New Methodology and Analysis of Determinants for Mixed Layer Depth

-- a Case Study in the Salish Sea

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Abstract

A new method, based on the minimum of the first derivative of Brunt–Väisälä frequency and two Quality indices, is established to find Mixed Layer Depth (MLD) from ocean profiles. Unlike previous methods that analyzes the oceanic profiles with a single proxy parameter (temperature, salinity, density etc.), the new method uses a conceptual metric that physically describe stability dynamics of MLD. The algorithm also ensures MLD quality by directly using a quality index (QI) and introducing a second quality index (QI2). The new method is evaluated in the Salish Sea, using CTD profiles from the Pelagic Ecosystem Function (PEF) program and Salish Cruise. By visual inspection comparing with other methods, the new method can identify an accurate Mixed Layer Depth in 90.4% of PEF profiles and xxx% Salish Cruise Profiles. To study the dominant factors of Mixed Layer Depth in Salish Sea, oceanographic variables were calculated from the same CTD profiles, and atmospheric variables were obtained from ERA5 reanalysis product. The correlation coefficient and p-value between the variables and Mixed Layer Depths show that Salinity and Wind are the most controlling factors in San Juan Archipelago with PEF profiles; Wind and salinity are still the two most dominant determinants in each sub-region, with temperature playing a relatively more important role than in the PEF study area. However, different wind components and salinity components are dominant in different sub-region as a result of the highly dynamic and diverse system in Salish Sea.

Key words: Mixed Layer Depth, stability, buoyancy frequency, Salish Sea, factors
1. Introduction

Mixed Layer (ML) is a worldwide well-mixed layer, and commonly refers to the near-surface mixed layer. Corresponding to the literal name, Mixed Layer is characterized by vertical well-mixing processes, with ocean tracers almost uniformly distributed in the water column. The Mixed Layer Depth (MLD) is defined as the bottom of the mixed layer, where mixing status below the MLD is distinct from the mixed layer. The Mixed Layer formation starts from the transmission of atmospheric fluxes into the ocean, where winds and heat loss further drive vertical ocean mixing (CHERESKIN & ROEMMICHI, 1991). Energized by atmospheric motions, the vigorous turbulent mixing state is maintained by horizontal momentum and vertical buoyancy fluxes (Lorbacher et al., 2006).

The Mixed Layer gains attention attributed to its significance to the climate system, ocean trend in mixed layer budget, and oceanic ecosystems. As the layer interacting with the atmosphere, the thickness of mixed layer corresponds to the storage of heat, dissolved gas such as carbon dioxide, and mechanical inertia in the ocean. Most biological activities are restricted to the euphotic zone, where the mixed layer depth is a key component in determining the net productivity of the surface ocean ecosystem. Therefore, the mixed layer depth is critical in understanding surface ecosystem dynamics (Carvalho et al., 2017). What’s more, mixed layer depth is a key factor of surface-deep ocean transport processes such as the biological pump and the solubility pump, which determines the strength of ocean mitigation against climate change (Primeau, 2005).

Despite the significance, the surface turbulent mixed layer depth shows highly temporal and spatial variation – In some places, heat exchange in winter could drives deep ocean circulation that pushes mixed layer depth to even 2000 meters; while in summer the water column could be
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highly stratified with no mixed layer depth (Marshall & Schott, 1999). What’s more, the turbulent mixing signal are often interfered by the complicated processes in ocean surface, making it hard to identify mixed layer depth. There have been numerous methods invented to estimate mixed layer depth, some of which have been proved to be precise in most cases. And considering that the importance of mixed layer depth has been widely recognized, new methods keep being published.

The most common, also the simplest, methods are categorized as threshold method. These methods, using either temperature or density profiles, search for the depth with a pre-defined threshold change relative to the surface (Holte & Talley, 2009). In global scale, the optimal temperature threshold was 0.2 °C, with a corresponding optimal density threshold of 0.03 kg/m³ (de Boyer Montégut, 2004), when the reference depth is 10m without diurnal cycle impact. Similarly, the gradient methods use a pre-defined value as the threshold for critical slope value to find mixed layer depth. The current optimal density gradient values are 0.0005 and 0.001 kg/m⁴, or within the range from 0.0005 to 0.05 kg/m⁴ (Brainerd & Gregg, 1995; Dong et al., 2008).

However, both the threshold and gradient methods require a pre-defined constant. As one single threshold is almost impossible to cover ocean profiles in all the places nor all the time, later research turns to more complex methods to improve the prediction accuracy. The curvature method uses second derivatives to identify the ‘curve’ (Lorbacher et al., 2006). And the method using linear Optimal Linear Fitting(OLF) and maximum angle was developed to deal with noisy profiles (Chu & Fan, 2010, 2011), which was later improved with Exponential leap-forward gradient method with shannon information entropy (Chu & Fan, 2017). And the method with maximum of buoyancy frequency was showed to be better in describing the mixing of chlorophyll (Carvalho et al., 2017).
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Despite so many brilliant and precise methods, most of them are still using one physical property as a proxy to describe the ocean mixing state. Here we’d like to provide a method that finds mixed layer depth by directly describing the mixing state and stability, and hopefully this could be a prompt for future work. The method starts from the physical definition of mixed layer -- the surface layer with turbulent mixing, or in other word, mixing below the layer is not as active. And mixed layer depth, as the boundary of active mixing and not-mixing, is the depth at which stability changes fastest. Therefore, we use the current optimal density threshold method of 0.03 kg/m³ to ensures the existence of mixed layer depth; the local minimum of first derivative of buoyancy frequency to find the fast-stability change layer; and the mixed layer depth quality index (QI) and other constraints to find the best mixed layer depth. And with CTD profiles from Pelagic Ecosystem Function program and NVS Salish Cruise in 2004-2021, we examined the method in Salish Sea. With intricate network, river input, and tidal mixing, it becomes an ideal test region for its ability to simulate various type of coastal situations.

