Soft sensing of water quality parameters in indoor shrimp farming using machine learning models

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Abstract: The objective of the paper is to explain how we used soft sensing based on machine learning models to estimate some water quality parameters in lined pond conditions from an indoor commercial shrimp (*Litopenaeus vannamei*) farm in Vietnam. Specific water quality parameters provide valuable insight into shrimp pond conditions which are critical for managerial decision making. Some parameters can be easy to measure using relatively inexpensive hand-held sensors submerged in the water and require minimal experience. Other parameters are far more expensive to measure because they require experienced labour, time consuming processes such as laboratory analyses of pond water samples, and ongoing materials costs.

Soft sensing refers to the process of estimating a variable from other directly measured variables. In this case, estimating variables that are difficult or time consuming to measure (ammonia, settling solids and total suspended solids) from variables that are easy and quick to measure along with pond input data. The aim is to reduce the time, cost, and requirement for experienced labour to monitor key pond water quality parameters. The study summarises the machine learning models we adopted and the accuracies we achieved in estimating key water quality parameters using soft sensing for commercial, super-intensive indoor shrimp farming.

We investigated different machine learning models to accurately estimate the target parameters. We investigated several different machine learning models for predicting the above target variables including Neural Network, long short-term memory Networks, Recurrent Neural Network, and Convolutional Neural Network etc. But these deep learning models did not produce good estimation results. This is most likely because these algorithms require huge volumes of data for effective training and the current data set is very small. Support Vector Regression was a good choice for modelling on small data sets. However, SVR models sometimes generate negative values that makes it unsuitable for estimation of WQ parameters. We used an ensemble tree-based modelling (Random Forest) approach that produced accurate as well as positive predictions hence making it suitable for these datasets.

We conducted multiple validation process to understand the effectiveness of the machine learning models. We used a leave-out-one-pond cross validation approach where we left one pond for testing and used the remaining ponds within a trial for model training. These validations were performed within a single trial (called 'within trial'). In another validation approach, we trained models on ponds from one or multiple trials and tested on ponds from a separate trial (called 'cross trial').

Ammonia estimation results based on machine learning models indicate that more accurate estimations were achieved using the 'within trial' validation than the 'cross trial' validation. This variability of ammonia among ponds in initial trials lead to relatively worse 'cross trial' estimation performance. However, 'cross trial' validations at later stages provided the highest accuracy. This demonstrates that as protocols are managed more consistently, estimating ammonia with high accuracy could become very likely.

For total suspended solids estimation, the predicted value provided a reliable enough estimate for pond managers to make informed decisions about the total suspended solids concentrations in the pond. There are some occasions where total suspended solids was underestimated. In occasions where this occurred, the estimation aligned itself with the actual values within the next few samples. Therefore, using the more frequently measured turbidity values to estimate total suspended solids might provide a more realistic indicator of the changes in pond conditions from day to day. Estimation of settling solids was highly inaccurate compared to total suspended solids and further investigation is needed on this front.

Keywords: Water quality, machine learning, Litopenaeus vannamei, automation, decision support tools

1. INTRODUCTION

The global demand for protein is increasing with a growing population, and farmed shrimp are considered as a suitable source to help meet such demand. Farmed shrimp are considered as a healthy food source by a variety of health experts because of their many nutritional benefits, including high-quality protein, vitamins, minerals, and long-chain fatty acids. Farmed shrimp accounts for 55% of the shrimp produced globally. The total global production increased 86% in the past 10 years, reaching more than 6.5 million tons in 2019 and a value of nearly US\$40 million. To keep up with this growth, the industry needs to carry out sustainable production strategies, most of the times switching from extensive to more intensive practices. However, its success is dependent not only on the nutrition and genetics, but also the culture environment and water quality.

It is important to maintain water quality (WQ) within certain ranges for optimal health and growth of shrimp in commercial farms (Rahman et al. 2019). The quality of pond water is regularly monitored (two to three times daily for some parameters) using handheld sensors, laboratory analyses of water samples or in some cases, permanently mounted sensors. Commonly measured water quality parameters in super-intensive conditions include temperature, dissolved oxygen, salinity, pH, turbidity, settling solids, total suspended solids, alkalinity, total ammonia, nitrite, and nitrate (Rana et al. 2021). These parameters provide critical insight into the health of the pond environment. Deviation of these water quality parameters from optimal ranges may result in compromised growth and health, increased pathogens risks, disease, and ultimately large-scale shrimp mortalities if the deviation is significant enough. Maintaining optimal water quality is a high priority for farmers to maximise production and profits but also avoid incidents of large-scale stock loss which could be catastrophic. One of the other benefits of soft sensor data is that the data can usually be generated in real time as opposed to traditional lab methods which often require at least 24 hours to generate data. Also, many locations require these soft-sensing techniques due to the health and safety risks, lack of resources etc.

