepsilon \sigma \left[ \left( 9.37 \times 10^{-6} (T_a + 273.15)^6 \right) \left( 1 + 0.17C^2 \right) \right]
\]

(3.28)

In EFDC temperature module, a slightly different version of Swinbank (1963) longwave incoming radiation formula is used:

\[
H_L = \varepsilon \sigma \left[ \left( 9.467 \times 10^{-6} (T_a + 273.15)^6 \right) \left( 1 + 0.0017C^2 \right) \right]
\]

(3.29)

where,

- \( H_L \) = longwave incoming solar radiation heat flux (W/m\(^2\));
- \( \varepsilon \) = emissivity (overall atmospheric emissivity considering cloudiness; \( \varepsilon = 0.96 \));
- \( \sigma \) = Stefan-Boltzmann constant = 5.67e\(^{-8}\) W m\(^{-2}\) K\(^{-4}\);
- \( T_a \) = air temperature (°C);
- \( C \) = cloud cover fraction (0 to 1; 0 = clear sky; 1 = overcast sky).

**Longwave back (outgoing) radiation** is the reflected radiation (back to atmosphere) from water surface and is defined by Stefan-Boltzmann law:

\[
H_B = \varepsilon \sigma T_w^4
\]

(3.30)

where,

- \( H_B \) = longwave outgoing solar radiation heat flux (W/m\(^2\));
- \( \varepsilon \) = emissivity (here, \( \varepsilon = 0.97 \) for water);
- \( \sigma \) = Stefan-Boltzmann constant = 5.67e\(^{-8}\) W m\(^{-2}\) K\(^{-4}\);
- \( T_w \) = water temperature (°C).

**Evaporative heat flux** is the loss of heat from water body associated with evaporation, by which water at the water surface is converted from the liquid to the vapor
state. It requires a large amount of energy for this change of state to happen, and so latent heat due to evaporation is the major heat loss for a water body. The average value of the latent heat of water required to evaporate 1 gram of water is 2400 Joule. This large heat flux is supplied directly from heat stored within the water body. Evaporative heat flux is a function of overlying air temperature, water temperature, wind speed and vapor pressure gradient. Various theoretical and empirical formulas have been proposed to estimate the latent evaporative heat flux; the formula based on the Mass Transfer approach (Dingman, 2012) is used in EFDC:

\[ H_E = FW \left[ e_{sw} - e_{aa} \right] \]  \hspace{1cm} (3.31)

where,

\[ H_E \] = latent heat flux (W/m²);

\[ FW \] = factor based on wind speed; calculated as:

\[ FW = 9.2 + 0.46 \left( wsp \right)^2 \]  \hspace{1cm} (3.32)

\[ wsp \] = wind speed at 10 m (m/s),

\[ e_{sw} \] = saturated vapor pressure at water surface (mbar); calculated using following empirical formula in EFDC:

\[ e_{sw} = 10^{\left(0.7859 + 0.03477T_w/(1+0.00412T_a)\right)} \]  \hspace{1cm} (3.33)

\[ e_{aa} \] = actual vapor pressure at overlying air (mbar); calculated using similar empirical formula mentioned above for vapor pressure at water surface, equation (3.33):

\[ e_{sw} = 10^{\left(0.7859 + 0.03477T_w/(1+0.00412T_a)\right)} \times R_h \]  \hspace{1cm} (3.34)

\[ T_w \] = surface water temperature (°C);

\[ T_a \] = air temperature (°C);
It is noted from Equation (3.31) that vapor pressure gradient, \([e_{sw} - e_{aa}]\) (based on air temperature and water temperature) is the primary factor to determine if evaporation or condensation (water changes to liquid from vapor state). Because if saturated vapor pressure of water \((e_{sw})\) > saturated vapor pressure of air \((e_{aa})\), water will be evaporated from water surface to overlying air. But if saturated vapor pressure of water \((e_{sw})\) < saturated vapor pressure of air \((e_{aa})\), vapor will actually condense from overlying air to waterbody and hence adding released heat in the condensation process to water surface instead of losing heat due to evaporation.

**Sensible heat exchange (conduction)** is the heat flux transferred between the water surface and overlying air interface by turbulence activities due to a temperature difference between water and air. The heat exchange occurs only within a very thin layer of air-water boundary and takes place by conduction and convection (Ji, 2008). The heat exchange can be upward (from the water surface to overlying air) or downward (from overlying air to water surface), depending on the air-water temperature difference. The empirical formula for sensible heat flux calculation in EFDC is as follow:

\[
H_C = k_cFW[T_w - T_a]
\]  

(3.35)

where,

- \(H_C\) = sensible heat flux \((\text{W/m}^2)\);
- \(FW\) = factor based on wind speed; calculated as mentioned in equation (3.32)
- \(T_w\) = surface water temperature \((\circ\text{C})\);
- \(T_a\) = air temperature \((\circ\text{C})\);
$k_c = \text{sensible heat transfer factor; calculated as (Ji, 2008): } \quad k_c = C_B \frac{P_{atm}}{P_o} \quad (3.36)$

$C_B = \text{Bowen coefficient (}=0.62 \text{ mbar}/^\circ\text{C}); \quad P_{atm} = \text{atmospheric pressure (mbar)};

P_o = \text{reference atmospheric pressure at sea level (}=1013 \text{ mbar)};

An empirical value, $k_c = 0.47$ is used in EFDC.

This can be noted from equation (3.35) that, sensible heat transfer increases, as the temperature difference between water and air increases and with increasing wind speed. Wind speed is a dominant factor for turbulent transfer across the air-water interface.

When the temperature of discharge is significantly different from the temperature of the receiving water, the discharge can have thermal and ecological impacts on the receiving water. In the thermal modeling of Lake Ontario, inflow from Niagara has higher water temperature than average lake temperature. The heat energy added to a receiving water body can be estimated using (Ji, 2008):

$$H_T = Q_c \rho C_p \Delta T \quad (3.37)$$

where,

$H_T = \text{rate of heat energy exchange (J/s)}$;

$Q_c = \text{discharge rate (m}^3/\text{s)}$; $C_p = \text{specific heat of water};$

$\Delta T = \text{temperature difference between the discharged water and receiving water}.$

This heat flux is considered as advective heat flux, which implies that the heat is transported or advected by the flow of water (Spigel et al., 2003). Equation (3.37) can be used as the external heat source term, $Q_T$ in equation (3.11). In EFDC Lake Ontario modeling, no heat exchange with bed has been considered.
In addition to surface heat fluxes, the heat exchange on the interface of water column-sediment bed can also affect simulated temperatures in the water column. The heat exchange with the sediment bed is generally much smaller compared to surface exchange though it is significant for accurately simulating vertical temperature profiles (Ji, 2008). The formula for sediment bed heat flux is proportional to the temperature difference between the water and the sediment bed:

\[ H_{SB} = -k_b(T_{wc} - T_b) \]  

(3.38)

where,

- \(H_{SB}\) = heat flux between water-sediment bed (W/m\(^2\));
- \(k_b\) = heat exchange coefficient (W/m\(^2\)/°C) =5.0e\(^{-7}\) W/m\(^2\)/°C used in this study;
- \(T_{wc}\) = water column temperature (°C);
- \(T_b\) = sediment bed temperature (°C);

The sediment bed heat exchange varies with seasonal changes in water temperature. In summer it is generally a very small percentage of the total heat flux of the water column. During the winter when the lake is ice-covered, and the water temperature is low, the sediment bed heat flux becomes significant (Ji, 2008).

All the heat fluxes described above within EFDC full heat balance mechanism are depicted in Figure 3.2 as a flowchart including all the meteorological variables, factors, coefficients pertinent to each heat flux component.
Figure 3.2: Full heat flux balance flow chart.
4.1 EFDC Lake Ontario Model

In this study, I performed numerical modeling of temperature profiles in Lake Ontario to demonstrate the spring thermal bar evolution and summer thermal stratification pattern, using the 3D hydrodynamic model - Environmental Fluid Dynamics Code (EFDC). Lake Ontario is modeled on a curvilinear grid with bathymetry interpolated onto the grid forced with hourly meteorological data and river flow data. This section provides a detailed description of the modeling grid, lake bathymetry, flow data and atmospheric forcing parameters. The simulations are carried out on high-performance computing servers in dual six-core AMD Opteron processors at Center for Research Computing (CRC), University of Notre Dame, Indiana. The model's time integration used a second-order accurate two-time level explicit finite difference scheme with an internal/external mode splitting technique. The mode ran with a constant, 2-second time step to satisfy the stability criterion of the Courant-Fredrichs-Lewy condition.

4.1.1 Lake Ontario Bathymetry

Lake Ontario domain is modeled on a structured curvilinear grid at 2-km horizontal resolution. The grid is generated using Delft3D-RGFGGRID software tool, fitting splines in parallel and perpendicular to lake contour lines. The grid is later
imported in EFDC and interpolated with lake bathymetry data from National Oceanic and Atmospheric Administration (NOAA). The bathymetric grids (from NOAA) consist of an array containing the average lake depths in 2-km squares which are consistent with our lake model grid size.

Lake bathymetry is shallow in a nearshore area with a gradient of 1m to 10m towards the inner part of the lake. In northern and western part, lake bathymetry gradually becomes deep from 10 m to ~ 100 m as it progresses towards mid-lake. In southern and eastern part, however, the lake has a steep gradient which changes from 10 m to 150 m within a short distance. In the upper northern-eastern part of the lake (Kingston basin area), the lake bathymetry is usually within 5 m to 30 m. The deepest part of the lake (depth > 200 m) is in the southern-eastern part of the lake.

Figure 4.1: Lake Ontario bathymetry.

Vertical layers are defined to the grid in EFDC through EFDC Explorer (the pre and post processing software for EFDC (Craig, 2005). Lake Ontario is a deep lake (maximum depth 244 m and mean depth 86 m); hence setting increased number of
vertical layers would help to capture vertical profile more accurately. However, finer resolution grid with a higher number of vertical layers is also computationally intensive. So I set 20 vertical layers to optimize both accuracy and intensity of computation.

Vertical layers are in bathymetry following sigma coordinate which means that every local depth will have 20 layers even in the shallow nearshore area. 20 equal bathymetry following vertical layers represents, each local depth (shallow or deep) will have 20 equally thick vertical layers; if local depth is 20 m it is divided into 1m thick 20 layers; if local depth is 100 m, it is divided into 5 m thick 20 layers. The model was initially set with 20 equally thick vertical layers; later the vertical grid was revised as 20 layers of gradually increasing thickness from top to bottom. The updated vertical grid was necessary for better capturing of the summer stratification pattern. Figures 4.2 shows the horizontal and vertical grid used in Lake Ontario EFDC model.
Figure 4.2: Lake Ontario (a) horizontal grid (b) vertical grid (East-West sectional profile).
4.1.2 Atmospheric Forcing Data

Lake Ontario EFDC model is forced with hourly meteorological data from weather stations surrounding Lake Ontario. Modeling of large lake systems requires high-quality data with sufficient temporal and spatial resolutions (Huang et al. 2010). Five buoys in Lake Ontario record weather data, but they are removed in winter when the lake gets snow-covered. Hence, hourly atmospheric data are used from land stations at Buffalo, Rochester, Oswego, Watertown, Hamilton, Toronto, and Kingston comprising: (1) wind speed and direction, (2) air temperature, (3) air pressure, (4) relative humidity, (5) shortwave solar radiation, (6) cloud cover, and (7) precipitation. Evaporation and condensation are internally computed in EFDC from these data. The data sources are:

- National Climate Data Center (NCDC),
- National Solar Radiation Database (NSRDB),
- National Weather Service (NWS),
- Iowa Environmental Mesonet (IEM) Weather Service,
- Environment Canada,
- National Climate Data & Information Archive (NCD Canada),
- Great Lakes Observing system (GLOS).

All meteorological data except evaporation were obtained from the seven weather stations mentioned above and were interpolated over the lake using inverse-distance weighing method (power 1) using the formula as below:

\[
\hat{v} = \frac{\sum_{i=1}^{n} \frac{1}{d_i^{p}} v_i}{\sum_{i=1}^{n} \frac{1}{d_i^{p}}}
\]  

(4.1)
where,

\[ \hat{\theta} = \text{value to be estimated}; \]

\[ v_l = \text{known value}; \]

\[ d_{p_l} \ldots d_{p_n} = \text{distances from the } n \text{ data points to the estimated point (with power of } p = 1,2,3). \]

In Figure 4.3 below the locations of the weather stations around Lake Ontario are shown. The atmospheric weighing factor mapping over the lake domain based on an inverse distance weighing method for each station is shown as well in Figure 4.3.
Figure 4.3: Seven weather stations around Lake Ontario and the mapping of weighing factors over the lake domain from each station.
Functional importance of each atmospheric forcing parameter on lake thermal process is described below:

**Wind speed** is a major forcing parameter in lake modeling. Wind adds kinetic energy to the lake and reorganizes the potential energy. Wind exerts a drag on the water surface which is conducive in flow circulation, generating turbulence, creating local upwelling/dowelling effect. Wind stress is defined as the tangential force per unit area due to the horizontal movement of the wind over the water surface (Ji, 2008):

\[
\tau = C_D \rho_a U^2
\]  
(4.2)

where, \( \tau \) = wind stress (N/m²);
\( U \) = wind speed at 10m above water surface (m/s);
\( C_D \) = drag coefficient (increases with wind speed); \( \rho_a \) = air density (kg/m³).

