A mini review of machine learning methods for predicting gas adsorption capacity of coal

Wei Zhao[1,2], Yujia Wan [1,2], Dan Zhao[1,2], Chenmin Zhang[1,2], Kai Wang[1,2,*] and Jingzhe Yu[1,2]

1 School of Emergency Management and Safety Engineering, China University of Mining & Technology (Beijing), Beijing, 100083, China.

2 Beijing Key Laboratory for Precise Mining of Intergrown Energy and Resources, China University of Mining & Technology (Beijing), Beijing, 100083, China.

* Corresponding Author. School of Emergency Management and Safety Engineering, China University of Mining & Technology (Beijing), Beijing, 100083, China; E-mail: kaiwang@cumtb.edu.cn

Abstract

Intelligent utilization of fossil energy has become a pivotal topic in contemporary energy development. The quantification of coal seam methane adsorption capacity is crucial for assessing Coalbed Methane (CBM) reserves and methane-related greenhouse effects. Currently, experimental procedure for methane adsorption isotherm measurement remains challenging because of its extended equilibrium durations and procedural complexity. Moreover, the conventional adsorption model constrained by restrictive assumptions and has limited application with alternative adsorption conditions. Given their effective problem-solving capabilities, artificial intelligence algorithms are increasingly adopted by researchers. This work systematically reviews of recent advancements in intelligent algorithms used for predicting gas adsorption characteristics, e.g., Artificial Neural Network (ANN), Deep Neural Network (DNN), Recurrent Neural Network (RNN), Support Vector Machine (SVM), etc., focusing on three key areas: experimental measurement of adsorption

isotherms, development of mathematical models for adsorption evaluation, and identification of dominant factors influencing coal adsorption. We further critically compare algorithmic strengths/limitations and identify future research directions. These findings enable improved CBM reserve assessment and inform greenhouse gas emission strategies.

Keywords: Gas adsorption; Isothermal adsorption model; Greenhouse effect; Machine learning algorithms; Neural network

Nomenclature

List of Abbreviations

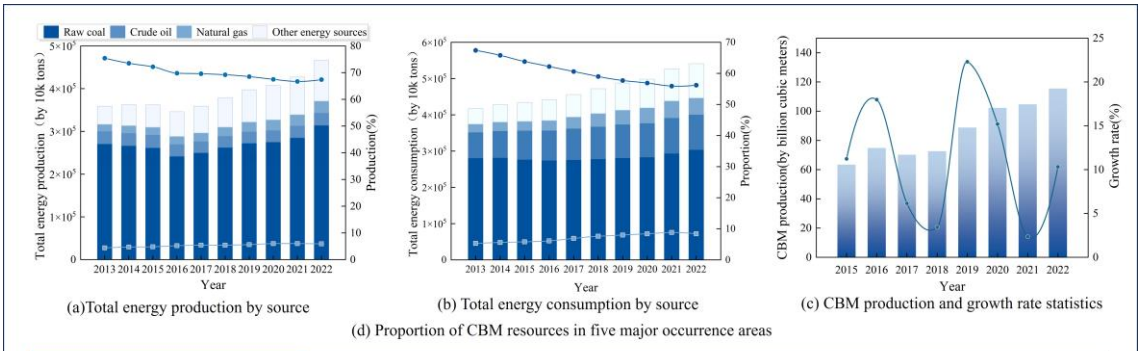
Acronym	Definition
ANN	Artificial Neural Network
ACE	Alternating Conditional Expectation
BP	Back-Propagation
BP-ANN	BP Artificial Neural Network
BET	Brunauer-Emmett-Teller
CBM	Coalbed Methane
CNN	Convolutional Neural Networks
DNN	Deep Neural Network
D-A	Dubinin-Astakhov
D-R	Dubinin-Radushkevich
GBDT	Gradient-Boosted Decision Tree
KNN	K-nearest Neighbor
LP-N_2GA	Low-Pressure Nitrogen Gas Adsorption
MIP	Mercury Intrusion Porosimetry
ML	Machine Learning
RF	Random Forest

RNN	Recurrent Neural Network
RL	reinforcement learning
SVM	Support Vector Machine
SDR	Supercritical Dubinin–Radushkevich
SL	supervised learning
TL	Transfer learning

1. Introduction

The typical characteristic of China's energy framework is "rich in coal, poor in oil and less in gas"(Li *et al.* 2024). Coal persistently dominates China's energy production and consumption structure(Zhao *et al.* 2024). As reported in the official statistics published by the National Bureau of Statistics("China Statistical Yearbook" 2024), national green energy policies have progressively reduced coal's share, yet it maintains >50% of production and consumption(Fig.1). This confirms coal's ongoing strategic importance in China's energy supply system(Zhao *et al.* 2025).

Coalbed Methane (CBM), a coal-associated greenhouse/geohazard gas, offers triple benefits, including mitigating atmospheric greenhouse gas emissions, enhancing coal mine safety, and augmenting domestic natural gas reserves(Yu *et al.* 2024). Global CBM production shows sustained growth (Chattaraj *et al.* 2019). China has developed five typical CBM basins, achieving production growth from 0.3 billion m^3 in 2003 to 11.55 billion m^3 by 2022(Sang *et al.* 2024). Therefore, the exploration and exploitation of CBM not only align with contemporary trends and comply with relevant national regulations but also substantially cater to the diverse needs of humanity.



(d) Proportion of CBM resources in five major occurrence areas

Major occurrence areas	Northwest	Qinghai-Tibetan	South	North China	Northeast
Production of CBM resources(100 million m³)	27.09	0.01	19.03	48.44	10.12
Proportion of CBM resources (%)	25.87	0.01	18.18	46.27	9.67

Figure 1 Profiles of coal and natural gas production and consumption

Methane exists in coal in two forms: adsorbed state and free state. Most of methane is present in coal seams through physical adsorption(Zhang *et al.* 2020). However, CBM adsorption characteristics are influenced by pore structure characteristics, distribution pattern, and other reservoir properties, thereby posing challenges in accurately estimating the gas content of coal seams. Therefore, achieving an accurate characterization of gas adsorption characteristics is important.

Gas adsorption refers to the phenomenon that gas adheres to the surface of solids and the adsorption process is exothermic(Kang *et al.* 2022), with its adsorption quantity increasing under elevated pressure and reduced temperature conditions. The isotherm theory is commonly employed for describing these adsorption properties(Kim *et al.* 2019). Currently, the experimental techniques employed for methane adsorption isotherm measurements include pressure, weight, and volume quantification methods(Busch & Gensterblum 2011). Although these methods differ in their principles for determining adsorption characteristics, each method necessitates critical operational steps, typically involving sample conditioning, adsorption equilibrium establishment, and subsequent data extrapolation. These multistep procedures introduce errors and extend

timelines. Furthermore, the fitting models employed to process the experimental data possess certain limitations, and conventional adsorption models such as Langmuir, Dubinin-Astakhov (D-A), Dubinin-Radushkevich (D-R), and Brunauer-Emmett-Teller (BET) models have been conventionally utilized for fitting methane adsorption experimental data over numerous years(Zhou *et al.* 2019). Despite their accuracy in fitting laboratory-derived adsorption curves, classical isothermal models' scope remains bound to predefined temperature regimes, coal petrographic classifications, and simplified theoretical premises, with experimental validation necessitating resource-intensive protocols. Therefore, it is urgent to establish a model with fewer restrictions and easy to characterize the coal adsorption capacity quickly.