In this study we present the results of some investigations to understand if some difficult-to-measure WQ parameters can be estimated from other easy-to-measure WQ parameters. They can be broadly classified under the category of *soft sensing*. Soft sensing refers to estimating a parameter from other measured signals/parameters rather than directly measuring them (Dabrowski et al. 2018). This is primarily done to reduce cost, but also developed as a decision support tool. In this study, we investigated the estimation of three difficult–to–measure parameters namely total ammonia nitrogen (TAN), settling solids (SS), and total suspended solids (TSS). These parameters require either time consuming laboratory-based analyses or pond-side processing of water samples. This is an expensive activity for a farm, resulting in infrequent data for decision making. Hence the *research problem* we investigated was how accurately WQ parameters like TAN, TSS, and SS can be estimated from other relatively easy-to-measure WQ parameters by sensors.

Machine learning (ML) models are ideal for studying such interactions (Rana et al. 2021). Machine learning in general provides a mechanism to learn a mapping between a set of inputs to a target. Given historical data from sensors and lab results, ML algorithms can learn such mapping by optimizing a set of parameters. In this paper we summarise the investigation of several machine learning models to learn these interactions. We discuss our models (based on ML) and findings on each of the three research problems (estimating TAN, SS and TSS) in the following sections. Our investigations revealed promising results as detailed in the manuscript.

2. DATA COLLECTION

The project was conducted in the Mekong Delta at Viet-Uc's commercial site in Nha Mat, Bac Lieu Province, Vietnam, and utilized two greenhouses that were solely dedicated to R&D experiments for the project. Between March 2018 and February 2021, six commercial-scale trials were completed, with each trial utilizing between 20 and $24 \times 500 \text{ m}^2$ plastic lined, indoor ponds, shade mesh covered to reduce ~80% of light exposure (Figure 1), and running for 90 to 100 days of culture (single phase, from ~PL10 to harvest), with stocking densities varying from 150 to 600 shrimp m⁻². This led to a total of 129 experimental ponds being ran through to harvest, whereby a comprehensive data collection regime was implemented to enable in-depth analysis of the pond environment and shrimp performance which is then used to identify the key constraints on production.

The trials were each conducted over a 14-week period with two trials conducted each year. Trials 1, 3 and 5 were conducted during the Spring/Summer months, whereas Trials 2, and 4 were conducted during the Autumn/Winter months. We exclude the data from Trial 4 in analysis due to analytical issues during sample processing. The trials mainly followed Biofloc Technology or BFT (minimum water exchange (Emerenciano et al. 2016; Schveitzer et al. 2013). However, Clear Water or CW (regular water exchange) protocols were experimented in the first two trials.

Rahman et al., Soft sensing of water quality parameters in indoor shrimp farming





Figure 1. Aerial view of Viet-Uc Nha Mat farm, Bac Lieu, Mekong Delta, and commercial greenhouses utilized in this study

WQ parameters dissolved oxygen (DO), temperature (Temp), and pH were measured using handheld sensors three times a day at 8 am, 2 pm, and 10 pm. Salinity (Sal), turbidity, oxidation reduction potential (ORP) and settling solids (SS) (Imhoff cones) were measured using handheld sensors once per day. SS was measured only for BFT ponds. TSS and TAN were measured twice per week. Bacteria counting (total aerobic heterotrophic bacteria named as "total bacteria", and total vibrio counting, including yellow and green colonies) were conducted once per week using TSA and TCBS plates (Hoang et al. 2018).

3. DATA ANALYSIS METHODS

We pose the soft sensing problem as estimating an expensive-to-measure target WQ parameter y as a function of relatively easy-to-measure WQ parameters $x_1, x_2, ..., x_m$. The set of easy to measure parameters can be represented by $\mathbf{s} = (x_1, x_2, ..., x_m)$. Given a set of input samples $\mathbf{s}_1, \mathbf{s}_2, ..., \mathbf{s}_n$ and corresponding targets $y_1, y_2, ..., y_n$, a machine learning algorithm finds a mapping f between s and y as $y \approx f_{\theta}(\mathbf{s})$. Depending on the learning algorithm, the set of parameters θ is optimized that reduces the overall difference between y and the estimated value $f_{\theta}(\mathbf{s})$.

