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Artificial neural network approach for prediction of ammonia emission from field-applied manure and relative significance assessment of ammonia emission factors

Youngil Lim[a,*], Young-Sil Moon[a], Tae-Wan Kim[b]

[a] *Research Center of Chemical Technology (RCCT), Department of Chemical Engineering, Anseong-si, Seokjung-dong 67, Gyonggi-do 456-749, Republic of Korea*

[b] *Faculty of Plant Life and Environmental Sciences, Anseong-si, Seokjung-dong 67, Gyonggi-do 456-749, Republic of Korea*

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Abstract

This article presents a systematic method for enhancing the estimation accuracy of ammonia emission from field-applied manure and for assessing the relative significance of ammonia emission factors, using the feedforward-backpropagation artificial neural network (ANN) approach.

The multivariate linear regression (MLR) method well describes the ammonia emission tendency with the emission factor variation. However, ammonia emission from manure slurry is too complex to be captured in a linear regression model. This necessitates a model which can describe complex nonlinear effects between the ammonia emission variables such as soil and manure states, climate and agronomic factors. In the present study, a principle component analysis (PCA) based preprocessing and weight partitioning method (WPM) based postprocessing ANN approach (called the PWA approach) is proposed to account for the complex nonlinear effects.

The ammonia emission is predicted with precision by the 11 emission factors, using the nonlinear ANN approach. The relative importance among the 11 emission factors is identified using the elasticity analysis in the MLR method and using the WPM in the ANN approach. The relative significance obtained quantitatively by the PWA approach in the present study gives an excellent explanation of the most important processes controlling NH_3 emission.

Keywords: Ammonia emission; Livestock manure; Michaelis–Menten equation; Multivariate linear regression (MLR); Artificial neural network (ANN); Principle component analysis (PCA); Weight partitioning method (WPM)

1. Introduction

The ammonia (NH_3) emission from animal wastes has become one of the major air pollution problems in recent years and is a major concern world-wide (Ni, 1999). In Europe, ammonia from animal wastes and fertilizer was believed to constitute about 90% or more of the anthropogenic NH_3 release (Ni, 1999). In most Asian countries, the estimated NH_3 release from fertilizer and livestock accounted for about 77% of the total anthropogenic NH_3 release and the release from livestock alone accounted for about 30% (Zhao and Wang, 1994). In UK, NH_3 losses following land spreading have been estimated at approximately 70 ktonnes/year (nitrogen basis in NH_3), accounting for 30% of the total emission from UK agriculture (Misselbrook et al., 2000).

Ammonia volatilization from field-spread animal manure leads to a significant reduction in the fertilizer value of the manure. Although many technical attempts have been made to reduce emissions, the reduction potential of the different techniques is not yet clear (Plochl, 2001). This is mainly because ammonia emission is influenced by many internal factors (e.g., manure dry matter content, pH value and ammonia concentration) as well as external factors (e.g., soil types, climate variables, application methods). Therefore, a better understanding of the mechanisms controlling NH_3 emissions from field-applied manure will contribute to the development of low-emission livestock production systems (Sommer et al., 2003).

The Michaelis–Menten equation involving two model parameters (total loss of ammonia and time to reach half of the total loss) has been used for the ammonia emission rate model

* Corresponding author. Tel.: +82 31 670 5207; fax: +82 31 670 5445.
E-mail address: limyi@hknu.ac.kr (Y. Lim).

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Nomenclature

a_i	linear regression model parameters for K_m or output values in ANN
A_i	exponential of linear regression model parameters for K_m
b_i	linear regression model parameters for N_{max} or biases in ANN
B_i	exponential of linear regression model parameters for N_{max}
K_m	time to reach half of N_{max} in the ammonia emission (h)
N_{max}	maximum ammonia emission based on nitrogen (kg/ha)
N_{NH_3}	nitrogen-based total ammonia loss (kg/ha)
$\dot{N}_{NH_3}$	nitrogen-based ammonia loss rate (kg-N/h ha)
p_i	independent input variables in ANN
P_{in}	independent input variable vector (or set) in ANN
$\bar{P}_{in}$	normalized input variable vector (or set) in ANN
P_{PCA}	input variable vector (or set) transformed by PCA
t	time
Δt	time interval
$v_{initial}$	initial ammonia emission rate (=N_{max}/K_m) (kg/h ha)
w	weights in ANN
x	independent variable
y	dependent variable

Greek letters

ε_{K_i}	elasticity of K_m to 11 input variables in MLR
ε_{N_i}	elasticity of N_{max} to 11 input variables in MLR
μ	mean value
σ	standard deviation
$\bar{\sigma}$	normalized standard deviation (= σ/μ)

by many researchers (Plochl, 2001; Søgaard et al., 2002; Misselbrook et al., 2005). The two model parameters of the Michaelis–Menten equation can be estimated by the linear regression method (Søgaard et al., 2002; Misselbrook et al., 2005) and the artificial neural network method (Plochl, 2001) on the basis of experimental data already performed.

Søgaard et al. (2002) present an ALFAM (ammonia loss from field-applied animal manure) model supported by theoretical consideration of impacts of the weather, soil characteristics and slurry composition on NH_3 volatilization from animal slurries applied on fields. The ALFAM (http://www.alfam.dk) database contains the experimental results obtained by 13 institutes from 7 European countries, where about 6000 experimental data are collected and over 20 ammonia emission factors are considered. In their study, the multivariate linear regression (MLR) method is used to estimate the Michaelis–Menten model parameters.

Misselbrook et al. (2005) assess the influence of a range of environmental, manure and management variables on ammonia emissions following application of different manure types to grassland and arable land, using the MLR method to estimate the Michaelis–Menten model parameters. The experimental measurements were conducted at six different sites in UK over a 3-year period, representing a range of soil types.

The artificial neural network (ANN) approach can take into account nonlinear characteristics between independent variables using a nonlinear transformation function (e.g., sigmoid function) and structuring a cross-linked network. The ANN method is widely used for the microbe growth rate prediction (Hajmeer et al., 1997), agronomical biology (Schultz and Wieland, 1997; Plochl, 2001) and reaction kinetics modeling (Molga, 2003). Plochl (2001) predicts the ammonia emission from field-applied manure using the artificial neural network trained and validated on the basis of 102 datasets measured in Europe. The review paper of Sommer et al. (2003) presents the relative importance of the ammonia emission factors in the qualitative way, using a hybrid approach between empirical and mechanistic models.

