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ORIGINAL ARTICLE

Comparative analysis of intelligent models for prediction of Langmuir constants for CO_2 adsorption of Gondwana coals in India

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Abstract An artificial neural network (ANN) is an artificial intelligence technique in which performance can be improved by adapting to the changes in the environment. The efficient manipulation of large amounts of data and the ability to generalize results are the main advantages of neural networks. Considering the advantages of this technique, this present paper aims to perform a comparison between linear methods like Multivariate Regression Analysis (MVRA) and different ANN techniques such as back propagation with regression analysis (BPNN), layer recurrent neural network (LRNN), generalized regression neural network (GRNN) and radial basis neural network (RBNN). This comparison was performed to predict the approximate values of Langmuir volume constant (LVC) and Langmuir pressure constant (LPC) for CO_2 adsorption in coal using proximate and maceral properties of India's major coalfield as input parameters. It is found that RMSE value for RBNN is least followed by GRNN, LRNN, BPNN and MVRA for both LVC and LPC models. Based on the best network, it is found that coal seams from Narayankuri coal mine has highest adsorbing capacity of CO_2 (0.0019791 mol/gm) as compared to other coal seams of this study.

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Keywords ANN · Sequestration · CO_2 · Gondwana coals · Langmuir volume constant · Langmuir pressure constant

1 Introduction

Coalbed methane (CBM) production with CO_2 injection combination is presently a worldwide topic of research and studies. The role of CO_2 injection is not only to enhance CBM production (ECBM) but also in subsurface storage of huge amount of CO_2 which are contributing in reduction of greenhouse gas percentage in atmosphere. Storing CO_2 in deep unminable coal beds has become one of the promising technologies of geological sequestration (Busch and Gensterblum 2011).

The entire methane gas in a Coalbed Methane (CBM) reservoir is stored into the micropores and cleats within the coal matrix in adsorbed form. For enhance purpose, the CO_2 captured is being injected into the subsurface coal beds which get adsorb to the coal pores surfaces. CO_2 can move in the finest pores and adsorb to the coal at a near-liquid density firmly with nominal chances of being released lately. (Krooss et al. 2002). Coal has higher affinity to CO_2 gas. Thus, CO_2 replaces adsorbed methane from the coal, accelerating methane recovery in ECBM process. Therefore, CO_2 for ECBM is a value-added selection. Although, relative sorption affinity of coal to methane and CO_2 is the primary parameter factor

which is needed to be consider for site suitability analysis of CO_2–ECBM (Dutta et al.,2011). A good understanding of methane and CO_2 sorption behavior on coal is an underlying requirement for the estimation of methane recovery and CO_2 storage capacity of a coal.

In coal matrix, mainly the CO_2 storage occurs by physical sorption (e.g. Harpalani and Chen 1997). There are many factors that are need to be considered for understanding the complexity of the interaction of CO_2 with coal in the cleat system and the coal matrix. Different aspects like moisture, volatile matter percentage, Ash content, depth of coal formation, Liptinite, Inertinite, Mineral Matter etc. that are obtained from the laboratory are minimum requirement to deal with CO_2 adsorption selectivity.

During CO_2-ECBM processes, the injected CO_2 flows through network of cleats by a complex mechanism of sorption/diffusion process (Mazzotti et al. 2009). It gets adsorb to the coal inner surface by replacing CH4 from the walls. This replacement occurs due to (1) by a reduction of the CH4 partial pressure or (2) by a higher selective sorption of CO_2 over CH4. Concentration gradient between CH4 in the matrix compared to the cleat system, results CH4 to diffuse from the coal matrix into the cleat system where, by pressure drawdown towards a production well, it is produced.

Many methods have been put up to model sorption isotherms on coal and Langmuir isotherm is among such simple methods. Langmuir isotherm is used to quantify the amount of gas adsorption on an adsorbent as a function of partial pressure or concentration at a certain temperature. The Langmuir volume constant and Langmuir pressure constant are the two constant that define the Langmuir isotherm model. It is well known approach in the ECBM industry and related reservoir simulations. It provides a reasonable fit to most experimental data:

$$n_{ads} = \frac{V_L * p}{P_L + p}$$

Here V_L is the Langmuir volume, representing the amount of gas sorbed at infinite pressure and P_L is the Langmuir pressure (Fig. 1), equivalent to the pressure at which half of the Langmuir volume V_L is reached (Crosdale et al. 1998a, b).

The adsorption of CO_2 in coal beds can be explained by the variation in Langmuir volume and Langmuir pressure constants (for CO_2). These two constant parameters help in determining of CO_2 adsorption tendency in coals. Generally it has been seen that the coal with higher Langmuir pressure constant value shows very high sorption capacity in low pressure range. It was observed that the adsorption isotherms of the coals if are steadily increasing and remain undersaturated within the experimental pressure range then these coals have comparable or even higher Langmuir volume constant.