This study also analyze the driven physical factors of mixed layer depth in each sub-region of Salish Sea with the new method, which could provide more insight into the dynamic of mixed layer depth and other hydrological processes in the Salish Sea region. With the same CTD profiles in 2004-2021, a regional model data in 2017-2021, and ERA5 reanalysis product in 2004-2017, we analyzed the importance of some potentially related factors – temperature, salinity, wind, and heat flux.
2. Data and Methods

2.1 Study Region

Salish Sea located in British Columbia Province of Canada and Washington State of United States (Figure 1a). Salish Sea covers about 18,000 square kilometers surface area, mainly composed of Georgia Strait, Strait of Juan de Fuca, Puget Sound, and other water bodies. The average depth of the study region is around 130 meters, with a maximum depth of 670 meters. Major rivers discharging into Salish Sea -- Fraser River, Skagit River, and Snohomish River – contribute to an overall mean discharge rate of more than 4500 m³/s. The seasonal change of river discharge rate and tidal strength create a variational salinity gradient. Combining with sophisticated topography, the intricately connecting channels, seasonal varied river discharge, and diurnal tidal activity, different mixing profiles could be observed in Salish Sea, which makes it an ideal region to study mixing.

2.2 Data

This study utilizes four datasets: (1) Pelagic Ecosystems Function Research Apprenticeship program (PEF) CTD profiles of San Juan Archipelago in 2004-2021; (2) NVS Salish Cruise CTD profiles of Strait of Juan de Fuca and Puget Sound in 2004-2021; (3) LiveOcean regional model oceanic and atmospheric variables in 2017-2021; (4) ERA5 reanalysis product atmospheric variables in 2004-2021.

PEF program has been held every year from September to December in Friday Harbor Laboratory (FHL) since 2004. In each year, there are six cruises arranged among the weeks of fall transitions. And during each cruise, Seacat Model SBE-19 CTD are deployed for oceanic profiles at several stations. During the 18 years, in total 14 stations are sampled (Table 1), only 5
stations (A B C N S) have more than 10 samples (Figure 1b), and only the north station
(48.583N, -123.043W) and the south station (48.420N, 122.943W) have been sampled
continuously each year.
NVS Salish Cruise program has been collecting data seasonally in 58 stations that spread over
Strait of Juan de Fuca, Puget Sound, and Washington Coast since 1998 (Figure 1a). Providing
thousands of CTD profiles, Salish Cruise data is extremely valuable for studying the highly
dynamic and various water properties in Puget Sound. In addition, the data of Salish Cruise
covers water bodies with different degrees of mixing in different seasons of the year, which
provides both spatial and temporal insights.
LiveOcean is a regional model developed by Parker MacCready and UW modelling groups with
hourly data available from 2017. In the study region, LiveOcean provides a 500m horizontal
resolution oceanic and atmospheric data for all variables required in this study. And for 2004-
2017 atmospheric data, we use ERA5 reanalysis product with 0.25 degrees resolution.

2.3 Mixed Layer Depth Estimation
We developed the method to estimate mixed layer depth from the definition – in an ideal model,
above the MLD is a turbulent mixing layer, with relatively low stability; and below the MLD is a
non-mixing layer of stratification, with relative high stability; and the MLD is expected to be the
depth at which stability changes fastest. The Brunt–Väisälä frequency, also known as buoyancy
frequency (Equation 1), is used to quantify stability against vertical displacement:

\[ N_z = \sqrt{-\frac{g}{\rho} \frac{d\rho}{dz}} \]  
\[ (e.q. 1) \]

At any given depth, \( z \) is the geometric height, \( \rho \) is potential density, \( g \) is the local acceleration of
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gravity. As the average depth of the study region is only 130 meters, the gravitational acceleration is assumed to be constant with depth.

The method also includes mixed layer depth quality index (QI) (Equation 2):

\[
QI_{mix} = 1 - \frac{\sigma(\rho_n - \bar{\rho})_{(h_{ref}, h_{mix})}}{\sigma(\rho_n - \bar{\rho})_{(h_{ref}, 1.5 \times h_1)}}
\]  
(\text{e.q. 2})

Where \(h_{ref}\) is the reference depth, \(h_{mix}\) is the mixed layer depth, \(\sigma()\) stands for the standard deviation from the vertical mean of \(\bar{\rho}\) from reference depth to the MLD or \(1.5 \times MLD\), respectively (Lorbacher et al., 2006), where potential density here is equal to density minus 1000. Regarding QI values, the calculated MLD could be categorized as well-defined (\(QI_{mix} > 0.8\)), uncertain (\(0.5 < QI_{mix} < 0.8\)), and not-existent (\(QI_{mix} < 0.5\)) (Lorbacher et al., 2006).