The three studies described above (Plochl, 2001; Søgaard et al., 2002; Misselbrook et al., 2005) have several differences in the ammonia emission factor selection. Søgaard et al. (2002) focused on understanding effects of several manure application methods on the reduction of ammonia loss. Plochl (2001) concentrated on effects of the climate factors (air temperature, wind speed, radiation and precipitation) but the soil type and manure application method were not considered. Misselbrook et al. (2005) took soil conditions and weather information into account for the surface-applied cattle and pig manures, measuring the ammonia emission rate with time by the wind tunnels.

This study aims at the development of a method for accurately predicting ammonia emission and systematically identifying the relative significance of the ammonia emission factors, applying the method to the database ALFAM used by Søgaard et al. (2002). The Michaelis–Menten model parameters are estimated on the basis of ALFAM database, using 11 variables which may influence ammonia emission such as soil types, weather, manure characteristics, agronomic factors and measuring technique (see Table 1). The MLR method and ANN approach are also employed to estimate the two model parameters. This article quantitatively assesses the relative significance (or importance) of the NH_3 emission factors in each estimation method.

Section 2 explains the Michaelis–Menten equation, the ammonia emission factors, the multivariate linear regression (MLR) method and the artificial neural network (ANN) approach used in this study. Section 3 presents the results and discussion.

2. Prediction models for ammonia emission from field-applied livestock manure

The Michaelis–Menten type equation is one of the widely used model to predict the ammonia emission from field-applied manure (Sommer and Ersboll, 1994; Søgaard et al., 2002; Plochl, 2001; Misselbrook et al., 2005). The Michaelis–Menten equation is:

$$N_{NH_3}(t) = N_{max}\frac{t}{t + K_m} \tag{1}$$

Table 1
Eleven independent variables influencing ammonia volatilization from field-applied pig manure

Variables	Index	Range	Units or variable description
Soil			
1. Type	p_1	[1, 3]	1 = sandy, 2 = clay, 3 = loam
2. pH	p_2	[5, 8]	
Weather			
3. Air temperature during experiment	p_3	[0, 28]	°C
4. Wind speed	p_4	[0, 6.5]	m/s
Manure			
5. Dry matter	p_5	[1.0, 11.5]	%
6. TAN[a]	p_6	[1.5, 6.5]	(g-nitrogen)/(kg-manure)
7. pH	p_7	[6.5, 8]	
Agronomic factors			
8. Manure application method	p_8	[0, 3]	0 = broad spread, 1 = band spread, 2 = trailing shoe, 3 = open-slot injection
9. Application rate	p_9	[7.5, 60]	(ton-slurry)/(ha-field)
10. Crops type	p_{10}	[1, 4]	1 = grass, 2 = stubble, 3 = bare soil, 4 = growing crops
11. Measuring technique	p_{11}	[1, 3]	1 = wind tunnel, 2 = micrometrological mass balance technique, 3 = JTI or equilibrium concentration method

N_{max} (kg/ha) = 25.9 (standard deviation = 22.9); K_m (h) = 8.35 (standard deviation = 12.26).
[a] TAN: total ammoniacal nitrogen (= $NH_3 + NH_4^+$).

where N_{NH_3} (kg/ha) is the accumulated ammonia loss at a time (t), N_{max} (kg/ha) the maximum ammonia loss, and K_m (h) is the time to reach half of the maximum ammonia loss ($N_{max}/2$). Here, the quantity of ammonia loss is based on the nitrogen weight. The two model parameters (N_{max} and K_m) can be estimated by an empirical equation regressed from experiments.

The ammonia loss rate ($\dot{N}_{NH_3}$) is obtained by the differentiation of Eq. (1) (Søgaard et al., 2002):

$$\dot{N}_{NH_3}(t) \equiv \frac{dN_{NH_3}}{dt} = N_{max}\frac{K_m}{(t+K_m)^2} \tag{2}$$

It is noted that the initial ammonia loss flux is defined by the ratio of N_{max} to K_m:

$$v_{initial} \equiv \dot{N}_{NH_3}(0) = \frac{N_{max}}{K_m} \tag{3}$$

Eq. (1) and (2) are used for the Michaelis–Menten model parameter estimation from experimental data. However, the equation popularly employed for the parameter estimation within a given time interval, $t + \Delta t$ (Sommer and Hutching, 2001; Søgaard et al., 2002; Misselbrook et al., 2005) is:

$$\dot{N}_{NH_3}(t, \Delta t) = N_{max}\frac{K_m}{(t+K_m)(t+\Delta t+K_m)} \tag{4}$$

and is used in the present study for the Michaelis–Menten model parameter estimation.

In the Michaelis–Menten type equations, the two model parameters (N_{max}, K_m) depend on soil condition, climate, livestock manure state, and agronomic factors. In this study, the ammonia emission with respect to these factors is predicted on the basis of ALFAM datasets, using a multivariate linear regression (MLR) and artificial neural network (ANN) approaches for the Michaelis–Menten model parameter estimation.

2.1. Independent variables influencing the ammonia loss

Factors which may influence the ammonia emission are the variables controlling the physical, chemical and biological manure decomposition. The factors consist of soil conditions, weather, manure characteristics, application method, land types, etc. (Søgaard et al., 2002). The ALFAM database (Sommer, 2000) collected in seven European countries contains about 6000 experimental data showing the ammonia emission rate ($\dot{N}_{NH_3}$) with time for pig and cattle manure slurries under specific experimental conditions (Søgaard et al., 2002). In the present study, 83 datasets of the pig manure slurry were selected for the model parameter estimation (see Table A1), in which 11 independent variables had been commonly measured (see Table 1). The 83 datasets contains about 500 experimental data provided by DIAS (Denmark), IMAG (The Netherlands), IGER (UK), ADAS (UK) and CRPA (Italy).

In Table 1, the 11 independent variables are classified by soil (two variables), weather (two variables), manure (three variables), agronomic factor (three variables) and measuring technique (one variable). Their boundary, unit and description are in detail presented in Sommer (2000). The mean values of the two model parameters are N_{max} = 25.9 kg/ha (corresponding to about 16% of the total nitrogen applied to the field) and K_m = 8.35 h for the 83 datasets. Thus, the initial ammonia loss flux is $v_{initial} = 3.1$ kg/ha h. The standard deviations of the two model parameters are relatively high, since the experiments were carried out at different experimental conditions in several European countries. The next section shows how K_m and N_{max} are estimated from a given dataset.