This paper has a linear and nonlinear mathematical models like Multivariate regression analysis (MVRA), Artificial Neural Network (ANN), Radial Bias neural network (RBNN), and Layer Recurrent method which are used to calculate Langmuir constants (for CO_2) using coal proximate and macerals properties like moisture, volatile matter, ash content, fixed carbon composition, vitrinite, semi-vitrinite, liptinite, inertinite, mineral matter, mean and depth (Dutta et al. 2011). These parameters are taken as input parameters for these mathematical models. The main objective of this study is to develop intelligent models to calculate coal having best adsorption capacity towards CO_2 gas for ECBM process.

2 Study area and data set

A previous study is the source of this study data set (Dutta et al. 2011). Fourteen coal samples were taken from the India's major coal mining and CMB exploration activity regions. Eight samples are from the Raniganj coalfield, four samples are from the Jharia coalfield, and the remaining two are from the South Karanpura Coalfield (Fig. 2). Dry samples are the source for analysis. The residual moisture of samples is being represent by the moisture content of a coal sample. The ash content is high in the samples which strongly reduces the adsorption of a coal for CO_2 gas. It is found out that the Raniganj formation coals have higher moisture content and lower ash content than other samples. 32–45 % of Volatile matter content has been found out in the coal samples. Other parameters like carbon percentage, Liptinite and Inertinite which are helping in knowing organic percentage in coal etc. have also been obtained from experiments to understand sorption capacity of coal for CO_2 gas (Verma and Sirvaiya 2015) (Table 1).