Near the lake, surface wind is responsible for surface waves and surface currents. Strong winds (above about 3 m/s) also induce Langmuir circulations, large-scale counter-rotating helical vortices. Langmuir circulation is largely responsible for mixing of the surface layer and deepening of the epilimnion. The wind-induced basin-scale currents at the water surface are responsible for horizontal mixing and result in a basin-scale circulation, as the bottom water must flow upwind to satisfy mass conservation. When the wind stops, basin-scale internal waves, called seiches, and other internal waves develop which also result in boundary currents and boundary mixing.

As spring heating proceeds, wind forcing plays a role in mixing of water throughout the lake and continues until the lake is fully stratified in summer. Both sensible and latent heat fluxes rely on wind and turbulence in the air to transfer heat flux.
and water vapor from the lake surface to overlying atmosphere (and vice versa). Wind thus plays a crucial role in mixing heat downward in the water column.

Figure 4.4: Hourly wind speed with directional components (U-wind and V-wind) for the year 2011 (interpolated and spatially averaged over the lake domain).

Wind direction is important as wind speed vary with variation of time scales (hourly, daily, seasonal) including diurnal variations (sea-land breeze), and the seasonal change in prevailing directional wind profile. The diurnal variation is important for lake heat flux since during daytime, cool sea breeze flow towards warm land and at night the direction reverses. Seasonal wind profile can generate persistent circulation patterns in a water system. The south shore of Lake Ontario to the right of the prevailing southwesterly winds in summer is considered warm shore. The north shore of the lake is
colder due to frequent upwelling by wind effect (Beletsky et al., 1999; Hall, 2008).

Figure 4.4 shows the hourly wind speed data (with directional U and V component) interpolated and spatially averaged over the lake domain.

Air temperature is a dominant factor in surface water temperature simulation since both evaporation (or condensation) and conduction processes rely on the temperature difference between the air-water interface (formula described in Section 3.3). Hence air temperature plays a key role in the computation of surface heat flux (sensible and latent heat flux) and also moisture exchange through evaporation (or conduction) process. In addition to diurnal changes, the air temperature has strong seasonal variations, especially over Lake Ontario. Since Lake Ontario is in higher latitude, it is greatly affected by atmospheric (overlying air) temperature: lake surface frozen in winter, ice melts way in spring and water get heated as overlying air temperature get warm as well. Figure 4.5 shows a historical seasonal correlation between air temperature and water temperature over Lake Ontario.
Air pressure (or atmospheric pressure) plays a role in the computation of both latent and sensible heat flux. Relative humidity is important for actual vapor pressure computation for overlying air, hence in turn affects evaporation process. Figure 4.6 shows the hourly air pressure, air temperature, and relative humidity data, interpolated and spatially averaged over the lake domain.
Cloud cover plays an important role for computation of incoming longwave radiation heat flux, (another heat source for the lake). It is expressed as percentage relating to the cloudiness of atmosphere (with clear sky = 0 and overcast = 1). Figure 4.7 shows the hourly solar radiation and cloud cover data, interpolated and spatially averaged over the lake domain.

Solar radiation (shortwave incoming) is considered most important heat flux component that acts as a heat source to a water body. Unlike the other heat flux components (longwave radiation, latent and sensible), which all occur only at the water
surface, incoming shortwave solar radiation is penetrative, distributing heat content through the water column.

Solar radiation has diurnal variations; peaks at noon (for water body peak lags a time delay compared to land) and diminishes as night sets in. As expected it also has a seasonal variation, immensely effective for Lake Ontario being in a temperate latitude. In a water body, distribution of solar radiation is affected by some certain coefficients named solar radiation attenuation coefficient (also called light attenuation coefficient). Figure 4.7 shows the hourly solar radiation and cloud cover data, interpolated and spatially averaged over the lake domain.

**Solar radiation attenuation coefficients** can be expressed quantitatively as the rate which light energy is depleted as it descends through the water column (Lee and
Rast, 1997). The light intensity at any given depth in a water body is computed by (Lee and Rast, 1997):

\[ I_z = I_o e^{-k_d z} \]  \hspace{1cm} (4.3)

where,

- \( I_z \) = light intensity (%) at depth \( z \); \( I_o \) = light intensity (100%) at surface;
- \( k_d \) = light (solar radiation) attenuation coefficient.

The EFDC model requires a user-specified value for the attenuation coefficient \((k_d)\), for downwelling irradiance in the water column. The decreasing light intensity with depth is a function of the concentration of light scattering and light absorbing constituents (Turbidity, Color, Suspended Solids [TSS] and Dissolved Matter [TDM], Chlorophyll-a etc.) in the water column. Light attenuation coefficient plays an important role in determining the depth of thermocline and the strength of temperature stratification in lakes. Lakes with higher values of light attenuation coefficient trap solar radiation at shallower depths, leading to warmer surface layers and cooler water at depth. In clear lakes, with smaller values of light attenuation coefficient, solar radiation penetrates to deeper depths, thereby spreading the solar heat over greater volumes of water, leading to deeper thermocline (Spigel et al., 2003). Lake Ontario is a mesotrophic lake (intermediate productivity level), hence EPA recommended value for light attenuation coefficient for Lake Ontario is 0.15-1.2 m\(^{-1}\) (Horne and Goldman, 1994). For this study however, I computed specific solar radiation attenuation coefficient for Lake Ontario, based on Turbidity, Color, Suspended Solids (TSS) and Chlorophyll-a (Armengol et al., 2003; Lee and Rast, 1997).
Precipitation is the input of freshwater to a water body. It is associated with lake water level. For a large lake like Lake Ontario, volumetric precipitation is an important factor in lake water balance. Change in lake heat flux gets influenced by stored/added/withdrawn volume of water in a water body. The impact of rain drops influence lake kinetic energy as well; as cold rain water falls on a warm lake surface, density currents can be induced, creating changes in kinetic and potential energy. Figure 4.8 below shows the hourly precipitation rate, spatially averaged over the lake domain.

![Hourly precipitation data for the year 2011](image)

**Figure 4.8: Hourly precipitation data for the year 2011 (interpolated and spatially averaged over the lake domain).**

Evaporation (rate of vaporization of water from the lake) is internally computed within EFDC since observed pan evaporation rate is very rare data source. In EFDC, the evaporation rate is computed using the Mass Transfer approach. The algorithm is as follow:

\[
E = k_e \frac{\text{wsp} \left[ e_{sw} - e_{atm} \right]}{P_{atm}}
\]  

(4.4)

where,

- \(E\) = rate of evaporation (m/s; multiply with 24*3600 for units in m/day);
- \(k_e\) = coefficient of evaporation;
\text{wsp} = \text{wind speed at 10 m (m/s)}; \\
e_{sw} = \text{saturated vapor pressure at water surface (mbar); calculated using following empirical formula in EFDC (same as equation 3.33):}
\[
e_{sw} = 10^{\left[ (0.7859 + 0.03477T_w)/(1 + 0.00412T_w) \right]}
\]
(4.5)
\[e_{aa} = \text{actual vapor pressure at overlying air (mbar); calculated using similar empirical formula mentioned above for vapor pressure at water surface, (same as equation 3.34):}
\[
e_{aa} = 10^{\left[ (0.7859 + 0.03477T_a)/(1 + 0.00412T_a) \right]} \times R_h
\]
(4.6)
\[T_w = \text{surface water temperature (°C)}; \]
\[T_a = \text{air temperature (°C)}; \]
\[R_h = \text{relative humidity (%).} \]

As mentioned in Section 3.3 for evaporation vapor pressure gradient, \(e_{sw} - e_{aa}\) (based on air temperature and water temperature) is the primary factor to determine if evaporation or condensation (water changes to liquid from vapor state). Because if saturated vapor pressure of water \(e_{sw}\) > saturated vapor pressure of air \(e_{aa}\), water will be evaporated from water surface to overlying air. But if saturated vapor pressure of water \(e_{sw}\) < saturated vapor pressure of air \(e_{aa}\), vapor will actually condense from overlying air to waterbody. In large lakes located in higher latitude like Lake Ontario with onset of summer, air temperature \(T_a\) increases fast compared to lake surface temperature \(T_w\). Hence, when overlying air temperature \(T_a \gg\) surface water temperature \(T_w\); saturated vapor pressure of water \(e_{sw}\) becomes less than saturated vapor pressure of air \(e_{aa}\), and so water vapor get condensed from overlying air. The value of \(k_e\) is affected by atmospheric stability condition (stable/neutral/unstable). In
Chapter 5 evaporation process will be further discussed, as EFDC computed evaporation rate was producing anomalous result and so the evaporation algorithm has been updated. All heat flux computation involving the forcing parameters mentioned above is discussed in the previous chapter, Section 3.3.

4.1.3 Flow Data

Lake Ontario flow boundary includes inflow from Niagara River at the south-western zone of the lake and outflow into St. Lawrence River at the upper north-eastern zone of the lake. Both flow boundaries are forced with hourly flow rate (m$^3$/s) from respective rivers. Flow rate for Niagara River (2011) is obtained from US Army Corps of Engineers, Buffalo District, New York. Flow rate for St. Lawrence River (2011) is obtained from New York Power Authority, New York, (Figure 4.9).

EFDC model uses inflow temperature for Niagara River as input to account for the advective heat flux (due to temperature difference between inflow and lake, discussed in Section 3.3). The term implies that the heat is transported or advected by the flow of water (Spigel et al., 2003). The hourly water temperature data for Niagara River is obtained from NOAA-National Data Buoy Center (NDBC), (Figure 4.9).
4.1.4 Input Data Formatting and Cleaning Up

The quality of the simulations depends on the accuracy of the meteorological data and on how well they represent conditions above the water surface of the lake. This section describes the necessary adjustments were made to input data to assemble a good meteorological dataset before modeling could begin.

1. Formatting diverse data: Input meteorological data exist in different file formats. So formatting data to required input format for EFDC was necessary. Unit conversion for variables was done where required.

2. Averaging multiple records for a single hour: Data was always not available in hourly time-step. Sometimes data was recorded in every 10, 15 or 30 minutes; automation program was used to average all records for a single hour and to make a new output dataset.

3. There are missing data in the dataset:
a. If data is missing for a single hour: There were some datasets where every 24th-hour data was missing. So an automated program was developed to average 23rd and next 1st hour data and put the averaged value for 24th hour. A similar approach was used when data is missing for less than 5 hours; (averaging previous and next hourly recorded data to fill data gaps).

b. If data is missing for a large period: Sometimes data were missing for a longer period (~10, 20, 30 hours of data went missing or not recorded). Therefore I needed a second source of the dataset for the same location (data sources mentioned in Section 4.1.2 and 4.1.3). Block of missing data was compared to the second set of data and the missing hours was replaced.

4. Finally, all meteorological variables were plotted against time-step to check for any anomalous/outlier value in the data. Following considerations were made for cleaning up anomalous/outlier data:

a. There should be no zero value or extremely low value for atmospheric pressure (usually ranges within 900-1100 mbar for Lake Ontario region).

b. Air temperature is low in winter/spring months, gets high in summer months. So there cannot be any zero value in summer months. The assessment was made to negative air temperature on spring months (April-May), especially after high positive temperatures. However, in the region of Lake Ontario sometimes a sudden sharp drop in temperature is observed in late April through mid-May.

c. Wind direction ranges within 0 to 360 degree (any other value is anomalous).

d. Relative humidity (%) cannot be zero and cannot be more than 100.

e. Solar radiation has a diurnal variation (high at noon, zero at night).

f. Cloud cover is often mentioned as a visibility condition; was converted to numerical value following guidelines by NOAA.
CHAPTER 5:
EFDC MODEL IMPROVEMENT FOR REPLICATING LAKE’S MIXED PHASE AND THERMAL BAR FORMATION

5.1 Overview

The scope of this research project is to demonstrate the spring thermal bar evolution and summer thermal stratification in Lake Ontario. The thermal bar formation begins in spring (late April to mid-May) and disappears (late June to early July) as the lake starts to get stratified in summer. Hence, the simulation period was initially set from early April to late July 2011. To capture the hydrothermal behaviors of Lake Ontario during spring to summer transition period, the model needed improvements to simulate lake temperatures as close as possible to those of observed in nature. EFDC Lake Ontario model is updated with evaporation algorithm (Quinn, 1979; Croley, 1989) to ensure accurate simulation of evaporation rates and latent heat fluxes and the model was calibrated for appropriate solar radiation attenuation coefficients and horizontal mixing coefficients. In this section, the necessary improvements made to the model are discussed, with the demonstration of (1) simulated temperature profiles during lake's mixed (homogeneous temperature) phase and (2) thermal bar formation.

5.2 Initial Condition

SNL-EFDC does not include a rigorous ice model although one is available in the proprietary version. Hence, simulations commenced once the lake was ice free. The
weekly total ice coverage (percentage) over Lake Ontario for the winter of 2010-2011 (from Environment Canada) indicated that the lake was ice free by early April 2011 as shown in Figure 5.1.

