RESEARCH ARTICLE

A CALPUFF model study for environmental pollution analysis in animal husbandry in Japan

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The California PUFF model (CALPUFF) is a widely used Lagrangian PUFF model system for predicting the diffusion of atmospheric pollutants. However, owing to limitations in parameterization schemes, errors in meteorological fields, and uncertainties in emission inventories, its standalone application consistently produces systematic prediction biases. Animal husbandry is one of the main sources of ammonia emissions in Japan's atmosphere. Analyzing the diffusion characteristics of this gas is crucial for environmental pollution analysis and control. This study integrated the CALPUFF with the random forest algorithm to analyze the diffusion characteristics of odorous gases from animal husbandry farms. Based on the analytical results, it proposed suggestions for environmental pollution control to mitigate emissions from these sources. The results demonstrated that the optimized model achieved a prediction accuracy exceeding 98% for the diffusion of various gases with a root mean square error of only 0.1233, which was lower than that of other models. This study analyzed the actual test results obtained from the Suisan Research Center for Livestock Production of the Agriculture and the Forestry and Fisheries Department of Okinawa Prefecture. The findings denoted that the diffusion of odorous gases from animal husbandry farms exhibited a seasonal distribution. In summer, under high temperature and low wind conditions, the pollution diffusion was nearly circular and uniform with a wide impact range but low concentration. In winter, under low temperature and high wind conditions, the diffusion range was concentrated but more directional, and the overall pollution range was reduced by 30 - 40% compared to summer. The proposed model analyzed environmental pollution from animal husbandry farms in Japan and provided a basis for environmental pollution control in these farms.

Keywords: Japan; animal farms; environmental pollution analysis; malodorous gases; random forest algorithm; California PUFF model.

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Introduction

Animal husbandry plays an important role in Japan's agricultural economy. However, according to statistics from the Japanese environmental protection department, animal husbandry is also one of the main sources of atmospheric ammonia emissions in Japan, accounting for 30% of the total emissions [1]. As the scale of animal husbandry continues to expand, the numbers of pollutants such as manure and wastewater generated during the breeding process are increasing daily and produce a large amount of malodorous gases,

thus causing environmental pollution [2]. Most of the current environmental pollution analysis of farms focuses on the total amount of pollutants and the monitoring of conventional pollution indicators, ignoring the analysis of the distribution of malodorous gases, resulting in poor environmental pollution control [3]. Predictive models are now used in various scenarios to predict various gases, pollutants, and other indicators [4]. Therefore, using predictive models to predict the diffusion of malodorous gases in farms and obtain their environmental pollution diffusion mechanism can help farm managers control pollution emissions and purify the environment around farms [5]. In addition, with the development of computer technology, some intelligent algorithms have been used for environmental pollution analysis.

eXtreme Gradient Boosting (XGBoost) has been used to analyze environmental pollution, but this method still has the problems of high data quality requirements and weak ability to process complex data [6]. Researchers introduced the XGBoost algorithm to analyze environmental pollution and found that, although the XGBoost algorithm could achieve an accuracy of 92.1% in analyzing environmental pollution, it still had the problem of insufficient interpretation of the spatiotemporal dependence characteristics of pollutants [7, 8]. Subsequently, some studies introduced genetic algorithms, particle swarm optimization, and differential evolution to analyze air pollution, but those algorithms had the problem of complex parameter settings [9]. Praveenchandar *et al*. used the genetic algorithm to analyze environmental pollution and found that, although the addition of the genetic algorithm could optimize the model combination to a certain extent and thus improve the prediction accuracy, the algorithm had a slow convergence speed and was prone to getting trapped in local optima [10]. Nikpour *et al*. designed an environmental pollution analysis model based on the particle swarm algorithm. The results showed that the model could improve the analysis accuracy to 93.2%, but its analysis accuracy in multi-source datasets was only 82.3% [11]. The California PUFF m(CALPUFF) is a non-steady-state Lagrange smoke plume model system used to predict the transport, diffusion, deposition, and chemical transformation of atmospheric pollutants. It is widely used in environmental impact assessment, emergency warning, and regional air quality research. In recent years, some scholars used the CALPUFF to analyze or reduce environmental pollution [12]. Tagliaferri *et al.* introduced the CALPUFF to analyze environmental pollution and found that it could improve the accuracy of environmental pollution analysis by 10.2%, but the CALPUFF alone still had the problem of large prediction bias [13]. Bayraktar *et al*. also used the CALPUFF to analyze environmental pollution and received similar results [14]. RF can capture the nonlinear relationship between multisource heterogeneous data and target variables to calculate the bias and thus correct the model bias. This method has also been used in various models and algorithms. Jiang *et al*. used the Random Forest (RF) algorithm to calibrate the bias of the gesture decoding model and found that, after calibration, the calculation accuracy of the model improved by 12.7% [15]. In addition, Bargam *et al*. used the RF algorithm to calibrate the bias of the support vector machine algorithm. The results also showed that the computational accuracy of the algorithm increased significantly after calibration [16]. Although CALPUFF can analyze most environmental pollution, as a physical mechanism model, it still has parameterization limitations, meteorological field errors, and emission inventory uncertainties. Therefore, the feasibility of using the CALPUFF alone is poor [17].