With the advent of the era of big data, deep learning methods such as ANN and Random Forest (RF) have been introduced into the prediction of gas adsorption characteristics in porous material(Skrobek *et al.* 2020; Guo *et al.* 2022; Skrobek *et al.* 2022; Mashhadimoslem & Ghaemi 2023). Based on previous research, a deep learning model can be developed to predict the gas adsorption capacity of coal by analyzing the characteristics of its matrix and pore structure(Mirzaei *et al.* 2020). Therefore, the establishment of a deep learning model with good performance has practical significance for reducing time-consuming and cost-consuming adsorption isotherm measurement work, which will be conducive to CBM development, natural gas mining and reserve assessment, thus assisting decision-making, optimizing production plans, and improving natural gas mining efficiency.

2. Traditional methods to predict gas adsorption capacity

Data is the basis of intelligent prediction. It is essential to clarify the traditional methods and influencing factors for gas adsorption capacity prediction. Scholars both domestically and internationally have conducted extensive field and laboratory tests, meticulously cross-referencing the collected empirical data with

fundamental theoretical knowledge. Consequently, they have unequivocally ascertained that the process of coal adsorption gas can be classified as a physical adsorption phenomenon(Tagliabue *et al.* 2009). Persistent progress technology and theory has precipitated substantial heterogeneity in methodological approaches across studies investigating gas adsorption. However, in general, the research scale is gradually refined, and the research methods are gradually expanded from a single experimental measurement to theoretical calculation. Furthermore, attempts are being made to establish simulation models based on various cutting-edge theories. Emerging technological innovations are enabling increasingly detailed comprehension of gas adsorption mechanisms. In general, scholars are most concerned about the research of coal adsorption experimental determination, theoretical model and influencing factors(Huang 2020).

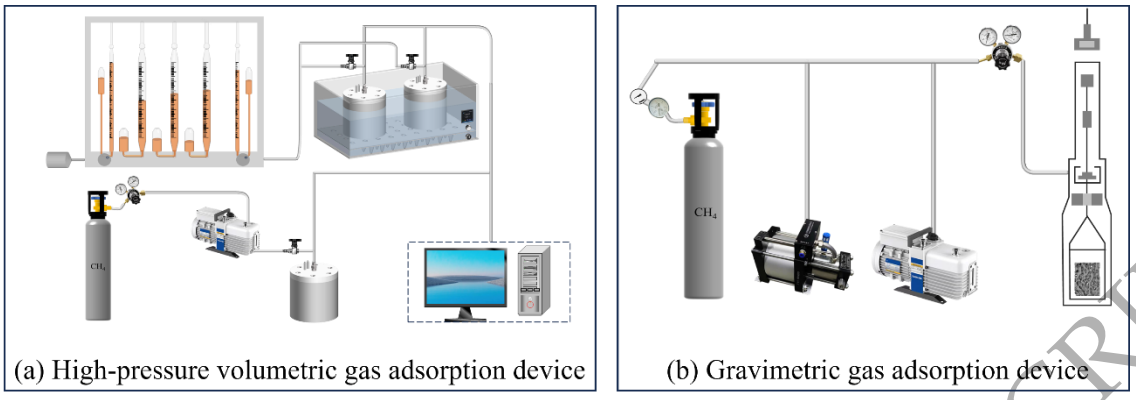
2.1 Experimental methods

Isothermal sorption assays conducted on coal serve as a validated framework for estimating the adsorption capacity of gas. Adsorption isotherm profiles enable the determination of gas-phase critical pressure thresholds, precise quantification of coal-rock sorption saturation limits, and empirical modeling of gas extraction yield dynamics. In contemporary gas analysis workflows, measurement protocols bifurcate into direct versus indirect methodologies(Wang *et al.* 2022). The direct method quantifies the coal gas content acquired during drilling operations by employing the volumetric desorption method to measure the volume of desorbed gas, lost gas, and residual gas(Sun *et al.* 2018). Because the direct method uses *in-situ* sampling, it is considered to be more reliable than the indirect method. The direct method, however, relies predominantly on experimental scenarios and presents the following limitations: (ⅰ) Quantifying fugitive gas leakage during gas-lift wellbore operations poses significant challenges. (ⅱ) The entire testing process typically entails a considerable duration, ranging from several hours to weeks; (ⅲ) Measurement costs are comparatively higher.

Therefore, numerous scholars have made improvements on the direct method. An *et al.* (2019) proposed a novel approach for determining gas content in coal based on gas desorption rate. Benchmarking the novel methodology against conventional direct approaches, validating operational reliability in engineering applications. Yu (2020) utilized a 3D Max software to construct a three-dimensional model of the experimental scene and the instrumentation, and completed the gas adsorption test by taking virtual simulation as the main experimental method. Jiao *et al.* (2023)designed a negative-pressure fixed-point sampling test system to address the challenges of difficult fixed-point sampling in soft coal seams and large errors in gas content measurements.

In contrast, indirect methods quantify the maximum gas adsorption capacity on the coal surface by analyzing the adsorption characteristics and pressure-dependent adsorption isotherms(Chen *et al.* 2019). Although indirect methods are relatively time-saving, they offer easier access to results. However, a drawback of this approach is that crushing the coal sample into appropriately sized lumps alters its physical properties such as ash content, moisture, fissure distribution, and pore structure. Indirect methods for measuring gas adsorption include volumetric and gravimetric methods(Zhou *et al.* 2017). Pressure-controlled adsorption quantification constitutes the core principle of volumetric determination, while the gravimetric method directly measures mass changes in the reactor under constant pressure conditions. The volumetric method is more susceptible to gas non-ideality and dead volume errors, making it suitable for adsorption studies under medium-low pressure conditions with small molecules. The gravimetric method demonstrates significant advantages in high-pressure and corrosive gas environments, though buoyancy correction and mechanical stability remain bottlenecks, rendering it preferable for precise measurements of strong adsorption systems. Method selection requires trade-offs among material properties, pressure ranges, and error tolerance. For high-precision research, cross-validation of both methods is recommended, complemented by molecular

simulations to elucidate the underlying mechanisms. The volumetric method is predominantly employed in research to determine the content of adsorbed gas(Zhao *et al.* 2020; Chen *et al.* 2021; Dai *et al.* 2023). Device diagrams for both volumetric and gravimetric approaches are shown in Fig. 2.



(a) High-pressure volumetric gas adsorption device (b) Gravimetric gas adsorption device

Figure 2 Volumetric and gravimetric gas adsorption units

2.2 Theoretical models

Over the years, numerous scholars have developed mathematical models for gas adsorption in coal based on three fundamental aspects: kinetic theory, thermodynamics, and potential energy theory. While these models provide valuable frameworks, their applicability to complex coal matrices remains contested due to oversimplified assumptions. For instance, the Langmuir equation—derived from kinetic adsorption theory (Zhao & Tang 2002) with assumptions of homogeneous surfaces, monolayer coverage, and negligible intermolecular forces—fails to capture methane adsorption behavior in heterogeneous coals, particularly under high-pressure conditions where multilayer adsorption occurs. Experimental and theoretical analyses demonstrate that the adsorption of methane on coal does not conform to the monomolecular adsorption assumption stipulated by the Langmuir equation(Sang *et al.* 2005). However, the isotherm of coal adsorption methane shows the characteristics of the *Class I* adsorption isotherms, so the adsorption process is described by the Langmuir equation has achieved a better effect(Wu & Pan 2017; Pajdak *et al.* 2019). Therefore, the

model is widely applied in gas adsorption research(Wang *et al.* 2023). The BET model extended Langmuir's framework to multilayer adsorption (Kołodziejek *et al.* 2013) but introduced new limitations by neglecting capillary condensation hysteresis in moisture-saturated coals. After that, Dubinin's model advanced micropore filling theory yet assume rigid pore structures, contradicting coal matrix swelling/shrinking during adsorption/desorption cycles (Dubinin 1960; Guo *et al.* 2006). In 1970, Dubinin & Astakhov (1971)extended the DR model to the DA model, which incorporated the influence of adsorbed molecules on microporous surface forces and pore structure (Busch *et al.* 2003). This resulted in a more precise description of gas adsorption behavior within a narrower range of pore sizes. Polanyi's potential theory effectively describes adsorption in ideal micropores but overlooks temperature-dependent potential shifts in swelling-prone coals above critical temperatures(Zhao *et al.* 2022; Li *et al.* 2003). processes. Even the Freundlich model(Vigdorowitsch *et al.* 2021), while accommodating heterogeneity, lacks physical basis for pore-network coupling effects observed in coal lithotypes. Collectively, these models reveal a persistent challenge: theoretical elegance often compromises geologically-grounded realism. Mounting evidence urges hybrid approaches integrating adsorption dynamics with coal's multiscale structural evolution—the focus of our proposed model.