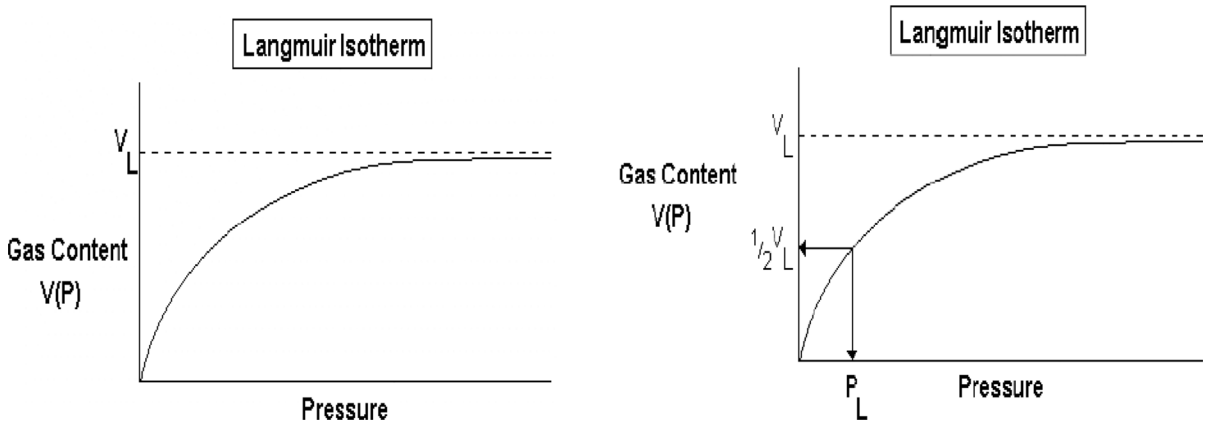

Fig. 1 Typical langmuir volume and pressure curve

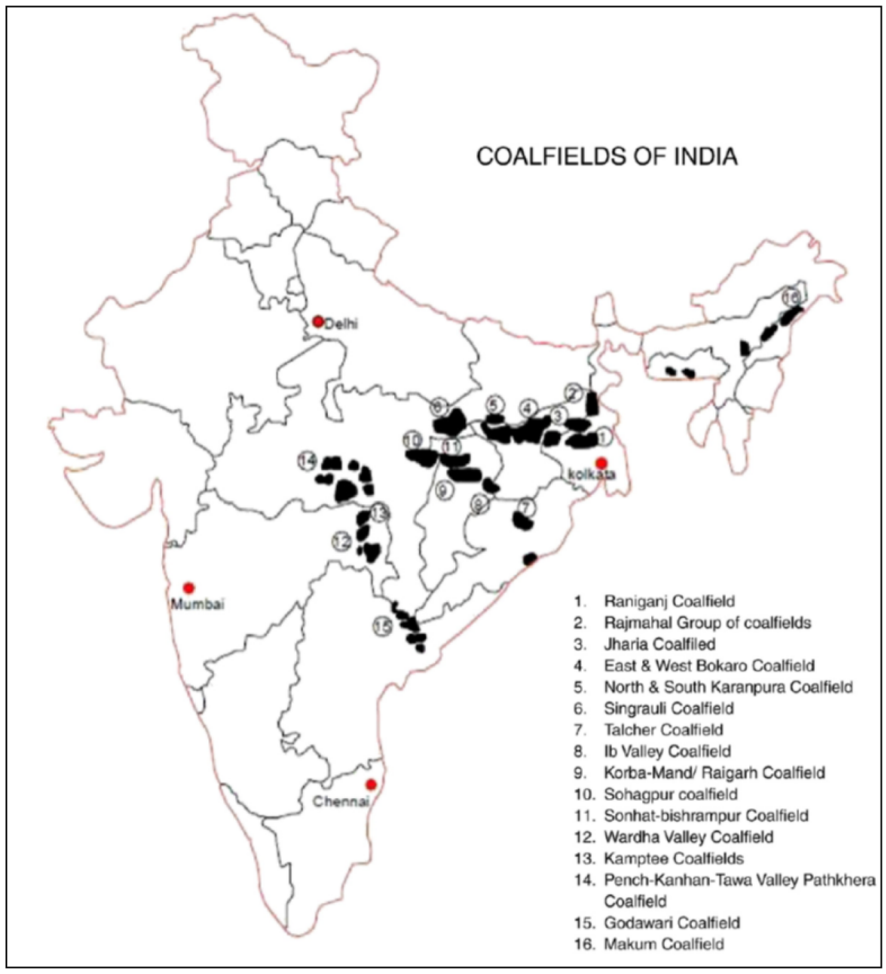

Fig. 2 Location of coal samples from coalfields in India (Dutta et al. 2011)

Table 1 Petrophysical properties and langmuir constants of coal samples for the study

Locations	Name of the coal mines	Moisture (%) (m)	Volatile matter (%) (v)	Ash (%) (a)	Fixed carbon (%) (f)	Vitrinite (%) (k)	Semi-vitrinite (%) (s)	Liptinite (%) (l)	Inertinite (%) (i)	Mineral matter (%) (z)	Mean ro % (w)	Depth (m) (d)	Langmuir volume constant (V_L,mL/g)	Langmuir pressure constant (P_L.MPa)
Raniganj formation of Raniganj coalfield	Bogra	7	38	10	45	73.9	0.4	4.2	15.8	5.7	0.64	160	74	2.732
	Kenda	4	40	12	44	65.3	1	9.7	16.6	7.4	0.62	107	68	2.406
	Narayankuri	7	41	15	37	73.8	0.8	6	11.4	7.9	0.64	46	89	2.586
	Satgram	4	40	17	39	49.7	0.8	11.3	27.2	11	0.61	190	58	1.976
Barakar formation of Raniganj coalfield	Kalimati	1.2	36	28	34.8	12	1.3	7.3	61.3	18.1	0.96	172	25	1.074
	Local II	2.3	41.5	22	34.2	2.9	1.8	5.8	62.1	17.4	1.01	118	18	0.8
	Mehaladih	1.1	35	30	33.9	16.7	2.3	8.3	64.6	8.1	0.96	201	31	1.271
	Mugma special	2.2	38	27	32.8	7.7	0.7	12.8	61.9	16.9	1.06	109	26	1.167
South Karanpura coalfield	SKAC 1	1.4	34	31	33.6	9.3	0.5	0.3	53.4	36.5	1.94	914	33	0.841
	SKAC 3	1.8	32	48	18.2	0.2	0	0	18.6	81.2	1.3	996	41	0.984
Jharia coalfield	15th Seam	1.2	45	20	33.8	86.1	0.2	0.2	5.5	8	1.29	520	35	1.082
	16th Top seam	1.6	36.5	24	37.9	62	1.4	0.3	29.5	6.8	1.22	650	42	1.418
	16th Bottom seam	6	35	34	25	58.4	2.3	0.3	33.7	5.3	1.11	450	42	1.231
	18th Seam	0.5	38	22	39.5	84.2	0.5	1	9.8	4.5	0.97	380	39	1.161

3 Multivariate regression analysis

Multivariate regression analysis is a statistical method used in estimation the relationship between a dependent variable and one or more independent variables (Alexopoulous 2010). It comprises of many technique for analysis and modelling of the dependent and independent variables. In other words, the regression analysis purpose it to calculate Y on the basis of X or to define the dependency of Y on X i.e.

$$X_1,\ X_2, \ldots, X_k \Rightarrow Y$$

The X_i (X_1, X_2, …, X_k) are "independent" variable, while Y is a "dependent" variable.

A Linear regression is made to estimate the coefficients of the linear equation which are involving one or more independent variables so that best prediction of the value of the dependent variable can be made quantitatively.

In the multivariate linear regression model, Y has normal distribution with mean

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_\rho X_\rho + \sigma(\Upsilon)$$

The parameters $\beta_0 + \beta_1 + \cdots + \beta_\rho$ and σ are estimated from data.

$\beta_0 =$ intercept

$\beta_1 \ldots \beta_\rho =$ regression coefficients

$\sigma = \sigma_{res} =$ residual standard deviation

In the equation $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_\rho X_\rho$, β_1 is the mean increase in Y per unit increase in X_i, when other X_i's are kept fixed. In general, β_i is influence of X_i corrected (adjusted) for the other X's. This estimation method follows the least squares criterion.

If b_0, b_1, …, b_ρ are the estimates of β_0, β_1, …, β_ρ then the "fitted" value of Y is

$$Y_{fit} = b_0 + b_1 X_1 + \cdots + b_\rho X_\rho$$

The b_0, b_1, …, b_ρ are computed such that $\Sigma(Y - Y_{fit})^2$ to be minimal. Since $(Y - Y_{fit})$ is called the residual; one can also say that the sum of squared residuals is minimized.