This study employed the RF algorithm to capture systematic biases in the CALPUFF. Based on the nonlinear relationship between the bias and meteorological and topographical conditions obtained through RF, the output of the CALPUFF was corrected, improving the model's accuracy in analyzing environmental pollution. The constructed RF-CALPUFF was used to predict the distribution of odorous gases in livestock farms,

thereby analyzing environmental pollution and proposing reasonable suggestions to mitigate it. This research designed RF-CALPUFF. Machine learning algorithms were used to correct the biases in CALPUFF, improving the accuracy of CALPUFF's prediction of odorous gases. A multi-dimensional bias feature vector system was constructed using diverse heterogeneous data such as meteorological conditions, topographic features, emission source characteristics, and temporal characteristics, providing feature support for model bias correction.

Materials and methods

Composition of the CALPUFF system

CALPUFF consisted of four parts including a preprocessing module, a meteorological module, a diffusion module, and a post-processing module. The preprocessing module performed geographic information processing, pollution source data organization, observation data quality control, and network system construction. In geographic information processing, parameters such as terrain height, slope, and aspect were extracted from the collected data. Different areas such as water bodies, farmland, forests, and cities were distinguished, and a computational domain coordinate system was established. Subsequently, the pollution source data was systematically organized including determining the farm's geographical location, pollutant emission intensity, and pollution source type, while distinguishing the differences between daytime and nighttime emissions and analyzing their seasonal variation patterns. Observation data quality control involved importing meteorological station data for subsequent meteorological field diagnosis and importing air quality monitoring data as a benchmark for model validation. In network system construction, horizontal resolution and vertical stratification were defined, the core farming area was covered with a fine-grained network, and sensitive receptor points such as residential areas, schools, and hospitals were marked. The meteorological module was an important component of the CALPUFF, used to generate the meteorological input data required for model operation. This module could process meteorological station observation data, generate a three-dimensional meteorological field through interpolation and extrapolation, and generate key meteorological parameters such as wind speed, wind direction, temperature, and humidity. The diffusion module was the core calculation engine of the model, which used the Lagrange smoke plume method to track the entire process of pollutants from the source to the receiver point. The concentration of pollutants at a certain receiver point was calculated as follows.

$$C = \frac{Q}{2_y} g\ exp(\frac{d_a^2}{2_x^2})\ exp(\frac{d_c^2}{2_y^2}) \quad (1)$$

where *C* was the ground-level concentration of the pollution source. *Q* was the source intensity of the pollutant. d_a was the downwind distance. d_c was the lateral clustering. *x*, *y*, and *z* were the diffusion coefficients. g was the vertical term of the Gaussian equation and was calculated as below.

$$g = \infty exp[\frac{(He+2nh)^2}{2_2^2}] \quad (2)$$

where He was the effective height. n was the stratification number. h was the mixing layer height. The post-processing module mainly performed result analysis, processing, and visualizing the output data generated by CALPUFF. When using CALPUFF to predict pollutant emissions from livestock farms, the parameters of CALPUFF were first set to determine the prediction time, prediction area, regional center point, pollution source elevation, and overall area of the pollution source. Then, local topographic and meteorological data were input. The CALPUFF calculated the odor concentration based on the input data, identified the pollution source, and thus analyzed the environmental pollution from the livestock farm.