Regarding the fitting of methane adsorption in coal using various adsorption theory models, researchers have conducted comparative analyses on the accuracy of Langmuir's theoretical model, BET model, DR model, and DA model along with their extensions and modifications (Wei & Liu 2023). The findings from these studies vary slightly, but a majority of them suggest that the microporous filling theory's DR or DA models exhibit superior accuracy in fitting methane adsorption in coal (Wang Z F *et al.* 2023; Abdulsalam *et al.* 2020; Han *et al.* 2020; Liu *et al.* 2023).

The study of gas adsorption in coal has seen major progress in modeling techniques recently. Zhang *et al.*

(2008) developed a novel integrated temperature-pressure adsorption model for gas adsorption in coal based on the theory of adsorption potential. They also provided a method to determine the characteristic constants in this model. Perera *et al.* (2012)proposed a new descriptive model for gas adsorption capacity in coal as a function of the effective factors. However, the developed model is valid only for the coal with less than around 85% fixed carbon content .Sheng *et al.* (2014) proposed the DA-Langmuir isothermal adsorption model when exploring the adsorption mechanism of methane gas by shale and verified the applicability of this model. Additionally, Song *et al.* (2018) proposed an optimized L-SDR model by combining the Supercritical Dubinin–Radushkevich (SDR) model with the Langmuir model to estimate supercritical gas adsorption of shale. The results demonstrated that this optimized model exhibited higher accuracy and effectively described the behavior of shale's methane adsorption at different temperatures. The Langmuir-Freundlich and DR adsorption formulas were combined by Song *et al.* (2018), Dong *et al.* (2020) to develop an enhanced high-pressure isothermal adsorption model. Comparative analysis with eight previous models confirmed that the improved adsorption formula yielded the most accurate adsorption model.

The diversity of methane isothermal adsorption models is illustrated in Table 1, which summarizes the commonly used models along with their applications, comparisons, and optimizations. However, it should be noted that the adsorption of CH_4 in coal can occur in various forms including monomolecular layer adsorption, multimolecular layer adsorption, micropore-filled form, or even a combination of multiple forms simultaneously(Hao *et al.* 2014; Charoensuppanimit *et al.* 2015; Miao *et al.* 2017). Therefore, relying on a single model may not accurately characterize the adsorption isotherms. Furthermore, it is important to acknowledge that all aforementioned models are only valid for particular thermal conditions and specific types of coal. Henceforth, constructing an intelligent model capable of overcoming these limitations holds significant practical value.

Table 1 Overview of common mathematical models of gas adsorption in coal

Author	Theoretical model	Mathematical equation	characteristic
Freundlich (1907)	Freundlich model	$V = KP^{\frac{1}{n}}$	Purely empirical equations with no clear physical meaning, but simple in form and easy to use.
Polanyi (1916)	Adsorption potential theory	$\varepsilon = RT\ln(\frac{P_0}{P})$	Good at describing the adsorption of gases on microporous solid surfaces, the adsorption process at different temperatures are described by the same characteristic curve.
Langmuir (1916)	Monolayer adsorption theory	Langmuir: $\frac{P}{V} = \frac{P}{V_L} + \frac{P_L}{V_L}$	Applies to the state of monomolecular adsorption on solid surfaces, and cannot rationally account for multilayer adsorption and capillary coalescence in coal.
Brunauer *et al.* (1938)	Multilayer adsorption theory	BET: $\frac{P}{V(P_0 - P)} = \frac{1}{V_m C} + \frac{C-1}{V_m C} \times \frac{P}{P_0}$	The application assumes that the gas is adsorbed by multimolecular layers on a completely uniform coal surface.
Dubinin (1960)	Microhole filling theory	DR: $V = V_0 \exp\left\{-\left[\frac{RT}{\beta_0 \mathrm{E}_0}\ln\left(\frac{P_0}{P}\right)\right]^2\right\}$	Describe the microporous filling behavior that occurs inside micropores.
Dubinin & Astakhov (1971)		DA: $V = V_0 \exp\left\{-\left[\frac{RT}{\beta_0 \mathrm{E}_0}\ln\left(\frac{P_0}{P}\right)\right]^n\right\}$	The effect of adsorbed molecules on the microporous pore surface forces and pore structure is considered.
Zhang *et al.* (2008)	Temperature-pressure integrated adsorption model	$V = De^{mRT\ln\frac{P}{P_C}}\left(\frac{Tc}{T}\right)^k$	It is possible to predict the methane adsorption capacity of coal at a certain depth and temperature, and to estimate deep CBM resources.
Song *et al.* (2018)	L-SDR model	$V = \begin{cases} V_0 \times \frac{b_1 \times \rho_{gas}}{1 + b_1 \rho_{gas}}, & when\ P < P_t \\ \alpha_1 \times V_0 \times \frac{b_2 \times \rho_{gas}}{1 + b_2 \rho_{gas}} + \alpha_2 \times V_m \times \exp\left\{-D \times \left[\ln\left(\frac{\rho}{\rho_{gas}}\right)RT\right]^2\right\}, & when\ P \geq P_t \end{cases}$	The model can accurately describe the process of supercritical methane adsorption in shale, and can also describe the behavior of methane adsorption in shale at different temperatures.
Dong *et al.* (2020)	Langmuir-Freundlich+ DR	-	A good fit to the high-pressure isothermal adsorption curve for shale methane.

2.3 Influencing factors

Methane adsorption in coal reservoirs is co-governed by geogenic properties of coal matrices and environmental operational variables. Structural features of coal including pore topology (volume, size, surface area) combine with coal rank, microscopic constituents, and industrial characteristics. Additionally, external factors such as particle size, temperature, pressure, and tectonic activity also play significant roles(Zhang & Zhang 2008; Zhao *et al.* 2023).

(1) Pore structure

It is generally believed that micropore determines specific surface area of coal(Cai *et al.* 2013; Liu 2022), and the larger the pore volume, the larger the pore specific surface area of coal. Furthermore, gas adsorption capacity demonstrates proportional enhancement with specific surface area elevation. Li *et al.* (2023)believed that specific surface area and volume of mesopores and macropores, measured by Low-Pressure Nitrogen Gas Adsorption (LP-N_2GA) and Mercury Intrusion Porosimetry (MIP) methods respectively, were found to have a weaker correlation with the adsorption constant "*a*". However, it exhibited a stronger correlation with micropores measured using the CO_2 adsorption method. Li *et al.* (2021) hypothesized that pore size distribution exhibits a higher degree of continuity and homogeneity, thereby resulting in a substantial enhancement in gas molecule mobility within micropores and consequently augmenting coal's gas adsorption capacity. It is evident that micropore proliferation combined with pore constriction systematically increases coal's available adsorption interfaces.