The QI normally is used to evaluate MLD estimates, but here we use it as a tool to determine the best MLD in each profile by filtering out the fast stability change depth that poorly estimate MLD. Here we expanded the QI definition to accommodate shallow MLD – when the MLD is close to the reference depth, there could insufficient points in the mixed layer for the standard deviation calculation, which could lead to biased QI value. Therefore, we assume that when MLD is shallower than a 5-meter threshold, the reference depth will be set to the surface:

\[
QI_{mix} = \begin{cases} 
1 - \frac{A_1}{A_2} = 1 - \frac{\sigma(\rho_n - \bar{\rho})_{(h_{ref}, h_{mix})}}{\sigma(\rho_n - \bar{\rho})_{(h_{ref}, 1.5 \times h_1)}}, & MLD \geq 5 \\
1 - \frac{A_1}{A_2} = 1 - \frac{\sigma(\rho_n - \bar{\rho})_{(0, h_{mix})}}{\sigma(\rho_n - \bar{\rho})_{(0, 1.5 \times h_1)}}, & MLD < 5 
\end{cases}
\]  
(\text{e.q. 2a})

(\text{e.q. 2b})

To ensure that the standard deviation was from the reference depth to \(1.5 \times MLD\) is mainly attributed to the stratification below MLD, rather than the difference of average value between the two layers, here we propose a Second Quality Index (QI2) (Equation 3)
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\[ Q_{I2} = \frac{\sigma(\rho_n - \bar{\rho})|_{h_{ref},h_{mix}}}{\sigma(\rho_n - \bar{\rho})|_{h_{mix} - 1.5 \times h_t}} \]  

(e. q. 3)

We also assume that for a well-defined MLD, the QI2 should be no larger than 1, or that the variation within the mixed layer should be clearly smaller than the layer below.

Using the concepts introduced above, logic of the method is presented below:

2.3.1 Reference Depth and Data Smoothing

For reference depth, the 10 meters value was applied when estimating for the global ocean to avoid strong diurnal cycle (de Boyer Montégut, 2004). In estuaries with an average depth of 130 meters, highly stratified and shallow mixing cases are expected to be frequent. But it is pointed out that only top 2 meters data in CTD profiles are noisy and should be excluded in Puget Sound (Moore, Mantua, Kellogg, et al., 2008; Moore, Mantua, Newton, et al., 2008). Therefore, we choose 2 meters as the reference depth in this study.

To remove extra noise, we choose to smooth CTD-derived potential density, numerically calculated buoyancy frequency and its first derivative (Moore, Mantua, Newton, et al., 2008).

2.3.2 Determine mixing state

In a shallow water body like Salish Sea, extremely strong forcing whole water is capable of turbulently mixing the whole water column. However, looking for relative stability change, our method could not tell if the water body is well-mixed or not. Therefore, a threshold is required to indicate the mixing state. Here we use the optimal density threshold of 0.03 kg/m$^3$ (de Boyer Montégut, 2004) -- If the potential density range below the reference depth is smaller than the threshold, there will be no need to go through all the process below, with the MLD set to be the deepest depth in this profile.

2.3.2 Find local minimum of first derivative of buoyancy frequency
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After compiling the buoyancy frequency profile using the smoothed potential density profile and equation 1, we defined buoyancy frequency at the unstable depth -- where there is a positive density gradient in z direction and complex buoyancy frequency -- to be the mode of its value. Then the first derivative of buoyancy frequency is calculated numerically with backward propagation (Equation 4):

\[
\frac{\partial N}{\partial z} \bigg|_{z_1} = \frac{N_{z_1} - N_{z_2}}{z_1 - z_2}
\]

where \( z_1 \) is the shallower iterative depth, \( z_2 \) is the deeper iterative depth, \( N_{z_1} \) and \( N_{z_2} \) are the buoyancy frequency at \( z_1 \) and \( z_2 \) respectively. In this study, we define a local minimum, or a local peak, as data sample that is either larger than its two neighboring samples or is equal to infinite. With this method, we find all the local minimum of buoyancy frequency, and where local stability changes fastest in the shallower depth direction at these depths. Then we filter out those local minimums at which buoyancy frequency is negative or the first derivative of buoyancy frequency is positive.

**2.3.3 Use the two Quality Indices to find MLD**

We first filter out the local minimums with a corresponding QI2 value (Equation 3) bigger than 1. Then we calculate the QI (Equation 2) to determine the final mixed layer depth. For profiles that have local minimums with highest QI that is bigger than 0.8, we define the one with the smallest first derivative of buoyancy frequency as the MLD. For profiles with highest quality index that falls in the range from 0.5 to 0.8, we choose the one with maximum QI value as mixed layer depth. For profiles with highest QI that is smaller than 0.5, we define MLD as the shallowest depth in this profile, and marked it as ‘highly-stratified’.

**2.3.4 Define highly stratified**
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If the final MLD is within the reference depth $MLD < h_{ref}$, we define the station as highly-stratified. This is because water above the reference depth should be turbulent and noisy, thus any MLD above it should be viewed as invalid.

2.3.5 Evaluation

We use visual inspection to evaluate the method: For each profile, we plot the density profile, the calculated MLD from the method we proposed in this paper, the MLD from 0.03 kg/m$^3$ density threshold method, the MLD from maximum buoyancy frequency method, the MLD from 0.2 °C temperature threshold method, and several random lines as ‘additional methods’. To ensure the objectiveness, we asked 5 oceanography students from the University of Washington and 2 atmospheric science student from the Ocean University of China to help to identify ‘Best Method(s)’ from their perspective from 1546 profiles – they could choose none, one, two, or any combinations of methods. Then we statistically analyze the results to find which methods could make the best estimations.

