Article

ANN-Based Estimation of Low-Latitude Monthly Ocean Latent Heat Flux by Ensemble Satellite and Reanalysis Products

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Abstract: Ocean latent heat flux (LHF) is an essential variable for air–sea interactions, which establishes the link between energy balance, water and carbon cycle. The low-latitude ocean is the main heat source of the global ocean and has a great influence on global climate change and energy transmission. Thus, an accuracy estimation of high-resolution ocean LHF over low-latitude area is vital to the understanding of energy and water cycle, and it remains a challenge. To reduce the uncertainties of individual LHF products over low-latitude areas, four machine learning (ML) methods (Artificial Neutral Network (ANN), Random forest (RF), Bayesian Ridge regression and Random Sample Consensus (RANSAC) regression) were applied to estimate low-latitude monthly ocean LHF by using two satellite products (JOFURO-3 and GSSTF-3) and two reanalysis products (MERRA-2 and ERA-I). We validated the estimated ocean LHF using 115 widely distributed buoy sites from three buoy site arrays (TAO, PIRATA and RAMA). The validation results demonstrate that the performance of LHF estimations derived from the ML methods (including ANN, RF, BR and RANSAC) were significantly better than individual LHF products, indicated by $R^2$ increasing by 3.7–46.4%. Among them, the LHF estimation using the ANN method increased the $R^2$ of the four-individual ocean LHF products (ranging from 0.56 to 0.79) to 0.88 and decreased the RMSE (ranging from 19.1 to 37.5) to 11 W m$^{-2}$. Compared to three other ML methods (RF, BR and RANSAC), ANN method exhibited the best performance according to the validation results. The results of relative uncertainty analysis using the triangle cornered hat (TCH) method show that the ensemble LHF product using ML methods has lower relative uncertainty than individual LHF product in most area. The ANN was employed to implement the mapping of annual average ocean LHF over low-latitude at a spatial resolution of 0.25$^\circ$ during 2003–2007. The ocean LHF fusion products estimated from ANN methods were 10–30 W m$^{-2}$ lower than those of the four original ocean products (MERRA-2, JOFURO-3, ERA-I and GSSTF-3) and were more similar to observations.

Keywords: latent heat flux (LHF); artificial neutral network; machine learning methods; triangle cornered hat
1. Introduction

Ocean latent heat flux (LHF) plays a key role in the transformation of energy and vapor at the interface of the atmosphere and ocean [1–3]. Knowledge of ocean turbulent fluxes is important for understanding the mechanism of global heat and freshwater budget and is helpful in various research, including on atmospheric issues, oceanic problems and weather prediction. The study of sea–air heat flux can deepen the understanding of the ocean circulation driving model, elucidate the role of the ocean in balancing global energy and develop numerical prediction work on climate change. Both the atmospheric model and the ocean model require accurate LHF estimates for numerical simulation and forecasting [4–7]. Thus, accurate LHF estimation of low-latitude regions is essential for climate and hydrology applications. Among them, ocean LHF in low-latitude regions has an important impact on global climate change.

Low-latitude areas within 30° N to 30° S, including tropical and subtropical regions, account for approximately half of the Earth’s surface area. Because it is covered by the ocean and receives concentrated solar radiation, low-latitude areas store a large amount of water vapor and heat. The LHF transferred from low-latitude oceans to the atmosphere is the main source of atmospheric circulation energy [8–10]. Thus, accurate LHF estimation of low-latitude areas plays a key role in climate and hydrology applications [11]. Accurate estimation of high spatial resolution ocean LHF is vital for researching climate change, and it remains a challenge.

Continuous ocean LHF monitoring is mainly located in low-latitude areas, which can improve the accuracy of ocean LHF estimates. Many experiments have been carried out to promote the study of air–sea turbulent fluxes [12–15], such as the Global Energy and Water Cycle Experiment (GEWEX) [16] and Joint Global Ocean Flux Study (JGOFS) [17]. Based on a large amount of experimental observations, the parameterization scheme of the turbulence flux algorithm has developed rapidly, and global ocean turbulence flux products with different scales and spatial and temporal resolutions have been produced. Satellite and reanalysis data can provide us with spatially and temporally continuous ocean LHF observations at various scales. At present, various satellite and reanalysis LHF products with moderate or coarse spatial resolution have been produced, including Japanese Ocean Flux Data Sets with Use of Remote Sensing (J-OFURO) [18], Goddard Satellite-Based Surface Turbulent Fluxes (GSSTF-3) [19], the Hamburg Ocean Atmosphere Parameters and Fluxes from Satellite Data (HOAPS) [20], Modern-Era Retrospective analysis for Research and Applications (MERRA), ERA_Interim, etc. However, compared with the observations obtained from buoy sites or experimental ships, satellite-based LHF products present large discrepancies. Brunke et al. [21] concluded that satellite-based products have generated large uncertainty in the process of inversion by comparing various turbulent flux products and four satellite products (GSSTF2, GSSSF2b, J-OFURO and HOAPS). Some satellite-based products provide accurate LHF estimates, but the study areas are limited to specific areas (e.g., SCS). Reanalysis products provide us with reasonable estimations of ocean LHF and have been successfully used in numerical weather prediction (NWP); however, they have notable errors owing to data assimilation schemes. Some reanalysis has a relatively high spatial and temporal resolution but tend to overestimate ocean LHF in most areas compared to buoy site measurements. Many studies have also indicated that ocean LHF estimates with a coarse spatial resolution (e.g., 1°) may lead to large errors due to the spatial heterogeneity of ocean LHF [22].