I then analyzed the lake surface temperature during late March to early April (2011) using AVHRR (Advanced Very High-Resolution Radiometer) satellite imagery (obtained from NOAA Great Lakes Environmental Research Laboratory, NOAA-GLERL). Daily, cloud-free average surface water temperatures (per pixel) available in ASCII format from the Great Lakes Surface Environmental Analysis (GLSEA) surface water temperature composite chart. The lake surface temperatures are derived from NOAA polar-orbiting satellite imagery obtained through the Great Lakes CoastWatch program. The surface temperature data (on a daily basis), is composited from valid available AVHRR SST satellite data from both daytime and nighttime orbits. Currently, NOAA CoastWatch program is using the non-linear split-window equation for daytime imagery and the linear triple-window equation for nighttime imagery.

It is observed from the satellite imagery that lake surface temperature is around ~2°C on 25th March when ice-coverage is almost disappeared and increases to ~3°C when ice-coverage is entirely gone by the beginning of April, (Figure 5.2).
Figure 5.1: Weekly (November 2010 - April 2011) total ice-coverage (%) for Lake Ontario (Environment Canada).

Figure 5.2: Daily surface temperature (SST %) based on NOAA satellite imagery for Lake Ontario, 2011.
To ensure that model is enforced with a realistic initial temperature throughout the lake, I analyzed the transect temperature profiles, (obtained from NOAA Great Lakes Environmental Research Laboratory, NOAA-GLERL) as well from 25th March to 8th April 2011 (Figure 5.3).

Based on the above analysis I decided to start the model on 4th April 2011 with corresponding initial temperature 3°C, throughout the lake. The hydrodynamic model was run from January 1\textsuperscript{st} and flows were recorded in a restart file on April 4\textsuperscript{th}. This file contains the initial flow conditions for the full thermo-hydrodynamic simulation beginning at midnight on April 4\textsuperscript{th}, 2011.

Figure 5.3 below shows the transect temperature profile from NOAA-GLERL Great Lakes Coastal Forecasting System (GLCFS) Nowcast model, for 4th April 2011.

![Figure 5.3: Temperature transect profile from NOAA-GLERL Great Lakes Coastal Forecasting System (GLCFS) Nowcast model, for 4th April 2011.](image)
5.3 Updated Evaporation Rate and Latent Heat Flux Estimates

Using the existing EFDC heat algorithm, an anomalous increase in simulated surface temperatures was observed starting in mid-May, 2011 as shown in Figure 5.4a. Heat flux components (longwave incoming and outgoing, sensible and latent heat fluxes) and meteorological data (air temperature, shortwave solar radiation, wind speed, precipitation, and evaporation) were individually extracted from the model to identify the source of the elevated simulated temperatures. Comparing the simulated evaporation rates to those from the NOAA Great Lakes Evaporation Model revealed that spurious condensation caused the temperature discrepancies as shown in Figure 5.4b. The Great Lakes do experience condensation, notably in summer months when overlying air temperatures are significantly higher than surface water temperatures, but continuous condensation is not observed. Anomalous evaporation/condensation affects the lake mass and heat balance:

- Lake mass balance and water level are affected by anomalous evaporation rate/persistent condensation process.

- Latent heat flux due to continuous condensation process adds up released heat (instead of losing heat) into net surface heat flux, leading to higher surface temperature increase.
Of the various evaporation algorithms investigated (Croley, 1989; Derecki, 1976; Harbeck, 1954; Phillips, 1978; Quinn, 1979), the bulk aerodynamic approach of Quinn (1979) with the wind speed factor empirical formula of Croley (1989) yielded the best agreement between the simulation and the NOAA Great Lakes Evaporation Model. Because no observed evaporation data are available for Lake Ontario, computed evaporation rates using the Quinn (1979) and Croley (1989) algorithms were verified against observed evaporation rates at Long Point on Lake Erie for May 2012- November 2013. Long Point on Lake Erie is the nearest location to Lake Ontario where evaporation data are available from Environment Canada. Evaporation rates at Long Point were computed using over-land meteorological data using a calibrated bulk evaporation
coefficient of $8 \times 10^{-4}$. As shown in Figure 5.5 evaporation rates computed from the algorithms of Quinn (1979) and Croley (1989) fit the observed data much better than the rates computed by the original EFDC algorithm.

![Simulated evaporation rates compared to observed data at Long Point in Lake Erie (2012–2013).](image)

**Figure 5.5:** Simulated evaporation rates (with original and updated algorithms) compared to those observed at Long Point in Lake Erie (2012–2013).

In the approach by Quinn (1979) evaporation from the water surface is related to the difference between specific humidity near the water surface and the overlying air as:

$$E = \left( \frac{\rho_a}{\rho_w} \right) C_e w_{sp} (q_{sw} - q_{as})$$  \hspace{1cm} (5.1)

where $E$ (m/s) is the evaporation rate, $\rho_a$ (kg/m$^3$) is the air density, $\rho_w$ (kg/m$^3$) is the water density, $C_e$ is the bulk evaporation coefficient, $w_{sp}$ (m/s) is the wind speed 10 m above the lake, $q_{sw}$ is the specific humidity of water based on the saturation vapor
pressure at the water surface, and \( q_{sw} \) is the specific humidity of air based on the vapor pressure of the overlying air:

\[
q_{sw} = \frac{0.622 e_{sw}}{P_{atm} - 0.378 e_{sw}}
\] (5.2)

\[
q_{aa} = \frac{0.622 e_{aa}}{P_{atm} - 0.378 e_{aa}}
\] (5.3)

where \( e_{sw} \) (mbar) is the saturated vapor pressure at the water surface temperature, \( T_w \) (°C); \( e_{aa} \) (mbar) is the actual vapor pressure at the overlying air temperature, \( T_a \) (°C); and \( P_{atm} \) (mbar) is the atmospheric pressure. This bulk aerodynamic approach accounts for atmospheric stability through the iteratively computed evaporation coefficient, \( C_e \), as a function of non-dimensional wind speed, potential temperature gradients, and the Monin-Obukhov length (Stull, 1988). For this study, however, I used the calibrated value (calibrated for Long Point, Lake Erie) of bulk evaporation coefficient, \( C_e \) \((8 \times 10^{-4})\).

Saturated vapor pressure at water surface, \( e_{sw} \) (mbar) and actual vapor pressure at overlying air, \( e_{aa} \) (mbar) are calculated using same empirical formula mentioned before (equation 3.33-3.34 and equation 4.5-4.6):

\[
e_{sw} = 10^{[(0.7859+0.03477T_w)/(1+0.004127T_w)]}
\] (5.4)

\[
e_{aa} = 10^{[(0.7859+0.03477T_a)/(1+0.004127T_a)]} \times R_h
\] (5.5)

where, \( R_h = \) relative humidity (%).

Croley (1989) suggested an adjustment to the wind speed in Quinn’s (1979) algorithm to implement an over-land to over-lake bias correction for the Great Lakes. Phillips and Irbe (1978) used over 7,000 observations from Lake Ontario in 1972 to come up with a regression equation for an adjusted wind speed factor:

\[
F_{wup} = 1.607 + 0.92 w_{wp} - 0.28 (T_a - T_w)
\] (5.6)
The preceding equation includes the effects of temperature differences between the overlying air and water surface along with wind speed. This adjusted wind speed factor influences the evaporation (condensation) rate better because the evaporation rate is not only linearly related to the wind speed but also to the temperature difference at the air-water interface.

Combining Croley’s (1989) adjustment of wind speed with Quinn’s (1979) algorithm yields updated equations for the evaporation rate and latent heat flux:

\[
E = \left( \frac{\rho_a}{\rho_w} \right) C_e F_{wp} \left( q_{sw} - q_{aa} \right) \\
H_E = \rho_w E\lambda_v
\]

where \( H_E \) (MW/m\(^2\)) is the latent heat flux and \( \lambda_v \) (MJ/kg) is the latent heat of vaporization:

\[
\lambda_v = 2.50 - 2.36 \times 10^{-3} T_w
\]

The original evaporation algorithm in EFDC is based on a mass transfer approach with governing equations:

\[
E = C_{wsp} \left( e_{sw} - e_{aa} \right) \\
H_E = F_{wefdc} \left( e_{sw} - e_{aa} \right) \\
F_{wefdc} = 9.2 + 0.46 w_{sp}^2
\]

Both the original EFDC evaporation algorithm and the evaporation algorithm by Quinn (1979) and Croley (1989) are fundamentally based on mass transfer approach. However, an over-water adjustment for wind speed was developed in the latter, (5.4), which considers the difference between the overlying air and water temperatures. This
approach improves the accuracy of estimated evaporation (condensation) processes. Using $F_{W_{up}}$ also improves estimates of sensible heat flux. In the original EFDC algorithm, $F_{W_{efdc}}$ is quadratically related to the wind speed in (5.10), resulting in an overestimation of evaporation (or condensation). The latent heat flux computation in the original EFDC algorithm does not explicitly consider $\lambda_v$ in (5.9), which is necessary for accurate simulation of latent heat fluxes. Hence, in the original EFDC algorithm, rates of evaporation and evaporative heat flux are computed separately in two different subroutines and values do not correspond. Figure 5.6 compares the evaporation rates in Lake Ontario, calculated using the original and updated EFDC formulations to the evaporation rates obtained from the NOAA Great Lakes Evaporation Model. This updated algorithm outperformed the original EFDC formulation and improved surface temperature simulations.

The updated evaporation algorithm regulated the rate of evaporation and condensation process as it is happening in real Lake Ontario environment in summer months. Hence, this updated corrected net heat flux balance over the lake surface and simulated surface water temperature.
Figure 5.6: Simulated evaporation rates (with original and updated algorithms) compared to those from NOAA (April–July 2011) in Lake Ontario.

Figure 5.7 below show the impact of updating evaporation algorithm on surface temperature compared with GLOS observed data, for nearshore, shallow WG location and offshore, deep 20NMB location. The surface temperatures from the original evaporation algorithm were notably higher than those observed during mid-May to mid-June, notably at the nearshore WG and the offshore 20NMB buoy. The updated evaporation algorithm yielded surface temperatures much closer to the observed data; RMSEs improved significantly for nearshore buoys: from 2.46 to 1.11°C for WG and from 2.60 to 2.01°C for 20NMB.
5.4 Sensitivity Analysis of the Solar Radiation Attenuation Coefficients

In a water body, the distribution of solar radiation through the water column is described as an exponential function of water depth according to the Beer-Lambert law (Ji, 2008):

\[
H_s = ISR_{\text{net}} \left[ f_r \exp^{-\beta_f H(1-z)} + (1 - f_r) \exp^{-\beta_S H(1-z)} \right]
\]  

(5.13)

where \( H_s \) (W/m\(^2\)) is the shortwave incoming solar radiation heat flux, \( ISR_{\text{net}} \) (W/m\(^2\)) is the incoming net shortwave solar radiation heat flux, \( \beta_f \) (1/m) is the fast-scale light attenuation coefficient, \( \beta_S \) (1/m) is the slow-scale light attenuation coefficient, \( f_r \) is the

Figure 5.7: Improved surface temperature with updated evaporation algorithm, compared with GLOS observed data (April-July 2011) for (a) WG, nearshore shallow location and (b) 20NMB, offshore deep location.
fast-to-slow distribution fraction between 0 and 1, $H$ (m) is the water depth, and $Z$ is the normalized vertical sigma layer depth.

Solar radiation attenuation coefficients describe the light energy depletion rate through the water column (Lee and Rast, 1997) that play an important role in determining the depth of the thermocline and the degree of temperature stratification. EFDC requires user-specified values for the attenuation coefficients to estimate downwelling irradiance in the water column. For this study, the solar radiation attenuation coefficients for Lake Ontario were based only on TSS (mg/m$^3$) and chlorophyll-$a$ ($\mu$g/l) concentrations (Armengol et al., 2003; Gallegos and Moore, 2000). The solar radiation attenuation coefficient based on TSS is (Armengol et al., 2003):

$$\beta = 6.45 \times 10^{-5} TSS + 0.4806$$

(5.14)

while the combination of TSS and chlorophyll-$a$ concentrations yields (Gallegos and Moore, 2000):

$$\beta = 0.32 + 0.016 Chl - a + 0.094 TSS$$

(5.15)

Table 5.1 lists estimated concentrations of TSS and chlorophyll-$a$ for Lake Ontario and the corresponding solar radiation coefficients. The estimated solar radiation attenuation coefficients range from 0.4 to 1.45/m, and vary both spatially (nearshore/offshore) and periodically (annual/seasonal). The higher the radiation attenuation coefficient, the less radiation is absorbed deeper in the water column – more is absorbed near the surface. USEPA (Horne and Goldman, 1994) recommended range for radiation attenuation coefficients is 0.15 m$^{-1}$ to 1.2 m$^{-1}$, since Lake Ontario is a mesotrophic (medium productivity) lake. Constrained by the range of solar radiation
attenuation coefficients (Table 5.1), the values for this study were calibrated to yield best matches to observed temperatures.

Malkin et al. (2010) analyzed the solar radiation attenuation coefficients for Lake Ontario based on Secchi depths from 1995 to 2008. Their study showed that the summer solar radiation attenuation coefficient values were higher than the spring values. Therefore, another sensitivity analysis was performed with a temporally varying $\beta_f$. I set $\beta_f = 0.3/m$ for spring (April-May) and $\beta_f = 0.5/m$ for summer (June-July).