4 Back propagation neural network

To develop the understanding on functioning of human brain and desire of building a machine that can capable for solving complex problems has result in Artificial neural network. It function as similar to a human brain works and architecture is complex like any human neural network. Neural network are used to learn from the large data set.

ANN consists an input layer, output layer/Target layer and one or more hidden layers (Cilimkovic 2015; Santos et al. 2013). Input Layer, hidden layers and output layers or Target layer are connected to each other by nodes. Number of hidden layers and nodes vary from the require training and result required. Every connection has some weight associated with them. Input parameters whose value remain same throughout the network are assigned to input layer. Hidden layer accept the data from input layer which are send down to the nodes in hidden layer. Hidden layer uses input values from input layer and modify them using some weight value and then new values are transferred to the output layer where it also modify by some weight from connection between hidden and target layer. Target layer process the values from the hidden layer and produce new values called as output. After that, these output are processed by activation function to give the results. The nonlinearity is introduce by the activation function. There are three types of activation function (1) linear function (2) threshold function and (3) sigmoid function. In this paper we have use sigmoid activation function. The architecture can be seen in following figure.

Output 'y' can be calculated, if each neuron has x inputs by equation

$$y = f\left(\sum_{i=1}^{n}(w_i * x_i + b)\right)$$

where x_i are the ith input, w_i are the ith weight, b is the bias and f is the activation function for the neuron.

The new information to be obtain was get only when the network is being trained. In this paper we have use back propagation algorithm which is the most robust and versatile technique in all algorithm. It results in efficient learning method for multilayer perception (MLP) neural networks.

When the received inputs are forwarded through the all others next layer to obtain the output then it is known as feed forward back-propagation neural network (BPNN). The learning capability of back propagation networks depend upon the internal mapping of the characteristic signal features in the process

of network training onto the hidden layer. The stored mappings in this layer during the training phase of the network gets automatically retrieved during its application phase.

When the network is trained, data processed from input to hidden layer and hidden to output layer. At output layer, the output is compared to the measured values (target values) and the error is processed back through the network by updating weights and biases of distinct neurons. The network is trained until minimum network error is reached (Verma and Sirvaiya 2015). The error is calculated from root mean square error (RMSE).

In the paper, transfer function are nonlinear sigmoid function (LOGSIG, TANSIG) and linear function (POSLIN, PURELIN). The logarithmic sigmoid function (LOGSIG) is defined as

$$f = \frac{1}{1 + e^{-e_x}}$$

whereas the tangent sigmoid function (TANSIG) is defined as [7]

$$f = \frac{e^{e_x} - e^{-e_x}}{e^{e_x} + e^{-e_x}}$$

where e_x is the weighted sum of the inputs for a processing unit.

The sample values of proximate and macerals parameters are taken as input data and sample values of Langmuir volume constant and Langmuir pressure constant of CO_2 are consider as target data (Table 2; Fig. 3).

5 Generalized regression neural network

A Generalized Regression Neural Network (GRNN) is a variation of the radial basis neural networks which does not require an iterative training procedure like back propagation networks needed (Hannan et al. 2010). Hidden or kernel regression networks is a basis of GRNN. Any arbitrary function between input and output vectors are approximated by GRNN. As the training set seize tends to a higher value, the function estimation error approaches to zero, with minor constraints on the function.

GRNN has input layer, pattern layer, summation layer and output layer as in figure The number of the observation parameters define number of input units.

Table 2 Ranges of the input and output parameters used to develop intelligent models

Parameters	Unit	Range	SD
Input			
Moisture	%	0.5–70	2.26
Volatile matter	%	32–45	3.44
Ash	%	10–48	9.92
Fixed carbon	%	18.2–45	6.92
Vitrinite	%	0.2–86.1	32.90
Semi-vitinite	%	0–2.30	0.73
Litinite	%	0–12.8	4.56
Intertinite	%	5.5–64.6	22.31
Mineral matter	%	4.5–81.2	20.37
Mean	Ro %	0.61–1.94	0.35
Depth	M	46–996	309.25
Target			
Langmuir volume constant	mL/gm	18–89	20.5
Langmuir pressure constant	kPa	0.8–2.732	0.66

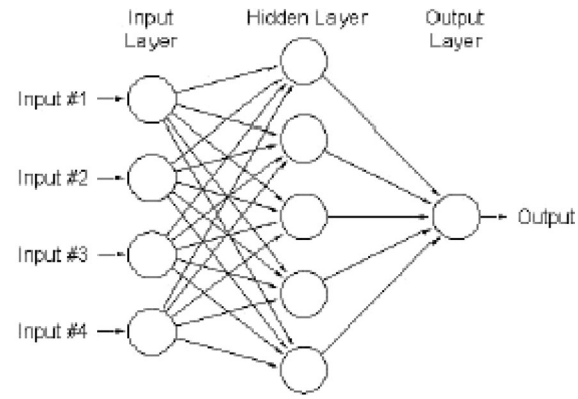

Fig. 3 A schematic diagram of neural network

In Pattern layer each neurons presents training pattern and output from the layer. Summation layer is next to the pattern layer. Summation layer with the output layer perform a normalization of output set. Radial basis and linear activation functions are used in hidden and output layers while training the network. The structure of GRNN is shown in Fig. 4.