Over the last forty years, many methods have been developed to implement ocean LHF estimates. To date, the methods used for estimating ocean LHF can be calculated by: (1) physically-based methods [23–25]; (2) data assimilation methods [26–30]; and (3) bulk aerodynamic algorithms [31–34]. Physically-based methods, including eddy covariance methods and inertial dissipation methods [35–38], are considered the most reliable methods in estimating ocean LHF. However, these methods require high-frequency instruments that can only be implemented for site-scale observations; further, such observations are limited in temporal and spatial distribution. Data assimilation methods can provide a reasonable simulation of the ocean LHF, but the difference in the parameterization scheme may introduce significant uncertainty to ocean LHF estimates [39–41].
Widely used bulk aerodynamic algorithms utilize air temperature, sea surface temperature, air specific humidity and wind speed as input bulk quantities to calculate ocean turbulent fluxes. Even though these methods can be used everywhere on Earth, there are still significant uncertainties from different models [23,42,43]. These methods are widely used to estimate ocean $LHF$ at various temporal and spatial resolutions. However, the ocean $LHF$ estimates derived from these methods differ substantially from observations [44–46].

Recently, multiple product ensembles using machine learning (ML) methods have been successfully applied to estimate terrestrial latent heat flux ($LE$). For example, Yao et al. [47] used support vector machine (SVM) to integrate three satellite-based LE products to improve global terrestrial evapotranspiration ($ET$) estimation and found that the SVM method was superior to all other physical methods. Fan et al. [48] developed four tree-based ensemble models ($RF$, $M5Tree$, $GBDT$ and $XGBoost$) to estimate daily $ET$ using limited meteorological data; the developed $XGBoost$ and $GBDT$ models have accurate predictions, strong model stability and low calculation cost. Shang et al. [49] applied four ML methods (Extremely Randomized Trees ($ETR$), Gradient Boosting Regression Tree ($GBRT$), Random Forest ($RF$) and Gaussian Process Regression ($GPR$)) to improve terrestrial $LE$ estimations over Europe based on five individual terrestrial $LE$ product; the validation results illustrate that the $LE$ estimation using $ETR$ method increased $R^2$ and decreased RMSE. Even though the ML methods have been widely used to estimate terrestrial biophysical variables, there is a lack of experiments on dataset fusion to improve ocean $LHF$ estimates by combining multiple $LHF$ products.

In this study, we used the Artificial Neutral Network (ANN) method to improve ocean $LHF$ estimation over low-latitude areas by using four individual $LHF$ products. We had three objectives: (1) evaluate the performance of the ANN and three other ML methods ($RF$, Bayesian Ridge Regression ($BR$) and Random Sample Consensus ($RANSAC$)) by using four $LHF$ products based on the moored buoy array of TAO, the Research Moored Array for African-Asian-Australian Monsoon Analysis and Prediction ($RAMA$) and the Prediction and Research Moored Array in the Tropical Atlantic ($PIRATA$); (2) assess the relative uncertainties among of the ocean $LHF$ products based on the triangle cornered hat ($TCH$) method; and (3) use ANN to map the average ocean $LHF$ with 0.25° spatial resolution for the period of 2003–2007 by using an ensemble of four $LHF$ products.

2. Data

2.1. Satellite and Reanalysis Ocean LHF Products

The $LHF$ products used in this study include the following: MERRA-2 [50], European Centre for Medium-Range Weather Forecasts (ECMWF) interim reanalysis ($ERA-I$) [51], Japanese Ocean Flux Data Sets with Use of Remote Sensing ($J-OFURO$) [18] and Goddard Satellite-Based Surface Turbulent Fluxes (GSSTF-3) [19].

Monthly ocean latent heat flux estimates derived from MERRA-2 [52], with a spatial resolution of 0.5° latitude × 0.625° longitude, from January 2003 to December 2007, was launched aboard the EARTHDATA at https://earthdata.nasa.gov/. The $ERA-I$ data [53] were produced by the data assimilation system using 4-dimensional variational assimilation (4D-Var), with a spatial resolution of 0.25° latitude × 0.25° longitude. $J-OFURO$ was produced by the School of Marine Science and Technology at Tokai University and was calculated by the COARE 3.0 method with an improved spatial resolution of 0.25°. Compared to the previous versions, GSSTF-3 is an improved version with corrected surface specific humidity ($Qair$) data retrieved by removing the effect of the Earth incidence angle ($EIA$) drifting [23]. These data were obtained from Goddard Earth Science Data and Information Services Center’s (GES DISC) website, with an advantage of a high spatial resolution of 0.25°.

The objectively analyzed air–sea fluxes product ($OAFlux$) [6,54] was used to validate the accuracy of the fusion product. It has been reported that the $OAFlux$ dataset is a reliable product for ocean turbulent flux research. The $OAFlux$ data have an advantage in that they combine satellite-derived data and reanalysis data by using the objective analysis method; however, these data have a coarser
spatial resolution of 1°. To estimate the monthly global ocean LHF products at a spatial resolution of 0.25° from 2003 to 2007, we used the bilinear interpolation method. Detailed information for each product mentioned above is summarized in Table 1 and detailed input variable datasets of each LHF product is summarized in Table 2.