2.4 Analyze Dominant Factors

2.4.1 Study Region Division

For PEF stations, we conduct an integrated analysis for all available profiles and subordinate analysis for each station where there are more than 10 available stations. For Salish Cruise stations, different hydrological properties are expected between stations in each Puget sound sub-basin, between stations in Puget Sound and Strait Juan de Fuca, and between stations in the Salish Sea and Washington coast. Due to these spatial differences, it is more reasonable to divide the study region into geographical regions – Washington coast, Strait of Juan de Fuca, Admiralty Inlet, Hood Canal, Main Basin, Whidbey Basin, Central Sound, South Sound. This provides
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more insights into the difference between the region, which is more meaningful than an integrated analysis of the whole Salish Sea.

2.4.2 MLD Factors Derivation and Analysis

For oceanic factors, as the mean depth is 130 meters, we assume a two-layer model – above the MLD is the mixed layer, and below the MLD is the bottom layer. We considered mixed layer average salinity and temperature, bottom layer average salinity and temperature and for atmospheric factors, we calculated the 24-hour-average wind speed and heat flux, as well as different wind components and different heat flux components during the cruise time.

We plotted each factor as independent factors and its corresponding MLD as dependent factors then using regression analysis, determined the R-values and p-values to infer factor importance.
3. Results

3.1 MLD Evaluation Summary

Following the visual inspection procedure, we counted the number of stations that MLD from each method are selected by the volunteers. For PEF, MLD derived from our method was chosen as the ‘best method’ or one of the ‘best method’ from 272 out of 301 profiles, or an equivalent percentage of 91%. While the second ranked method, the 0.03 kg/m³ density threshold method was selected less than 30% of the time (89 of 301 profiles) (Table 1, Figure 2a).

For Salish Cruise, MLD derived from our method was chosen as ‘best method’ from 1068 out of 1204 profiles, or an equivalent 88.7%. The second most selected method, the optimal density threshold method, was selected in 832 out of 1244 profiles (69.1%) (Table 2, Figure 2b).

3.2 MLD Determinant Analysis Summary

Following the analysis procedure, we describe only the factors with P<0.05, whose correlation with MLD are significant. And we classify 3 degrees of significance based on P value ranges: low (0.01<p<0.05), moderate (0.001<p<0.01), and high (p<0.001).

3.2.1 PEF stations

In San Juan Archipelago with all PEF Stations, temperature and salinity in both layers and all wind components -- wind speed, meridional wind that along longitude, zonal wind that along latitude -- show significant correlation with MLD (Table 3). Among all factors, mixed layer averaged salinity has the highest R value (R = 0.32, p < 0.001). For winds, the overall wind speed has a R value 0.191 with MLD, with a moderate significance. Among all wind components, it is the meridional wind that has both the highest R value (0.223), and lowest P value falls in high significance range.
In station A B C, although some factors show relatively high correlation coefficient, but uniformly low significance. In Station N S, correlations between the average salinity in both layers and MLD have either moderate or high significance. And in North Station, the meridional wind shows a relatively high correlation to MLD, with a R value of 0.307 and a moderate significance.

### 3.2.2 Salish Cruise stations

In Washington coast, only zonal wind shows a moderate significance, and the oceanic factors are not significant (p > 0.5), and therefore are not significantly correlated with MLD (Table 4). In Strait of Juan de Fuca, it is the bottom averaged salinity that have the largest R value of 0.403 and the lowest P value falls in moderate significance range. And the bottom average temperature also shows a relatively high correlation (R=-0.388) in moderate significance. What’s more, the zonal wind is also relatively high correlated with MLD with a R value of -0.358 with a moderate P value.

In Admiralty Inlet, the bottom average temperature and salinity are the only significant factor, while both sit in the low P value range. And the R values of the two factors, -0.627 for bottom temperature and 0.625 for bottom salinity, are very high and in a similar value.

In Hood Canal, the overall wind speed (R=0.434) and zonal wind (R=-0.401) are highly significantly relatively-highly correlated with MLD. For oceanographic factors, the bottom average temperature shows a relatively high correlation with R value of -0.307 in the high significance range. And bottom average density has a R value of 0.222 and a moderate P value of 0.0018. And two heat flux components are low correlated with MLD with low R values.
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In Whidbey Basin, only the overall wind speed (R=0.361) and zonal wind (R=-0.299) have moderate R values, which are both highly significant. The correlation between MLD and other significant components, such as surface mean salinity (R=0.140), are all weak.

In South Sound, the mean salinity in both layers have high R values over 0.5 and highly significant P values. The average bottom temperature also presents a relatively high correlation coefficient but in low significance. Similarly, the overall wind speeds (R=0.530) and zonal wind (R=-0.470) are relatively highly correlated with MLD, on high and moderate significance respectively.

While in Central Sound and Main Basin, none of the factors show significant correlation.
4. Discussion

4.1 Difference between the newly proposed method and the curvature method

The curvature method, commonly used to identify MLD, uses the second derivative of either temperature or density profiles to find the shallowest curvature and identify the MLD (Lorbacher et al., 2006). Buoyancy frequency is a function of first derivative of density, so the first derivative of buoyancy frequency also contains the second derivative of density. Similarly, the new method is also not using derivative, and it also shows capability to identify ‘curve’. However, the method proposed in this paper should be considered as a different method from motivation, mathematical expression, and constraints perspective.

4.1.1 Motivation & Approach

First, the motivations for the two methods are completely different. Assuming temperature is uniformly distributed in the mixed layer, the curvature method aims to describe the shape of the depth profile of temperature or density and defines MLD from the curvatures. In comparison, the new method raised in this paper starts from the mixed layer definition perspective by referencing the stability difference indicated by the mixed layer and stratification definition. Finding the curvature is not the purpose, but the inevitable result of the new method – the curvature is where the MLD should be.