The predicted value Y'_i generated from an unknown input vector x can be given by equation:

$$Y'_i = \frac{\sum_{i=1}^{n} y_i \cdot \exp(-D(x, x_i))}{\sum_{i=1}^{n} \exp(-D(x, x_i))},$$

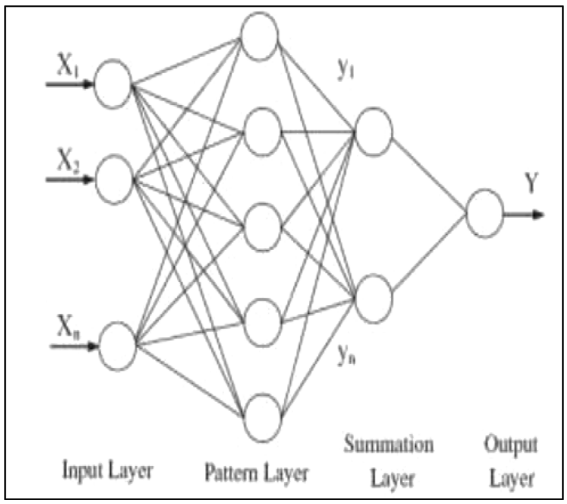

Fig. 4 A schematic diagram of generalized neural network

$$D(x, x_i) = \sum_{k=1}^{m} \left(\frac{x_i - x_{ik}}{\sigma} \right)^2$$

where y_i is the weight connection between the ith neuron in the pattern layer, n is the number of the training patterns, D is the Gaussian function, m is the number of elements of an input vector, x_k and x_{ik} are the jth element of x and x_i, respectively.

6 Radial basis neural network

RBF networks are similar to generalized regression neural networks. In generalized regression neural networks, there have one neuron for each point in the training file, whereas RBF networks have a variable number of neurons. These number of neuron in RBF is usually much less than the number of training points (Hannan et al. 2010).

RBFN comprises three layers (1) an input layer (2) hidden layer and (3) an output layer. All the layers are fully connected by the nodes. The input layer has assigned input parameters, and hidden layer neurons comprise Gaussian transfer functions which is used as radial basis function. The outputs from hidden layer are inversely proportional to the distance from the center of the neuron. Input Layer are direct to the hidden layer without any weights. The transfer function used is RBF which is symmetrical about a given mean or center point in a multidimensional space. The number of hidden nodes with RBF activation function in RBFN are connected in a feed forward parallel architecture. The optimization of the parameters associated with the RBF occurs in network training. When training network are accurately assumed then linear combination of RBFs can give no error at the training vector. This fitting of RBFs to data for function approximation is closely related by distance weight regression.

Moody and Darken (1989) has given a radial neural network in which they have selected exponential activation function for their radial basis function networks. The exponential activation function is similar to the Gaussian density function centered at c_i.

$$F_i = \exp\left(-\frac{||x_i - c_i||^2}{\sigma_i^2} \right)$$

where the function spread (σ_i) around the centre finds the ratio of the function decay with its distance from the centre. Spread constant value should be selected small enough in order to restrict the basis function spreading (Palit and Popovic 2005).

7 Layer recurrent neural network

A layer recurrent neural network (LRNN) is that type of artificial neural network where connections between units form a directed cycle. This results in an internal state of the network which permits it in exhibiting dynamic temporal behavior. In this network bi-directional data flow occurs. RNNs use their internal memory to process arbitrary sequences of inputs which is different from feedforward neural networks. There are feedback connections between units of different layers in RNN. This explain that the dependency of output of the network on both external inputs as well as on the state of the network in the previous time step as shown in Fig. 5. The model explain full feedback employment and interconnections between all nodes. Advantages like the capability to retain values from previous cycles of processing, which can be used in current computations allows RNNs to produce complex, time varying outputs in response to simple static inputs (Nkoana 2011).