2.2. Michaelis–Menten model parameter determination

The ALFAM database provides ammonia emission rate values ($\dot{N}_{NH_3}$: (kg-N)/(ha h)) with time at the measured inde-

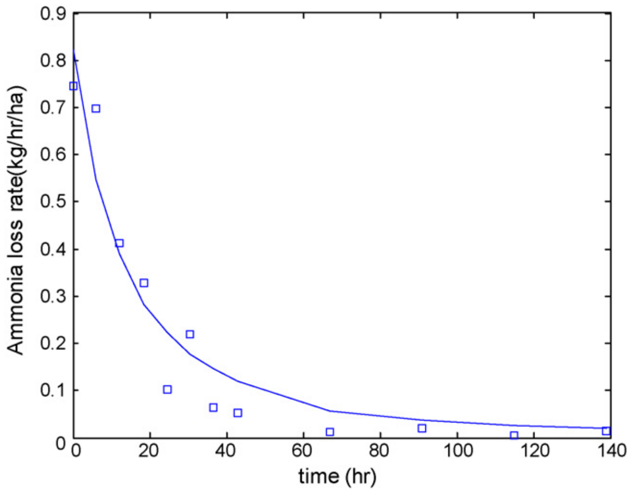

Fig. 1. Michaelis–Menten model parameter estimation from the experimental data for ammonia emission rate with respect to time (squares: experimental data, solid line: model estimation).

pendent variables. The two parameters of Michaelis–Menten equation (4) are determined for each dataset. Fig. 1 shows the ammonia emission rate with time, where the square points are 12 experimental data, and the solid line is the regression values using the Michaelis–Menten equation. The two parameters of the Michaelis–Menten equation are identified by minimizing the sum square error (SSE) between experiment (x_{exp}) and model (x_{model}) values:

$$\min_{N_{\max}, K_{\text{m}}} \quad \text{SSE} = \sum_{i=1}^{n} (x_{i,\text{exp}} - x_{i,\text{model}})^2,$$
$$\text{s.t.} \quad x_{i,\text{model}} = \frac{N_{\max} K_{\text{m}}}{(t_i + K_{\text{m}})(t_i + \Delta t_i + K_{\text{m}})} \tag{5}$$

The above optimization procedure is performed in the Matlab environment (Mathworks, USA, 2005) using a function called fminsearch. The results are shown in Table A1 with the values of the independent variables. Henceforth, these 83 values of K_{m} and $N_{\max}$ are called the measured or experimental values, in order to distinguish from the values estimated by the MLR and ANN approaches.

2.3. Multivariate linear regression (MLR) method

The multivariate linear regression (MLR) method is constructed by the exponential of the independent variables to have non-negative K_{m} and $N_{\max}$ values (Søgaard et al., 2002):

$$\ln K_{\text{m}} = a_0 + \sum_{i=1}^{11} a_i p_i, \qquad \ln N_{\max} = b_0 + \sum_{i=1}^{11} b_i p_i \tag{6}$$

where a_i ($i = 0, \ldots, 11$) and b_i ($i = 0, \ldots, 11$) are the model parameters to be estimated, and p_i ($i = 1, \ldots, 11$) are the input variables (or NH_3 emission factors). By rewriting these expressions, the input variable coefficients can be obtained:

$$K_{\text{m}} = A_0 \prod_{i=1}^{11} A_i^{p_i}, \qquad N_{\max} = B_0 \prod_{i=1}^{11} B_i^{p_i} \tag{7}$$

where $A_i = e^{a_i}$, $i = 0, \ldots, 11$ and $B_i = e^{a_i}$, $i = 0, \ldots, 11$.

In the MLR method, the elasticities of the two model parameters (ε_{K_i} and ε_{N_i} for K_{m} and $N_{\max}$, respectively) to the input variables are obtained as follows:

$$\varepsilon_{K_i} = \left.\frac{\partial \ln K_{\text{m}}}{\partial \ln p_i}\right|_{p_j, j \neq i} = \bar{p}_i \left.\frac{\partial \ln K_{\text{m}}}{\partial p_i}\right|_{p_j, j \neq i} = \bar{p}_i a_i,$$
$$i = 1, \ldots, 11 \tag{8}$$

$$\varepsilon_{N_i} = \left.\frac{\partial \ln N_{\max}}{\partial \ln p_i}\right|_{p_j, j \neq i} = \bar{p}_i \left.\frac{\partial \ln N_{\max}}{\partial p_i}\right|_{p_j, j \neq i} = \bar{p}_i b_i,$$
$$i = 1, \ldots, 11 \tag{9}$$

where $\bar{p}_i$ is the mean value of the 11 input variables for 83 experimental data (see Table A1). Since the elasticity ($(\mathrm{d}\ln y)/(\mathrm{d}\ln x) = (\mathrm{d}y/y)/(\mathrm{d}x/x)$, where x and y are the independent and dependent variables, respectively) means the relative variation of the dependent variable to that of the independent variable and has no unit, it can be used as a relative significance between the independent variables.

2.4. Artificial neural network (ANN) approach

The ANN approach is composed of one input layer, one or several hidden layers and one output layer. The neuron numbers of the input and output layers are equal to the input and output variable numbers, respectively. In this work, the neuron numbers of the input and output layers correspond to the 11 independent variables influencing the ammonia loss and the two model parameters of the Michaelis–Menten equation, respectively. The neuron number of the hidden layer is determined by minimizing the MSE (or performance index). The mean square error (MSE) is given by

$$\text{MSE} = 0.5\left[\frac{1}{83}\left(\sum_{i=1}^{83}(K_{\text{m,exp},i} - K_{\text{m,ann},i})^2\right) + \frac{1}{83}\left(\sum_{i=1}^{83}(N_{\max,\text{exp},i} - N_{\max,\text{ann},i})^2\right)\right] \tag{10}$$

where $K_{\text{m,exp}}$ and $N_{\max,\text{exp}}$ are the values obtained from the experimental data, and $K_{\text{m,ann}}$ and $N_{\max,\text{ann}}$ are the values predicted by the artificial neural network. All of the 83 data are used for training the ANN to assess the relative importance of the ammonia emission factors.