Figure 5.8 compares simulated vertical temperature profiles in a shallow region of the lake to those of Environment Canada. The RMSEs were less than 0.5°C in the mixed phase (April 25th to May 10th) for all combinations of solar radiation attenuation coefficients. As the lake became stratified in the nearshore later in May (after May 10th), RMSEs increased. The temporally varying fast-scale attenuation coefficients, $\beta_f = 0.3/m$ (spring, April-May), $\beta_f = 0.5/m$ (summer, June-July), and temporally non-varying fast-scale attenuation coefficient, $\beta_f = 0.5/m$ both yielded the similarly low RMSEs (< 0.5°C) during the lake mixed phase. However, temporally varying $\beta_f$ were selected for production runs to be consistent with the fact that summer attenuation coefficient values are typically higher than those in the spring (Malkin et al., 2010).
TABLE 5.1
SOLAR RADIATION ATTENUATION COEFFICIENTS FOR LAKE ONTARIO
COMPUTED BASED ON TSS AND CHLOROPHYLL CONCENTRATIONS

<table>
<thead>
<tr>
<th>Time period and location</th>
<th>TSS (mg/l)</th>
<th>Chlorophyll-(a) ((\mu g/l))</th>
<th>Computed (\beta) (m(^{-1})), (TSS only)</th>
<th>Computed (\beta) (m(^{-1})), (TSS and Chl-(a))</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lake spatial average in summer, 2011</td>
<td>2.2</td>
<td>1.75</td>
<td>0.62</td>
<td>0.55</td>
<td>Limnotech (2011); Yurista et al. (2012)</td>
</tr>
<tr>
<td>Nearshore annual (2002-2010) mean (from tributaries)</td>
<td>11.62</td>
<td>1.75 (lake spatial average)</td>
<td>1.23</td>
<td>1.44</td>
<td>Coleates and Hale (2008); Yurista et al. (2012); Zevin et al. (2011)</td>
</tr>
<tr>
<td>Nearshore annual (2003-2009) mean (30m depth)</td>
<td>0.7</td>
<td>2.1</td>
<td>0.52</td>
<td>0.42</td>
<td>Makarewicz et al. (2012)</td>
</tr>
<tr>
<td>Offshore annual (2003-2009) mean (100m depth)</td>
<td>0.8</td>
<td>2.7</td>
<td>0.53</td>
<td>0.44</td>
<td>Makarewicz et al. (2012)</td>
</tr>
</tbody>
</table>
5.5 PEST Calibration

After early manual calibration efforts, the automated Parameter ESTimation software, PEST (Doherty, 2009, 2010), was applied to the Lake Ontario model. The software is based on a robust implementation of Gauss-Marquardt-Levenberg algorithm and adjusts the model parameters by weighted least squares and yields parameter uncertainty and sensitivity information during estimation (Doherty, 2009).

Observed temperature data are supplied to PEST, and adjustable parameters are iteratively updated to yield the closest match to these data (minimized weighted squared residuals between simulated and observed temperatures). The parameter range that PEST
was constrained to interrogate, the initial values, and calibrated parameters are listed in Table 5.2. Unit weight was applied to each observation.

**TABLE 5.2**

PEST CALIBRATION PARAMETERS FOR THE EFDC LAKE ONTARIO MODEL

(MIXED PHASE)

<table>
<thead>
<tr>
<th>Parameter type</th>
<th>Parameter name</th>
<th>Range</th>
<th>Initial value</th>
<th>Calibrated value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solar radiation attenuation coefficients</td>
<td>Fast-scale coefficient, $\beta_f$</td>
<td>0.2–1.3 m(^{-1})</td>
<td>0.5 m(^{-1})</td>
<td>0.53 m(^{-1})</td>
</tr>
<tr>
<td></td>
<td>Slow-scale coefficient, $\beta_s$</td>
<td>0.1–0.5 m(^{-1})</td>
<td>0.15 m(^{-1})</td>
<td>0.14 m(^{-1})</td>
</tr>
<tr>
<td></td>
<td>Distribution factor, $f_r$</td>
<td>0.3–1.0</td>
<td>0.5</td>
<td>0.7</td>
</tr>
<tr>
<td>Vertical mixing parameters</td>
<td>Vertical eddy viscosity</td>
<td>$10^{-4}$–0.1 m(^2)/s</td>
<td>$10^{-2}$ m(^2)/s</td>
<td>$8.35 \times 10^{-3}$ m(^2)/s</td>
</tr>
<tr>
<td></td>
<td>Vertical diffusivity</td>
<td>$10^{-8}$–0.01 m(^2)/s</td>
<td>$10^{-6}$ m(^2)/s</td>
<td>$1.05 \times 10^{-6}$ m(^2)/s</td>
</tr>
<tr>
<td>Horizontal mixing parameters</td>
<td>Background horizontal eddy viscosity</td>
<td>0–0.25 m/s</td>
<td>0.25 m/s</td>
<td>0.1 m/s</td>
</tr>
<tr>
<td></td>
<td>Dimensionless momentum diffusivity</td>
<td>0.1–5.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Solar radiation attenuation coefficients were calibrated through PEST to appropriately reflect the absorption of incoming radiation through the water column. The PEST-calibrated values were similar to manually calibrated values (Table 5.2). In
addition, horizontal and vertical mixing coefficients were calibrated. These coefficients were interrogated from a range of 0 to 0.25 m$^2$/s for the background horizontal eddy viscosity (Smagorinsky coefficient) and from 0.1 to 5 for the dimensionless horizontal momentum diffusivity. The simulated temperature profiles were least sensitive to the horizontal mixing coefficients; therefore, they were fixed at a horizontal eddy viscosity of 0.1 m$^2$/s and a dimensionless horizontal momentum diffusivity of 1. Calibration of vertical mixing coefficients spanned ranges of $10^{-4}$–0.1 m$^2$/s for vertical eddy viscosity and $10^{-8}$–0.01 m$^2$/s for vertical diffusivity. Best results were achieved when vertical eddy viscosity was $8.35 \times 10^{-3}$ m$^2$/s, and vertical diffusivity was $1.05 \times 10^{-6}$ m$^2$/s.

The most sensitive parameters are, not surprisingly, the solar radiation attenuation coefficients because these directly affect the temperature profiles. Next most sensitive are the vertical mixing parameters, which is intuitive given the importance of their role in establishing or diminishing vertical temperature gradients. Temperature profiles were least sensitive to horizontal mixing parameters. In future efforts to refine this calibration, the focus will be on establishing improved vertical mixing parameters through the implementation of a new vertical mixing algorithm in EFDC.

5.6 Simulated Temperature Profiles for Lake Ontario

Simulated temperatures were compared against (1) observed surface time-series temperatures from three buoys that were part of the Great Lakes Observation System (GLOS), (2) observed vertical temperature profiles from two buoys monitored by Environment Canada, and (3) lake-wide surface temperatures from remotely sensed AVHRR images from NOAA similar to the approach used by de Alwis (1999). Monitoring buoy locations are shown in Figure 5.9. Surface temperatures were compared
at nearshore locations West Grimsby (WG, 25 m deep) and Prince Edward Point (PEP, 74 m deep) and offshore location 20NM Buoy (20NMB, 140 m deep). Vertical temperature profiles were compared at a nearshore location, Shallow Point (SP, 19 m deep), and an offshore location, Deep Point (DP, 177 m deep).

![Diagram showing locations of temperature observations in Lake Ontario](image)

**Observed Surface Temperature Location (Great Lakes Observing System, GLOS):**
- WG (West Grimsby, 25m deep)
- PEP (Prince Edward Point, 74m deep)
- 20NMB (20 NM Buoy, 140m deep)

**Observed Vertical Temperature Location (Environment Canada):**
- SP (Shallow Point, 19m deep)
- DP (Deep Point, 177m deep)

**Figure 5.9:** Locations for observed temperature profiles in Lake Ontario.

After all of the adjustments to the EFDC model, the simulated surface temperature profiles were compared to observed surface temperature profiles from April to July 2011 in Figure 5.10. At nearshore location WG, the RMSE was 1.2°C indicating well-matched temperature profiles. At nearshore location PEP, RMSE was 1.88°C, and at offshore location 20NMB, RMSE was 1.93°C. Historically, RMSEs below 2°C are considered acceptable error statistics for Lake Ontario (Hall, 2008; Huang et al., 2010a; Rao et al., 2004; Wilson et al., 2013). At nearshore location PEP and offshore location 20NMB, increased discrepancies between the simulated and observed temperature
profiles were noticed in July (see Figure 5.10) when the lake was fully stratified. The model underestimated the surface temperatures of the stratified lake in July hence the overall RMSEs increased at PEP and 20NMB buoys.

![Figure 5.10: Simulated and observed (GLOS) surface temperatures in Lake Ontario, late April–July 2011.](image)

Simulated vertical temperature profiles are compared to observations at SP and DP buoys in Figures 5.11a and 5.11b. The simulated temperatures compared well with observed temperatures when the lake was in the mixed phase (the overall RMSEs for both the SP and DP were below 0.5°C). The lake began to stratify at SP and DP by May 20th and June 10th, respectively, but the model failed to capture this transition on these dates. At SP, the RMSE began to increase around May 20th and was 6.05°C by July 10th. At DP, the RMSE increased after June 10th, and by July 10th, the RMSE was 3.18°C. The vertical profiles in Figures 5.11a and 5.11b show that the model captured the mixed phase
(thermal bar formation phase) better than the stratified phase. The greatest RMSEs occurred when the lake transitioned to the stratified phase in the observations (late May/early June).

Deviations were observed primarily for depths less than 20 m, regardless of the local depth of the lake. This is the depth over which wind mixing imparts kinetic energy that mixes solar heating. This mixing mechanism governs the epilimnion transition. When wind-driven mixing decreases, the potential energy of the lake is re-oriented to re-stratify the lake; warm, lighter water migrates to the top, while colder, denser water sinks and a density-based thermocline appears. Thus it can be concluded from the measured profiles that the errors in simulating the development of the stratified layer and thermocline are associated with both wind mixing in epilimnion and the strong density gradients in the thermocline. To resolve these problems, the model was updated and refined with an alternative vertical mixing parameterization scheme, discussed in Chapter 6.
Figure 5.11: Simulated and observed (Environment Canada) vertical temperature profiles in Lake Ontario, late April–July 2011
(a) at SP, (b) at DP.
Because the model captured temperature profiles well in the mixed phase, lake-wide surface temperatures were compared with remotely sensed AVHRR images from NOAA (Figure 12) during formation of the thermal bar (late April to late May). NOAA images were georeferenced and superimposed upon images of EFDC simulated temperatures and the spatial distribution of temperature differences between the two sets of images are shown in Figure 12. From Figure 12, simulated temperatures were typically lower than the NOAA satellite measurements by 0.5 to 1°C. However, the simulated nearshore temperatures near the north shore were warmer than the corresponding NOAA data by 0.5 to 2°C. Note that on the north shore, colder deeper water upwells because of prevailing offshore winds from the north (Hall, 2008). Although upward velocities were simulated in this region, the model did not capture the magnitude of local upwelling events. The simulated temperatures in the deeper areas of the lake and the south nearshore area were cooler than those measured by NOAA by 0.5°C from late April to early May. Later in May, the difference between the two increased to 1°C in the deeper area and 2°C along the south shore of the lake. Consistent with Figure 12, the model under-predicted temperatures in deeper areas as the lake moved into the stratified phase. Nevertheless, the simulated surface temperatures were accurate (0.5 to 1°C different from NOAA) when the lake was in the mixed phase.
Figure 5.12: Lake-wide surface temperatures compared with satellite images from NOAA, late April–late May 2011 when the lake is in the mixed phase (during thermal bar evolution).
5.7 Formation of the Thermal Bar in Lake Ontario

The EFDC Lake Ontario model captured the temperature profiles well in the mixed phase (RMSEs were below 0.5°C for vertical temperature profiles) and so the evolution of the thermal bar was explored through simulated temperature profiles from late April to May 2011.

Figure 5.13 shows the thermal bar formation (4°C temperature throughout the water column) at SP consistent with observed data. Both model-simulated and observed thermal bar formation started approximately at day 113 (April 23rd). The simulated thermal bar was stationary at SP until day 119 (April 29th) in the simulated profile and until day 118 (April 28th) in the observed data. The simulated lake mixed phase continued until day 125 (May 5th) and until day 127 (May 7th) for observed data after which the lake began to stratify at this nearshore location. Wind speed data (obtained from land-based stations) during the thermal bar period at SP was low to moderate (3 to 8 m/s for days 113 to 135) and hence the simulated wind stress was low as well (0.015 to 0.15 N/m²). There was no strong wind to push the thermal bar into deep waters and minimal wind-energy-induced turbulent heat and mass exchange at the air-water interface. The wind direction was predominantly easterly. The simulated surface net heat flux (SNHF) at this location from day 113 to 125 was negative on some days and positive on other days (the values were between −30 and +65 W/m²), so there was no sudden heat loss or gain at the surface. After day 125, the simulated SNHF was positive (+25 to +105 W/m² for days 126-135) supporting thermal stratification at SP and facilitating progression of the thermal bar into deeper areas.
Figure 5.13: Time series (late April–late May 2011) of vertical temperature distributions and thermal bar formation (shaded in diagonal lines) at SP.