(2) Coal rank

Coal rank stratification creates pronounced adsorption variability across specimens. According to the conventional theory, the adsorption constant "*a*" follows a "*three-stage*" evolution pattern with increasing coal rank: it attains minimum and maximum values near 1.3% and 3.5% of maximum vitrinite reflectance ($R_{0,\,max}$),

respectively, and then diminishes during the middle and late stages of anthracite coal. However, statistical analysis on equilibrium water-containing coal samples from various grades reveals that the "*a*" value only reaches its peak around 4.5% of $R_{0,max}$, indicating an actual "two-stage" evolution pattern(Zhang 2022). The research conducted by Weniger *et al.* (2010), Feng *et al.* (2014) revealed a parabolic relationship between the maximum CH_4 adsorption capacity of coal and $R_{0,max}$. In contrast, Faiz *et al.* (2007) observed a negative correlation between Langmuir volume (V_L) and $R_{0,max}$ in the high to a medium rank range of bituminous coals. These previous studies have shown that simple coal-rank analysis is insufficient to evaluate coal adsorption capacity.

(3) Maceral

Regarding the influence of macerals on the gas adsorption capacity, extensive studies have been conducted by domestic and foreign scholars, leading to relatively consistent views with some detailed differences. The vast majority of research indicates that under the same coal rank conditions, the adsorption capacity (V_L) of vitrinite is significantly higher than that of inertinite(Zhang *et al.* 2005; Chalmers & Bustin 2007; Mastalerz *et al.* 2008; Zhang *et al.* 2017). The adsorption capacity of exinite remains controversial and complex. Levy *et al.* (1997)investigated coal samples from the Bowen Basin in Australia and found that the content of exinite was negatively correlated with V_L, indicating that its adsorption capacity was weaker than that of vitrinite. Prinz & Littke (2005)proposed that exinite in the early stage of thermal evolution ($R_0 < 0.8\%$) generates a large number of open pores due to hydrocarbon generation, which may endow it with higher pore connectivity and adsorption potential than vitrinite. Li *et al.* (2012)argued that the methane adsorption capacity of low-rank coal is negatively correlated with exinite content, while that of medium-rank coal shows a weak correlation with exinite.

(4) Proximate analysis components

The moisture content in coal is a crucial parameter that significantly influences the adsorption capacity. It has been observed that there exists a critical value of moisture content in coal, beyond which the relationship between moisture content and methane adsorption becomes more complex. Below this critical value, moisture primarily occupies the pores of coal, leading to a decrease in methane adsorption with increasing moisture content. However, above this critical value, the outer surface of coal particles starts to be occupied by moisture, resulting in reduced adsorbed moisture within the pore space and only minimal changes in methane adsorption(Chen *et al.* 2015). The findings of Clarkson & Bustin (2000) further supported this conclusion. Similarly, Li & Nie (2006) arrived at similar conclusions, suggesting that the interaction force between moisture molecules and coal surface molecules exceeds that of methane molecules, thus explaining this phenomenon. These observations are consistent with empirical theory. It is widely accepted that there is competition between moisture and gas adsorption; however, once the moisture content reaches a certain critical value, its incremental increase has minimal to negligible influence on coal adsorption.

The ash content of coal has a similar impact on gas adsorption as the moisture content does. Early studies (Gürdal & Yalçın 2000; Dutta *et al.* 2011) have consistently indicated a negative correlation between the methane adsorption capacity in coal and its ash content, with the latter exerting an even greater influence than coal rank(Laxminarayana & Crosdale 2002). The volatile fraction of coal refers to the thermally decomposed products of organic matter in coal, encompassing methane, carbon monoxide, carbon dioxide, nitrogen, hydrogen, hydrogen sulfide, and various complex organic compounds.

The volatile matter content of coal is a key indicator for categorizing coal rank. The effect of volatile matter on gas adsorption exhibits a “U-shaped” trend. In lower ranks of coal, both volatile matter and adsorption capacity decrease as the degree of coalification increases(Cheng *et al.* 2017; Busch *et al.* 2019).

However, in highly metamorphosed coals, adsorption capacity gradually increases as volatile matter decreases. Furthermore, there exists an inverse correlation between the volatile content and "*a*", which contrasts with the correlation between $R_{0,max,}$ and "*a*"(Yuan 2021).

The effect of volatile matter on methane adsorption exhibits a “U-shaped” trend. In lower ranks of coal, both volatile matter and adsorption capacity decrease as the degree of coalification increases. However, in highly metamorphosed coals, adsorption capacity gradually increases as volatile matter decreases.

(5) External factors

In addition to various internal factors, coal reservoir adsorption dynamics are predominantly governed by ambient constraints including stress, pressure, temperature, and particle size. Both theory and experiments have demonstrated that higher pressures in coal reservoirs result in greater methane adsorption, while lower temperatures favor the adsorption of CBM. Under the combined effects of temperature and pressure, there is a critical point where the impact of temperature on adsorption surpasses that of pressure (Yao *et al.* 2018; Zhang 2019). The gas adsorption capacity of coal was observed to increase with decreasing particle size under specific conditions, as reported by Nie *et al.* (2013). However, once a certain particle size threshold is reached, the gas adsorption capacity shows no significant change.

Numerous previous studies have extensively investigated the adsorption and desorption characteristics of coal, as well as their influencing factors. The main factors that affect coal adsorption are shown in Fig. 3. Although some results remain controversial, most studies consistently show an overall trend. Existing investigations predominantly address gas adsorption responses to isolated geological parameters, whereas systematic analysis of sorption mechanisms under coupled geological constraints remains inadequate. In this study, we simulate changes in coal adsorption resulting from the combined effects of these aforementioned multiple factors.

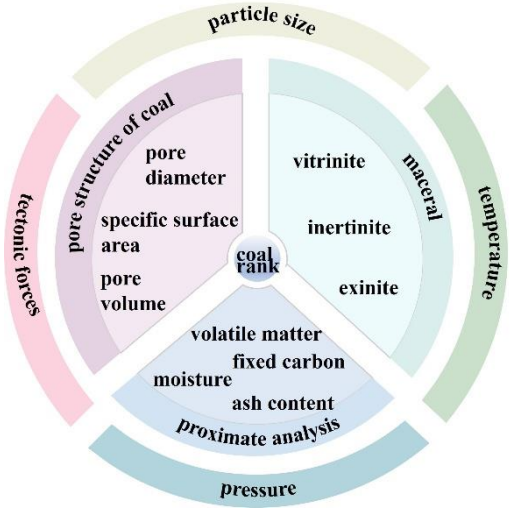


Figure 3 Factors affecting gas adsorption

3. Current status of Intelligent prediction for gas adsorption capacity

Machine Learning (ML) is a computational process in which computer programs autonomously acquire knowledge and adapt to new data by constructing mathematical models(Chang *et al.* 2024). Initially, ML constructs a learning algorithm based on the history data, subsequently using this algorithm to generate a predictive data model capable of extracting relevant information related to the target variable. Ultimately, it enables pattern recognition and behavioral identification . With the development of big data and deep learning, machine learning algorithms such as K-nearest Neighbor (KNN), Decision Tree Regression, RF, BP neural network, and SVM have made significant progress in fields like image recognition, natural language processing, medical diagnosis, or autonomous driving (Raschka & Mirjalili 2019; Sarker 2021; Xiouras *et al.* 2022; Wu *et al.* 2021). Applying machine learning algorithms to coal methane adsorption experiments enables training models with large datasets to predict methane adsorption in coal(Meng *et al.* 2020). By processing massive amounts of data, these algorithms have greatly improved prediction accuracy and operational efficiency while reducing the need for manual intervention. Among these algorithms, the most commonly used one is neural network, which is a computational model that simulates the behavior of human brain neurons. In the human brain, there are billions of cells called neurons, which are interconnected to form a neural network. Serving as the elementary part of the neural network, the neuron is used to receive, process and transmit information. This is similar to the principle of the neural network computing model, and the neuron model is a model that contains input, output and computing functions. A classic neural network structure and schematic diagram are depicted in Fig.4. The deep learning algorithm based on neural networks is characterized by its use of deep networks, including DNN, Convolutional Neural Networks (CNN), and RNN(Alzahrani *et al.* 2024; Raschka & Mirjalili 2019).