Second, the two approaches used to find MLD are also distinct. Targeted in finding the curvature of variable vertical profile, the curvature method estimates MLD by signal analyzing of a proxy, such as temperature and density, of the profile. For the new method, though it also contains the second derivative, the first derivative of buoyancy frequency also has its own physically meaning -- direct description of the mixed layer property relative to stability. Hence, it is not targeted in getting the second derivative of density.
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To summarize, though this new method contains the second derivative of density and is capable to find curvature, this method approaches through definition quantification rather than signal analysis, and the MLD are gained at the curvature as it is where MLD should be at but not because the algorithm targets to find the curvature.

4.1.2 Mathematical Expression

Although buoyancy frequency is a function of the first derivative of density, the relationship is not simply linear. By taking the derivative of buoyancy frequency (Equation 1), we get the mathematically formula of first derivative of buoyancy frequency (Equation 5):

$$\frac{\partial N}{\partial z} = \sqrt{-\frac{g}{4 \frac{\partial \rho}{\partial z} \cdot \rho^3} \cdot \left[ \rho \cdot \frac{\partial^2 \rho}{\partial z^2} - \left( \frac{\partial \rho}{\partial z} \right)^2 \right]} \quad (e. q. 5)$$

Although the second derivative of density is a major component in the first derivative of buoyancy frequency, the contribution from other components is non-negligible theoretically. Therefore, the complicated relationship support that the first derivative of buoyancy frequency is different from the second derivative of density based on the mathematically derivation.

4.1.3 Constraint

After finding the potential MLD, the curvature method chooses the shallowest depth curvature as the MLD. In comparison, our method applies two quality indices to find the best MLD, ensuring the quality of the chosen MLD.

4.2 Importance of Second Quality Index (QI2)

From equation 2 and 3, both quality indices are a measure of the ratio between standard deviation in the mixed layer and the layer including stratification. If so, what is the difference between the quality indices? Why do we need QI2? And could one cover the other by altering its
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thresholds? To simplify illustration, we hereinafter use ‘mixed layer’ to refer to the layer from reference depth to MLD, and ‘1.5 mixed layer’ refers to the layer from reference depth to 1.5 times MLD.

4.2.1 Issue Identification and Introduction of QI2

With the selection using only QI (Equation 2), the method is capable of picking MLD close to visual inspection. However, volunteers reported the derived MLD are ‘in the middle of stratification’ and are deeper than their estimation. When invented, the QI was used to find depth above which has ‘quasi-homogeneous properties’, and below which ‘property variance increase rapidly’ (Lorbacher et al., 2006). And using standard deviation ratio is an effective way to quantify this property. Nevertheless, when including the stratified layer below, the mean property value in 1.5 mixed layer will deviate from the mean property value in the mixed layer. Therefore, the larger standard deviation in the 1.5 mixed layer than in mixed layer is partly, but not sure how much degrees, contribute to the standard deviation ‘inflation’ from mixed layer depth points. This uncertainty also leads to instability of MLD quality, which potentially leads to larger QI values. Thus, the MLD could become a ‘moderate’ one even resides clearly deeper than MLD inside the stratification layer (Figure 3).

Therefore, the QI2 is introduced. Using the standard deviation of the layer from MLD to 1.5 times MLD in the denominator, the QI2 directly compare the variance in and below the mixed layer. After ensuring the standard deviation in the 1.5 mixed layer is mainly attributed to the variance below the MLD, the local minimum inside stratification layer could be filtered out before QI selection.

4.2.2 QI and QI2
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Despite the necessity of the QI2, it is a question that if the QI could be manipulated, such as changing or adding more threshold, to include the QI2 or vice versa. It might counter-intuitive that the two quality indices are inextricable – the standard deviation is calculated relative to the expected mean value, where the change of mean and the subsequent each components change are unpredictable. To give a more straightforward example, the correlation coefficient between all Quality indices and second quality indices is only -0.11 in PEF stations, denoting that the two quality indices are not linearly correlated. What’s more, QI2 not only works in low QI stations or high QI stations. For example, in the 2008 Oct 12 South station, QI value as high as 0.65, and QI2 value was only 1.2, while in the 2008 Oct 02 O station, QI value is as low as 0.5081, and QI2 value as high as 2.37.

To summarize, there appears to be no clear relationship between the quality indices, and using QI alone is insufficient for reliable MLD determination. Therefore, it is necessary to introduce a complementary QI2 to ensuring the accuracy for identifying MLD.

4.3 New Method - Issues, Limitations and Potential Improvements

From table 1 and table 2, the new method, though works for most of the situations, are still not considered the ‘best’ or ‘most accurate’ in some profiles. And in this section, we will propose some internal issues of the method, related limitations that leads to the inaccuracy, and further potential improvements.

4.3.1 Empirical Constants – Reference Depth and Well-mixing Threshold

Even though trying to avoid pre-defined empirical thresholds, the method in this paper still includes some constants derived in previous works statistically.
First, the well-mixing determination applies the optimal density threshold of 0.03 kg/m$^3$ (de Boyer Montégut, 2004). As our method find the relatively fast stability change depth, a pre-method check of the mixing status is necessary to ensure that the potential stratification could resist at least some degree of interference. Therefore, we use the optimal density threshold – if the density threshold could not identify a MLD in the profile, no MLD should be expected. Although being optimal, the 0.03 kg/m$^3$ threshold is derived from empirical and statistical summary, which leads to biases and errors in at least some cases. For instance, when the profile density range is only slightly larger than the threshold, the ‘best’ MLD derived from our method are often biased.