8 Result and discussion

8.1 Multivariate regression (MVRA) analysis to predict LVC and LPC

The macerals parameters are taken as ‘y’ variable (independent variable) and LVC/LPC are taken as ‘x’

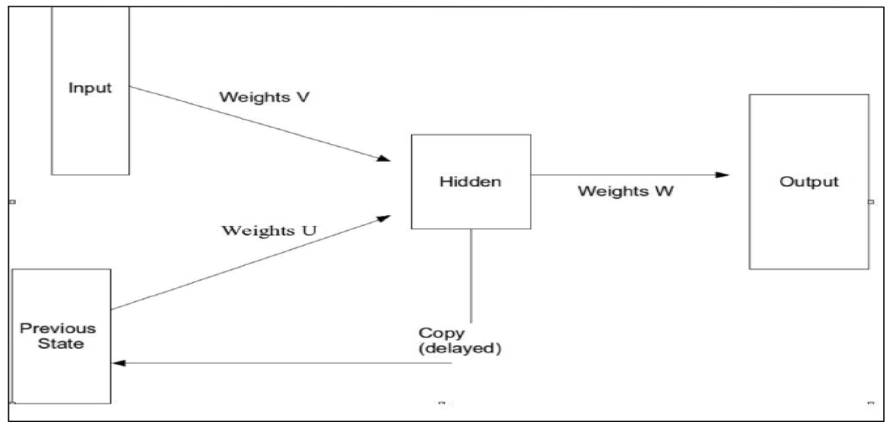

Fig. 5 A simple recurrent network

variable (dependent variable) to develop MVRA model. A correlation has been generated for each Langmuir constant with the given macerals paramters (Moisture, Volatile matter, Ash, Fixed carbon, Vitrinite, Semi-vitinite, Litinite, Intertinite, Mineral matter, Mean Ro% and Depth).

Multivariate linear equation for each LVC and LPC are obtained. The equations are :

$$\begin{aligned} LVC = {} & (4.553826842 * m) + (0 * v) \\ & + (-0.627388513 * a) + (1.345670812 * f) \\ & + (2.603845223 * k) + (17.11085324 * s) \\ & + (2.997470493 * l) + (1.931219754 * i) \\ & + (3.490123182 * z) + (22.0153635 * w) \\ & + (-0.030223317 * d) \end{aligned}$$

And

$$\begin{aligned} LPV = {} & (0.119074233 * m) + (0 * v) \\ & + (* - 0.039505654 * a) + (0.030893488 * f) \\ & + (0.090233506 * k) + (0.404806961 * s) \\ & + (0.09012357 * l) + (0.084394968 * i) \\ & + (0.112784163 * z) + (-0.213303844 * w) \\ & + (-0.000263957 * d) \end{aligned}$$

8.2 Artificial neural network (ANN)

Several researchers have used ANN to predict rock parameters like oil flow rate of reservoir, permeability, dynamic elastic constants, compressive strength, creep parameters, ground vibration etc. (Tahmasebi and Hezarkhani 2012; Ahmadia et al. 2013; Verma and Singh 2013; Singh and Verma 2010; Verma and Singh 2009; Singh and Verma 2011).

In this paper, different type of neural network are considered to predict LVC and LPC governing the nature of Langmuir isotherms which associate the adsorption of carbon dioxide gas molecules on a coal surface to gas pressure or concentration at a fixed temperature. The architect of all different neural network are optimally optimized.

ANN application has some issues also and the most common one is to define optimum number of hidden layers, the number of neurons in these hidden layers, functional relations between input and output parameters, learning algorithm and avoiding overfitting. So, different neural network has been considered in study and a simulation has been done on the same problem.

The RMSE method has been used to determine the optimal model parameters. The RMSE is more sensitive to the larger relative errors which are resulted due to the low valued so that it offers a balanced evaluation of the goodness of fit of the model. The perfect model will have a RMSE value approaching to zero. The formula for determining the RMSE is:

$$RMSE = \sqrt{\frac{(O_i - T_i)^2}{N}}$$

where, Ti is measured output (Target),Oi is the predicted output and N represent the number of input–output data pairs.

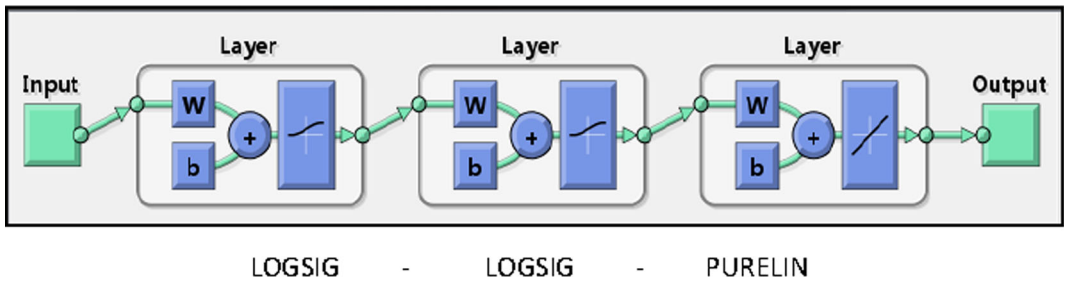

Fig. 6 Optimum ANN Network with typical feed-forward back propagation

Table 3 Comparison of the different ANN architecture based on RMSE values

S. no.	Transfer function	Model	RMSE
1.	Tansig-purelin	11-7-2	3.4058
2.	Tansig-purelin	11-20-2	3.0854
3.	Logsig-purelin	11-20-2	2.7874
4.	Tansig–tansig-purelin	11-15-5-2	0.3633
5.	Logsig-logsig-purelin	11-15-10-2	0.0022
6.	Logsig-poslin	11-15-2	6.2289
7.	Tansig-tansig-purelin	11-7-15-2	1.5198
8.	Tansig-tansig-poslin	11-15-20-2	4.1952
9.	Logsig-logsig-purelin	11-10-5-2	0.7368
10.	Tansig-logsig-purelin	11-10-20-2	4.8785