Table 2 presents the principles, characteristics, and applications of these three models.

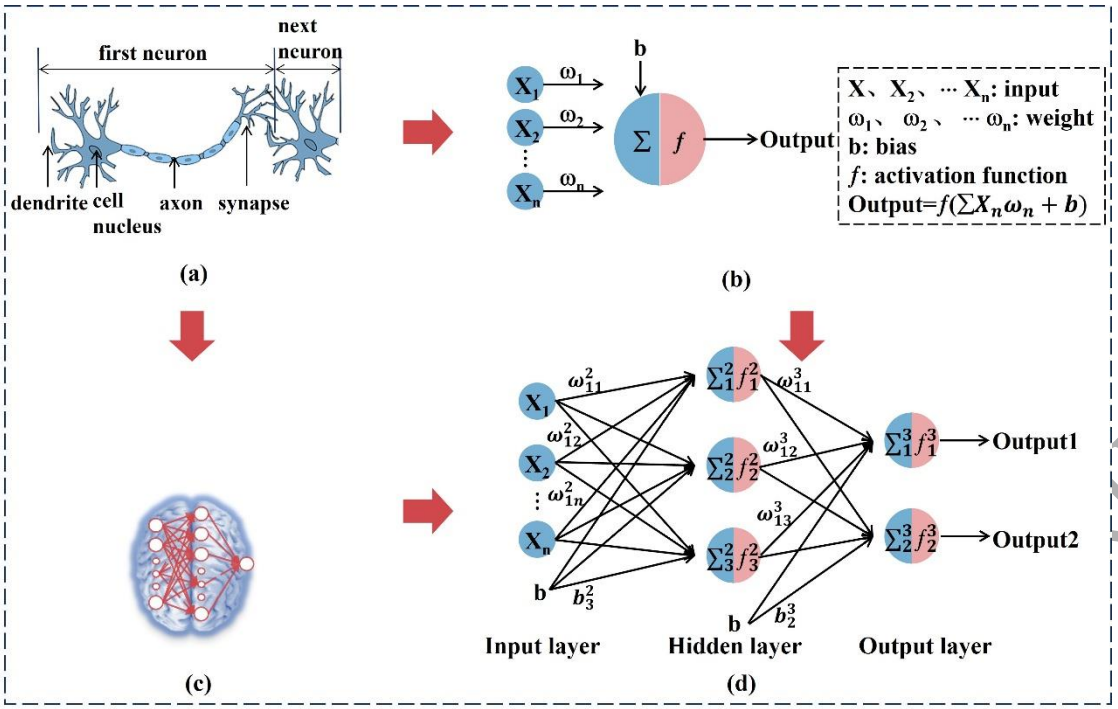
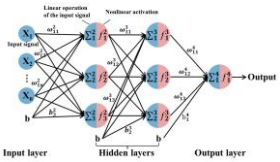
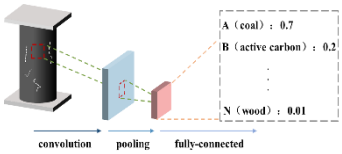
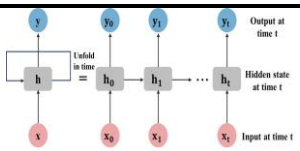


Figure 4 Neuron and neural network structure:(a) Biological neuron structure(Jin 2007). (b) Artificial neuron structure(Zhou F Y *et al.* 2017). (d) Neural network model(Marcus & Papaemmanouil 2019).

Table 2 Principles, characteristics and applications of typical deep learning models

Neural network	DNN	CNN	RNN
Rationale	The network structure contains three layers with multiple hidden segments. Input data flows successively through the initial layer, undergoes processing in intermediate layers, then terminates at the final layer. All layers integrate adjustable synaptic weights and activate nonlinear functions for computing predictions.	The core of this approach lies in the recognition of patterns, which encompasses three fundamental layers. Convolutional layer: to preserve the features of the picture information; Pooling layer: data dimensionality reduction to avoid overfitting; Fully connected layer: performs classification or regression tasks to yield specific results.	Networks handling time-series data incorporate feedback connections, where computational units use prior step's signals to generate current outputs, preserving historical state awareness.
Characteristics	**Advantages**: The model exhibits robust nonlinear fitting capabilities, demonstrates strong feature extraction abilities, showcases high latitude data processing capabilities, and possesses fault tolerance. **Disadvantages**: The model lacks the ability to explain functional meanings and network operation characteristics; Additionally, it imposes stringent requirements on data quality and necessitates complex hyperparameter settings.	**Advantages**: Pioneering in the field of image recognition, this approach enables direct utilization of images as input, eliminating the need for feature extraction and data reconstruction processes; The utilization of shared weights reduces training parameters, simplifies the structure, and enhances adaptability. **Disadvantages**: This method requires significant computational resources and is constrained by fixed input image sizes, thereby limiting its applicability in embedded device scenarios.	**Advantages**: Proficient in processing time series data, exhibiting a robust capability to extract temporal features; Demonstrating versatility across various application scenarios; Exhibiting commendable predictive performance. **Disadvantages**: Encountering high training complexity; Facing challenges such as gradient vanishing and exploding, leading to ineffective retention of long-term historical information; The computational process exhibits strong interdependence and poses difficulties for parallelization.
Application scenarios	Medical diagnostics, artificial intelligence, natural language processing, stocks and weather forecasting.	Image retrieval and classification, target location detection and segmentation, face recognition and object detection.	Text generation, speech recognition, machine translation, generating image descriptions and video marker.

Schematic diagram			
	Figure 5 Schematic diagram of the DNN model(Marcus & Papaemmanouil 2019)	Figure 6 Schematic diagram of the basic architecture of the CNN model (Raj & Kos 2025)	Figure 7 Architecture of RNN (left) and architecture of RNN unfolded in time (right) (Chemali *et al.* 2018)

Quantitative analysis of the impact of multiple factors on adsorption falls within the realm of traditional multiple-parameter regression methods. However, these conventional approaches require prior assumptions about the functional forms of independent and non-independent variables, which can lead to erroneous or misleading outcomes if the functional forms are not appropriately matched. In contrast, ML models offer a novel approach to multivariate parametric regression in this context(Xie *et al.* 2023). By leveraging sufficient data, ML-based models can incorporate all relevant variables, thereby addressing the limitations inherent in traditional adsorption models that are restricted to specific temperatures, hypothetical conditions, and coal ranks while also avoiding the complexities associated with experimental procedures. The basic idea of utilizing ML techniques to predict methane adsorption capacity is illustrated in Fig.8. Firstly, a suitable model should be established for the nonlinear regression problem. Then, the input data should consist of basic physical parameters of coal, pore structure characteristics, and other experimental parameters. The output data should be the methane limit adsorption amount (V_L). By training the model to achieve a good fitting effect, accurate prediction of V_L can be achieved. Additionally, although V_L can also be measured experimentally, this paper focuses on predicting gas adsorption capacity using ML methods due to limitations associated with experimental approaches.