Fig. 2 shows a simple ANN structure called ANN r-1-1 (input variable number, hidden layer neuron number, and output variable number), where the input variables (p), weights (w), biases (b) and output variables (a) are indicated. When the sigmoid function as transformation is used for the hidden layer and the purelinear function for the output layer, the output variables are

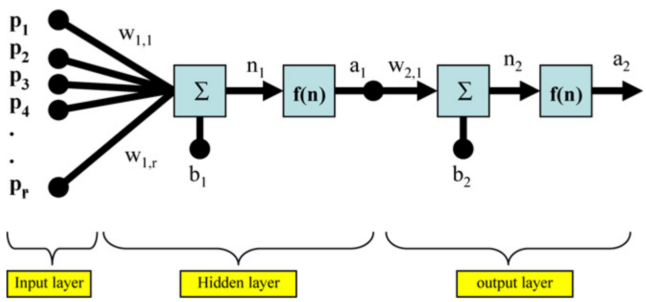

Fig. 2. Components in a typical ANN (artificial neural network).

obtained as follows:

$$a_1 = f_{\text{sigmoid}}(w_1 p + b_1) \tag{11a}$$

$$a_2 = f_{\text{purelinear}}(w_2 a_1 + b_2) \tag{11b}$$

Since the output variables (a) are calculated in the feed-forward direction and the weights (w) are regulated in the opposite direction minimizing the MSE, the ANN is called the feedforward-backpropagation artificial neural network (ANN) method (Hajmeer et al., 1997; Schultz and Wieland, 1997; Plochl, 2001; Molga, 2003). The ANN is used to estimate the two model parameters of the Michaelis–Menten equation in this work. The ANN approach is preprocessed by the principle component analysis (PCA; Jackson, 1991) to reduce the eventual correlation between the 11 independent input variables and to normalize these 11 input variables.

The input vector (P_{in}: 83 × 11 matrix) is normalized so that their mean is $\mu = 0$ and the standard deviation is $\sigma = 1$. The normalized data ($\bar{P}_{\text{in}}$: 83 × 11 matrix) are transformed by the principle component analysis (PCA) so that the elements of the input vector would be uncorrelated and the size of the input vector may be reduced by retaining only those components which contribute more than a specified fraction (= 0.012 in this study) of the total variation in the dataset. In this case, the 11 components are reduced into 10 components. The vector transformed by the PCA (P_{PCA}: 83 × 10) is used for training the ANN.

The output of the ANN approach is postprocessed by the weight partitioning method (WPM; Garson, 1991; Goh, 1994; Hajmeer et al., 1997) to assess the relative significance of 11 ammonia emission factors. The WPM partitions the weights between the hidden and output layers into the input variables (Garson, 1991).

The attempt is called the PWA approach: principle component analysis (PCA) based preprocessing and weight partitioning method (WPM) based postprocessing *A*NN approach. Fig. 3 shows the calculation procedure of the PWA approach with the matrix size in the parenthesis.

Table 2
Correlation coefficient (R^2) and mean square error (MSE) in MLR and PWA approaches

Model	R^2 for K_m	R^2 for $N_{\max}$	MSE
MLR			
This study	0.3680	0.6631	141.04
DIAS[a]	0.77	0.80	–
PWA 11-10-26-2	0.9941	0.9985	0.8333

[a] DIAS: referred to Søgaard et al. (2002).

3. Results and discussion

The calculation is performed on the statistics and neural network toolboxes of Matlab (Mathworks, USA, 2005). Table 2 shows the correlation coefficients (R^2) of the two model parameters and the mean square errors (MSE) using the two model parameter estimation methods proposed above. The nonlinear regression method (i.e., PWA approach) shows a higher correlation coefficient value than the MLR method, because nonlinearity between the independent variables (p_i) and the model parameters (K_m and $N_{\max}$) is better considered. It is noted that the PWA approach predicts quasi perfectly the measured K_m and $N_{\max}$ values (see Fig. 7) even without information of NH_3 emission factors excluded in the model (e.g., soil moisture, radiation, total nitrogen in manure, etc.). However, the prediction is valid for the used 83 datasets.

The linear regression results are reported in Table 3 and are compared with the measured model parameters in Fig. 4. The exponentials of the input variable coefficients (A_i and B_i) for K_m and $N_{\max}$ are compared with those of Søgaard et al. (2002). It is worth noting that the 83 datasets used in this study (see Table A1) are different from the datasets used by Søgaard et al. (2002) and not specified in their paper. It is, however, observed from Table 3 that A_i and B_i of this study have a good agreement with those of Søgaard et al. (2002), except for the TAN value. In this study, the cumulated ammonia loss ($N_{\max}$) increases with the TAN value and the K_m value decreases with increasing the TAN value. These results are in agreement with the linear regression model of Misselbrook et al. (2005) for the application of pig-slurry to the arable land. This is due to the fact that the partial pressure of NH_3 in the air immediately adjacent to the slurry/soil surface is proportional to the TAN concentration in the mechanistic model (Sommer et al., 2003).

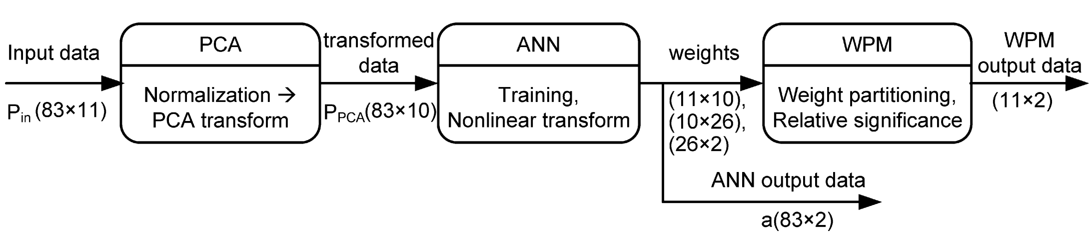

Fig. 3. Calculation procedure of the PWA approach.