Figure 5.14 illustrates the thermal bar progression rate at SP using temperature time-series (simulated and observed). Using the analytical formulation of Elliott and Elliott (1970), thermal bar progression rate is estimated as the ratio of bar displacement from its current position to another deeper location based on the assumption that heat entering the surface of a unit column remains within the column and the horizontal heat fluxes are negligible. By distributing the surface heat flux (considered constant in space and time) over the local depth and balancing this against the rate of temperature increase, Elliott and Elliott (1970) estimated the speed of the thermal bar as:

\[ S = \frac{QL}{\Delta T \rho c_p D} \]  

(5.16)
where $Q_s$ (cal/cm/sec) is the heat flux through surface, $L$ (cm) is the horizontal distance between the bar and some deeper reference position where the mean temperature is known, $D$ (cm) is the depth at the deeper position, $\Delta T$ ($^\circ$C) is the temperature difference between 4$^\circ$C and the mean temperature at the deeper position, and $\rho c_p$ is the density of water times its specific heat (1 cal/$^\circ$C/cm).

Figure 5.14: Estimated thermal bar progression rate using simulated and observed (Environment Canada) time-series (late April–late May 2011) temperature profiles.

Figure 5.14 shows that the thermal bar progression rate was overestimated using the simulated temperature time-series compared to the rate estimated using observed temperature profiles. This difference may be because the simulated temperature profiles neglected local mixing in the thermal bar zone. The estimated progression rates (in Figure 5.14) show two distinct phases of thermal bar progression (Malm et al., 1993; Zilitinkevich et al., 1992): an initial slow phase (until mid-May) and a subsequent fast
phase (late May). However, theoretical models over-estimate the progression rate of the thermal bar during the early phase. In the later phase, models that incorporate the effect of horizontal heat flux in the thermal bar region (Malm et al., 1993; Zilitinkevich et al., 1992) capture the significant increase in progression rate (Rao and Schwab, 2007; Rao et al., 2004). Directly observed progression rates of the thermal bar were not available to compare with the estimated rates. The estimated progression rate didn't capture the thermal bar stationary phase at SP (April 23rd to April 29th). This is probably because an average heat flux was used, and horizontal heat fluxes were not considered in the analytical formula.

Figure 5.15a showed the surface flow circulation on Lake Ontario on May 7th when the lake was in the mixed phase, and the thermal bar formed nearshore. Figure 5.15b shows vertical temperature profiles during thermal bar formation at the north shore (25 m deep) and south shore (33m deep) locations (locations marked as N and S in Figure 5.15a). Both at north and south shore the water column was homogeneously mixed with ~4°C temperature indicating the thermal bar formation at respective locations. Figure 5.13 depicts the thermal bar formation at SP from April 23rd to April 29th. The north shore location in Figure 5.15b is about ~10 km from SP. As stratification began with positive heat flux at SP in early May, the thermal bar progressed towards the deeper position.
Figure 5.15: (a) Surface velocity profile at Lake Ontario during the thermal bar formation at nearshore (b) Vertical temperature profiles at the north shore (N in Figure 5.15a) and south shore (S in Figure 5.15a).
Figure 5.15a shows surface flows convergence towards the thermal bar in opposite directions: counter-clockwise in stratified nearshore and clockwise in deep water where water is still mixing. Converging surface flow patterns toward thermal bar have been observed and analyzed in several studies (Holland and Kay, 2003; Malm, 1995; Zilitinkevich et al., 1992). In general, density-induced horizontal circulation in large, temperate lakes in the northern hemisphere is counterclockwise in the stably stratified nearshore region, and clockwise in the deep water region (Rao and Schwab, 2007). In the study by Rao et al. (2004), it was confirmed that the observed circulation within a zone between the shore and the thermal bar is predominantly shore-parallel and counter-clockwise. This two-cell thermal bar circulation is important because flows converging at the thermal bar suppress most cross-frontal exchange thereby inhibiting horizontal mixing (Gbah and Murthy, 1998; Holland and Kay, 2003).

Figure 5.16 demonstrates the effect of thermal bar formation on horizontal mixing coefficients in nearshore areas. Figure 5.16 shows that horizontal eddy viscosity (m$^2$/s) significantly decreased during the thermal bar phase (18 m$^2$/s) compared to pre-thermal bar (30 m$^2$/s) and post thermal bar periods (25 m$^2$/s) at SP, whereas thermal bar formation has no considerable effect on horizontal eddy viscosity value (5-12 m$^2$/s) at DP. At SP, horizontal mixing coefficients were higher near the surface (18-30 m$^2$/s) than corresponding subsurface values during pre-, post- and thermal bar periods. At DP, horizontal mixing coefficients were elevated near the water surface and at the bottom (8-12 m$^2$/s) with lower values (3-7 m$^2$/s) in the mid-water column. Lower values of horizontal mixing coefficient at SP during the thermal bar phase, compared with the pre- and post- thermal bar periods, support the hypothesis that the thermal bar plays an
important role in reducing horizontal mixing in nearshore areas. Similar observations were reported by Rao et al. (2004) as they found that during the thermal bar phase, the magnitude of both alongshore and cross-shore exchange coefficients decreased when the bar was in the nearshore.

Figure 5.16: Depth variation of horizontal mixing coefficient (eddy viscosity, m²/s) during the pre-thermal bar, thermal bar, and post-thermal bar periods at SP and DP.
CHAPTER 6:
AN IMPROVED VERTICAL MIXING SCHEME FOR SIMULATING SUMMER STRATIFICATION

6.1 Overview

Lake Ontario has two distinct lake phases: (1) a mixed phase (early April through late May), during which convective mixing dominates, and the evolution of the thermal bar progresses from near-shore areas to the deepest portions of the lake and (2) density-stratified phase (late May through mid-October), during which the thermal bar disappears and warm, lighter water rises to form the epilimnion (Figure 6.1). Cold, denser water sinks to form the hypolimnion and remains largely isolated from the warmer water above by a density-gradient-driven thermocline within the water column.

In general, both local and global mixing and stratification processes in a lake are driven by winds and solar radiation, with the latter generates stable stratification while the former (wind stress) erodes the stratification. Solar radiation and other heat inputs (e.g. advective heat flux, sensible and latent heat fluxes) warm surface waters (reducing the density) play a conducive role in setting summer stratification. The wind transfers horizontal momentum to the water body, creating currents (Stewart, 2008), and the resulting vertical shear associated with currents promotes mixing (Djoumna et al., 2014).
It is important to understand the vertical mixing processes that govern not only
the thermal structure but also nutrient exchanges and distribution of dissolved and
particulate matter between the different parts of the lake (Bonnet et al., 2000). Simulation
of the vertical temperature profile of the water column is crucial for the assessment of
climatic effects on lake physics, biology, and water quality (Huang et al., 2010b).
Appropriate vertical mixing parameterizations are necessary to accurately simulate
vertical temperature profiles.
Vertical eddy diffusivity and eddy viscosity are the mixing coefficients that regulate mixing and stratification phenomena. Turbulent (eddy) diffusion enhances the transport of mass, heat, and momentum within a system due to random and chaotic time-dependent motions (Stewart, 2008). It occurs when turbulent fluid systems reach critical conditions in response to shear flow, which results from a combination of steep concentration gradients, density gradients, and high velocities (Csanady, 1973). Turbulent diffusion occurs much more rapidly than molecular diffusion and is therefore extremely important for problems concerning mixing and transport. Eddy viscosity is an expression for the transfer of momentum of mean motion which is increased by turbulence. The magnitude of the eddy viscosity depends on the size and intensity of the eddies—that is, on the magnitude of the exchange of masses between adjacent layers. In the case of vertical turbulence, the effective exchange of masses is related to small eddies in a vertical plane. The eddies are oriented random, only their vertical components produce any effect on the mean motion (Sverdrup et al., 1942).

This chapter describes the improvement to EFDC model’s ability in simulating the summer thermal stratification accomplished through an alternate vertical mixing parameterization scheme. The simulation is run from April 5th to October 15th, 2011. The performance of EFDC's original vertical mixing scheme Mellor and Yamada (1982) and a review of other mixing schemes applied in thermal simulations in the Great Lakes region are discussed in the next section.

6.2 Background for Updating Vertical Mixing Parameterization

McCormick and Meadows (1988), Huang et al. (2010b) and Djoumna et al. (2014) conducted notable comparative studies on hydrodynamic models simulating
thermal stratification of the Great Lakes. McCormick and Meadows (1988) simulated vertical temperature profiles and mixed-layer depths in Lake Erie using four one-dimensional mixed-layer models. When diurnal physical processes are of interest, they found that the model’s ability to simulate the mixed-layer depth is crucial for the overall success of the predictions.

Huang et al. (2010b) compared three 3D hydrodynamic models with three different mixing schemes for simulating thermal behavior in Lake Ontario: the Princeton Ocean Model (POM) with the Mellor-Yamada 2.5 Level scheme (Mellor and Yamada, 1982), the Canadian Version of Diecast Model (CANDIE) with the modified K profile (KPP) scheme (Large et al., 1994), and the Estuary, Lake, and Coastal Ocean Model (ELCOM) with the 3D mixed-layer approach (Hodges et al., 2000b). In the Mellor and Yamada (1982) scheme, the vertical diffusivities for momentum and heat are related to the turbulent length scale, turbulent kinetic energy (TKE), and the gradient Richardson number (details are provided in Section 3.2). In the KPP scheme (Large et al., 1994), the vertical viscosity and diffusivity are related to the wind stress in the upper mixed layer and the gradient Richardson number in the stratified interior (Djoumna et al., 2014). The 3D mixed layer mixing scheme is based on mixing energy budgets to simulate the vertical eddy fluxes in momentum and transport equations (Hodges et al., 2000b).

Huang et al. (2010b) found that all three models underestimated the mixed layer depths compared to observations at mid-lake stations, and the errors were large (peak RMSEs of 5 – 6°C) for simulated thermocline temperatures. The models, however, performed better near the coast. They suggested that the differences in the simulated
temperature distribution may be related to differences in the parameterization of vertical mixing, rather than the vertical numerical discretization.

Djoumna et al. (2014) performed a sensitivity analysis of the parameterization of vertical mixing and radiative fluxes on the seasonal evolution of Lake Erie’s thermal structure using the Massachusetts Institute of Technology general circulation model (MITgcm) and the General Estuarine Transport Model (GETM). They studied three approaches for the parameterization of vertical mixing: the Mellor-Yamada 2.5 Level scheme (Mellor and Yamada, 1982), the KPP scheme (Large et al., 1994), and the Generic Length Scale (referred to as GLS) closures. The GLS scheme considers the energetics of the mixing and solves transport equations for turbulent kinetic energy and length scale (Umlauf and Burchard, 2003). They found that both MITgcm and GETM with the Mellor-Yamada 2.5 Level scheme produced deeper mixed layers than observed at a station located in the eastern basin, yielding large errors in simulated thermocline temperatures. MITgcm with the KPP scheme produced a peak RMSE of 4.5°C and GETM with the $k$-$\varepsilon$ scheme produced RMSEs between 3 and 3.7°C in the thermocline. They emphasized the need for more accurate parameterization schemes for vertical turbulent exchange processes in large lakes.
I analyzed the vertical temperature profiles simulated using EFDC's original mixing scheme Mellor and Yamada (1982) at two buoy locations over Lake Ontario: a nearshore, shallow point (SP, 19 m deep) and an offshore, deep point (DP, 177 m deep), as shown in Figure 6.2. From Figure 6.3, simulated and observed temperatures (obtained via personal communication with Dr. Ram Yerubandi Rao from Environment Canada) compared well when the lake was in the mixed phase; overall RMSEs at both SP and DP were below 0.5°C. At SP from May 20th, the RMSE started to increase, and by July 10th it was 6.05°C while at DP from June 20th, RMSE started to increase and by July 10th it was 3.18°C. The increases in RMSEs are because from late May and late June, lake stratification set in at SP and DP, respectively. It is also evident from Figure 6.3 that the existing vertical mixing scheme does not capture the shape of the stratification pattern as
three distinct layers: epilimnion, metalimnion (with thermocline formation) and hypolimnion, as observed in SP profiles from June 10\textsuperscript{th} onward.

Figure 6.3: Simulated (with Mellor-Yamada vertical mixing parameterization) and observed (Environment Canada) vertical temperature profiles in late-April to July 2011 (a) at SP and (b) at DP.
I implemented parameterizations for vertical eddy diffusivity following Vinçon-Leite et al. (2014) and vertical eddy viscosity following Pacanowski and Philander (1981). I chose the particular mixing schemes because they are fairly simple to implement. Moreover, the eddy diffusivity parameterization by Vinçon-Leite et al. (2014) follows the lake's thermal structure; the algorithm uses different eddy diffusivity formulation above and below the thermocline to accurately simulate the thermocline formation. Based on the review of recent research approaches (summarized above) on simulating summer stratification patterns in the Great Lakes region, I discarded the vertical mixing schemes those already have been implemented and tested for Great Lakes' thermal simulation.