The other empirical constant leading to issue is reference depth. Used in both local minimum hunting and quality indices calculation, reference depth is a critical but arbitrarily decided constant. This study once set reference depth to 5 meters, where the derived MLD from every method present non-negligible difference from the current MLD derived from a 2 meters reference depth. Reference Depth choice is particularly important in this study because the limitation resides in both quality indices, where the layers property standard deviation plays a major role. Therefore, when local minimum depth is close enough to the reference depth, the insufficient data could make the quality indices biased. Even though we could include the noisy and turbulent layer above reference depth, it could lead to other issues.

Lastly, the quality indices thresholds are also chosen arbitrarily. Although the current threshold is reasonable, more efficient and proper thresholds are always helpful.

To summarize, the two empirical constant, well-mixing threshold and reference depth, leads to the method malfunctioning in some extreme situation of near well-mixed and highly-stratified samples respectively. Future research should pay more attention on not only determining more
accurate empirical values, but also how to theoretically derive a reasonable value from individual profiles.

**4.3.2 MLD Evaluation with Visual Inspection**

As an evaluation method, visual inspection could lead to biased statistically result. First, evaluation by human decisions can easily become subjective. In this study, although the volunteers are not informed about the exact MLD methods, the colors for each method are not switched frequently. Therefore, the evaluators might assume a ‘best’ method (with a certain color) based on the previous profiles in their subconsciousness, and consequently prefer that method in later profiles. What’s more, volunteers could have their own preference for a certain color, leading to more frequent choice of a certain method.

Second, we asked the volunteers to ‘choose the best MLD(s) based on your estimation from density profile’ – in a single profile, there could be a best MLD, two equivalently good MLD, or no good MLD estimation. However, besides the ‘best prediction’, other methods predictions could still be relatively accurate with small error. Nevertheless, volunteers report that they are sometimes reluctantly to choose those ‘moderately good but not very accurate’ MLD when there is an extremely accurate one. Also, one volunteer says he is more willingly to choose two methods when they are visually stacked rather than close in distance. This is particularly obvious when evaluating Salish Cruise Stations in Puget Sound, where most of profiles have shallow MLD and most methods predictions are visually near surface. Another method for evaluation is to estimate exact MLD during visual inspection (Holte & Talley, 2009). Despite needing an additional evaluation method, this could greatly decrease the subjectiveness in the result. Therefore, a more objective and statistically scientific method is need for evaluation in future research.
4.3.3 Potential Application for Deep Mixed Layer

Although developed for finding surface mixed layer depth, the new algorithm internally finds the boundaries of different layers. Therefore, the new algorithm could also be used to find the deeper mixed layers – the layer between two fast stabilities change depth and is relatively low in standard deviation. To achieve that, we need to find both the local minimum and maximum and change the quality indices to focus on a certain layer. With similar procedures, the sub-surface mixed layer and its boundaries could be identified.

4.4 MLD Comparison for Factor Analysis

Before analyzing the significance of MLD factors, this part will compare the MLD derived from the new method and the most commonly used optimal methods with ANOVA, which could help determine if using the new method MLD for factor analysis is convincing. And to compare with new method MLD, we choose the MLD from 0.03 kg/m³ density threshold method, the MLD from maximum buoyancy frequency method, and the MLD from 0.2 °C temperature threshold method. Although not flawless, the optimal methods have been tested accurately in most of cases (de Boyer Montégut, 2004) and have been recognized as good method world-wide. We evaluate our new MLD method to make sure it performs at least as well as these published optimal methods.

Figure 4a shows the ANOVA and Multi-comparison result from PEF CTD profiles. And the t-test only can’t reject the null hypothesis, that the two categorized are different, between the 0.03 kg/m³ optimal density threshold method and the new method. As the P value is 0.0847, the MLD derived from the two methods are though similar, but with considerable difference. And the
correlation coefficient between the MLD derived from the two methods are as high as 0.69, further support the similarities of the two groups of MLD.

Figure 4b shows the ANOVA and Multi-comparison result from Salish Cruise CTD profiles. And the t-test also only can’t reject the null hypothesis of between the 0.03 kg/m$^3$ optimal density threshold method and the new method. Nevertheless, this time it shows a P value as high as 0.9956. This is because most of Salish Cruise stations are highly stratified, and both methods are expected to predict MLD in a shallow depth range. The average MLD of the 1204 stations is only 3.92 meters from density threshold method, and 4.18 meters from new method (Table 5), where both methods predict MLD mostly near the surface (Figure 5). Nonetheless, the correlation coefficient between MLD derived from the two methods are only 0.27, and the standard deviation of new method (7.78) is clearly larger than the standard deviation of the optimal density threshold method (1.85), which is attribute to a few outliers of very deep MLD from new method.

To summarize, the new method MLD are not significantly different from the optimal density threshold MLD, especially in profiles with significant stratification and shallow MLD, which is supported by the Salish Cruise Evaluation results. Therefore, it is convincing to use new method MLD for factor analysis.

4.5 MLD Factor Analysis

4.5.1 San Juan Archipelago

When analyzing all San Juan Archipelago with all PEF stations, meridional wind and mean salinity features are showed to be significantly correlated with MLD (Table 3).
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For the oceanic factors, there are significant correlations between MLD and mean salinity in both the surface mixed and bottom layer, which is consistent with the prediction – sitting at the convergence of Georgia Strait and Strait of Juan de Fuca, the hydrological properties in San Juan archipelago are impacted by both the currents with oceanic properties and the Fraser River discharging with riverine properties. What’s more, the diurnal tidal, the topography, and the narrowing Cattle point contribute to the different degrees of mixing in the PEF profiles. And MLD most significantly correlates with mean salinity of surface mixed layer in North Station and of bottom layer in South Station – because the north station is located in the San Juan Channel, which is more susceptible to Fraser River discharge from surface layer; and the south station resides south of Cattle Point and closer to the Strait of Juan de Fuca, where ocean currents bring more oceanic water from Washington coast.