Environmental pollution analysis model based on RF-CALPUFF

While the CALPUFF could predict the diffusion of odorous gases in livestock farm environments and determine the distribution of pollutants, it suffered from systematic bias and required improvement. The RF algorithm could calibrate the CALPUFF error based on the deviation between the predicted and actual observations, thereby improving the accuracy of CALPUFF predictions. The RF calibration process consisted of two stages including deviation feature extraction and correction. In deviation feature extraction, the CALPUFF first obtained the predicted value based on the input data and then calculated the concentration deviation value based on the actual value measured by the instrument as below.

$$\Delta C^{i,t} = C_{obs}^{i,t} - C_{sim}^{i,t} \quad (3)$$

where $\Delta C^{i,t}$ was the concentration difference at the i-th monitoring point at time t. $C_{obs}^{i,t}$ was the observed concentration at that point. $C_{sim}^{i,t}$ was the predicted concentration at that point. Furthermore, to capture the nonlinear causes of the bias, a multidimensional feature vector was constructed, which included meteorological condition features, topographic features, emission source features, and temporal features. Meteorological condition features included wind speed, wind direction, atmospheric stability level, mixing layer height, temperature, and relative humidity. Topographic features included the monitoring point's altitude, slope, and aspect. Emission source features included emission height and emission temperature. Temporal features included seasonal and diurnal characteristics. During the calibration phase, RF constructed multiple decision trees using the bootstrap aggregating (Bagging) method, which consisted of four steps including data preprocessing, Bootstrap sample generation, decision tree construction, and model ensemble. During data preprocessing, the various feature data predicted by CALPUFF were first cleaned and standardized to remove outliers. Continuous features were standardized using Z-score. The standardization was done as follows.

$$x_{norm} = \frac{X-\mu}{\sigma} \quad (4)$$

where μ was the feature mean. σ was the standard deviation. X was the original dataset. x_{norm} was the standardized dataset. The training dataset for the RF was constructed by using calculated concentration bias as the target scalar and combined with the various features predicted by CALPUFF. When generating bootstrap samples, N samples were first drawn with replacement from the original training set to form the bootstrap sample set of the low k decision trees. Weights were initialized for each sample in the bootstrap sample set to ensure a uniform weight distribution for each tree. When constructing the decision tree, each decision tree was recursively split from the root node, while the purity of the node was calculated first. For the sample set of the node, the variance of the target variable was used as the measure of impurity as follows.

$$Var(S) = \frac{1}{|S|}\sum_{m\in S}(\Delta C_m - \Delta \bar{C}_S)^2 \quad (5)$$

where $Var(S)$ was the impurity measure. S was the current node sample set. $|S|$ was the number of samples in the sample set. m was the m-th sample index. $\Delta \bar{C}_S$ was the mean deviation within the node. Subsequently, when splitting a node, multiple features were randomly selected from all features as candidate features. The number of features selected was determined below.

$$m_{try} = \sqrt{M} \quad (6)$$

where M was the total number of features. m_{try} was the number of selected features. After the candidate features were selected, the midpoint of the sorted features was chosen as the split point. For each split point, the sample was divided into a left subset and a right subset, and the variance reduction after splitting was calculated. The feature and split point that

maximized the variance reduction were selected as the optimal split point as follows.

$$\Delta Var(\theta, j) = Var(S) - \frac{|S_L|}{|S|} Var(S_L) - \frac{|S_R|}{|S|} Var(S_R) \quad (7)$$

where θ was the candidate split point. S_L was the left subset. S_R was the right subset. j was the number of different values of the feature within the node. After selecting the optimal split point, the left and right child nodes were repeatedly split according to the selection method until the decision tree reached the maximum threshold. The above process was repeated to generate multiple decision trees and perform model integration. After inputting data, RF output the average value of the prediction results of all decision trees as follows.

$$\Delta\tilde{C}(Y) = \frac{1}{K}\sum_{k=1}^{K} T_k(Y) \quad (8)$$

where $T_k(Y)$ was the bias prediction value of the k-th decision tree for the input feature Y. K was the total number of decision trees. After obtaining the bias of the RF prediction, the original prediction result of CALPUFF was dynamically corrected to obtain the corrected concentration value and was calculated below.