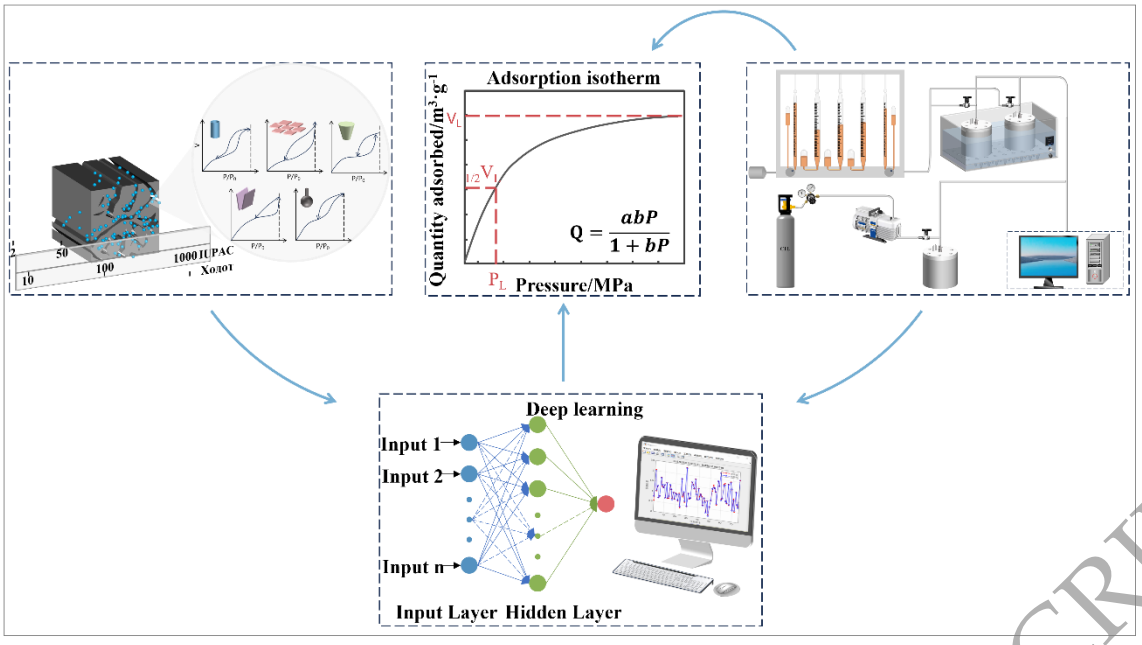


Figure 8 Flowchart of predicting gas adsorption capacity based on ML methods

Based on 139 sets of experimental data, Feng *et al.* (2014) proposed to utilize the Alternating Conditional Expectation (ACE) algorithm to predict V_L. The independent variables considered in this model include proximate analysis, maceral composition, $R_{0,max}$, and temperature of coal. The resulting correlation coefficient reached 0.91, demonstrating the robustness of the model. Cao *et al.* (2015); (Liu & Li 2018)utilized BP neural network to achieve prediction of coal and gas outburst, and combined principal component analysis to optimize the dimensions of influencing factors, reduce the correlation between variables, select main control factors, improve the prediction efficiency of the entire model, and the prediction accuracy of the optimized model is also high. To address the limitations of the Langmuir correlation model, which is restricted to temperature and coal rank, Meng *et al.* (2019)proposed an innovative adsorption model based on an ANN, demonstrating its remarkable efficacy in predicting coal adsorption characteristics. Zhang *et al.* (2019)proposed the utilization of a DNN for accurately predicting CO_2 adsorption, and their findings demonstrated excellent agreement between the predicted and actual CO_2 limit adsorption values. Zhang J Y *et al.* (2020) proposed an ensemble ML method, specifically a Gradient-Boosted BP (GBDT), for accurate

estimation of methane adsorption isotherms based on coal properties in the Qinshui Basin of China. The GBDT algorithm underwent performance benchmarking against two prevalent predictive models: ANN and SVM. The results confirmed the superior accuracy and robustness of GBDT. Subsequently, Palle *et al.* (2022) achieved similar results using a comparable approach, further validating the reliability of deep learning in gas adsorption prediction. Gao F *et al.* (2023)developed a Back-Propagation (BP) neural network-based multifactorial model for predicting CO_2 adsorption. The results demonstrated that both the training and test sets achieved a coefficient of determination greater than 0.98, meeting the required prediction accuracy. Subsequently, the RF method was employed to simplify the input variables of the model, resulting in an optimized fit with improved performance compared to the original multifactorial model. It merits emphasis that the study was restricted to predicting V_L values, leaving Langmuir pressure (P_L) determination—a critical parameter controlling adsorption isotherm curvature—unaddressed. Therefore, the proposed model's predictive capability is confined exclusively to maximal uptake quantity estimation rather than comprehensively predicting adsorption isotherms. The difficulty in accurately estimating P_L may arise from its uncertain correlation with coal properties. For example, Busch *et al.* (2019) in their study involving approximately 1000 samples, observed a highly scattered pattern between P_L and $R_{0,max}$. However, Chen (2020) analyzed 89 coal samples from the Qianxi region, demonstrating a fluctuating trend of P_L with increasing coal deterioration degree. In contrast, A summary of the models mentioned in this text can be found in Table 3 for comparative purposes.

Transfer learning (TL) is the revolutionary method of supervised learning (SL). TL can greatly reduce the cost of data annotations, and construct accurate structure-activity relationships, which can achieve great prospects in molecular and materials.TL has shown remarkable potential in addressing data scarcity and domain shift challenges in material science(Zhang *et al.* 2022; Chen *et al.* 2024). Li *et al.* (2020)proposed a

GAN model using semi-supervised learning, which achieved remarkable results based on logging curves. However, this method is only specialized in identifying shale and sandstone, leading to limited practicality. Theoretically, TL can leverage knowledge from large datasets of similar porous materials (e.g., shale, activated carbon) or simulated molecular dynamics data to improve prediction accuracy under limited coal-specific training samples. However, current applications of TL in coal adsorption remain limited, and future research should focus on cross-domain knowledge transfer between different coal ranks and geological conditions.

The basic idea of reinforcement learning (RL) is that the Agent adjusts its strategies continuously based on rewards from environmental feedback during interaction with the environment to achieve optimal decision-making, which is primarily used to solve decision optimization problems(Ma *et al.* 2018). Currently, the application of reinforcement learning in the field of coalbed methane remains in the exploratory stage, with relatively few direct studies, but it has shown potential application prospects. Gao X Y *et al.* (2023)introduced an algorithm based on Q-learning to solve the CBM well maintenance tasks scheduling. Future research could focus on combining physical models with RL to construct more efficient hybrid intelligent systems.

Although scholars have been active in the field of gas adsorption prediction for coal, and existing literature has demonstrated the feasibility of this approach through well-fitted data, there is still a lack of research on gas adsorption prediction models for coal. By utilizing ML techniques and analyzing a large amount of historical literature and experimental data, we can propose new adsorption models to predict CH_4 adsorption capacity in coal.

Table 3 Overview of intelligent predictive models and their applications

Model	Model characteristic	Data Requirements	Parameter variable	Evaluation indicators and accuracy	Feature Processing Capability	Application	Ref
ACE algorithm	The magnitude of individual predictors' impacts on the target metric is quantifiable through numerical analysis	Low(139 samples)	**Input**: ash, fixed carbon, moisture, vitrinite content, $R_{0,max}$, temperature; Output: V_L	coefficient of determination (**R^2**)=0.91	Only handles monotonic relationships	Single-parameter prediction (V_L)	(Feng *et al.* 2014)
ANN	Contains three processing units (input, hidden, and output layers) with highly nonlinear global roles	Medium	**Input**: pressure, porosity, $R_{0,max}$, chitinite, vitrinite, hydrogen, inertinite; **Optimized**: porosity, $R_{0,max}$; **Output**: Excess adsorption of CO_2	Pre optimization: **R^2**=0.9694 After optimization: **R^2**=0.9977	Automatic dimensionality reduction	Multi-level coal types	(Meng *et al.* 2019)
DNN	An ANN with multiple hidden layers	High (＞100 samples)	**Input**: BET specific surface area, micropore and mesopore volume; **Output**: CO_2 adsorption capacity	**Average error**:0.43	Automatic learning of nonlinear relationships	High-precision adsorption prediction for porous materials	(Zhang *et al.* 2019)
GBDT	GBDT is an ensemble method that combines multiple basic estimators (decision trees) with a gradient boosting algorithm	Medium (1320 samples)	**Input:** coal properties (ash, fixed carbon, moisture, vitrinite, $R_{0,max}$) and experimental conditions (pressure,	Average absolute error(**MAE**)=0.53; Mean relative error (**MRE**)=3.85; Root mean square	Automatic collinearity handling	Prediction of adsorption isotherms for complex coal qualities	(Zhang J Y *et al.* 2020)