**Table 1.** Summary of the five ocean LHF products in this study for 2003–2007.

| Products   | Variables | Spatial Resolution | Time Span     | References          |
|------------|-----------|--------------------|---------------|---------------------|
| MERRA-2    | LHF       | 1/2° × 2/3°        | 1980–present  | Rienecker et al., 2011 |
| ERA-interim| LHF       | 0.125°             | 1979–present  | Dee et al., 2011    |
| GSSTF-3    | LHF       | 0.25°              | 1987–2008     | Shie 2012           |
| J-OFURO    | LHF       | 0.25°              | 1988–2013     | Tomita et al., 2018 |
| OAFLUX     | LHF       | 1°                | 1958–present  | Yu et al., 2004     |

**Table 2.** Summary of input variable datasets for each LHF product.

| Product   | Variable                           | Source                                                                                      |
|-----------|------------------------------------|--------------------------------------------------------------------------------------------|
| MERRA-2   | Surface winds                      | SSM/I; QuikSCAT; ERS (ERS-1 and ERS-2);                                                     |
|           | Rain rate                          | SSM/I; TRMM Microwave Imager (TMI);                                                        |
|           | Radiances                          | SSM/I; GOES sounder; TIROS Operational Vertical Sounder (TOVS) and Advanced TOVS (ATOVS); |
|           | Upper-level winds                  | geostationary satellites and MODIS                                                         |
|           | ozone                              | SBUV                                                                                       |
|           | Surface winds; Ocean wave height   | ERS (ERS-1 and ERS-2);                                                                      |
| ERA-I     | Radiances                          | VTPR; High Resolution Infrared Sounder (HIRS); Stratospheric Sounding Unit (SSU); MSU; AMSU-A; |
|           | Upper-level winds                  | Meteosat-2                                                                                 |
|           | Ozone profiles                     | SBUV                                                                                       |
|           | clear-sky radiances                | Meteosat-2                                                                                 |
|           | Surface wind speed; Column water   | SSM/I                                                                                      |
|           | vapor                               | radio occultation (RO) CHAMP; COSMIC; GRACE                                                 |
| GSSTF-3   | wind speed (U)                     | SSM/I                                                                                      |
|           | surface air specific humidity (Qair)| corrected SSM/I brightness temperature (Tb)                                               |
|           | Radiances                          | SIRS, HIRS, VTPR, and TOVS;                                                                |
|           | Upper-level winds                  | geostationary satellites                                                                   |
| JOFURO-3  | wind speed (U)                     | SSM/I; TMI; WindSAT; AMSR-E; AMSR2; ERS (ERS-1 and ERS-2); QuikSCAT; ASCAT-A; ASCAT-B; OSCAT |
|           | Qair                               | SSM/I; TMI; AMSR-E; AMSR2                                                                 |
|           | SST                                | MGDSST; OSTIA-NRT; AMSR-E; MW; OISST; AMSR; TMI; WindSAT; GMI; OSTIA-RA                     |
| OAFLUX    | wind speed (U)                     | SSM/I; AMSR-E; QuikSCAT;                                                                    |
|           | Qair                               | SSM/I                                                                                      |
|           | SST                                | NCEP-OI; NCEP–NCAR; NCEP–DOE; ERA-40                                                       |
2.2. Buoy Observations

Buoy observations were used as the reference data to evaluate the performance of the ocean LHF estimation. The monthly ocean latent heat observations were collected from 115 moored buoy sites [55–58].

Among 115 moored buoy sites, 67 buoys were collected from the Tropical Atmosphere Ocean/Triangle Trans Ocean Buoy Network (TAO/TRITON, https://tao.ndbc.noaa.gov/), 18 buoys were collected from the Prediction and Research Moored Array in the Tropical Atlantic (PIRATA, http://www.brest.ird.fr/pirata/) and 12 buoys were collected from the African-Asian-Australian Monsoon Analysis and Prediction (RAMA, https://www.pmel.noaa.gov/tao/dispersel/). All ocean turbulent fluxes were calculated by the COARE 3.0 method; these data covered the period from 2003 to 2007. Buoy observations were mainly located in tropic areas. Figure 1 shows buoy site locations and information about the three buoy site arrays. Although the moored buoy footprints varied from the pixel size of the reanalysis and satellite-based products, we still regarded the buoy site observations as “ground truth” in this study.

![Figure 1. Distribution of 115 buoys sites for different buoy sites arrays over low-latitude area. “Train” represents training sites and “Test” represents the validation sites.](image)

3. Methods

3.1. Artificial Neural Network

An Artificial Neutral Network (ANN) [59] can be considered a network that consists of a series of adaptive connected simple neuron nodes to simulate the human biological nervous system in response to input signals (Figure 2). Different from logistical regression, which is composed of an input and an output layer, the ANN comprises three layers: the input layer, the hidden layer and the output layer. Various datasets are considered the input data; the input data are weighted in the hidden layer by means of flexible mathematical algorithms, and the prediction dataset is produced in the output layer. Based on self-adaptation and self-learning, the ANN method causes the input and output data to establish a nonlinear relationship.

Within the hidden layer, the fully connected neurons receive input signals from other neurons; these input signals are passed through a weighted connection.

\[ y_j = \sum_{n=1}^{m} w_{nj}b_n \]  

(1)

where \( y_j \) refers to the \( j \)th neuron output data, \( w_{nj} \) is the connection weight of the \( n \)th neuron in the hidden layer and the \( j \)th output layer neuron and \( b_n \) is the output of the \( n \)th neuron in the hidden layer.
The total input signal value received by the different neurons is used to compare with the threshold of the neuron node,

\[ y_j = f(\beta_j - \theta_j) \]  

(2)

where \( f \) is the activation function of the neural network, \( \beta_j \) is the output received by the \( j \)th neuron in the output layer and \( \theta_j \) is the threshold of the \( j \)th neuron in the output layer.

Then, the output data of the neuron are easily generated by the activation function. The learning process of ANN is used to adjust the connection weight between neurons and the threshold of each neuron based on the results of the training data.