$$C_{cor}^{i,t} = C_{sim}^{i,t} + \Delta\tilde{C}(Y^{i,t}) \quad (9)$$

where $C_{cor}^{i,t}$ was the corrected gas concentration. Based on the odor gas diffusion prediction results of RF-CALPUFF, the environmental pollution around the farm could be analyzed, and reasonable suggestions could be made based on the analysis results. The analysis process consisted of five stages including data input and preprocessing, CALPUFF prediction, RF bias correction and model optimization, comprehensive environmental pollution analysis, and control recommendations. In the data input and preprocessing stage, basic geographic information data, land use data, and vegetation cover data of the study area were collected to construct a three-dimensional topographic database. Simultaneously, local meteorological observation data were acquired, and data on the farm's scale, manure treatment methods, and emissions of odorous gases were compiled. Finally, an environmental monitoring network was deployed with monitoring stations being set up at sensitive target points around the farm to acquire real-time data for model validation. The preprocessed data was input into the CALPUFF, which output the concentration distribution of odorous gases based on the preprocessing, meteorological, diffusion, and post-processing modules. In the RF bias correction and model optimization stage, a bias feature dataset was constructed using RF, and an RF bias correction model was trained. This model was then used to correct the bias in the CALPUFF, yielding the corrected concentration distribution. Based on the corrected concentrations, the environmental pollution around the farm was analyzed, examining the impact of different temperatures, wind directions, and wind speeds on the distribution of odorous gases. High-concentration areas and pollution points were identified. Based on the pollution analysis results, targeted environmental management recommendations were proposed for control and management.

Dataset and environment configuration

The predictive performance of RF-CALPUFF was tested on a Dell PowerEdge R750 server with a 10 TB SSD high-speed storage array and an Ubuntu 20.04 LTS (64 bit) operating system. Python 3.9.7 (https://www.python.org/downloads/release/python-397/) was employed as the machine learning framework, while NumPy 1.24.3 (https://pypi.org/project/numpy/1.24.3/) was used for data processing. CALPUFF version 7.2.1 (https://www.calpuff.org/) was applied for model construction. For testing, the Kincaid dataset (https://www.harmo.org/jsirwin/KincaidHourlyDiscussion.html) from the Classic Tracer Datasets (https://www.harmo.org/jsirwin/Tracer_Data.html) was selected, which contained 350 hours of tracer experiments, as well as hourly and 5-minute SO_2 and SF_6 concentrations, and meteorological data to test the predictive performance of the RF-CALPUFF

on gas distribution. 171 hours of data from this dataset were selected as the model performance test dataset and divided into training, test, and validation sets at 8:1:1 ratio. For actual testing, topographic data, meteorological data, pollution source emission data, and air quality monitoring data from an animal farm in Japan were collected as the actual test dataset. During testing, the number of decision trees in the RF model was set to 200, the maximum depth to 15, the minimum number of split samples to 5, and the random seed to 42. The Kincaid dataset was selected for ablation testing of the model to verify whether introducing RF could improve the performance of CALPUFF. The prediction performance of the RF-CALPUFF gas diffusion prediction model was then compared with existing gas diffusion prediction models based on Physical-Informed Neural Network-Convolutional Neural Network (PINN-CNN) (https://deepxde.readthedocs.io/en/latest/), Computational Fluid Dynamics-Pressure Implicit with Splitting of Operations (CFD-PISO) (https://www.openfoam.com/), and Temporal Convolutional Network-Residual Network (TCN-ResNet) (https://arxiv.org/abs/2104.10122). The Mean Square Error (MSE), Root Mean Square Error (RMSE), and Mean Absolute Error (MAE) of four models were analyzed.

Real practical test

The pig farm of the Cattle Research Center in Okinawa Prefecture served as the test subject, which Located in Jinbei-ken, Kintoku-gun, Okinawa Prefecture, Japan with the geographical coordinates of 26°41'13"N and 127°56'24"E. This farm was chosen because it represented the mainstream model of intensive farming in Japan, and its scale and facilities were typical among similar farms in Japan. Furthermore, the farm located in a hilly basin with significant topographical variations, which effectively validated the applicability of the CALPUFF. The farm also belonged to a Japanese agricultural cooperative, possessing comprehensive production records and environmental monitoring infrastructure. Additionally, environmental monitoring stations were in the farm area, providing continuous meteorological and air quality observation data to support model construction and analysis.

Statistical analysis

SPSS 26.0 (IBM, Armonk, NY, USA) was employed to verify whether the difference in prediction error between the RF-CALPUFF and other comparison models was statistically significant. One-way ANOVA on the MSE, RMSE, and MAE of the four models were performed. Tukey HSD test was applied for pairwise comparison. *P* value less than 0.05 was defined as statistically significant difference.