Once WQ parameters for the whole growing season have been captured, we first generate samples and targets by combining the input and target WQ parameters at different time scales. This is done as different WQ parameters are measured at different time scales. Once the dataset is ready, we train and test machine learning models to understand their performance in terms of estimation error. From here, we split the dataset into training and test set. The training set is used to optimize the parameters of the machine learning model by reducing estimation error. The performance is obtained for estimation errors of the test set that is unknown to the model during training. Different methods were used for generating training and test sets. Different input WQ variables and data integration approaches are used for TAN, SS, and TSS estimation as detailed next:

- *TAN*: Two types of inputs were explored for predicting TAN: (i) WQ parameters (DO, Temp, pH, Salinity, and ORP) and bacteria count, and (ii) only WQ parameters (DO, Temp, pH, Salinity, and ORP). The target was set as TAN. Data from all the ponds were combined into a single dataset. There were some missing data in the combined data set, so we used data imputation method (*k*-nearest neighbour) to fill in the missing data before the machine learning training process. The readings of WQ and vibrio (i.e., bacteria count) on a given day is used to estimate TAN for the same day and no past values are used. While using the bacteria count, we developed two different versions of input features for the machine learning algorithms. In one version (no feature engineering) we used *Total Bacteria*, *Vibrio Y*, and *Vibrio G* input features. In another version (feature engineering) we derived the following features from *Total Bacteria*, *Vibrio Y*, and *Vibrio G*: Vibrio G is Vibrio G is the machine learning and Vibrio Y is the machine learning model.
- SS and TSS: During the project, the turbidity of the ponds was measured, and results demonstrated that turbidity was highly correlated with TSS and SS. Once the initial capital investment in the sonde is made, measuring turbidity is quick and easy with immediate results. Therefore, we aim to estimate TSS and SS from turbidity using machine learning models.

We investigated several different machine learning models for predicting the above target variables. Deep learning algorithms like NN (Neural Network), LSTM (Long short-term memory) (Tan et al. 2022), RNN (Recurrent Neural Network) (Tan et al. 2022), and CNN (Convolutional Neural Network) (Ajit et al. 2020) etc. did not produce good estimation results. This is most likely because these algorithms require huge volumes of data for effective training and the current data set is very small. Support Vector Regression (SVR) (Hearst et al. 1998) was a good choice for modelling on small data sets. However, SVR models sometimes generate negative values that makes it unsuitable for estimation of WQ parameters. We used an ensemble tree-based modelling (Random Forest) approach (Ho et al. 1995) that produced accurate as well as positive predictions hence making it suitable for these datasets.

4. **RESULTS AND DISCUSSIONS**

4.1. Ammonia (TAN) estimation

We conducted several validation approaches on data from Trials 1, 2 and 3. We used a leave-out-one-pond cross validation approach where we left one pond for testing and used the remaining ponds within a trial for model training. These validations were performed within a single trial. In another validation approach, we trained models on ponds from one or multiple trials and tested on ponds from a separate trial. The mean absolute error represents the average error in mg L⁻¹ of estimating each ammonia reading in the test set.

Table 1 presents the 'within trial validation' and Table 2 presents the 'cross trial validation'. More accurate estimations were achieved using the 'within trial' validation than the 'cross trial' validation. In addition, estimations were more accurate for trials 3 and 5, compared to trials 1 and 2. This is potentially because TAN was highly variable between the CW and BFT treatments in trials 1 and 2. This idea is further supported by the 'cross trial' validations whereby training on Trial 3 data to estimate TAN in Trial 5 provided the highest accuracy. This potentially demonstrates that as protocols produce more consistent results, the accuracy of estimating TAN increases. These models could then be applied to other 'difficult or expensive' to measure parameters such as nitrite and alkalinity.

When WQ and bacteria were both included as an input, the TAN estimations for each trial were slightly more accurate for 'within trial' validations. However, for 'cross trial' validations, the inclusion of bacteria as an input only improved estimations for Trial 3 when trained on data from Trial 1 and 2, and Trial 5, when trained on data from Trial 3. Future research should investigate combinations of other input measures to determine whether they can improve accuracy. The inclusion of feature engineering did not improve the accuracy of TAN estimations. In this situation, the ratio of total bacteria, total vibrio and green colony vibrio added no benefit. When the 'estimated' versus the 'actual' TAN readings for Pond 5 are plotted over time for Trial 3 (Figure 2) and Trial 5 (Figure 3), the results demonstrate that the estimated value could be reliably used as a tool to monitor TAN for most of the culture period, with the occasional 'spot check' with a photometer. This would significantly reduce labor and laboratory costs.