3.2. Other Machine Learning Methods

3.2.1. Random Forest

RF [59] is an ensemble method that is widely applied for regression issues. It uses classification regression tree (CART) as a regressor for the decision tree and bootstrap sample methods to select different training datasets for different decision trees. Further, it randomly selects features to perform attribute splitting on internal nodes when constructing a single tree. Therefore, the RF method can better exclude noise interference and has better performance for classification and regression. Generalization is the ability of the Random Forest to correctly predict data outside the training set, and the generalization error is the probability of a misclassification of the data outside the training set by the regression. The generalization error of a Random Forest depends on the regression ability of a single tree and the correlation between any two trees. Research results show that the generalization error of the RF converges to a finite value; thus, as the number of classification trees in the forest increases, the Random Forest does not cause overfitting.

3.2.2. Bayesian Ridge Regression

In addition to the RF and ANN methods, we also applied two other linear regression methods to predict ocean LHF flux. Compared to other ML methods, the linear regression method is fast in
Sensors 2020, 20, 4773 7 of 24

modeling, and the calculation method is simple. Therefore, even if the amount of input data is large, the calculation speed is fast.

Considering the high correlation among the input variables in this paper, we used the Bayesian Ridge Regression (BR) [60] to estimate ocean LHF flux. Generally, the linear regression algorithm uses the least squares method to optimize the coefficients. Ridge regression obtains the optimal parameters by penalizing the coefficients to reduce the impact of highly correlated input variables. The Bayesian Ridge Regression (BR) method, which combines the Bayesian method and the ridge regression method, has a strong self-adaptation ability to the input datasets, which not only avoids the overfitting of datasets but also promotes a high utilization rate of data samples.

3.2.3. Random Sample Consensus

The RANSAC regression [61] model can obtain valid sample data from the observation dataset containing “outliers” and iteratively estimate the mathematical model parameters. In short, the RANSAC method process is as follows: first, randomly extracted samples from the datasets build “interior points”; second, the remaining datasets test the model training by “interior points” and add the sample points that fall within a predetermined tolerance range to the “interior points”; finally, it fits the model with all the “interior points” and uses “interior points” to estimate the error. The process is terminated if the model performance reaches expectations.

3.3. Triangle Cornered Hat Method

TCH [62] can estimate relative uncertainty without prior knowledge. The TCH method is an improved version of the Triangle Cornered (TC) method and can be used to calculate the relative uncertainty among three or more independent products. Quantifying uncertainty by removing “true values” from different variables (assuming the input variables all contain true values) is a difference method. This method has been successfully used in gravity fields [63], evapotranspiration [64] and soil moisture [65] at different scales. Here, we applied the TCH method to quantify the relative uncertainty among ocean heat fluxes from different products.

The TCH method treats the time series of input products as \{X_i\}, i = 1,2, \ldots, N. The subscript i represents the ith product among all sorted products and N represents the total number of products. \{X_i\} can be divided into two parts, including the “true value” \{X_t\} and the error term \{\varepsilon_i\}:

\[X_i = X_t + \varepsilon_i, \forall i = 1,2,\ldots,N\] (3)

Due to an unknown true value, it is difficult to obtain the error term \{\varepsilon_i\}. Thus, the first step in the TCH method is to determine the difference among the N products and reference dataset. First, choose one time series LHF product as reference data \{X_R\} and calculate the differences \{D_{i,M}\} between reference data \{X_R\} and other LHF datasets \{X_i\}.

\[D_{i,M} = X_i - X_R = \varepsilon_i - \varepsilon_R \forall \varphi = 1,2,\ldots,N - 1\] (4)

where \(D_{i,M}\) represent the difference matrix between the reference dataset \{X_R\} and the input dataset \{X_i\}. Next, calculate the \((N-1) \times (N-1)\) covariance matrix \(S = \text{cov}(D)\) and determine the covariance matrix of the noise matrix \(G\) through the S matrix:

\[S = M^T \cdot G \cdot M\] (5)

\[M = \begin{bmatrix} A & -\mu^T \end{bmatrix}\] (6)

where \(A\) is the identity matrix and \(\mu\) is the vector of \([1 \ 1 \ 1 \ldots \ 1]\). To minimize the global correlation of errors, Premoli and Tavella [66] proposed a free parameter selection criterion to maintain the positive definiteness of \(G\). According to the constraint minimization problem proposed by the Kuhn–Tucker
theorem, it can be used to determine the unique solution of the matrix $G$, and the random error of each group of data can be calculated.

3.4. Evaluation Metrics

The squared correlation coefficient ($R^2$), root-mean-square-error (RMSE) and bias are used as metrics to evaluate the performance of the LHF estimations against reference dataset. The matching degree between the evaluated estimations $\{x_i\}$ and the reference dataset $\{r_i\}$ can be judged by the metrics mentioned above, and they are written as:

$$R^2 = \frac{\left(\sum_{i=1}^{N}(x_i - \bar{x})(r_i - \bar{r})\right)^2}{\sum_{i=1}^{N}(x_i - \bar{x})^2 \sum_{i=1}^{N}(r_i - \bar{r})^2}$$

(7)

$$\text{Bias} = \frac{\sum_{i=1}^{N}(x_i - r_i)}{N}$$

(8)

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N}(x_i - r_i)^2}$$

(9)

where $N$ represents the number of samples. The King–Gupta efficiency ($KGE$) is a comprehensive evaluation metric that can be calculated as follows:

$$KGE = 1 - \sqrt{(R - 1)^2 + \left(\frac{ST_e}{ST_o} - 1\right)^2 + \left(\frac{E_e}{E_o} - 1\right)^2}$$

(10)

where $R$ denotes the correlation coefficient between the LHF estimation and reference dataset; $ST_e$ and $ST_o$ represent the standard deviation of the LHF estimation and reference dataset, respectively; and $E_e$ and $E_o$ are the mean value of the LHF estimation and reference dataset, respectively. The closer $KGE$ is to 1, the closer the LHF estimation is to the reference dataset.