8.2.1 Backpropagation feed forward neural network (BPNN)

To determine the optimal architecture, two and three hidden layer in network has been considered for carrying out parametric simulation. In each hidden layer, number of neurons has been changed to determine the optimum model based on minimum value of RMSE. The 80 % dataset is used for training, 10 % for validation and 10 % for testing. The network with architecture 11–15–10–2 with transfer function 'logsig–logsig-purelin' has been found to have the minimum RMSE of value 0.0022 (Fig. 6; Table 3).

8.2.2 Generalised regression neural network (GRNN)

The generalized regression neural network is considered and input parameters are assigned to input data and measured LVC and LPC value are assigned to target data. Input has been simulated with different spread constant of 1, 5, and 10. The outputs are obtained and RMSE value has been calculated from obtained output to study the optimum of the network. The network view for generalised neural network is as follows (Fig. 7; Table 4).

8.2.3 Radial basis neural network (RBNN)

The radial basis network is considered and input parameters are assigned to input data and measured LVC and LPC value are assigned to target data. Input has been simulated with different spread constant of 1, 10, and 100. Output for both Langmuir isotherm constant has been obtained. There is no change in output with the change in value of spread constant. The network view for radial basis neural network is as follows (Fig. 8).

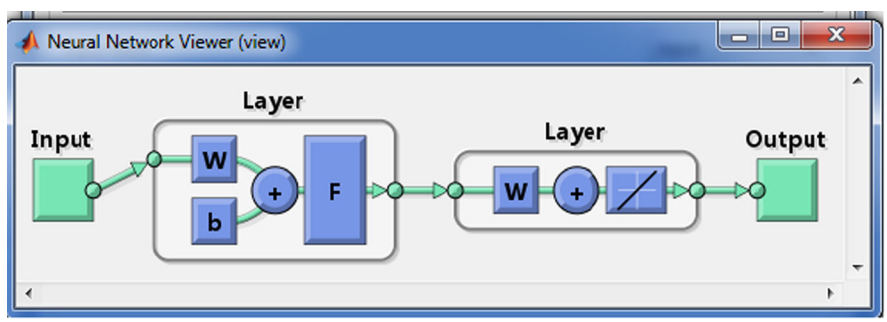

Fig. 7 Optimum GRNN network

8.2.4 *Layer recurrent neural network (LRNN)*

Input data are simulated with different training function and adaption learning function in Layer recurrent neural network. The training function considered are TRAINLM, LEARNGDM and TRAINLM whereas adaption learning function considered are LEARNGDM and LEARNGD. The performance function is MSE. The number of Layers are 2 with 15 neuron in 1st Layer and transfer function as logsig-purelin. The network view for recurrent neural network is as (Fig. 9; Table 5):

The optimized model is for network with training function = TRAINLM, Adaption Learning Funtion

Table 4 Comparison of the different GRNN architecture based on RMSE values

Spread constant	RMSE
5	0.0099
10	0.4431

Table 7 RMSE of different prediction models for LPC

Model	Root mean square error (RMSE)
MVRA	8.1305
BPNN	0.0970
GRNN	0.00064
RBNN	2.3e−23
LRNN	0.00443

Table 6 RMSE of different prediction models for LVC

Model	Root mean square error (RMSE)
MVRA	279.6838
BPNN	1.2570
GRNN	0.0140
RBNN	1.4e−20
LRNN	1.23