Results and discussion

Model performance testing

CALPUFF's prediction accuracies for SO_2 and SF_6 gas concentrations in the dataset were 82.1% and 81.9%, respectively, indicating a relatively large prediction error (Figure 1a). After introducing RF, RF-CALPUFF improved its prediction accuracies for SO_2 from 82.1% to 98.2% and SF_6 gas concentration by 16.7% (Figure 1b). The results demonstrated that introducing RF significantly improved the prediction accuracy of CALPUFF. RF algorithm could enhance the performance of CALPUFF. The MSE, RMSE, and MAE of the four prediction models PINN-CNN, CFD-PISO, TCN ResNet, and RF-CALPUFF demonstrated that RF-CALPUFF had an MSE of 0.0152, an RMSE of 0.1233, and an MAE of 0.0896, exhibiting extremely small errors. The PINN-CNN prediction model had an MSE of 0.0289, an increase of 0.0137 compared to RF-CALPUFF. Simultaneously, the RMSE and MAE of the PINN-CNN model also increased. The MSE, RMSE, and MAE values of the CFD-PISO and TCN-ResNet models also increased (Figure 2). These results indicated that the proposed RF-CALPUFF performed better in predicting gas concentration diffusion than other gas concentration diffusion models. Therefore, this study selected RF-CALPUFF for predicting gas concentrations in aquaculture farms.

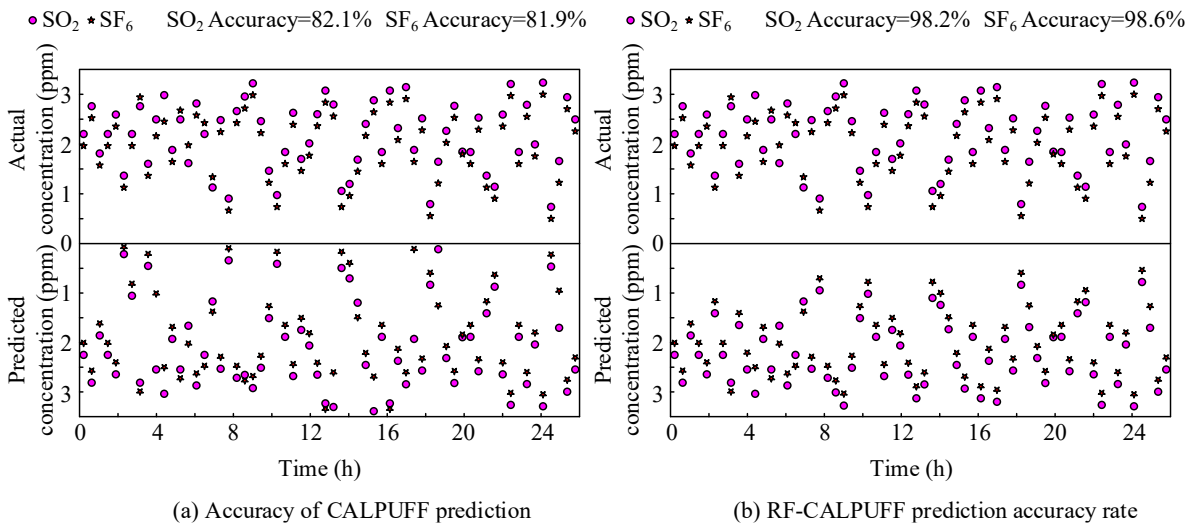


Figure 1. Comparison of model performance between CALPUFF and RF-CALPUFF.