For the atmospheric factors, despite impact MLD through the universal wind-drive mixing, meridional winds also determine freshwater transportation from Fraser River. Therefore, when meridional winds blow northward, freshwater transport to San Juan Archipelago is impeded, and the north station will be better mixed with a deeper MLD. Therefore, the correlation between meridional wind and MLD is positive.

4.5.2 Salish Cruise Stations

Although spread from Puget Sound to Strait of Juan de Fuca to Washington Coast, some of the sub-regions covered by Salish Cruise still have some common features – overall wind speed, zonal wind speed, and bottom mean properties show uniformly significant correlation with MLD.

For the oceanographic factors, most of the sub-regions show significant correlation between the mean bottom layer properties with MLD. Admiralty Inlet directly connects Strait of Juan de Fuca
and Puget Sound, whose narrow width leads to extremely active mixing by the diurnal tidal currents. Therefore, the degree of mixing and MLD are highly susceptible to seawater property changes, which lead to highest correlation coefficient in this study; Similarly, Eastern Strait and Strait of Juan de Fuca are also highly oceanic, therefore, correlates better with bottom layer average properties; The South Sound or South Basin have significant strong correlation with mean salinity in both mixed layer and bottom layer, because the considerable river input and also non-negligible oceanic mixing. The oceanic feature in the South Sound could be largely attributed to the two Stations near the Tacoma Narrow, which actively mixing the passing water. Hood Canal is relatively special, which is more significantly and more strongly correlated with bottom layer mean temperature than bottom layer mean salinity. Hood Canal is a fjord and doesn’t have as much river input as other sub-basins of Puget Sound, leading to a slow turnover time. Therefore, Hood Canal is relatively calm and is more susceptible to oceanic changes; For Whidbey Basin, we predicted that the surface layer mean salinity would be a dominant factor, based on the importance of Skagit river. However, it is only a moderate significant factor with a relatively low P value of only 0.140. This might be due to the fact that most of the Salish Cruise Station in Whidbey Basin lies in the Saratoga Passage, rather than near Port Susan where Skagit river directly discharge into.

For the atmospheric factors, the overall wind speeds and zonal wind are significantly correlated with MLD in some sub-regions. The importance of overall wind speed is expected due to its role in driving mixing, while we failed to predict the high zonal wind correlation with MLD. Zonal wind is a significant factor in every sub-region where overall wind speed is important; and in Strait of Juan de Fuca and Washington Strait, zonal wind is even a more significant and stronger factor than the overall wind speed, where zonal wind lines up with the Strait of Juan de Fuca.
Therefore, we hypothesized that this is attributed to the zonal wind function in driven oceanic water into Salish Sea, which is similarly to the meridional wind role in driven Fraser river fresh water to PEF North Station.

4.6 Limitations and Potential Improvements in MLD Factor Analysis

4.6.1 Data

In this study, none of the oceanic or atmospheric data is comprehensive:

For oceanic data, the analysis in San Juan Archipelago is not completed as the PEF program only provides data in fall. Although including the fall transition with changing properties each year, it is still limited for analyzing factors with highly seasonal variation, such as temperature. And Salish Cruise data, though collected in different seasons each year, will be better if stations are sampled more frequently. And it will be helpful if there are more stations in some sub-region such as Whidbey Basin Port Susan and South Sound.

For atmospheric data, the ERA5 reanalysis product has a relatively coarse resolution of 0.25 degrees compared to diverse hydrological properties in the study region. This might lead to biased factor analysis in this study.

Therefore, the next step of the MLD factor analysis should find data with higher spatial and temporal resolution, and we plan to use the oceanographic and atmospheric variables in LiveOcean model for a more comprehensive analysis.

4.6.2 Method

This study uses correlation coefficient and corresponding P-value to study the factors relationship. Nevertheless, not all factors are linearly correlated with MLD. What’s more, one factor might have a significant P value because it has the same trend with a true MLD factor, but
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it doesn’t relate to any physical processes that impact MLD. Therefore, a more scientific and more comprehensive analysis method is needed for future studies. And we plan to start with Principle Components Analysis (PCA) that was used in previous studies (Moore, Mantua, Newton, et al., 2008).

4.6.3 Tidal Impact

Tidal current is a potentially dominant MLD factor in short timescale, which not only directly related to turbulent mixing but also plays a significant role in water transportation. Therefore, how tide impacts and relates MLD will be an interesting topic for future study.
5. Concluding Remarks

To summarize, this paper presents a new methodology that found that Mixed Layer Depth from the stability dynamics perspective with buoyancy frequency and two quality indices. And it works well in 89.04% of all profiles in the study region. The MLD values are consistent with the optimal density threshold method of 0.03 kg/m³, especially in thin mixed layer profiles with MLD near reference depth. This paper also shows salinity and wind are the two dominant factors determining MLD in the study region. In San Juan Archipelago, meridional wind and both surface and bottom salinity are important, which corresponds to the hydrological feature that enormous fresh water is discharging nearby. Thus, MLD is dynamic, with non-negligible portion of both highly-stratified and well-mixing; In Puget Sound and Strait of Juan de Fuca, most sub-regions are impacted by zonal wind, overall wind speed, bottom temperature, and bottom salinity. This is attributed to the strong tidal current and oceanic features in the region. Looking at all Salish Cruise Stations, there are relatively thinner mixed layer with average mean MLD around 4 meters, corresponding to the continuously strong stratification over the whole water column. The result is also consistent with previous study using gradient threshold method (Moore, Mantua, Newton, et al., 2008).
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Reference

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https://doi.org/10.1007/s10872-017-0418-0
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**Figure Captions:**

**Figure 1:** Maps with all Salish Cruises stations and the most commonly sampled PEF stations (A B C N S). Salish Cruise stations are annotated in yellow dots; and PEF stations are annotated in pink starts. (a) the entire study region in Salish Sea; (b) the zoom-in PEF study sites in San Juan Archipelago.