	to improve the robustness of a single estimator.		equilibrium moisture, temperature); **Output:** V_L	error(**RMSE**)=0.73; $\mathbf{R^2}$=0.977			
BP-ANN	Neural parameters are iteratively refined via error backpropagation to optimize network performance through gradient-based loss reduction	Medium		**MAE**=0.61; **MRE**=4.44 **RMSE**=1.06; $\mathbf{R^2}$=0.952	Manual feature selection required	Rapid modeling for small-scale datasets	
SVM	Converting a nonlinear regression problem in real space to a linear approximation in high-dimensional feature space by minimizing a regularized loss function	Low (effective for small samples)		**MAE**=0.84; **MRE**=6.74 **RMSE**=1.19; $\mathbf{R^2}$=0.94	Sensitive to feature scaling	Small-sample high-dimensional data	
BP	This methodology effectively analyzes diverse structural attributes, multifaceted influencing variables, and nonlinear interdependencies	Low (126 samples)	**Input**: pore specific surface area, volume, average pore size, mineral content, moisture; **Optimized**: moisture, specific surface area, porosity; **Output**: CO_2 saturation adsorption capacity	$\mathbf{R^2}$=0.983; **RMSE**=0.055; **MAE**=0.045 After optimization: $\mathbf{R^2}$=0.988; **RMSE**=0.04; **MAE**=0.029	Dependent on feature engineering (normalization required)	Multi-factor coupling prediction under limited data	(Gao F *et al.* 2023)

4. Conclusions

In conclusion, given China's strategic commitment to actively promote the advancement of clean energy and intelligent mining infrastructure, there is an urgent need for precise quantification of gas adsorption capacity. Although the current experimental techniques and theoretical models can partially characterize the gas adsorption capacity, whether it is through indirect or direct methods of experimentation, or through continuous optimization and innovation of theoretical models, there are still certain limitations when measuring the gas adsorption capacity of coal. The main limitations lie in two aspects: ⅰ) Cumbersome experimental processes and long experimentation periods. ⅱ) Single or integrated models are constrained by specific influencing factors, such as coal grade and temperature. However, the multitude and complexity of factors affecting gas adsorption cannot be captured by a simple relationship. Traditional methods face significant challenges in establishing a unified adsorption model that transcends the limitations imposed by various factors (pressure, temperature, coal type).

Considering the aforementioned issues, the development of an efficient intelligent prediction model emerges as a crucial research direction for investigating gas adsorption characteristics in the future. Intelligent prediction can avoid the defects of experimental measurement and break through the limitations of traditional fitting models. By inputting multiple factors affecting coal adsorption characteristics, gas adsorption capacity can be quantitatively predicted, and the model can be continuously optimized to achieve prediction effect. However, research on ML methods for predicting gas adsorption in coal seams remains limited up to now. Therefore, it is necessary to further explore the use of ML for predicting gas adsorption in coal seams as it has practical value in improving prediction accuracy, reducing experimental costs, accelerating research progress, and aiding decision-

making processes. The main research focus can be summarized as follows:

(i) The basis of intelligent prediction is data. To achieve exceptional prediction results, it is imperative to rely on robust historical experimental data. In the future, there is a pressing need for establishing an extensive database encompassing gas adsorption characteristics, which needs to cover internal factors such as coal type, pore size and composition, as well as environmental factors such as pressure, stress, temperature, particle size and moisture.

(ii) The key of intelligent prediction is algorithm. However, the current intelligent algorithms are predominantly based on data sets with minimal variations in data structure, resulting in static indicator values. This limitation hinders the practical application of intelligent algorithms. For the field application, in addition to the influence of static factors such as coal type and gas content, the gas content is also affected by dynamic characteristics such as dynamic stress and crushing degree. Consequently, the collected data is likely to comprise a combination of dynamic and static information with time series attributes. Therefore, it is imperative to develop an intelligent algorithm that is multimodal, capable of handling large volumes of data across multiple time periods.

(iii) The purpose of intelligent prediction is application. Currently, the intelligent prediction of gas adsorption characteristics in coal is still at the laboratory stage, and obtaining input parameters for field applications remains challenging. In the future, it is essential to comprehensively compare the effectiveness of intelligent prediction algorithms under different working conditions and identify algorithms that meet engineering timeliness and hardware requirements to truly support field gas content prediction.

Acknowledgements

This research was supported by the National Natural Science Foundation of China (grant nos. 52374250, 52130409, 52121003), the Fundamental Research Funds for the Central Universities (grant no. 2025ZKPYAQ02), and Innovation and entrepreneurship training program for college students (grant no. 202412027). Comments from all anonymous reviewers are highly appreciated.

Conflict of interest statement

None declared.

Data availability

The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

References

Abdulsalam J,Mulopo J,Bada SO,Oboirien B. 2020. Equilibria and Isosteric Heat of Adsorption of Methane on Activated Carbons Derived from South African Coal Discards. *ACS omega,* **5:** 32530-9.http://dx.doi.org/10.1021/acsomega.0c04744.

Alzahrani MK,Shapoval A,Chen ZX,Rahman SS. 2024. MicroGraphNets: Automated characterization of the micro-scale wettability of porous media using graph neural networks. *Capillarity,* **12:** 57-71.http://dx.doi.org/10.46690/capi.2024.09.01.

An FH,Yuan Y,Chen XJ. 2019. A new method for gas content determination based on gas desorption r atio. *Safety in Coal Mines,* **50:** 34-7.http://dx.doi.org/10.13347/j.cnki.mkaq.2019.09.010.(in Chine se)

Brunauer S,Emmett PH,Teller E. 1938. Adsorption of Gases in Multimolecular Layers. *Journal of the American Chemical Society,* **60:** 309-19.http://dx.doi.org/10.1021/ja01269a023.

Busch A,Gensterblum Y. 2011. CBM and CO2-ECBM related sorption processes in coal: A review. *Int ernational Journal of Coal Geology,* **87:** 49-71.http://dx.doi.org/10.1016/j.coal.2011.04.011.

Busch A,Gensterblum Y,Krooss BM. 2003. Methane and CO2 sorption and desorption measurements on dry Argonne premium coals: pure components and mixtures. *International Journal of Coal Ge ology,* **55:** 205-24.http://dx.doi.org/10.1016/S0166-5162(03)00113-7.

Busch A,Han F,Magill CR. 2019. Paleofloral dependence of coal methane sorption capacity. *Internatio nal Journal of Coal Geology,* **211:** 103232.http://dx.doi.org/10.1016/j.coal.2019.103232.

Cai Y,Liu D,Pan Z,Yao Y,Li J,Qiu Y. 2013. Pore structure and its impact on CH4 adsorption capacity a nd flow capability of bituminous and subbituminous coals from Northeast China. *Fuel,* **103:** 258-6 8.http://dx.doi.org/10.1016/j.fuel.2012.06.055.

Cao B,Bai G,Li H. 2015. Prediction of gas content based on PCA-GA-BP neural network. *Prediction o f gas content based on PCA-GA-BP neural network,* **11:** 84-90. (in Chinese)

Chalmers GR,Bustin RM. 2007. On the effects of petrographic composition on coalbed methane sorpti on. *International Journal of Coal Geology,* **69:** 288-304.http://dx.doi.org/10.1016/j.coal.2006.06.0 02.