3.5. Experimental Setup

Before model construction, we extracted LHF variable from four products and in situ measurements. More than 4000 observations from 115 buoy sites were collected as target variable, and LHF variable extracted from four products (JOFERO-3, GSSTF-3, ERA-I and MERRA-2) were used as predictor variables. To build the model, the datasets (both target dataset and predictor dataset) were randomly divided into two groups: 70% to train the model and the remaining 30% to validate the trained model. The best parameters which can provide the highest correlation coefficient were selected in the training data through cross validation. The obtained optimal parameters were then used in the model to estimate LHF.

We constructed the ANN, RF, BR and RANSAC model based on sklearn modules by using the Python platform. The main parameters of ANN models include the learning_rate, hidden_layer_sizes, n_estimators and min_samples_split. The performance of RF method in the scikit-learn toolbox is mainly influenced by n_estimators and max_features. The main parameters of BRR are n_iter and lambda. The main parameters to adjust when using RANSAC are max_trials, min_samples and residual_threshold. Obtaining the optimal parameters of the model can not only improve the accuracy of model estimation but also improve efficiency and shorten model running time.

To find the optimal parameter for each ML method, we applied the GridSearchCV module. GridSearchCV method is a parameter tuning method. It tries every possibility through loop traversal among all parameter combinations and selects the optimal parameter combination based on the performance of the results. The main disadvantage of this method is that it is time-consuming.
Optimal parameter combinations for each ML methods were determined by GridSearchCV method in optional parameters, as shown in Table 3.

| Method | Parameters     | Optional                  | Interval        | Selection of GridSearchCV |
|--------|----------------|---------------------------|-----------------|---------------------------|
| ANN    | activation     | “identity”, “logistic”, “tanh”, “relu” |relu            |                           |
|        | learning_rate  | “10”, “1”, “0.1”, “0.01”, “0.001”, “0.0001” |0.01            |                           |
|        | hidden_layer_sizes | “(10, 50)”, “(10, 100)”, “(20, 80)”, “(20,150)”, “(30,100)”, “(50,100)” |(20, 80)        |                           |
|        | batch_size     | 50–300                    | 50              | 150                       |
| RF     | min_samples_split | 2–6                       | 1               | 4                         |
|        | n_estimators   | 5–50                      | 3               | 40                        |
|        | max-features   | 1–10                      | 1               | 6                         |
| BR     | n_iter         | 20–300                    | 20              | 240                       |
|        | lambda         | “0.1”, “0.01”, “0.001”, “0.0001” |“0.000001”      |                           |
| RANSAC | max_trials     | 30–120                    | 5               | 105                       |
|        | min_samples    | 80–300                    | 20              | 260                       |
|        | residual_threshold | 5–100                     | 5               | 45                        |

4. Results

4.1. Validation of the Five Ocean LHF Products against Buoy Observations

At the site scale, the five ocean LHF products exhibited substantial differences in ocean LHF estimation, as shown in Figure 3. For the TAO buoy site array with the most observations, the monthly ocean LHF estimation of ERA-I product correlated best with the observations, indicated by an $R^2 = 0.80$ ($p < 0.01$); however, the RMSE and bias both exceeded 25.2 W m$^{-2}$. Similarly, MERRA also showed good performance with an $R^2 > 0.75$ ($p < 0.01$) but highly overestimated ocean LHF as indicated by the highest RMSE and bias among all ocean LHF products. In contrast, the OAFlux product showed relatively lower RMSE and the lowest bias; the lower correlation ($R^2 = 0.56$, $p < 0.01$) may be caused by its coarse spatial resolution (approximately 1°). GSSTF-3 performed least satisfactorily in estimating ocean LHF, with disperse distribution of validation points and relatively high overall estimates. Compared to other observation arrays, all ocean LHF products performed better with higher $R^2$ and lower bias in the PIRATA buoy site array.
Figure 3. Validation of five products against buoy observations from 115 sites during the period from 2003 to 2007 (unit W m$^{-2}$).

Figure 4 shows the $R^2$, RMSE, bias and KGE statistics of five ocean LHF products against observations from different buoy sites. For all buoy site arrays, reanalysis products (MERRA and ERA-I) have the highest $R^2$ ranging from 0.39 to 0.83. However, the magnitude of average monthly LHF derived from reanalysis is much higher than that of buoy-measured LHF, as indicated by biases exceeding 25 and 32 W m$^{-2}$, respectively. When considering the KGE (ranging from 0.5 to 0.83) and RMSE (ranging from 18 to 31 W m$^{-2}$), the JOFLIRO-3 product is superior to others. This indicates that different parameterizations of ocean LHF products affect the accuracy of ocean LHF estimates. The performance of OAFlux products is lower than JOFLIRO-3 but better than GSSTF-3; this is probably caused by the coarse spatial resolution of OAFlux, which has a spatial resolution of 1°.
Figure 4. The evaluation parameters ($R^2$, RMSE, bias and KGE) comparison between the five ocean LHF products against buoy sites observations (unit W m$^{-2}$).