6.3 Vertical Eddy Diffusivity Parameterization Update

I have implemented the uni-dimensional vertical model for eddy diffusivity parameterization that uses different eddy diffusivity formulations above and below the thermocline (Vinçon-Leite, 1991; Vinçon-Leite et al., 2014). The model originates from the work of Simons (1981) on Lake Ontario. The large size of this lake (19,000 km$^2$) justified the use of oceanic equations for eddy diffusivity. Henderson-Sellers (1985) adapted these equations and applied them to Lake Windermere, UK (14.7 km$^2$). For relatively small lakes, these equations seem to work adequately even if they are only strictly valid for the ocean and very large lakes. Tassin (1986) adapted this approach using different equations for the eddy diffusivities in the epilimnion and hypolimnion and implemented it on Lake Geneva, Switzerland, and France (580 km$^2$). It was then implemented in Lake Bourget, France (42 km$^2$) (Vinçon-Leite, 1991; Vinçon-Leite et al., 2014; Vinçon-Leite et al., 1989). Bonnet et al. (2000) used this uni-dimensional model to
study the vertical temperature profiles for an artificial lake (i.e. a reservoir) located in France. I will refer to this uni-dimensional model as Vinçon-Leite et al. (2014) algorithm hereafter.

The algorithm is based on the horizontally averaged diffusion equation for temperature:

$$\frac{\partial T(z,t)}{\partial t} = \frac{1}{A(z)} \frac{\partial}{\partial z} \left[ A(z) K(z,t) \frac{\partial T(z,t)}{\partial z} + \frac{A(z) SS(z,t)}{\rho \cdot C_p} \right]$$ (6.1)

where $T(z,t)$ is the local water temperature (°C) at time $t$ (s), $A(z)$ is the horizontal area ($m^2$) of the lake at depth $z$, $K(z,t)$ is the vertical diffusion coefficient ($m^2 s^{-1}$), $SS(z,t)$ is the heat source/sink ($W m^{-2}$), and $C_p$ is the specific heat of water at constant pressure (4,180 J kg$^{-1}$ K$^{-1}$). Because vertical eddy diffusivity is instrumental for vertical transport of heat (temperature) through the water column, its proper parameterization is important when simulating thermal mixing and stratification patterns.

In this parameterization, the thermocline depth $Z_{therm}$ is defined by the location of the maximum density gradient and different formulae are used for the eddy diffusivity above and below the thermocline. The boundary between the metalimnion and the hypolimnion at depth $Z_{meta}$ is defined by the location where density gradient exceeds a threshold value of $10^{-5}$ kg m$^{-4}$ (Vinçon-Leite et al., 2014).

From the surface to the thermocline:

The eddy diffusivity from the surface to the thermocline is first calculated for neutral conditions (homogeneous density along the vertical) as:

$$K_o(z) = \gamma \delta u^* \exp \left( - \frac{z}{\gamma u^*} \right)$$ (6.2)
where \( z \) is the water depth (m), \( u_s^* \) is the surface friction velocity (m s\(^{-1}\)), and \( \gamma \) and \( \delta \) are calibration parameters.

Following Simons (1981), who decoupled the impacts of wind and stratification, eddy diffusivity in stratified conditions is taken as the product of the eddy diffusivity in neutral conditions (the preceding equation) and an empirical function of the Richardson number, \( Ri(z) \):

\[
K(z) = \frac{K_0(z)}{1 + \sigma Ri(z)}
\]  
(6.3)

where \( \sigma \) is a calibration parameter.

Richardson number, \( Ri(z) \), is defined in more general form (using the stability factor or Brunt-Väisälä frequency, \( N(z) \) as done in oceanography), as the ratio of the buoyancy and shear influences (Stewart, 2008; Turner, 1973). This function sharply reduces eddy diffusivity close to the thermocline (Vinçon-Leite et al., 2014). \( Ri(z) \) and \( N(z) \) (Hz) are computed as:

\[
Ri(z) = N(z)\left(\frac{\partial u}{\partial z}\right)^2 = \left(N(z)\gamma\delta\right)^2 \exp\left(\frac{2z}{\gamma u_s^*}\right)
\]  
(6.4)

\[
N(z) = -\sqrt{\frac{g}{\rho(z)}} \left| \frac{\partial \rho}{\partial z} \right|
\]  
(6.5)

where \( g \) is gravitational acceleration (m s\(^{-2}\)), \( \rho(z) \) is the local water density (kg m\(^{-3}\)), \( u(z) \) is the average horizontal current velocity (m s\(^{-1}\)). Surface friction velocity \( u_s^* \) (m s\(^{-1}\)) is:

\[
u_s^* = C_d \frac{\rho_s U}{\rho_0}
\]  
(6.6)

where \( \rho_0 \) is the average water density (1,000 kg m\(^{-3}\)), \( \rho_a \) is the average air density (1.293 kg m\(^{-3}\)), \( C_d \) is the wind drag coefficient (1.8\(\times\)10\(^{-3}\) J kg\(^{-1}\) K\(^{-1}\)), and \( U \) the wind speed 10 m above the water surface.
Below the thermocline:

Below the thermocline, the wind acts indirectly on mixing particularly through internal waves (Lorke, 2007; Vinçon-Leite et al., 2014). A different formulation for the eddy diffusivity is required, which is a power function of the Brunt-Väisälä frequency as:

$$K(z) = \alpha K(z_{\text{therm}}) \left[ \frac{N(z_{\text{therm}})}{N(z)} \right]^{2p_2} \quad \text{for} \quad z_{\text{therm}} < z < z_{\text{meta}}$$

(6.7)

where $Z_{\text{therm}}$ is the thermocline depth, $Z_{\text{meta}}$ is the boundary depth between the metalimnion and hypolimnion; the fitting parameter $\alpha$ is introduced to reduce the eddy diffusivity because the complex processes of energy dissipation are not physically described in the model and $p_2$ is a calibration parameter (Vinçon-Leite et al., 2014). Here, $N(z)$ is interpreted as the vertical frequency excited by a vertical displacement of a fluid parcel, which is the maximum frequency of internal waves in the ocean (Stewart, 2008). If $N(z)^2 > 0$, stable stratification exists and if $N(z)^2 < 0$, stratification is unstable. In this case, overturning or convection ensues.

A (linearly) depth-dependent reduction factor is applied in the hypolimnion to reach a zero-flux condition at the lake bottom (Tassin, 1986; Vinçon-Leite, 1991; Vinçon-Leite et al., 2014).

$$K(z) = \frac{z_{\text{max}} - z}{z_{\text{max}} - z_{\text{meta}}} K(z_{\text{meta}}) \left[ \frac{N(z_{\text{meta}})}{N(z)} \right]^{2p_2} \quad \text{for} \quad z_{\text{meta}} < z \leq z_{\text{max}}$$

(6.8)

where $Z_{\text{max}}$ is the maximum water column depth. Here, the geothermal flux at the lake bottom was neglected. The numerical values for all calibration parameters are listed in Table 6.1.
TABLE 6.1
CALIBRATION PARAMETERS USED IN THE EDDY DIFFUSIVITY PARAMETERIZATION

<table>
<thead>
<tr>
<th>Calibration parameter</th>
<th>Numerical value (Vinçon-Leite et al., 2014)</th>
</tr>
</thead>
<tbody>
<tr>
<td>σ</td>
<td>9.46</td>
</tr>
<tr>
<td>γ</td>
<td>570 sec</td>
</tr>
<tr>
<td>δ</td>
<td>0.015</td>
</tr>
<tr>
<td>α</td>
<td>0.173</td>
</tr>
<tr>
<td>$p_2$</td>
<td>0.605</td>
</tr>
</tbody>
</table>

6.3.1 Adding Convective Velocity to Friction Velocity Computation

The simulated temperature profiles are compared with observed profiles after updating the vertical eddy diffusivity parameterization (Figures 6.7-6.10). At SP, the simulated temperatures matched the observed profiles quite well until 240 days (August 29th), after which the observed water column was thoroughly mixed at 15 to 20°C, and the model failed to capture this transition (Figures 6.9 and 6.10). I investigated the meteorological parameters at SP to determine the reason for this discrepancy (Figure 6.11), a detailed discussion is presented in Section 6.5.

The air temperature and solar radiation both decreased past day 235 at SP (Figure 7) indicating the possibility of a convective overturning event; thus I added additional stirring in terms of a convective velocity, modified based on the work on Deardorff (1970). The expression for convective velocity is:
\[ u_{cv} = \begin{cases} \left[ C_{cv} \left( g \alpha_T \Delta T_{z_{\text{max}}} \right)^{1/2} \right] & \Delta T > 0 \\ 0 & \Delta T \leq 0 \end{cases} \]  \tag{6.9}

where \( C_{cv} \sim O(1) \) is a tuning parameter, \( \alpha_T = 69 \times 10^{-6} \text{ K}^{-1} \) is the linear thermal expansion coefficient at 20°C, and \( \Delta T \) is the difference between the surface water temperature and air temperature. When air temperature exceeds the surface water temperature, convective mixing takes place along with wind-mixing, otherwise convective velocity is zero, leaving only wind-mixing.

This convective velocity term is added to the surface friction velocity yielding a composite velocity of (Deardorff, 1983):

\[ u_{\text{comp}} = \left[ u_s^3 + u_{cv}^3 \right]^{1/3} \]  \tag{6.10}

6.3.2 Calibrating Bed Heat Flux Parameters

I investigated the parameters pertaining to bed heat flux (the heat exchange on the interface of water column-sediment bed; details are described in Section 3.3) computation and calibrated them. I set spatially varying bed temperature for the lake domain; 4°C for areas where depth is less than or equal to 50 m and 3°C for areas where depth is more than 50 m. This is more realistic than having a uniform constant bed temperature over the whole lake domain. I set a minimal value (0.1) for the dimensionless coefficient for computing convective heat transfer between the bed and water column (HTBED1) to check excessive heat loss through bed heat flux. If I set HTBED1 = 0, hence completely shutting off the convective heat exchange, it yielded excessive heat in the water column even at the surface.
6.4 Vertical Eddy Viscosity Parameterization Update

The eddy viscosity is updated following the method mentioned in Rao and Murthy (2001) and Rao et al. (2004); using the simple empirical formula suggested by Pacanowski and Philander (1981), where eddy viscosity is related to the Richardson number.

\[ K_v(z) = \frac{K_{vo}(z)}{(1 + 5Ri(z))^2} + K_{vb} \]  \hspace{1cm} (6.11)

where, \( K_{vo}(z) \) = an adjustable parameter \( (10^{-2} \text{ m}^2 \text{s}^{-1}) \); \( K_{vb} \) = background value \( (10^{-6} \text{ m}^2 \text{s}^{-1}) \); \( Ri(z) \) = Richardson number; \( z \) is local depth (m).

6.5 Simulated Temperature Profiles with Updated Vertical Mixing Parameterization

Observed vertical temperature profiles from late May to late September for both DP and SP are compared to simulated vertical temperature profiles in Figures 6.4 and 6.6. Temperature time-series from late April to mid-October for certain depths are shown in Figures 6.5 and 6.7.
Simulated profiles using the Vincon et al. (2014) scheme (V scheme) matched the observed temperature profiles at DP, better than simulated profiles using the Mellor-Yamada (1982) scheme (M-Y scheme), (Figures 6.4 and 6.5). RMSEs for transect temperature profiles using the V scheme were 0.6 to 1.61°C from late May to late September (Figure 6.4) and were lower than the RMSEs obtained using the M-Y scheme. RMSEs for temperature time-series using the V scheme were ~2°C at 1 m and 10 m depths and are ~0.5°C at 50 m, 100 m, 180 m depths (Figure 6.5). The 10 m depth profile was in the thermocline formation depth-zone, implying that the new vertical parameterization (V scheme) captured thermocline formation at DP; whereas the RMSE for 10 m depth profile using the M-Y scheme was 6.10°C.
Replicating thermocline formation with simulated temperatures is challenging because, within the thin (with respect to local water-column depth) depth-zone of the thermocline, temperature and density change more rapidly with depth than they do in the layers above or below. In the updated eddy diffusivity parameterization by Vinçon-Leite et al. (2014), the thermocline depth is marked as the depth of maximum density gradient. Up to thermocline depth, the stratification/mixing pattern is related to the function of Richardson number $Ri(z)$. If the buoyancy flux dominates due to a high-density gradient, $Ri(z)$ will be high, and eddy diffusivity for the stratified fluid will be low. If the wind-mixing dominates, $Ri(z)$ will be low, and eddy diffusivity for the mixed fluid will be high.
It usually takes strong wind-induced mixing or convective mixing to break the density gradient barrier in the thermocline. Below the thermocline, eddy diffusivity parameterization is related to buoyancy factor Brunt-Väisälä Frequency. By definition of the Brunt-Väisälä Frequency, a liquid (nearly incompressible) fluid is expected to be stable with positive $N(z)^2$ when the density of the fluid increases with depth, and so stable stratification develops in the metalimnion below the thermocline. Convective mixing will follow if $N(z)^2$ becomes negative with lighter (reduced density) fluid particle, leading to unstable stratification.

The simulated temperature profiles using the V scheme replicated the stratification pattern from late May to late September at SP with higher RMSEs of 1.25
to 3.7°C (Figure 6.6). The new vertical parameterization scheme captured the thermocline formation structure which was not previously captured by the Mellor-Yamada scheme (Figure 6.6), temperature increase was almost linear from the bottom towards the surface. Hence, the RMSEs using the M-Y scheme were higher than those from using the V scheme. The temperature time-series using the V scheme at SP showed that the simulated temperatures matched the observed profiles well until 240 days (August 29th), RMSEs were 1.8 to 3.2°C (computed, not shown in Figure 6.7). From September, the observed profiles at SP were thoroughly mixed at 15 to 20°C, whereas the simulated profiles stayed as stratified water column (Figure 6.6 and 6.7). Hence the overall RMSEs for temperature time-series using the V scheme at SP increased for 9 m, 15 m, 19 m depths and were 4.20 to 5.27°C (Figure 6.7). RMSEs for temperature time-series using the M-Y scheme were higher than those from the V scheme for all depths at SP (Figure 6.7).
I investigated the meteorological parameters at SP to determine the reason for this discrepancy (Figure 6.8). The 1 m and 19 m depth profiles in Figure 6.8 at SP show the thoroughly mixed water column past day 240 highlighted with a dotted yellow box.