4.2. TSS estimation

We analyzed data from trials 3, 4, and 5 using the machine learning models for SS and TSS estimation. Turbidity and SS data were collected daily whereas TSS data was collected weekly. We thus integrated turbidity and SS at daily scale whereas turbidity and TSS at weekly scale. The integrated dataset from all the ponds within a trial was used to develop training and test data sets. We conducted modelling and testing within each trial. The modelling and validation were conducted within each trial (not across trials like ammonia). Within each trial, a Leave-Out-One-Pond cross validation was used where each pond becomes a test set in turn and the remaining ponds are combined into a training set. The mean absolute error (MAE) represents the average error in mg L^{-1} of estimating each TSS reading through the trial. The error as a percentage is calculated from the MAE divided by the average TSS for the trial multiplied by 100.

Table 1. Leave-out-one-pond (LOOP) validation (within trial validation). 'No feature engineering' means we used *Total Bacteria*, *Vibrio Y*, and *Vibrio G* as input features. 'Feature engineering' means we used $\frac{\text{Vibrio G}}{\text{Vibrio Y}}$

Validation setup			Mean absolute error (mg L ⁻¹)
WQ only, Vibrio not		Trial 1	0.95
as Input		Trial 2	0.37
		Trial 3	0.04
		Trial 5	0.09
WQ and Vibrio as	No Feature Engineering	Trial 1	0.90
Input		Trial 2	0.31
		Trial 3	0.03
		Trial 5	0.05
	Feature Engineering	Trial 1	1.14
		Trial 2	0.31
		Trial 3	0.03
		Trial 5	0.05

 $\frac{\text{Vibrio G}}{\text{Total Bacteria}} \text{ and } \frac{\text{Vibrio Y}}{\text{Total Bacteria}} \text{ as input features.}$

Table 2. Leave-out-one-trial (LOOT) validation (cross trial validation). 'No feature engineering' means we
used *Total Bacteria*, *Vibrio Y*, and *Vibrio G* as input features. 'Feature engineering' means we used
 $\frac{\text{Vibrio G}}{\text{Vibrio Y}}$,
 $\frac{\text{Vibrio G}}{\text{Total Bacteria}}$ and $\frac{\text{Vibrio Y}}{\text{Total Bacteria}}$ as input features.

Validation setup		Training	Test	Mean absolute error (mg L ⁻¹)
WQ only, Vibrio		Trial 1	Trial 2	1.33
not as Input		Trial 2	Trial 3	0.20
		Trial 1, Trial 2	Trial 3	0.81
		Trial 3	Trial 5	0.13
WQ and Vibrio	No Feature	Trial 1	Trial 2	1.41
as Input	Engineering	Trial 2	Trial 3	0.22
		Trial 1, Trial 2	Trial 3	0.56
		Trial 3	Trial 5	0.10
	Feature	Trial 1	Trial 2	1.09
	Engineering	Trial 2	Trial 3	0.34
		Trial 1, Trial 2	Trial 3	0.65
		Trial 3	Trial 5	0.12





Figure 2. Ammonia (TAN) prediction results for pond 5 from Trial 3. Both training and testing were done on ponds from Trial 3. The empty 'actual' readings indicate no ammonia data was recorded on that week.

Figure 3. Ammonia (TAN) prediction results for pond 5 from Trial 5. Both training and testing were done on ponds from Trial 5. The empty 'actual' readings indicate no ammonia data was recorded on that week.

For Trial 3 and 4, the mean absolute error was 38.95 and 25.55 mg L⁻¹, respectively (Table 3). This equates to a similar percentage error of 23.5% and 24.8%, respectively. For Trial 5, the error was much higher at 93.91 mg L⁻¹ resulting in a higher percentage error of 36.8%. However, there were concerns with the accuracy of the TSS data from Trial 5 and this higher error rate potentially justifies these concerns. Therefore, the Trial 5 TSS data will not be considered when evaluating the potential of these prediction models.

TSS Prediction results for Pond 5 from Trial 3 and Trial 4 are presented in Figure 4 and Figure 5 respectively. For most sample numbers, the predicted value provided a reliable enough estimate for pond managers to make informed decisions about the TSS concentrations in the pond. The main concern would be when the estimated value significantly underestimates the actual value, as higher than expected TSS can be problematic in extreme cases. However, in the few cases where this occurred, the estimation aligned itself with the actual values within the next few samples. It's also possible that sudden changes in TSS are from sampling or analytical variability rather than actual changes in pond conditions. Therefore, using the more frequently measured turbidity values to estimate TSS might provide a more realistic indicator of the changes in pond conditions from day to day.