Table 3
Michaelis–Menten model parameters and elasticity to ammonia emission factors in the MLR method

Variables	Index	K_m			N_{max}		
		A_i (this study)	A_i (DIAS[a])	ε_{K_i}	B_i (this study)	B_i (DIAS[*])	ε_{N_i}
Common factor	–	1.99695	1.038	–	0.79795	0.0495	–
Soil							
Type	p_1	0.45458	–	−1.82(2)	0.80211	–	−0.51
pH	p_2	0.81887	–	−1.37(3)	0.85167	–	−1.10(2)
Weather							
Air temperature during experiment	p_3	0.95045	0.960	−0.65	1.02011	1.0223	0.26
Wind speed	p_4	0.93825	0.950	−0.18	1.08578	1.0417	0.23
Manure							
Dry matter	p_5	1.10892	1.175	0.50	1.12782	1.108	0.59
TAN	p_6	0.85893	1.106	−0.51	1.0624	0.828	0.20
pH	p_7	1.5827	–	**3.46**(**1**)	1.49913	–	**3.05**(**1**)
Agronomic factors							
Manure application method	p_8	1.63855	–	0.21	0.58621	–	−0.23
Application rate	p_9	1.03489	1.0177	1.12(4)	1.03265	0.996	1.05(3)
Crops type	p_{10}	1.18551	–	0.41	0.73025	–	−0.77(4)
Measuring technique	p_{11}	0.80192	–	−0.33	1.26833	–	0.36

[a] DIAS: referred to Søgaard et al. (2002).

The MLR analysis confirms the results from the study of Søgaard et al. (2002) showing that the broad spreading as the manure application method increases N_{max} and decreases K_m (see B_8 and A_8 in Tables 3 and 1). The linear analysis indicates that the emission measured with the wind tunnels is lower than that of others (see B_{11} in Tables 3 and 1).

It is also evident from Table 3 that the initial loss rates in Eq. (3) increase with increasing the air temperature and wind speed: $B_3/A_3 = 1.07$ (1.06 in Søgaard et al., 2002), $B_4/A_4 = 1.14$ (1.10 in Søgaard et al., 2002). A high dry matter contents, manure pH and application rate will result in increasing both of K_m and N_{max}. From the linear analysis, it is considered that the 83 experimental datasets used in this study are a good representative set of about 300 pig-manure ALFAM datasets.

The elasticity is negative when the exponential of the regression parameters is less than 1. The manure pH value will influence N_{max} most significantly, since ε_{N_7} is the biggest one, compared to the remaining 10 input variables (see Table 3).

This study also supports that the mechanism controlling NH_3 emissions from slurry are too complex to be captured in a linear regression model (Sommer et al., 2003), as the linear regression model shows the low correlation coefficients as reported in Table 2.

In Figs. 5–7, the results related to the nonlinear ANN approach are shown. Fig. 5 illustrates the variations in MSE and the correlation coefficient (R^2) with the neuron number of the hidden layer for 500 training epochs using 83 experimental datasets. It is evident from Fig. 5 that the correlation coefficient

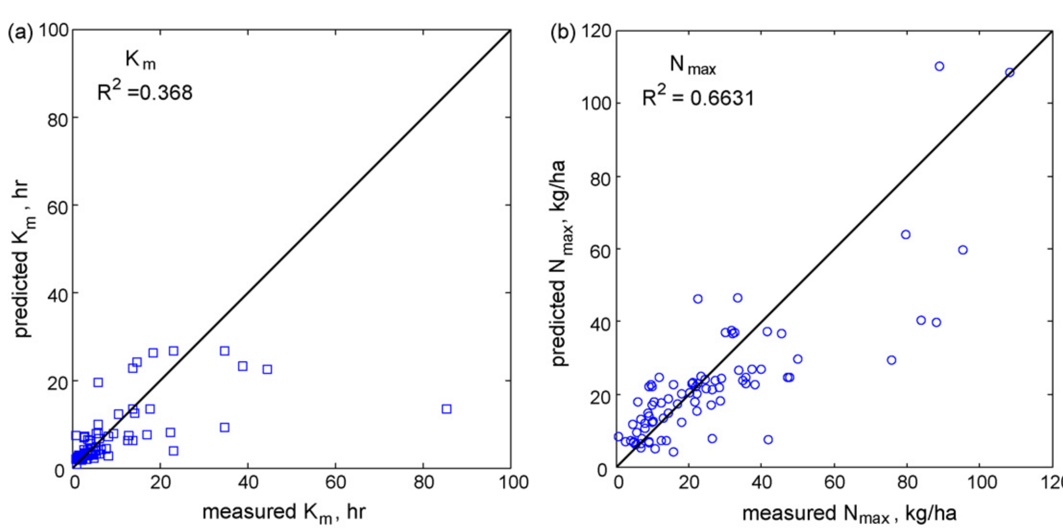

Fig. 4. Comparison of measured and predicted model parameters (K_m and N_{max}) obtained from the MLR method for 83 experimental data.

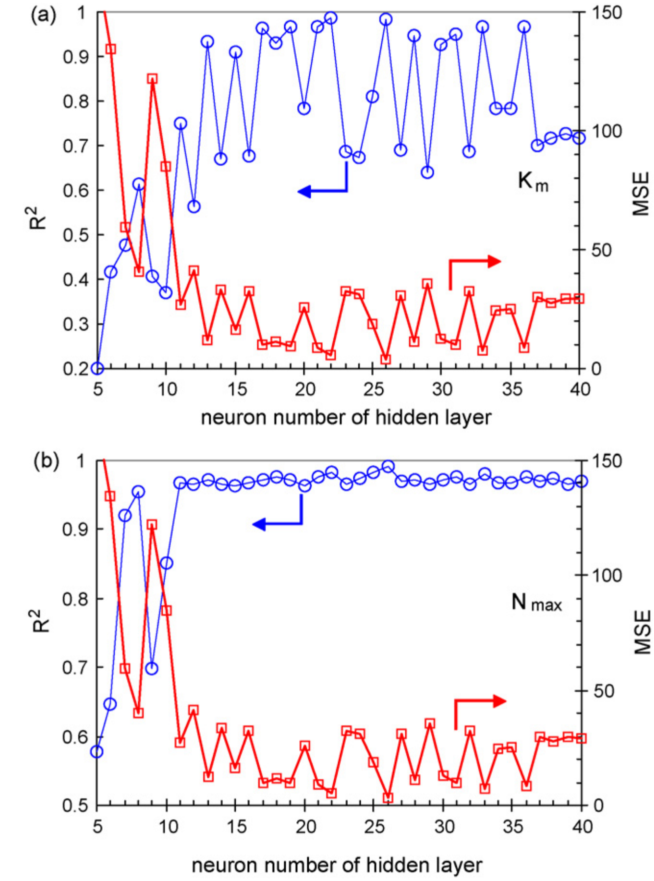

Fig. 5. The effect of the neuron number of hidden layer on the correlation coefficient (R^2) and the MSE of (a) K_m and (b) N_{max}, for 500 training epochs of 83 experimental data.