4.2. Ensemble of Four Ocean LHF Products from ANN and Other ML Methods

4.2.1. Model Training and Validation based on Buoy Observations

None of the individual ocean LHF products provides the best LHF estimates based on buoy observations. Thus, we used ANN and other ML methods (RF, BR and RANSAC) to calculate ocean LHF by an ensemble of four ocean LHF products: MERRA, ERA-I, JOFURO-3 and GSSTF-3. The reanalysis products are highly correlated with measurements but also highly overestimate ocean LHF. In contrast, the satellite-based product JOFURO-3 and objectively analyzed product OAFlux perform well with lower bias.

Figure 5 represents the training results of ANN, RF, BR and RANSAC for all buoy site observations. Estimated ocean LHF derived from four ML methods agreed well with buoy measurements and is consistent with the trend of buoy observations. Among the four ML methods, ANN has the highest $R^2$ and lowest RMSE in training datasets, as indicated by an $R^2$ exceeding 0.88. The RANSAC method has a slightly higher RMSE of 12.1 W m$^{-2}$ and a slightly lower $R^2$ than other ML methods.

Figure 6 shows the scatter plot for the ocean LHF observations and LHF estimations from four ML methods. The validation results show that ANN yields the best estimations of ocean LHF, as indicated by the highest $R^2$ of 0.87, the lowest RMSE of 10.9 W m$^{-2}$ and the highest comprehensive index (KGE) of 0.90, followed by RF and BR. Although RANSAC performed weakly as indicated by the lowest $R^2$ (0.82) and KGE (0.78), it is still superior to any individual ocean LHF product. Overall, these results illustrate that the ocean LHF fusion products derived from ML methods are superior to individual LHF products. In addition, the ANN model performs best among the four ML models.
Figure 5. The scatter plots for ocean LHF observations at 81 training buoy sites and LHF estimates from the ANN, RF, BR and RANSAC methods during 2003–2007 (unit W m\(^{-2}\)).

Figure 6. The scatter plot for ocean LHF observations from 34 validation buoy sites and the LHF estimations from the ANN, RF, BR and RANSAC methods during 2003–2007 (unit W m\(^{-2}\)).
4.2.2. Relative Uncertainties of Ocean LHF Over Low-latitude Areas

To quantify the performance of all four methods over the tropics, we used the TCH method to calculate the uncertainties of ocean LHF estimates derived from ML methods.

Figure 7 presents the distribution of relative uncertainties estimated from ocean LHF estimations based on four ML models. Generally, the ocean LHF estimated from ML methods perform better than those from ocean LHF products (MERRA, ERA-I, JOFURO-3 and GSSTF-3). Moreover, the LHF products tend to generate lower uncertainties in the area away from the coast due to the stable and uniform climatic conditions and have higher uncertainties in the area close to land. The ANN and BR perform well over low-latitude areas with lower relative uncertainties; BR has higher uncertainties than ANN in the west of South Africa and equatorial area. Among the LHF estimations based on ML methods, RF has the highest relative uncertainties, especially in the Kuroshio current region and Southern Hemisphere Subtropical area, which may be caused by the errors in the model estimation. For ocean LHF products, although the ERA-I outperforms the other three LHF products, it underperforms the ANN estimation in most areas.

Figure 7. Distribution of relative uncertainties from eight ocean LHF products (including four ocean LHF products and four ensemble LHF products) over low-latitude area (unit W m⁻²).

Figure 8 shows the relative uncertainties of ocean LHF estimations calculated by four ML methods. ANN outperforms the other LHF estimations with lower average relative uncertainties of 2.60 W m⁻², a median value of 2.39 W m⁻² and a maximum of relative uncertainties lower than 10 W m⁻². The BR is second to ANN with higher average relative uncertainties of 2.86 W m⁻² and a maximum of relative uncertainties of 20 W m⁻². Although the median values of relative uncertainties for RF and RANSAC are slightly higher than ANN as indicated by values of 3.15 and 3.95, respectively, they have higher relative uncertainties exceeding 30 W m⁻².

Overall, ANN slightly outperformed other ML methods according to validation against buoy observations and relative uncertainty evaluation based on the TCH method over tropical areas.
4.3. Mapping of Ocean LHF Over Low-Latitude Areas

4.3.1. Annual Patterns of the Ensemble Tropical Ocean LHF

We applied ANN, RF, BR and RANSAC driven by monthly ocean LHF products (MERRA-2, JOFURO-3, ERA-I and GSSTF-3) to estimate ocean LHF in low-latitude areas at 0.25° spatial resolution from 2003 to 2007. Figure 9 shows the spatial distribution of annual LHF averaged from different products during the years 2003–2007.
All of the ocean LHF products yielded lower LHF estimates over the equatorial region, especially over the East Pacific along South America and the East Atlantic along Africa. The highest ocean LHF exceeded approximately 200 W m\(^{-2}\) and occurred in the South Pacific with latitudes between 10\(^\circ\) and 20\(^\circ\) S. Even though ocean LHF products have similar spatial distribution in low-latitude areas, there are still significant differences between different products. As shown in Figure 9, MERRA-2 and GSSTF-3 products yielded higher LHF values in the South Pacific and South Indian Ocean. Compared with MERRA-2, JOFURO-3, ERA-I and GSSTF-3, OAFlux yielded lower ocean LHF values over low-latitude areas. In contrast, the spatial distribution of ANN, BR and RANSAC showed highly consistent characteristics. However, it is also noted that the ocean LHF estimation from RF cannot properly simulate the high ocean LHF values, which may be because the RF algorithm highly depends on the representativeness of the sample dataset; if the sample dataset does not include the high ocean LHF value, it may cause a deviation in LHF results. The ocean LHF of four ensemble products is much lower than that from the four individual ocean products, but close to that from the reference dataset (OAFlux product).