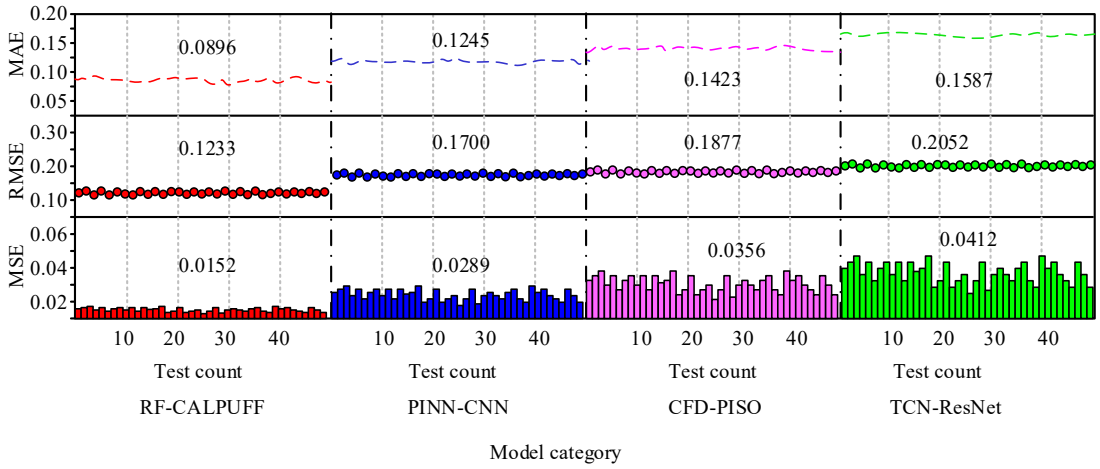
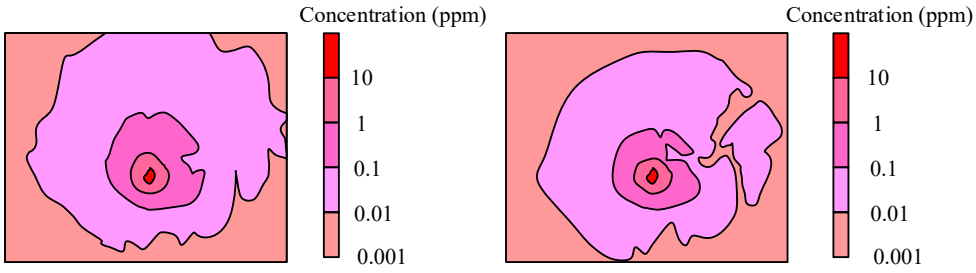


Figure 2. Comparison of different models' performance.

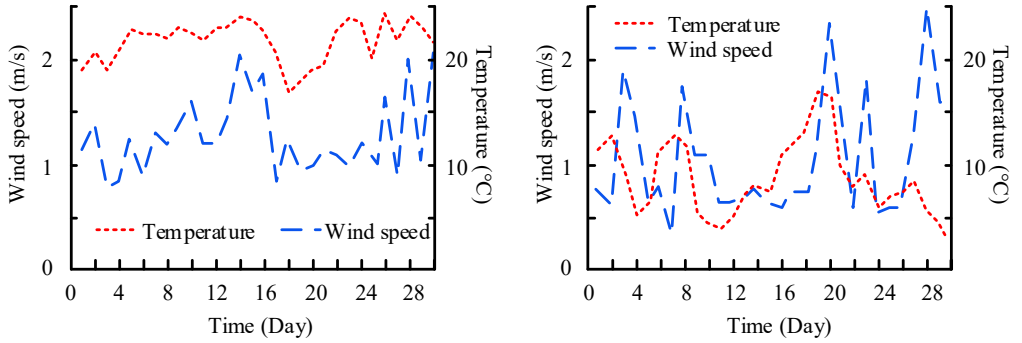
Pollution analysis results

RF-CALPUFF was then tested in a real-world setting to analyze malodorous odors in animal farms in June and November. The results showed that, in summer (June), the gas concentration at the central pollution source location of the farm reached over 10 ppm, and the area exhibited obvious power diffusion characteristics. The diffusion range was relatively uniform with similar extension distances in all directions, forming an approximately circular distribution (Figure 3a). In winter (November), the high-concentration core area was still located at the center of the pollution source, but its range was significantly reduced. Furthermore, the pollution source showed a clear directional distribution, extending far in the northeast-southwest direction (Figure 3b). Comparing summer and winter, the overall pollution impact range of the farm in winter decreased by 30 - 40%, and the pollutant diffusion direction no longer followed a concentric circle distribution but extended along the prevailing wind direction, indicating a significant influence from topography. Further predictions with wind speed and temperature changes in the region in June and November were performed to analyze the causes of pollution diffusion. The results showed that



(a) Average pollution dispersion forecast for June (b) Average pollution dispersion forecast for November

Figure 3. Distribution of pollution spread from livestock farms.