(R^2) of K_m fluctuates more strongly than that of N_{max}. This is because the normalized variation (i.e. the ratio of the standard deviation to the mean value, $\bar{\sigma} = \sigma/\mu$) is higher for K_m than for N_{max} ($\bar{\sigma}_{K_m} = 1.5$ and $\bar{\sigma}_{N_{max}} = 0.9$). Thus, the total MSE $(= (\mathrm{MSE}_{K_m} + \mathrm{MSE}_{N_{max}})/2)$ in Eq. (10) is much affected by

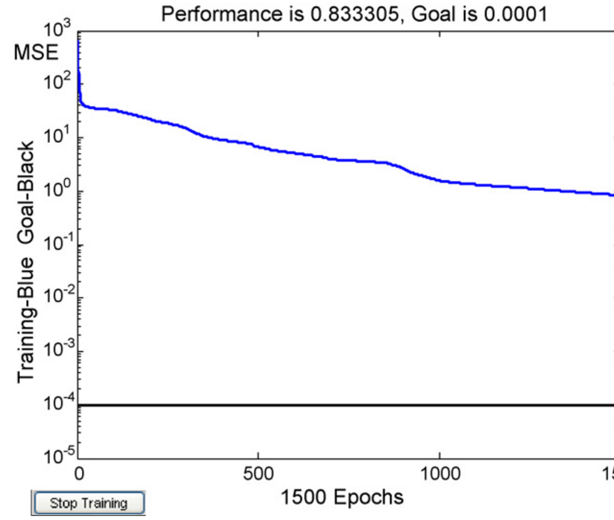

Fig. 6. Training performance of PWA 11-10-26-2 for 1500 training epochs of 83 experimental data.

the MSE of K_m (MSE_{K_m}). It is also observed in Fig. 5 that 26 neurons of the hidden layer give the lowest MSE and highest R^2. Therefore, the neuron number of the hidden layer is set to 26.

In Fig. 6, the MSE (or training performance) is plotted for 1500 iterations (or epochs) for PWA 11-10-26-2 (input variable number, PCA component number, hidden layer neuron number, and output variable number) structure. The solid line with a deep color is the goal of the MSE and the solid line with a light color is the MSE value with respect to the number of epochs. This figure was directly captured from the result of the Matlab execution.

The regressed values of K_m and N_{max} by the PWA approach for 1500 training epochs are compared with the measured values in Fig. 7. There is an excellent agreement with the predicted values and measured values for both K_m and N_{max} ($R^2 = 0.994$ and 0.999 for K_m and N_{max}, respectively). The result suports that the ammonia emission can be predicted with precision by the 11 emission factors, using the PWA approach.

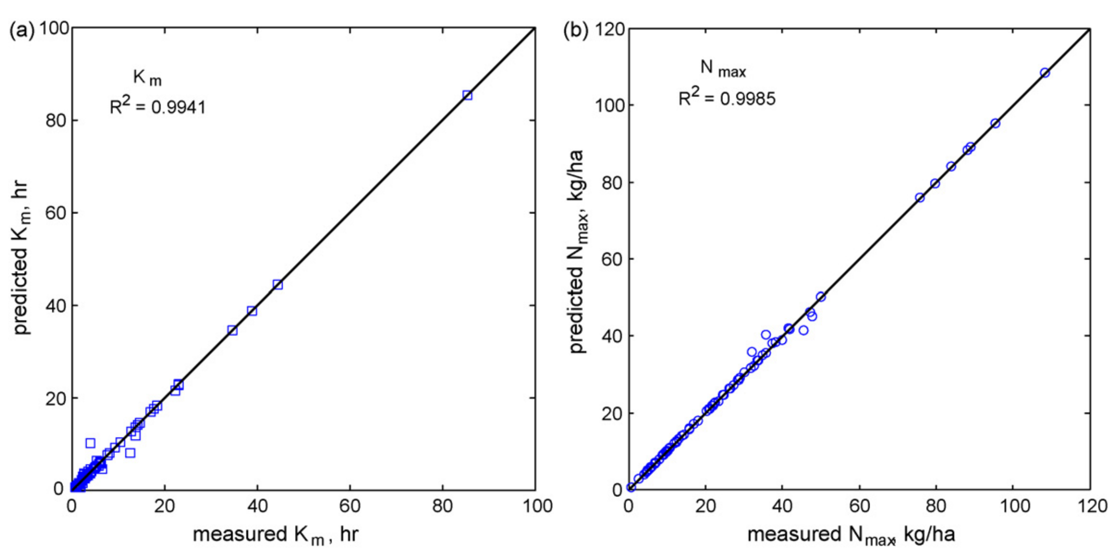

Fig. 7. Comparison of measured and predicted model parameters (K_m and N_{max}) regressed by PWA 11-10-26-2 for 1500 training epochs of 83 experimental data.

Table 4
Relative significance of 11 ammonia emission factors obtained from the PWA approach

Variables	Index	Significance (%) (PWA 11-10-26-2)
Soil (18.3 %)		
1. Type	p_1	8.57
2. pH	p_2	10.68(2)
Weather (29.9%)		
3. Air temperature during experiment	p_3	10.50(3)
4. Wind speed	p_4	19.36(1)
Manure (23.8 %)		
5. Dry matter	p_5	7.71
6. TAN	p_6	6.88
7. pH	p_7	9.25(4)
Agronomic factors (21.4 %)		
8. Manure application method	p_8	6.97
9. Application rate	p_9	6.96
10. Crops type	p_{10}	7.50
11. Measuring technique (5.6%)	p_{11}	5.62
Total		100

The relative significance of the 11 input variables to the N_{max} and K_m are obtained for PWA 11-10-26-2 by using the weight partitioning method (Garson, 1991). Table 4 shows that the wind speed, soil pH value, average air temperature and manure pH value are the highest significant factors.