Figure 10 shows the comparison of the annual average LHF from ANN versus that of the other three methods (RF, BR and RANSAC) over low-latitude areas. In general, the ocean LHF from ANN agrees best with BR, followed by RANSAC. The most prominent difference between ANN and BR is that the LHF values estimated by ANN were lower than those of BR when LHF was greater than 150 W m\(^{-2}\) and higher than those of BR when it was less than 50 W m\(^{-2}\). When the ocean LHF was lower than 10 W m\(^{-2}\), RANSAC poorly simulated LHF variability. The estimated LHF from ANN was higher than those of RF when ocean LHF was greater than 130 W m\(^{-2}\) and lower than those of RF when it was less than 20 W m\(^{-2}\). The discrepancies may be mainly caused by the difference in algorithm structure. As shown in Figure 9, the estimated ocean LHF from ANN was close to that from the other three ML methods, indicated by an \(R^2\) higher than 0.98 and bias less than 3.5 W m\(^{-2}\). As mentioned above, the estimated LHF from BR was closest to that of ANN, as characterized by the highest \(R^2\), the lowest RMSE and lowest bias.

![Figure 10. Comparison of monthly ocean LHF from ANN and other ML methods (unit W m\(^{-2}\)).](image-url)
Figure 11 shows spatial differences in annual ocean LHF over low-latitude regions between ANN and the other three ML methods (RF, BR and RANSAC). The differences in annual ocean LHF estimated by ANN and the other three ML methods were mainly distributed in the range of −10 to 10 W m$^{-2}$. The ensemble ocean LHF product from BR also showed a consistent spatial distribution with that of ANN; the difference was less than 5 W m$^{-2}$ in most areas. The ensemble LHF using RANSAC has the most significant variation in spatial distribution. RANSAC yields high ocean LHF mainly in the Equatorial East Pacific and Equatorial East Atlantic; this may be caused by the differences in different ML methods.

4.3.2. Seasonal Patterns of the Ensemble Tropical Ocean LHF

Figure 12 presents the multiyear average seasonal pattern of ocean LHF, which shows that strong regional variations occur in low-latitude areas. The variation in ocean LHF is affected by the climate and land–sea distribution. Lower wind speeds and lower sea temperatures due to proximity to land result in the lowest ocean LHF in the equatorial current region of the eastern Pacific. Moreover, the maximum ocean LHF occurs in the central Pacific.

In the northern hemisphere, ocean LHF increased from fall then decreased from spring to fall over tropical areas. The lowest ocean LHF in the southern hemisphere occurs in spring; there was a sharp increase in ocean LHF from spring to fall. In the winter of the northern hemisphere, the largest ocean LHF occurs in the Kuroshio Current, followed by the Gulf Stream; the average ocean LHF exceeds 200 W m$^{-2}$ in these regions. Ocean LHF values are large in the Kuroshio Current and Gulf Stream due to the large temperature differences at the air–sea interface. Similarly, the largest ocean LHF of the southern hemisphere occurs in the South Pacific, especially in the 10° and 20° south latitude.

Compared to the RF method, the ANN method exhibited a good ability to simulate spatial variability. RF performed poorly in simulating high ocean LHF in ocean current regions, such as the Kuroshio Current area in the northern hemisphere’s winter, and Australia’s bordering sea. This may be caused by the fact that RF has a different algorithm structure compared to those of the other ML methods. According to the ANN method, fall has the highest average ocean LHF (113.8 W m$^{-2}$), followed by summer (113.0 W m$^{-2}$), spring (112.7 W m$^{-2}$) and winter (111.2 W m$^{-2}$).
Figure 12. Maps of multiyear (2003–2007) average seasonality of ocean LHF estimations from OAFlux product and four ML methods (unit W m$^{-2}$).

Figure 13 illustrates the latitudinal variation in annual average LHF over low-latitude areas during 2003–2007. Despite the general differences in latitude distribution among different ocean LHF estimates, the latitudinal distribution of all ocean LHF estimations is bimodal, and the highest ocean LHF occurs at approximately 15° S, followed by 15° N. The minimum values appear in the equatorial region, and the LHF gradually increases with the increase in latitude. After reaching the maximum value at approximately 15°, ocean LHF gradually declines to the poles. There are still substantial differences between the seven ocean LHF estimates. Compared to reanalysis datasets that overestimate ocean LHF against buoy site observation, ANN is closer to OAFlux and JOFURO-3. Moreover, ANN-based ensemble LHF can capture more detailed information than OAFlux owing to its high spatial resolution. Although the estimated ocean LHF of four ML methods are very close, the estimated LHF using ANN is slightly higher than others by 3–5 W m$^{-2}$.

Figure 14 compares the monthly average ocean LHF derived from ANN and the other ML methods with other ocean LHF products over the tropics. All the ocean LHF estimates presented similar seasonal variability, and the magnitude of ocean LHF seasonal variation was less than 10 W m$^{-2}$. Ocean LHF increased from April to June then decreased from June to October due to the high ocean LHF in the
southern hemisphere. Figure 13 also illustrates that the reanalysis product (ERA-I) was 10–30 W m$^{-2}$ higher than others. The LHF derived from the four ML methods was closer and more than 10 W m$^{-2}$ lower than those derived from the other products. Among them, ANN is slightly higher than other ML methods by 1–3 W m$^{-2}$.