(a) Wind speed and temperature variations in June (b) Wind speed and temperature variations in November

Figure 4. Changes in temperature and wind speed at the farm in June and November.

average daily temperature fluctuated between 17 and 25°C in summer, remaining relatively stable overall. Significant temperature fluctuations occurred only between days 14 and 20. Summer wind speeds ranged from 0.84 to 2.1 m/s with wind speeds exceeding 1.8 m/s on days 10, 14, 16, 26, 28, and 30, totaling 6 days and representing a relatively low percentage (Figure 4a). The average daily temperature fluctuated between 3 and 17°C in winter, exhibiting a large range. Wind speeds varied between 0.4 and 2.5 m/s with significant variations occurring in November (Figure 4b). Further, the relationship between wind speed and temperature showed a negative correlation with decreasing temperature leading to increasing wind speed. Comparing summer and winter, the temperature and wind speed fluctuations in November were significantly greater than that in June. There was a causal relationship between the diffusion of odorous gases from livestock farms and meteorological conditions. In summer, the average daily temperature was between 17 and 25°C. The high temperature led to a mixing layer height of 1,500 – 2,000 m, resulting in strong vertical turbulence. Furthermore, summer wind speeds remained between 0.84 and 2.1 m/s. These high-temperature, low-wind-speed meteorological conditions diluted pollutants vertically, but the dilution capacity was weak horizontally, leading to a near-circular, uniform diffusion of pollutants around the pollution source. In contrast, in winter, the temperature fluctuated significantly, and wind speeds changed drastically. Intermittent cold air activity controlled the directional diffusion of pollutants along the prevailing wind direction, resulting in a clear directional distribution. Therefore, the diffusion of odorous gases from livestock farms exhibited a significant seasonal pattern as a wide impact area but low concentration in summer and a concentrated impact area but with

stronger directionality in winter. Based on the above pollution diffusion analysis results, the environmental pollution level was then analyzed. The environmental pollution level and pollution diffusion mechanism of livestock farms differed under different wind speed conditions in summer and winter. Reasonable environmental pollution control measures were proposed based on this risk level and pollution diffusion mechanism. According to the pollution diffusion mechanism under low wind speeds in summer, livestock farms were advised to stop manure removal operations at night and increase the frequency of biological deodorizing agent spraying to reduce the risk of pollution accumulation near the farm and minimize the impact on the surrounding environment. During windy weather in summer, livestock farms could carry out centralized manure collection and composting operations, taking advantage of the strong winds to accelerate the decomposition of organic matter in the compost. Meanwhile, by increasing the scale of processing, they could promote the resource utilization of livestock and poultry waste and ensure the stability of the surrounding environmental quality. On days with calm winds in winter, pollutant accumulation was severe, and the risk level was extremely high. Livestock farms needed to comprehensively reduce production to mitigate the degree of pollution accumulation. Sealed storage facilities and increased monitoring frequency at the plant boundary allowed for timely and accurate monitoring of pollutant concentration changes. If an abnormal increase in concentration was detected, immediate action could be taken to mitigate the serious harm of accumulated pollution to the farm and surrounding environment. During windy winter days, the risk level was extremely high. To reduce environmental pollution, farms needed to empty manure storage areas in advance to prevent the release of foul odors from waste during strong winds. Simultaneously, reinforced covering facilities were required to prevent dust generation, and protective measures were to be implemented for sensitive areas to prevent adverse effects from windy conditions on distant sensitive areas.

Conclusion

In response to the current lack of analysis on the diffusion of odorous gases and the low accuracy of analysis in environmental pollution analysis, this study optimized the CALPUFF using RF and constructed an RF-CALPUFF gas diffusion prediction model. The model was used to predict the diffusion of odorous gases in aquaculture farms, analyze the characteristics of gas diffusion, and thus analyze the environmental pollution of aquaculture farms. The results showed that RF-CALPUFF had good predictive performance. Tests conducted in actual animal farms illustrated that pollutants in Japanese animal farms were evenly distributed in a circular shape in summer with a balanced distribution in all directions. In winter, pollutants were controlled by intermittent cold air activity and spread in a directional manner along the dominant wind direction with a reduced overall impact range. The results suggested that the proposed model could accurately analyze the environmental pollution around animal farms in Japan and thus propose reasonable environmental control measures. However, the training of RF-CALPUFF relied on historical data, which limited its ability to predict extreme weather events. Future research should use attention mechanisms to construct temporal prediction modules and optimize the model again to improve its predictive ability.

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