Since atmospheric stability is affected by both wind speed and temperature profiles and atmospheric instability increases the NH_3 gas concentration in the liquid surface of manure (Sommer et al., 2003), the wind speed and temperature can play a major role for the ammonia emission from manure. In Misselbrook et al. (2005), the wind speed was identified as the most influenced variable on ammonia emission for pig slurry in particular. An increase in temperature will significantly increase emission of NH_3 and evaporation of water from the slurry. This will have a strong effect on the NH_3 concentration in manure slurry through the resultant increase in the TAN concentration (Sommer et al., 2003).

In our analysis, the pH values of manure and soil appears to be the most influenced emission factors. Slurry and slurry/soil pH is generally regarded to be a very important factor controlling NH_3 loss (Misselbrook et al., 2005; Sommer et al., 2003). The quantitative results obtained by the PWA approach in the present study gives an excellent explanation of the most important processes controlling NH_3 emission proposed by Sommer et al. (2003).

4. Conclusion

This study proposed a systematic method for enhancing the estimation accuracy of ammonia emission and for assessing the relative significance of ammonia emission factors.ed for enhancing the estimation accuracy of ammonia emission and for assessing the relative significance of ammonia emission factors.

The ammonia emission is predicted using the Michaelis–Menten type equation involving two model parameters (total ammonia loss and time to reach half of the total ammonia loss) and is estimated by the multivariate linear regression (MLR) and the artificial neural network (ANN) approaches on the basis of the 83 experimental datasets selected from the ALFAM database.

Using the proposed PWA approach, the relative significance of the NH_3 emission factors is well assessed and the potential of this approach is illustrated using 11 emission factors. The wind speed, soil pH value, average air temperature and manure pH value are the highest significant factors influencing the ammonia loss from field-applied pig manure. For more accurate prediction and the practical uses, it is needed to apply the proposed PWA approach into sufficient experimental data including most of the important ammonia emission factors.

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Appendix A

Table A1 shows 83 Michaelis–Menten equation parameters and experimental data measured at 11 input variables for field-applied pig manure (Søgaard et al., ALFAM, 2002). K_m and N_{max} are determined by the method explained in Section 2.2. The minimum, maximum, average and standard deviation of the two Michaelis–Menten model parameters and the 11 input variables are also shown.

Table A1
Michaelis–Menten equation parameters derived from experimental data measured at 11 input variables for field-applied pig manure (Sommer, 2000)

No.	K_m	N_{max}	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}
1	14.05	21.12	1	6.60	12.1	3.1	3.9	3.9	7.9	0	30	3	1
2	10.30	24.66	1	6.60	12.1	3.4	3.9	3.9	7.9	0	30	3	1
3	13.70	38.30	1	6.60	10.8	3	3.9	3.9	7.9	0	30	3	1
4	17.60	15.87	1	6.60	10.8	3.1	3.9	3.9	7.9	0	30	3	1
5	85.40	35.75	1	6.60	10.8	3.2	3.9	3.9	7.9	0	30	3	1
6	38.74	21.83	1	6.60	6.1	2.8	3.9	2	7.9	0	30	3	1
7	44.45	14.41	1	6.60	6.1	3.2	3.9	2	7.9	0	30	3	1
8	13.54	28.67	1	6.60	6.1	3	3.9	2	7.9	0	30	3	1

Table A1 (*Continued*)