4.3. SS estimation

The mean absolute error represents the average error in mL L⁻¹ of predicting each SS reading through the trial. The error as a percentage is calculated from the MAE divided by the average SS for the trial multiplied by 100. For Trial 3, the mean absolute error was 0.96 mL L⁻¹ (Table 4). However, the estimation improved for Trial 4 (0.40 mL L⁻¹) and Trial 5 (0.32 mL L⁻¹). In terms of a percentage, the estimation was not as accurate as the TSS prediction, ranging from 41.7% to 69.0%.

When the predicted values are compared against the actual values for different sample numbers throughout the culture period, the higher inaccuracy of estimating SS, compared with TSS, is particularly noticeable in some

ponds. For example, in pond 10, Trial 3, the estimated values were substantially lower than the actual values from sample 40 onwards. In Trial 4, the model did not estimate the sharp increase in SS around DOC 75 for ponds 5 and 10 or the peaks in SS for ponds 1 and 5 in Trial 5. This could be partially explained but the nature of these two parameters with higher expected variance in SS compared to TSS 0. According to these authors, the coefficients of correlation was higher in TSS × turbidity (0.98) as compared to TSS × SS (0.92) in a super-intensive shrimp culture with no water exchange. With more data collected over a greater number of ponds operating under a consistent protocol, the accuracy of these models is likely to improve greatly. While measuring SS might seem simple, it still requires a lot of labour and can be time consuming when accumulated over multiple greenhouses and crops. Therefore, further investment in the continual refinement of these models will be beneficial to large scale commercial operations in future.

Table 3. The mean absolute error (mg L⁻¹) and percentage error (%) for predicting Total Suspended Solids (TSS) throughout trials 3, 4 and 5

Trial	Mean absolute error for predicting TSS (mg L ⁻¹)	Error (%)
3	38.95	23.5
4	25.55	24.8
5	93.91	36.8

Table 4. The mean absolute error and percentage error (%) for predicting Settling Solids (SS) throughout trials 3, 4 and 5

Trial	Mean absolute error for prediction SS (mL L ⁻¹)	Error (%)
3	0.96	41.7
4	0.40	69.0
5	0.32	65.3



Figure 4. Total Suspended Solids (TSS) prediction results for Pond 5 from Trial 3. Both training and testing were done on ponds from Trial 3.



Figure 6. Settling Solids (SS) prediction results for pond 5 from Trial 3. Both training and testing were done on ponds from Trial 3.



Figure 5. Total Suspended Solids (TSS) prediction results for Pond 5 from Trial 4. Both training and testing were done on ponds from Trial 4.



Figure 7. Settling Solids (SS) prediction results for pond 5 from Trial 4. Both training and testing were done on ponds from Trial 4.

5. CONCLUSIONS

Efficient WQ management of super-intensive ponds for sustainable production of shrimp is the key mantra of success in this industry. An ideal pond environment within desirable WQ ranges will improve survival, sustain efficient growth, allowing production consistency and predictability. In this paper we presented our investigation on soft sensing for estimating ammonia (TAN), settling solids, and total suspended solids from dissolved oxygen, temperature, salinity, pH, ORP, total bacteria, total vibrio, and turbidity. A subset of feature engineered version of these input water quality parameters were investigated to find the best combination of input features that produces accurate estimations of the target variables.

TAN estimation results indicate that more accurate estimations were achieved using the 'within trial' validation than the 'cross trial' validation. This variability of TAN among ponds in initial trials lead to relatively worse 'cross trial' estimation performance. However, 'cross trial' validations at later stages (training on Trial 3 data to estimate ammonia in Trial 5) provided the highest accuracy. This demonstrates that as protocols are managed more consistently, estimating ammonia with high accuracy could become very likely.

For TSS estimation, the predicted value provided a reliable enough estimate for pond managers to make informed decisions about the TSS concentrations in the pond. There are some occasions where TSS was underestimated. In occasions where this occurred, the estimation aligned itself with the actual values within the next few samples. Therefore, using the more frequently measured turbidity values to estimate TSS might provide a more realistic indicator of the changes in pond conditions from day to day. Estimation of SS was highly inaccurate compared to TSS and further investigation is needed on this front.

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