No strong winds were observed at SP; the wind speed was moderate and below 10 m/s (Figure 6.8) and hence wind-induced break up of stratification is unlikely. However, there remains a possibility that local wind gusts (e.g., a thunderstorm) broke the stratification pattern around day 240 at SP, which is not properly accounted in the model forcing data.
Air temperature and solar radiation decreased past day 235 at SP (Figure 6.8). I further analyzed the air temperature for both shallow and deep points; the air temperature started cooling down from day 235 (August 24th) at both locations, so a convective cooling event could have taken place and mixed the water column. To account for this convective mixing event, a convective velocity term was added in the computation of surface friction velocity from day 235 (details are presented in Section 6.3.1).
Figure 6.9: Simulated with spatially varying bed temperature and convective velocity (from August 24th) and observed (Environment Canada) transect temperature profiles in Lake Ontario, 2011 at the shallow location, SP.

With spatially varying bed temperature (4°C for shallow location and 3°C for deep location), by reducing the convective heat exchange between bed and water column (by lowering the value for HTBED1 coefficient) and with convective mixing effective from day 235, the temperature time-series at SP improved with better RMSE values for 9 m, 15 m and 19 m depths (Figure 6.10). With convective mixing the simulated profiles at 1 m and 5 m depths deviated from the observed profiles and RMSEs increased. The transect temperature profiles for September 12th and 26th were thoroughly mixed at SP (Figure 6.9) due to convective mixing and reduced convective bed heat flux exchange but at a lower temperature than observed. The observed water column at SP was thoroughly mixed at ~15-20°C for September 12th and 26th profiles whereas the simulated water column got mixed at ~12-16°C. It appears that the model needs additional heat/energy
source to mix the water column thoroughly. Local wind forcing not captured by sparse land stations is another potential explanation. Increased bed temperature (4°C bed temperature at SP, was 3°C before) and reduced convective heat flux exchange between the bed and water column, however, heated the water column more and RMSEs increased for July 11th to August 14th profiles.

Figure 6.10: Simulated with spatially varying bed temperature and convective velocity (August 24th) and observed (Environment Canada) temperature time-series in Lake Ontario, 2011 at the shallow location, SP.

For DP, with the reduced convective heat flux exchange between the bed and water column, the simulated profiles were similar to previously simulated profiles until convective mixing took place. The bed temperature for DP is 3°C as before (not changed). The temperature time-series for 1 m and 10 m depths and the vertical temperature profiles matched nicely until the convective mixing became effective from
day 235 (August 24\textsuperscript{th}) (Figures 6.11 and 6.12). It is evident from Figures 6.11 and 6.12 that convective mixing is not required for the deep location. The temperature profiles at lower depths of 50 m, 100 m, and 180 m were not affected by convective mixing.

Figure 6.11: Simulated with spatially varying bed temperature and convective velocity (from August 24\textsuperscript{th}) and observed (Environment Canada) transect temperature profiles in Lake Ontario, 2011 at the deep location, DP.
Figure 6.12: Simulated with spatially varying bed temperature and convective velocity (August 24th) and observed (Environment Canada) temperature time-series in Lake Ontario, 2011 at the deep location, DP.

6.5.1 Advective Flow Input from Streams and Tributaries

Since the water column at SP was mixed with a relatively high temperature of 15-20°C, I speculated that the model was missing an additional heat source. I previously investigated individual heat fluxes and their components, and the model was improved with a new evaporation algorithm (Arifin et al., 2016). To account for additional heat input, the model was forced with flow and temperature data from 10 streams/rivers surrounding Lake Ontario (Figure 6.13).
Figure 6.13: Locations of streams and tributaries surrounding Lake Ontario.

The flow data for streams and tributaries were obtained from the United States Geological Survey (USGS) and the Environment Canada. Temperature input data were available for Niagara, Oswego, and Genesee Rivers. The temperature data for other streams/tributaries (where temperature data were not available) were assigned equal to those of the nearest River (Niagara, Oswego, or Genesee).
With additional advective heat flux, the transect temperature profiles at the shallow location shifted to increased temperatures (Figure 6.14), with shapes similar to the simulated profiles without stream flows. Corresponding RMSEs improved until June but then increased until September 26th. For temperature time-series at SP, I noticed a slight improvement in RMSEs for 9 m, 15 m, 19 m depth profiles (Figure 6.15).
For deep location, due to advective heat flux, overall RMSEs increased for transect temperature profiles (Figure 6.16). Because of the added heat flux, 1m and 10m temperature-depth profiles deviated from the observed time-series from late May (140 days) onwards (Figure 6.17). Implementation of an effective advection scheme that does not induce early onset of stratification may resolve the differences observed in the simulated temperature profiles with the streamflow. Integration of surface runoff with appropriate temperatures from a hydrology model could potentially improve the simulated lake temperatures.
Figure 6.16: Simulated with streamflow and observed (Environment Canada) transect temperature profiles in Lake Ontario, late May–late September 2011 at the deep location, DP.

Figure 6.17: Simulated with streamflow and observed (Environment Canada) vertical temperature time-series in Lake Ontario, late April–mid-October 2011 at the deep location at specific depths.
6.5.2 Simulated Surface Temperature Profiles

I analyzed surface temperature profiles from late April to mid-October at two nearshore locations: WG (25 m deep) and PWP (74 m deep) and at one offshore location: 20NMB (140 m deep), (locations are shown in Figure 5.8) for comparison to observed profiles (GLOS) in Figure 6.18.

The surface temperature profiles until May 25\textsuperscript{th} (while the lake was in mixed phase) were simulated using the Mellor and Yamada (1982) scheme and from May 25\textsuperscript{th} to mid-October (while the lake was stratified) were simulated using the Vinçon-Leite et
al. (2014) scheme. Running a single simulation using different mixing schemes is quite easy in EFDC. The mixing schemes are designated as scheme 1, scheme 2, …, etc. with a numerical parameter. The user has to select the parameter's numerical value to specify the desired mixing scheme and restart files can be generated to continue the simulation (without any disruption), with a different mixing scheme.

Overall, the simulated temperature profiles matched the observed profiles quite well. For nearshore locations WG and PWP, RMSE were 1.87 and 2.41°C respectively, and for offshore 20NMB location, the RMSE was 1.85°C. Historically, RMSEs below 2°C are considered as acceptable for Lake Ontario (Hall, 2008; Huang et al., 2010a; Rao et al., 2004; Wilson et al., 2013). I observed that from September 2011 (Figure 6.18), the simulated temperatures were under-predicted compared to observed temperatures in all three locations: WG, PEP, and 20NMB. I previously observed that from September the lake was in its mixed phase, and the model under-predicted observed temperatures, especially at SP. This is consistent with the previous observation that the model lacks a heat source at this time.
CHAPTER 7:
COMPARATIVE ANALYSIS USING NARR METEOROLOGICAL DATA

7.1 Baseline Research for Coupling of Climate-Lake Model

Results in previous chapters demonstrated that atmospheric conditions such as air temperature, wind profile, distribution of solar radiation attenuation, and rate of evaporation play important roles in the heat flux and water (mass) balance within the lake; significantly affecting the thermal structure, currents, and water level in large lakes (Gibson et al., 2006; Huang et al., 2010a). Except absorption of incoming shortwave radiation, all other heat flux transfer happens in the air-lake interface, understanding the mechanisms of these physical processes (the wind, waves, heat flux) occurring at the lake/atmosphere interface is important (Hall, 2008; Wüest and Lorke, 2003). Furthermore, recent studies have shown that atmospheric models coupled with 3D lake models could obtain more realistic local temperature, evaporation, and convergence patterns compared to simulations, for example, over Lake Victoria (Song et al., 2004) and Great Bear and Great Slave lakes (Long et al., 2007).

General circulation models (GCMs) have included idealized lake models (Lofgren, 1997), and regional climate model (RCMs) have included one-dimensional lake models (Hostetler et al., 1993). However, these lake models are fairly simple and only account for the vertical heat transfer by eddy diffusion and convective mixing, without
considering advective heat transfer between neighboring lake points in the horizontal direction. This kind of air-lake coupling may be justified for small lakes, but it is too simple to represent complex lake-air interactions over large lakes because of the significant spatial variability in the surface temperatures (Huang et al., 2010a).

Recently, a few attempts have been made to couple three-dimensional lake models with regional climate model RCMs (Long et al., 2007; Song et al., 2004). Their results show that fully coupled air-lake regional climate model systems provide a reasonable temporal evolution of lake surface temperature and heat exchange at the air-lake interface in large lakes, allowing important feedbacks between the atmosphere, adjacent land, and the lakes at fine resolutions. Huang et al. (2010a) used a one-way coupling of atmospheric forcing parameters from the regional version of the Canadian Operational Global Environmental Multiscale (GEM) model to drive a 3-D hydrodynamic model of Lake Ontario. The results of the model simulation are directly compared with observations from the lake, as well as with the results from another simulation using the observed atmospheric forcing interpolated onto the model grids. The comparison enables the evaluation of both the lake hydrodynamic model and the GEM model forcing. In a similar study, Wilson et al. (2013) used North American Regional Reanalysis (NARR) data to drive an unstructured grid Finite Volume Coastal Ocean Model (FVCOM) to simulate the 2006 summer hydrography of the Lake Ontario-Kingston basin system. They discussed that for long-term process studies, time series of surface fluxes and winds that span years and decades are required as forcing. They argued that the forcing used by Huang et al. (2010a) from the GEM model has only been
available in recent years, and the currently available data may not be adequate for performing decadal simulations. The NARR dataset was previously used for Great Lakes modeling successfully, as it was incorporated to force the Massachusetts Institute of Technology (MIT) General Ocean Circulation model on a 2-km uniform grid implemented in Lake Superior for 1979 to 2006 (Bennington et al., 2010).

To provide supporting facts for coupling of lake models with climate models, it is important to interpolate the atmospheric forcing parameters from the climate model over the lake domain and compare the simulated results with the observed data. In this chapter, I incorporated atmospheric forcing data from NARR dataset into the EFDC model to layout the baseline research for coupling EFDC-Lake Ontario model with a regional climate model.

7.2 Incorporating Atmospheric Forcing Data from North American Regional Reanalysis (NARR)

North American Regional Reanalysis (NARR) is a long-term, dynamically consistent, high-resolution, high-frequency, atmospheric and land surface hydrology dataset for the North American domain (Mesinger et al., 2006). NARR dataset assimilation has been validated for the period 1979-2003. It provides temporal coverage at 3 hourly, daily and monthly time-step from 1979 to present time. The dataset is available on a Northern Hemisphere Lambert Conformal Conic grid at ~32-km spatial resolution. The dataset provides 29 pressure level for the atmosphere along with monolevel coverage. The monolevel is a single level including surface and near surface,
top of atmosphere, and cloud height. Hence, for analyzing the physical processes at the air-lake interface, NARR monolevel atmospheric forcing dataset is much suitable.

I analyzed the atmospheric forcing parameters from NARR dataset and compared them to those obtained from weather stations around Lake Ontario. In the comparative study, I selected the grid points in NARR dataset which were over-lake only. I obtained spatially averaged (over the lake domain) time series profiles for the year 2011.

![Figure 7.1: 3-hourly air temperature, air pressure, and relative humidity data from NARR and weather stations for the year 2011 (spatially averaged over the lake domain).](image)

Analyzing both NARR data and station based data I found that air temperature and air pressure correlated very well between both datasets (correlation factor was above
0.9) (Figure 7.1). However, in Figure 7.1, the correlation factor for relative humidity was very poor (value is 0.33). This can have an impact on the rate of evaporation and latent heat flux calculations.

I compared wind speed and solar radiation at daily time-step between NARR and station based data over the lake domain (Figure 7.2). The correlation factor for wind speed was below 0.5; the difference in wind speed magnitude between the two datasets may have a pronounced impact on latent and sensible heat fluxes, mixing induced by wind stress and circulation of surface water.

![Figure 7.2: Daily solar radiation and wind speed data from NARR and weather stations for the year 2011 (spatially averaged over the lake domain).](image1)

From Figure 7.2, NARR solar radiation was well-correlated with the station based dataset (correlation factor is 0.77). However, I observe that NARR incoming solar radiation was much higher in magnitude compared to station based dataset. Shortwave
Solar radiation is not only a component of surface net heat flux but also the only heat flux that penetrates downward through the water column. So this difference in magnitude will influence both simulated surface and vertical temperature profiles.

I ran several case studies involving NARR dataset:

- To account for the over-land and over-lake based difference in atmospheric forcing parameters, I ran following case study simulations:
  - NARR grid points at over-lake locations only.
  - NARR grid points at surrounding over-land station locations.

- Since NARR solar radiation and wind speed data differ significantly from land station based data, I ran following case study simulations combining NARR and station based datasets:
  - NARR wind speed and other forcing data from land station dataset.
  - NARR solar radiation and other forcing data from land station dataset.