No.	K_m	N_{max}	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}
9	14.64	5.99	1	6.60	5.1	3	3.9	2	7.9	0	30	3	1
10	22.89	26.34	1	6.60	3.1	2.9	3.9	2	7.9	0	30	3	1
11	18.36	12.41	1	6.60	3.1	3.2	3.9	2	7.9	0	30	3	1
12	34.61	17.03	1	6.60	3.1	3	3.9	2	7.9	0	30	3	1
13	1.07	9.06	3	6.30	8.41	5.78	3.70	3.84	7.35	0	31.8	4	2
14	4.62	9.11	3	6.30	8.44	5.74	3.30	3.81	7.48	1	26.0	4	2
15	0.63	8.93	3	6.30	14	4.19	3.50	3.93	7.66	0	30.9	4	2
16	4.55	4.01	3	6.30	14.06	4.22	3.50	3.57	7.64	1	26.5	4	2
17	3.12	14.37	3	6.30	11.4	6.31	3.10	3.54	7.53	0	30.9	4	2
18	2.06	2.72	3	6.30	11.4	6.31	3.00	3.33	7.53	1	25.5	4	2
19	2.15	7.92	3	6.30	8.86	5.17	3.40	3.06	7.55	0	24.3	4	2
20	3.39	10.80	3	6.30	8.86	5.17	3.20	3.09	7.56	1	19.4	4	2
21	0.86	8.02	3	6.30	10.81	4.06	3.40	3.17	7.76	0	27.5	4	2
22	5.98	6.93	3	6.30	10.81	4.06	2.80	2.70	7.71	1	21.6	4	2
23	1.18	10.18	3	6.30	10.57	6.34	3.40	3.16	7.61	0	24.9	4	2
24	3.46	6.76	3	6.30	10.65	6.34	2.70	2.60	7.58	1	24.2	4	2
25	1.40	6.87	3	6.30	12.85	4.31	5.20	1.49	6.70	0	38.3	4	2
26	4.93	5.39	3	6.30	12.75	4.3	5.20	1.49	6.70	1	31.3	4	2
27	2.49	10.52	3	6.30	5.87	5.52	6.90	3.65	7.01	0	34.4	4	2
28	4.65	12.54	3	6.30	5.87	5.52	6.90	3.65	7.01	1	22.9	4	2
29	2.97	17.98	3	6.30	10.93	4.91	4.20	3.44	6.97	0	31.9	4	2
30	3.77	9.03	3	6.30	10.93	4.91	4.20	3.44	6.97	1	31.3	4	2
31	34.67	15.75	2	7.80	0.85	3.15	1.93	3.00	7.52	1	28.7	4	2
32	0.64	0.65	2	7.65	5.5	4.37	2.79	2.80	7.66	1	29.9	3	2
33	9.23	13.95	2	7.49	9.62	3.58	3.56	3.2	7.63	1	30.2	4	2
34	16.84	41.90	2	7.46	11.65	3.85	3.54	2.8	7.66	1	30.2	4	2
35	12.79	26.42	2	6.91	15.05	2.82	3.76	2.6	7.42	1	30.9	4	2
36	2.33	7.12	2	7.47	15.12	2.85	4.04	2.69	7.51	1	31.2	4	2
37	3.31	4.81	2	7.69	17.03	2.08	3.7	2.4	7.52	1	31.1	4	2
38	6.05	5.02	2	7.74	17.15	1.88	3.44	2.45	7.68	1	31.3	4	2
39	7.64	9.85	2	8.00	15.7	1.8	11.30	6.31	8.00	2	7.9	1	2
40	3.92	26.46	2	8.00	15.89	1.75	11.30	6.31	8.00	2	14.9	1	2
41	1.29	79.66	2	8.00	12.93	1.8	11.30	6.31	8.00	0	17.5	1	2
42	5.60	13.17	2	8.00	15.71	1.8	11.30	6.31	8.00	3	17.3	1	2
43	0.74	21.00	2	7.80	24	1.88	5.13	3.51	7.8	0	8.4	1	2
44	5.34	9.87	2	7.30	7.29	5.11	8.66	5.00	7.30	2	12.0	1	2
45	4.77	84.11	2	7.30	7.29	4.98	8.66	5.00	7.30	0	16.3	1	2
46	3.07	88.30	2	7.30	7.3	5.14	8.66	5.03	7.3	0	15.2	1	2
47	4.05	4.54	2	7.30	7.34	5.19	8.66	5.03	7.3	2	10.6	1	2
48	22.31	32.65	2	5.14	8.31	0.93	3.07	4.02	7.50	0	40.0	1	1
49	5.75	31.79	2	5.14	8.36	1.15	3.07	4.02	7.50	0	40.0	1	1
50	5.36	41.71	2	5.14	8.36	1.04	3.07	4.02	7.50	0	40.0	1	1
51	2.66	32.04	2	5.88	8.59	1.05	4.01	4.14	7.44	0	40.0	1	1
52	8.13	30.23	2	5.88	8.59	1.15	4.01	4.14	7.44	0	40.0	1	1
53	2.46	45.66	2	5.88	8.59	1.06	4.01	4.14	7.44	0	40.0	1	1
54	1.86	27.37	3	5.71	18.3	0.95	1.52	2.00	7.47	0	40.0	1	1
55	1.99	34.97	3	5.71	18.3	0.87	1.52	2.00	7.47	0	40.0	1	1
56	1.22	29.02	3	5.71	18.3	1.13	1.52	2.00	7.47	0	40.0	1	1
57	3.89	17.96	3	5.75	5.05	1.06	1.72	3.71	7.38	0	40.0	1	1
58	6.25	22.39	3	5.75	5.05	1.05	1.72	3.71	7.38	0	40.0	1	1
59	5.30	20.45	3	5.75	5.05	1.17	1.72	3.71	7.38	0	40.0	1	1
60	3.27	24.68	3	5.46	4.9	1.04	2.06	3.05	7.45	0	40.0	1	1
61	2.41	21.96	3	5.46	4.9	1.24	2.06	3.05	7.45	0	40.0	1	1
62	6.34	28.44	3	5.46	4.9	1.14	2.06	3.05	7.45	0	40.0	1	1
63	3.94	9.09	2	7.90	21.58	0.50	4.74	3.19	7.17	0	40	2	1
64	1.71	11.85	2	7.90	21.58	1.90	4.74	3.19	7.17	0	40	2	1
65	2.13	37.45	2	7.90	21.58	2.92	4.74	3.19	7.17	0	40	2	1
66	2.65	9.70	2	7.90	21.58	0.89	4.74	3.19	7.17	0	40	2	1
67	2.33	23.32	2	7.90	21.58	1.95	4.74	3.19	7.17	0	40	2	1
68	2.17	39.82	2	7.90	21.58	2.93	4.74	3.19	7.17	0	40	2	1
69	3.15	10.00	2	7.90	21.58	0.49	4.74	3.19	7.17	0	40	2	1
70	3.41	50.16	2	7.90	21.58	4.07	4.74	3.19	7.17	0	40	2	1
71	3.21	22.70	2	7.90	21.58	0.95	4.74	3.19	7.17	0	40	2	1

Table A1 (*Continued*)

No.	K_m	N_{max}	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}
72	2.78	75.87	2	7.90	21.58	4.01	4.74	3.19	7.17	0	40	2	1
73	5.82	5.77	3	7.50	17.02	0.82	10.50	3.75	7.77	3	40.0	2	1
74	5.35	33.62	3	7.50	17.02	0.73	10.50	3.75	7.77	0	40.0	2	1
75	5.03	22.59	3	7.50	17.02	0.69	10.50	3.75	7.77	0	40.0	2	1
76	1.92	108.42	3	7.50	27.31	1.38	4.36	2.58	7.85	0	58.0	1	3
77	1.51	89.03	3	7.50	27.31	1.38	4.03	2.56	7.99	0	58.0	1	3
78	8.02	95.34	3	7.50	27.31	1.38	3.96	2.50	7.82	1	58.0	1	3
79	13.55	47.31	3	7.60	17.81	0.76	11.00	3.70	7.77	1	35.0	2	1
80	12.49	47.78	3	7.60	17.81	0.85	11.00	3.70	7.77	1	35.0	2	1
81	3.79	35.79	3	7.60	17.81	0.82	11.00	3.70	7.77	1	35.0	2	1
82	1.90	33.74	3	7.60	22.39	0.77	6.17	2.49	7.25	0	45.0	2	1
83	22.85	22.42	3	7.60	22.39	0.66	6.17	2.49	7.25	1	45.0	2	1
Min.	0.63	0.65	1	5.14	0.85	0.49	1.52	1.49	6.7	0	7.9	1	1
Max.	85.40	108.42	3	8	27.31	6.34	11.3	6.31	8	3	58	4	3
Aver.	8.35	25.89	2.31	6.84	12.83	2.78	4.87	3.36	7.53	0.43	32.73	2.43	1.49
S.D.	12.26	22.88	0.71	0.85	6.53	1.76	2.73	1.03	0.31	0.70	9.97	1.23	0.57

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