**Figure 2:** Evaluation results of MLD derived from different methods with (a) All PEF profiles and (b) All Salish Cruise profiles

**Figure 3:** A Cartoon to explain QI and its limitation

**Figure 4:** ANOVA analysis of MLD derived from different methods with (a) All PEF profiles and (b) All Salish Cruise profiles.

**Figure 5:** Distribution of MLD derived Salish Cruise profiles with (a) new method and (b) Optimal density threshold 0.03 kg/m$^3$ method
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**Table 1**: Evaluation of MLD derived from different method with 301 PEF profiles

<table>
<thead>
<tr>
<th></th>
<th>Threshold 0.03 kg/m³</th>
<th>Threshold 0.2 °C</th>
<th>1st Derivate BuoyancyF</th>
<th>Maximum BuoyancyF</th>
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<td># Works Best</td>
<td>89</td>
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<td>272</td>
<td>40</td>
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<tr>
<td>% Works Best</td>
<td>29.57%</td>
<td>15.95%</td>
<td>90.37%</td>
<td>13.29%</td>
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Table 2: Evaluation of MLD derived from different method with 1204 Salish Cruise profiles

<table>
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<th>Maximum BuoyancyF</th>
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</thead>
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<tr>
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<tr>
<td>% Works</td>
<td>69.10%</td>
<td>13.04%</td>
<td>88.70%</td>
<td>12.21%</td>
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Mixed Layer Depth definition and determinants

Table 3: Correlation Coefficient between MLD and each MLD factors in PEF commonly sampled stations (ABCNS). Cell coloring depend on corresponding P values range (1) P>0.05 with no color for insignificance, (2) 0.01<P<0.05 with yellow for low significance, (3) 0.001<P<0.01 with green for moderate significance, and (4) P<0.001 with blue for high significance.

<table>
<thead>
<tr>
<th></th>
<th>All</th>
<th>A</th>
<th>B</th>
<th>C</th>
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<td>-0.14</td>
<td>-0.06</td>
</tr>
<tr>
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<td>0.18</td>
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</tr>
<tr>
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<td>-0.31</td>
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<td>0.03</td>
<td>0.18</td>
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<td>0.28</td>
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<tr>
<td>Surface Salinity</td>
<td>0.33</td>
<td>0.31</td>
<td>0.22</td>
<td>0.08</td>
<td>0.28</td>
<td>0.27</td>
</tr>
</tbody>
</table>
Mixed Layer Depth definition and determinants

**Table 4**: Correlation Coefficients between MLD and each MLD factors in Salish Sea sub-regions with Salish Cruise data. Cell coloring depend on corresponding P values range (1) P>0.05 with no color for insignificance, (2) 0.01<P<0.05 with yellow for low significance, (3) 0.001<P<0.01 with green for moderate significance, and (4) P<0.001 with blue for high significance.

<table>
<thead>
<tr>
<th></th>
<th>Admiralty Inlet</th>
<th>Central Sound</th>
<th>Easter Strait</th>
<th>Hood Canal</th>
<th>Main Basin</th>
<th>South Sound</th>
<th>SJA WA Coast</th>
<th>Whidbey Basin</th>
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</thead>
<tbody>
<tr>
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<td>0.23</td>
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<td>-0.40</td>
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<tr>
<td>Bottom Temperature</td>
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<td>-0.17</td>
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<td>0.12</td>
<td>0.29</td>
<td>0.55</td>
<td>-0.07</td>
<td>-0.09</td>
</tr>
</tbody>
</table>

p.s. ‘SJA’ stands for Strait of Juan de Fuca; ‘WA Coast’ stands for Washington Coast
Table 5: Summary of MLD derived from PEF and Salish Cruise profiles with Optimal density threshold 0.03 kg/m³ method and new method.

<table>
<thead>
<tr>
<th></th>
<th>MLD Mean [m]</th>
<th>MLD Standard Deviation [m]</th>
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<tr>
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<tr>
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<tr>
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</tr>
<tr>
<td>Salish Cruise</td>
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<td>New Method</td>
<td>4.18</td>
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<td>optimal density threshold</td>
<td>3.92</td>
<td>1.85</td>
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</tbody>
</table>
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Figure 1:
Mixed Layer Depth definition and determinants

Figure 2:

(a)

**PEF MLD Method Evaluation**

- Density
- Temperature
- d(BuoyancyF)
- max BuoyancyF

(b)

**Salish Cruise MLD Method Evaluation**

- Density
- Temperature
- d(BuoyancyF)
- max BuoyancyF
Figure 4:

(a) Multi-Compare PEF MLD

(b) Multi-Compare Salish Cruise MLD

2 groups have means significantly different from Rho MLD
Mixed Layer Depth definition and determinants

Figure 5:

(a) 

Salish Cruise MLD - New Method

(b) 

Salish Cruise MLD - Optimal Density Threshold Method (0.03 kg/m$^3$)