**Figure 13.** Latitudinal variation of annual average LHF over low-latitude area during 2003–2007, (unit W m$^{-2}$).

5. Discussion

ANN, RF, BR and RANSAC were used to estimate ocean LHF at a spatial resolution of 0.25°. Some of these four ML methods were successfully used to estimate a terrestrial LE fusion product, such as ANN and RF [49,67,68]. According to validation against buoy observations (Figure 4), our results illustrate that ensemble ocean LHF from ML methods performed much better than the estimated LHF from...
four individual ocean LHF products (MERRA-2, JOFURO-3, ERA-I and GSSTF-3). Compared to the individual LHF products, the $R^2$ of the ML methods was 3.7–46.4% higher and the bias decreased by approximately 15 W m$^{-2}$. Our results also show that some minor differences existed among the four ML methods, which are mainly affected by the structure of different fusion algorithms [69,70]. Sagi and Rokach [71] showed that the differences in structure of the ensemble methods may significantly affect the predictions, and the best ensemble method for a given problem needs to consider other factors (such as suitability to a given setting).

The ensemble ocean LHF from ANN showed great consistency with that of the other three ML methods. The difference in the spatiotemporal variation of ensemble LHF from the four ML methods was less than 5 W m$^{-2}$ and were all 10–30 W m$^{-2}$ lower than the individual ocean LHF products. In comparison with the RF, BR and RANSAC methods, the ocean LHF estimation using ANN performed better. This may be attributed to the fact that ANN is composed of a series of adaptively connected simple neuron nodes, which improves the accuracy of model estimation by adjusting the weights between different neurons [59,72]. Other studies also found that ANN presents a superior ensemble performance to other ML methods in many fields, such as ET, solar radiation and downscaling [67,73,74].

Similar to ANN, RF has a strong correlation with observations (Figure 4), but we found that ocean LHF estimations from RF performed poorly in simulating high LHF values in the spatiotemporal distribution. This is consistent with the conclusions drawn by Zhang et al. [75]; the regression prediction obtained by RF performs poorly, while ANN achieves the best estimation of the total biomass in four ML methods. This may be due to the fact that the training of RF not only requires a large amount of sample dataset [76] but also requires the sample dataset itself to be representative. Studies have shown that increasing the number and periodicity of sample datasets can improve the estimation accuracy of RF [77]. Considering that the buoy site observations cannot cover all the ocean LHF features in the study area, the RF method underperformed the other three ML methods in simulating the spatial and temporal distribution of LHF.

We also applied the TCH method to evaluate relative uncertainties among the four ocean LHF fusion products and four individual LHF products because the TCH method has been successfully used in territorial LE uncertainty evaluation [78–80]. All ML methods performed better than individual ocean LHF products as indicated by lower relative uncertainty. The relative uncertainty of the four ensemble products was approximately 5 W m$^{-2}$, while relative uncertainty of the individual ocean LHF products ranged from 7 to 20 W m$^{-2}$. ANN had the lowest average uncertainty, followed by BR. The average relative uncertainty of RF was the highest among the four ML methods.

In terms of the spatial distribution of relative uncertainty, the high relative uncertainty values of RF were mainly located in the extreme values of ocean LHF (Figures 7 and 12). The uncertainties of the ensemble LHF products mainly stemmed from the biases of the individual datasets [21], the errors in the buoy site observations [81], the mismatched spatial scales between datasets from different sources and the structure of ML methods [71,82,83]. Due to the measurement sensors and environmental disturbances, the uncertainties in ocean LHF observations obtained from buoy sites array were approximately 10 W m$^{-2}$ [44,56,81]. The representativeness of the buoy site ranges from tens to hundreds of meters, while the spatial resolution of LHF products was greater than 12.5 km, the spatial resolution mismatch may lead to uncertainties in the validation results. Additionally, the errors in the individual products will lead to an 8% error in ensemble LHF [21,84]. The mismatches among different data sources may also introduce a 5–7% uncertainty in ensemble LHF [85–87]. Although the ML methods do not require a priori knowledge, the structure of different ML methods may lead to large errors and poor generalization performance [84].

Our study provided future efforts to improve ocean LHF estimation using ML methods by an ensemble of multiple LHF products. ML methods performed better in estimating ocean LHF than the individual ocean LHF products (MERRA-2, JOFURO-3, ERA-I and GSSTF-3). All these products can be well trained by observations and then used for estimating ocean LHF. Importantly, different ML methods need to be fully evaluated in different studies. For example, RF has higher relative uncertainty
at the region of extreme LHF values, but that is not conclusive. In contrast, ANN presents lower relative uncertainty in global or regional ocean LHF estimations. Therefore, ANN can be considered an ideal method to replace RF when generating tropical ocean LHF products.

6. Conclusions

We applied ANN and three other ML methods (RF, BR and RANSAC) to improve tropical ocean LHF estimation by ensemble of satellite and reanalysis products (MERRA-2, JOFURO-3, ERA-I and GSSTF-3) and evaluate the performance of fusion products based on reference product (OAFlux) and buoy observations. The ML models used here were trained (tested) using observations from 81 (34) buoy sites over low-latitude areas from 2003 to 2007.

By merging individual LHF product, our results show that the ensemble LHF products derived from four ML methods were significantly superior to the individual LHF products with higher accuracy and lower bias. Among them, ANN performs best, indicated by the highest $R^2$ (0.88 and 0.87), the lowest RMSE (10.4 and 10.9) and the highest KGE (0.89 and 0.90) for training and testing, respectively.

By quantifying relative uncertainties by the TCH method, we found that the relative uncertainties of ensemble LHF products were also significantly lower than individual LHF product, which lead to the conclusion that the individual product’s uncertainties caused by errors in algorithm and input datasets can be reduced by merging multiple products. In addition, ANN generated lower relative uncertainty than the other three ML methods. The result demonstrates that ANN can be considered an ideal method to replace RF when generating tropical ocean LHF products.

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