Figure 7.3 shows NARR grid point locations over-lake and over-land surrounding Lake Ontario.
7.2.1 Simulated Vertical Temperature Profiles with NARR Data

Simulated temperature profiles using NARR over-lake and over-land data were compared to simulated profiles using land station based data and observed profiles in Figures 7.4 -7.7. All temperature profiles were simulated with the updated vertical mixing parameterization scheme.
Simulated profiles using NARR over-lake data matched well with observed data for the deep location, DP. RMSEs for transect temperature profiles from late May to late September were 0.37 to 1.58°C, which was lower than the RMSEs for respective profiles simulated using land station based data (Figure 7.4). RMSE for the time-series 1 m depth profile was 1.34°C (was 2.04°C for the land station based 1 m depth profile) and was 2.31°C for 10 m depth profile (was 2.1°C for the land station based 10 m depth profile) (Figure 7.5). The overall improvement was due to a couple of factors: (1) effect of directional wind speed over-lake, (2) higher incoming solar radiation (3) effect of over-
water air temperature and relative humidity (4) 16 evenly distributed grid points over-lake, effectively distributing atmospheric forcing parameters over the lake domain.

Figure 7.5: Simulated (using NARR over-lake and over-land data) and observed (Environment Canada) vertical temperature time-series in Lake Ontario, late April–mid-October 2011 at the deep location at specific depths.

Simulated profiles using NARR over-land data had overall higher RMSE values at DP. RMSEs for transect temperature profiles were 0.81 to 5.73°C (Figure 7.4), RMSE for time-series 1 m depth profile was 4.27°C and for 10 m depth profile was 6.2°C (Figure 7.5); which were higher than the RMSE values of respective profiles simulated using both land station based data and NARR over-lake data. I didn't investigate each
atmospheric forcing parameter from NARR over-land dataset individually, but overall it can be said that the forcing parameters were adding more heat fluxes to the lake domain, leading to increased simulated temperatures and early onset of thermal stratification (Figures 7.4 and 7.5).

![Simulated and observed transect temperature profiles in Lake Ontario](image)

Figure 7.6: Simulated (using NARR over-lake and over-land data) and observed (Environment Canada) transect temperature profiles in Lake Ontario, late May–late September 2011 at the shallow location, SP.

Simulated profiles using NARR over-lake and over-land data for the shallow location, SP were not as promising as those of DP. RMSEs for transect temperature profiles, simulated using NARR over-lake data were 1.26 to 8.95°C and using NARR over-land data were 2.0 to 7.80°C (Figure 7.6); which were higher than the RMSEs of
respective profiles simulated using land station based data. The thermocline formation and stratification pattern were deviated from the observed profiles. The lake was receiving more heat flux at this location by using NARR over-lake and over-land data. Especially the simulated profiles up to 5 m depth were getting heated faster, and I noticed the early onset of stratification (Figures 7.6 and 7.7). RMSEs for 1 m and 5 m depths time-series were 3.52 and 3.39°C respectively, for NARR over-lake data and were 4.02 and 3.97°C respectively, for NARR over-land data (Figure 7.7). These RMSEs were quite higher than the RMSEs for respective profiles (2.06°C for 1 m depth and 2.48°C for 5 m depth profiles) simulated using land station based data. Stratification developed as early as day 130 with NARR over-land data and at day 145 with NARR over-lake data (see 1 m depth profile in Figure 7.7).
Figure 7.7: Simulated (using NARR over-lake and over-land data) and observed (Environment Canada) vertical temperature time-series in Lake Ontario, late April–mid-October 2011 at the shallow location at specific depths.

However, even with more heat flux received at the shallow location, the simulated profiles did not match the observed profiles past day 240. The simulated profiles using NARR over-lake and over-land data were stratified whereas the observed profiles were mixed past day 240. Hence I noticed higher RMSE values for September 12th and 26th profiles in Figure 7.6 and for 9 m, 15 m, 19 m profiles in Figure 7.7.
I analyzed the wind speed data at six neighboring NARR grid points of the shallow location but did not observe any strong wind movement around day 240 (Figure 7.8). Convective cooling is one reason for mixing the water column, but it usually takes strong force (gusty wind or big wave, etc.) to break the density gradient barrier of the stratified water column. There remains the possibility a local thunderstorm or strong wind event was not included within 32 km-evenly-spaced NARR grid points.

Figure 7.8: Wind speed profiles (2011) at six neighboring NARR grid points of the shallow location, SP.
Figure 7.9: Simulated (using a combination of NARR solar radiation, wind speed, and other land station data) and observed (Environment Canada) vertical temperature time-series in Lake Ontario, late April–mid-October 2011 at the deep location at specific depths.

The comparative analysis of NARR and land station meteorological data revealed that the directional wind speed and incoming solar radiation differ significantly between the datasets (Figures 7.2). So I ran two case-study simulations combining land station meteorological data with (1) NARR over-land solar radiation and (2) NARR over-land wind speed and direction. The results are presented in Figures 7.9 and 7.10 for the deep and shallow location respectively.
At the deep location, I noticed the early onset of stratification during May 2011 at 1 m and 10 m depths with both NARR solar radiation and wind speed data (Figure 7.9). Hence, RMSEs increased at respective depth profiles compared to RMSEs obtained using land station data. The deeper profiles at 50 m, 100 m, and 180 m depths were not greatly affected by the use of NARR solar radiation or directional wind speed data because these forcings have little influence at these depths.

At the shallow location, the increased value of incoming solar radiation from NARR over-land dataset resulted in early stratification and hence the RMSEs slightly
increased at 1 m and 5 m depths (Figure 7.10). RMSE values did not improve for all depths with the NARR directional wind speed data (Figure 7.10). However, NARR directional wind speed data induced mixing in the water column, especially from September 2011. But this wind-mixing could not replicate the observed mixed water column with a high temperature of ~15-20°C.

7.2.2 Simulated Surface Temperature Profiles with NARR Over-Lake Data

Since, the simulated vertical temperature profiles using NARR over-lake data matched the observed profiles better than the simulated profiles using NARR over-land data, I analyzed surface temperature profiles in 3 buoy locations (locations shown in Figure 5.8) using NARR over-lake data from late April to mid-October. The simulated surface temperature profiles using NARR over-lake data were compared to the simulated profiles using land station based data and observed profiles (Figure 7.11) at two nearshore locations: WG (25 m deep) and PWP (74 m deep) and at one offshore location: 20NMB (140 m deep). All temperature profiles were simulated with the updated vertical mixing parameterization scheme.
Overall the simulated temperature profiles using NARR over-lake data matched the observed profiles better compared to the profiles using land station based data. For nearshore location PWP and offshore location 20NMB, RMSEs decreased to 1.61 and 2.05°C respectively, from RMSEs of 1.85 and 2.41°C obtained using land station based data. For nearshore location WG, RMSE was 1.97°C obtained using NARR over-lake data which was slightly higher than the RMSE of 1.87°C obtained using land station based data. I observed in the simulated surface temperature profiles using land station based data that from September 2011, the temperature profiles were under-predicted in all three buoy locations when the lake was getting mixed again. With NARR over-lake
data, the simulated temperature profiles particularly improved from September 2011 except for a few instances at WG and 20NMB in October 2011.
CHAPTER 8:
CONCLUSIONS

This thesis discusses improvements to the EFDC model for simulating temperature profiles and exploring the thermal behavior of Lake Ontario, including spring mixing, thermal bar evolution, and summer stratification. Simulated lake temperature profiles were substantially improved using new evaporation and vertical mixing algorithms and parameter calibration.

The EFDC Lake Ontario model was improved with a new evaporation algorithm following Quinn (1979) and Croley (1989) because EFDC’s original evaporation algorithm yielded anomalous evaporation rates and latent heat fluxes. The simulated surface temperature profiles were notably affected by anomalous latent heat fluxes. The updated evaporation algorithm corrected the computation of latent heat flux and an over-lake adjustment for wind speed improved the accuracy of the estimated evaporation (condensation) process. This update is recommended when EFDC is used to simulate similar lakes.

Lake Ontario is a mesotrophic lake, and appropriate solar radiation attenuation coefficients must be specified to ensure accurate solar radiation absorption by the water column. In this study, solar radiation attenuation coefficients specifically applicable for
Lake Ontario were computed based on TSS and chlorophyll-a concentrations and are 0.3/m (spring, April-May) and 0.5/m (summer, June-July) for $\beta_f$.

A sensitivity analysis was performed on solar radiation attenuation coefficients, horizontal mixing coefficients, and background values of vertical mixing coefficients using the Parameter Estimation Software PEST. Calibrated values of solar radiation coefficients were similar to initially computed values. Reasonable values were set for horizontal mixing coefficients although the model proves to be minimally sensitive to horizontal coefficients.

With the improvements summarized above, the Lake Ontario model performed well when the lake was in the mixed phase (especially during the thermal bar evolution period from April to late May). The RMSEs for vertical profiles were below 0.5°C (late April to late May 2011). The model captured surface temperature profiles with RMSEs of 0.5 to 2°C for the simulation period of April 4th through July 31st, 2011. Lake-wide surface temperatures were compared to data from satellite images from NOAA and the temperature differences between the two sets ranged from 0.5 to 1°C when the lake was in the mixed phase (thermal bar evolution period).

Because the model accurately simulated temperature profiles during the mixed phase (late April to late May 2011), thermal bar formation was explored nearshore. The simulated thermal bar showed the expected characteristics: a thoroughly mixed water column at 4°C, stationary from days 113 to 119 (April 23rd to 29th) at shallow location SP, two-phase thermal-bar progression rate, surface flow convergence towards the thermal bar, and decreased horizontal eddy viscosity during the thermal bar period.
The model including the improved evaporation scheme and calibrated solar radiation attenuation parameters still failed to closely capture the summer temperatures when the lake transitioned to the stratified phase (late May/early June and onward). Thermocline formation was not well captured in the simulated vertical profiles, highlighting the need for an improved vertical mixing scheme.

Deviating from EFDC's original Mellor-Yamada (1982) vertical mixing scheme, I added a new eddy diffusivity parameterization following Vinçon-Leite et al. (2014), and eddy viscosity parameterization following Pacanowski and Philander (1981). Eddy diffusivity parameterization plays a key role in temperature transport and vertical stratification. The formulation of eddy diffusivity by Vinçon-Leite et al. (2014) is primarily based upon the lake’s thermal structure, which is used to identify the depth of the thermocline. Different formulations were used for the eddy diffusivity above and below the thermocline. In addition, convective velocity was included in the surface friction velocity computation to incorporate convective mixing in the water column after day 235 (August 24th), 2011.

With the newly implemented vertical mixing parameterization, the model captured the summer thermal stratification with thermocline formation from late May to mid-October 2011. Simulated temperature profiles matched observed profiles well for the deep (DP, 180 m) location, with RMSEs of 0.6-1.6°C. The model captured the thermocline formation at the shallow (SP, 19 m) location, with higher RMSEs of 1.25-3.7°C. The model could not replicate the thoroughly mixed water columns at SP with ~15-20°C during September 2011. The inclusion of convective velocity mixing term
from day 235 (August 24\textsuperscript{th}) was able to thoroughly mix the water column at SP during September 2011 but at a lower temperature than observed. The improved EFDC model simulated overall surface temperature profiles well from late April to mid-October 2011, with RMSEs of 1.85-2.41°C at three buoy locations over Lake Ontario.

The model was forced with 10 stream/tributary flows surrounding Lake Ontario in addition to Niagara River inflow to supply additional heat source. This shifted the simulated vertical profiles at SP to higher temperatures. However, I suggest the model would benefit from the integration of surface runoff with appropriate temperature from a hydrology model.

The model was further augmented with meteorological forcing data from NARR regional climate model. Comparative analysis of simulated temperature profiles using NARR and land station data would provide a baseline for future coupled climate-lake model. Vertical temperature profiles using NARR over-lake data were simulated better compared to the profiles using NARR over-land data. Simulated vertical profiles at DP and surface temperature profiles using NARR over-lake data matched observed data better than the simulations forced by land station based data. RMSE values for surface temperatures using NARR over-lake data were 1.61-2.05°C, as compared to 1.85-2.41°C for land station based data. This improvement is because of the over-water effect of the meteorological parameters (e.g. air temperature, relative humidity, solar radiation and wind speed) and 16 evenly distributed grid points over the lake.

NARR solar radiation and directional wind speed showed a significant difference in magnitude in the comparative study to land station based data. However, use of (1)
NARR solar radiation, and (2) NARR directional wind speed with other meteorological forcing data from land stations did not improve the simulated temperature profiles.

NARR directional wind speed induced more mixing in the water column at SP but failed to replicate the thoroughly mixed water column as observed at SP.

Overall the EFDC Lake Ontario model was significantly improved in simulating temperature profiles by (a) updating the evaporation algorithm following Quinn (1979) and Croley (1989) (b) specifying appropriate solar radiation attenuation coefficients, and (c) updating the vertical mixing scheme following eddy diffusivity parameterization by Vinçon-Leite et al. (2014) and eddy viscosity parameterization by Pacanowski and Philander (1981).

Over-water meteorological forcing data from more buoy locations over Lake Ontario would be conducive to improve simulated temperature profiles. I could not continue the simulation to winter months because this version of EFDC is not equipped with an ice submodel. So this study has scope to provide more information about the thermal behaviors of Lake Ontario if these limitations are overcome in the future.
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