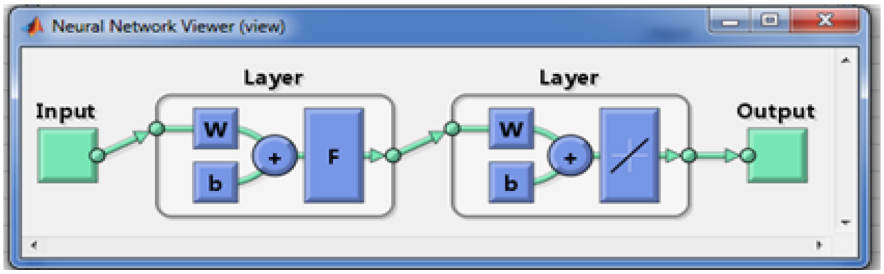

Fig. 8 Optimum RB network

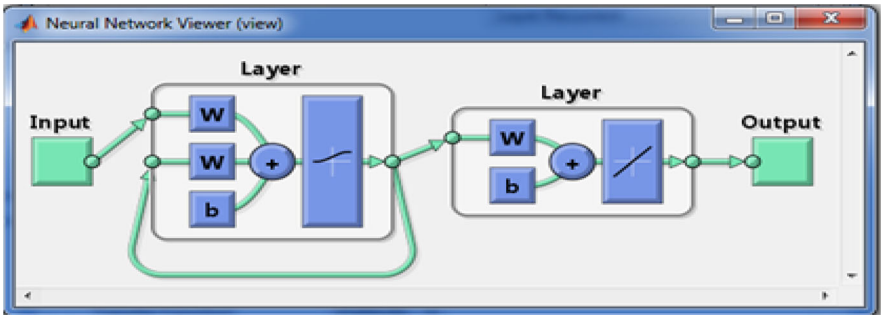

Fig. 9 Optimum recurrent network

Table 5 RMSE values for different network

S.No	Training function	Adaption learning function	Performance function	RMSE
1	TRAINLM	LEARNGDM	MSE	3.346640106
2	LEARNGDM	LEARNGDM	MSE	16.73320053
3	TRAINLM	LEARNGD	MSE	4.949747468

Table 8 Output from different networks

Name of coal mines	MVRA		BFFNN		GRNN		RBNN		LRNN	
	Langmuir volume constant (V_L, mL/g)	Langmuir pressure constant (P_L MPa)	Langmuir volume constant (V_L, mL/g)	Langmuir pressure constant (P_L MPa)	Langmuir volume constant (V_L, mL/g)	Langmuir pressure constant (P_L MPa)	Langmuir volume constant (V_L, mL/g)	Langmuir pressure constant (P_L MPa)	Langmuir volume constant (V_L, mL/g)	Langmuir pressure constant (P_L MPa)
Bogra	357.677	10.83493	73.8918	2.750737	74	2.732	74	2.732	74.0943	2.732
Kenda	354.4144	10.60786	68.04387	2.415283	68	2.406	68	2.406	68	1.9651
Narayankuri	358.3805	10.61225	88.87698	2.592906	89	2.586	89	2.586	89	2.586
Satgram	335.6095	10.1923	62.0752	2.255086	58	1.976	58	1.976	57.2921	1.5735
Kalimati	307.5902	9.34341	25.02697	1.073902	25	1.074	25	1.074	25	1.1054
Local II	297.7553	8.931138	18.03693	0.797207	18.037	0.8017	18	0.8	18	0.88108
Mehaladih	307.6106	9.286722	31.01909	1.269175	31	1.271	31	1.271	29.2149	1.2263
Mugma special	306.1793	9.215589	26.00152	1.167101	25.963	1.1653	26	1.167	26.9804	1.167
SKAC 1	311.4136	9.016909	35.33676	1.072078	33	0.841	33	0.841	33.7015	0.841
SKAC 3	320.9305	9.085995	41.00943	0.983649	41	0.984	41	0.984	41	1.0664
15th seam	317.8396	9.219093	34.96882	1.083854	35	1.082	35	1.082	36.8051	1.149
16th Top seam	317.44	9.426272	41.91868	1.417442	42	1.418	42	1.418	42.7282	1.418
16th Bottom seam	326.3686	9.457639	42.01276	1.23134	42	1.231	42	1.231	42	1.231
18th seam	316.9266	9.328285	38.87861	1.177016	39	1.161	39	1.161	37.7325	1.1817

Table 9 Moles of CO_2 adsorbed for each coal mines

Coal mines	No. of moles of CO_2 adsorbed/g
Bogra	0.001645516
Kenda	0.001512095
Narayankuri	0.001979066
Satgram	0.001289728
Kalimati	0.000555917
Local II	0.000400261
Mehaladih	0.000689338
Mugma special	0.000578154
SKAC 1	0.000733811
SKAC 3	0.000911705
15th Seam	0.000778284
16th Top seam	0.000933941
16th Bottom seam	0.000933941
18th Seam	0.000867231

= LEARNGDM and Performance function = MSE with RMSE value of 3.346640106.

The performance of LVC and LPC predicting models has been evaluated using the root mean square error (RMSE) criteria (Verma and Sirvaiya 2015) in Tables 6, 7, 8 shows output from different networks used in this study. Considering a coal mine with a coal seam at a pressure of 1305.342 psia, reservoir temperature of 536.67 deg. R (25 deg. C) and Z factor to be 0.36, the moles of CO_2 adsorbed for each coal mines are shown in Table 9.

9 Conclusion

In this study, neural network models were efficiently used to predict the CO_2 adsorption parameters like Langmuir volume constant and Langmuir pressure constants of sub-bituminous to high-volatile bituminous Indian Gondwana coals. These applications presented more accuracy in comparison with the statistical methods. It can be concluded that ANN is a useful resource to determine adsorption capacity of CO_2 gas in Indian Gondwana coal.

In this paper, multivariate regression model and different neural network models like back propagation with regression analysis, recurrent neural network, generalized regression neural network and radial basis function network (RBF) are developed and used to predict adsorption capacity through Langmuir isotherm. The Neural Network architecture is optimum with radial basis as best model. The target values and output values are coming almost same. Back propagation method and generalized regression also result in low RMSE. Based on the study, it is can be established that the neural network methods are the better option for better prediction of Langmuir constants of Indian Gondwana coals for CO_2 adsorption.

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