Chang Y,Yang D,He X. 2024. A deep learning operator-based numerical scheme method for solving 1 D wave equations. *Journal of Geophysics and Engineering,* **21:** 1194-215.http://dx.doi.org/10.109

3/jge/gxae062.

Charoensuppanimit P,Mohammad SA,Robinson RL,Gasem KAM. 2015. Modeling the temperature dependence of supercritical gas adsorption on activated carbons, coals and shales. *International Journal of Coal Geology,* **138:** 113-26.http://dx.doi.org/10.1016/j.coal.2014.12.008.

Chattaraj S,Mohanty D,Kumar T,Halder G,Mishra K. 2019. Comparative study on sorption characteristics of coal seams from Barakar and Raniganj formations of Damodar Valley Basin, India. *International Journal of Coal Geology,* **212:** 103202.http://dx.doi.org/10.1016/j.coal.2019.05.009.

Chemali E,Kollmeyer PJ,Preindl M,Ahmed R,Emadi A. 2018. Long Short-Term Memory Networks for Accurate State-of-Charge Estimation of Li-ion Batteries. *IEEE Transactions on Industrial Electronics,* **65:** 6730-9.http://dx.doi.org/10.1109/TIE.2017.2787586.

Chen A, Wang Z, Vidaurre KLL, Han Y, Ye S, Tao K, Wang S, Gao J, et al. 2024. Knowledge-reuse transfer learning methods in molecular and material science. *arXiv preprint arXiv:2403.12982,* **11:** 2304138.http://dx.doi.org/10.48550/arXiv.2403.12982.

Chen B,Qiao W,Yan WX,Xiang YB. 2019. Research progress on determination method of coal seam gas content in coal mine. *Mining Safety & Environmental Protection,* **46:** 98-103. (in Chinese)

Chen B,Yan WX,Sun BX,Liu H. 2021. Study on the mapping law of adsorption,porosity and deformation of gas bearing coal. *Safety in Coal Mines,* **52:** 25-9.http://dx.doi.org/10.13347/j.cnki.mkaq.2021.01.006. (in Chinese)

Chen SD. 2020. Permeable-storage mechanism and the development technical countermeasures for coalbed methane in multi-seams in western Guizhou. *Ph.D.*, *China University of Geosciences (Beijing)*.http://dx.doi.org/10.27493/d.cnki.gzdzy.2020.000067. (in Chinese)

Chen Y,Liu D,Yao Y,Cai Y,Chen L. 2015. Dynamic permeability change during coalbed methane prod

uction and its controlling factors. *Journal of Natural Gas Science and Engineering,* **25:** 335-46.http://dx.doi.org/10.1016/j.jngse.2015.05.018.

Cheng Y,Jiang H,Zhang X,Cui J,Song C,Li X. 2017. Effects of coal rank on physicochemical properties of coal and on methane adsorption. *International Journal of Coal Science & Technology,* **4:** 129-46.http://dx.doi.org/10.1007/s40789-017-0161-6.

China Statistical Yearbook https://www.stats.gov.cn/sj/ndsj/2024/indexch.htm. (in Chinese)

Clarkson CR,Bustin RM. 2000. Binary gas adsorption/desorption isotherms: effect of moisture and coal composition upon carbon dioxide selectivity over methane. *International Journal of Coal Geology,* **42:** 241-71.http://dx.doi.org/10.1016/S0166-5162(99)00032-4.

Dai L,Lei H,Cheng X,Li R. 2023. Prediction of coal seam gas content based on the correlation between gas basic parameters and coal quality indexes. *Frontiers in Energy Research,* **10**.http://dx.doi.org/10.3389/fenrg.2022.1096539.

Dong Y-t,Ju BS,Liu NN. 2020. Evaluation and improvement of high-pressure isothermal adsorption model for methane in shale. *Journal of China Coal Society,* **45:** 3208-18.http://dx.doi.org/10.13225/j.cnki.jccs.2019.0806. (in Chinese)

Dubinin M,Astakhov V. 1971. Description of adsorption equilibria of vapors on zeolites over wide ranges of temperature and pressure, **102:** 69-85, ACS Publications.http://dx.doi.org/10.1021/ba-1971-0102.ch044.

Dubinin MM. 1960. The Potential Theory of Adsorption of Gases and Vapors for Adsorbents with Energetically Nonuniform Surfaces. *Chemical Reviews,* **60:** 235-41.http://dx.doi.org/10.1021/cr60204a006.

Dutta P,Bhowmik S,Das S. 2011. Methane and carbon dioxide sorption on a set of coals from India. *In*

ternational Journal of Coal Geology, **85:** 289-99.http://dx.doi.org/10.1016/j.coal.2010.12.004.

Faiz M,Saghafi A,Sherwood N,Wang I. 2007. The influence of petrological properties and burial history on coal seam methane reservoir characterisation, Sydney Basin, Australia. *International Journal of Coal Geology,* **70:** 193-208.http://dx.doi.org/10.1016/j.coal.2006.02.012.

Feng Q,Zhang J,Zhang X,Shu C,Wen S,Wang S,Li J. 2014. The use of alternating conditional expectation to predict methane sorption capacity on coal. *International Journal of Coal Geology,* **121:** 137-47.http://dx.doi.org/10.1016/j.coal.2013.11.011.

Freundlich H. 1907. Über die adsorption in lösungen. *Zeitschrift für physikalische Chemie,* **57:** 385-470.http://dx.doi.org/10.1515/pch-1907-5723.

Gao F,Wang P,Wang D,Yang Y,Zhang X,Bai G. 2023. Model for Predicting CO2 Adsorption in Coal Left in Goaf Based on Backpropagation Neural Network. *Energies,* **16:** 3760.http://dx.doi.org/10.1007/s40789-017-0161-6.

Gao XY,Diao P,Kui GF,Pan J,Zuo X,Li FF. 2023. Reinforcement learning based optimization algorithm for maintenance tasks scheduling in coalbed methane gas field. *Computers & Chemical Engineering,* **170:** 108131.http://dx.doi.org/10.1016/j.compchemeng.2022.108131.

Guo B,Chang L,Xie K. 2006. Adsorption of Carbon Dioxide on Activated Carbon. *Journal of Natural Gas Chemistry,* **15:** 223-9.http://dx.doi.org/10.1016/S1003-9953(06)60030-3.

Guo W,Liu J,Dong F,Chen R,Das J,Ge W,Xu X,Hong H. 2022. Deep Learning Models for Predicting Gas Adsorption Capacity of Nanomaterials. *Nanomaterials,* **12:** 3376.http://dx.doi.org/10.3390/nano12193376.

Gürdal G,Yalçın MN. 2000. Gas adsorption capacity of Carboniferous coals in the Zonguldak basin (NW Turkey) and its controlling factors. *Fuel,* **79:** 1913-24.http://dx.doi.org/10.1016/S0016-2361(0

0)00050-8.

Han WC,Li AF,Fang Q,Memon A. 2020. Comparative analysis of isothermal adsorption models for co als with water content under supercritical conditions. *Journal of China Coal Society,* **45:** 4095-10 3.http://dx.doi.org/10.13225/j.cnki.jccs.2020.0292. (in Chinese)

Hao S,Chu W,Jiang Q,Yu X. 2014. Methane adsorption characteristics on coal surface above critical te mperature through Dubinin–Astakhov model and Langmuir model. *Colloids and Surfaces A: Phys icochemical and Engineering Aspects,* **444:** 104-13.http://dx.doi.org/10.1016/j.colsurfa.2013.12.0 47.

Huang RT. 2020. The influence of coal pore structure on adsorption and desorption characteristics of P ingdingshan No.10 coal mine. *Master*, *China University of Mining and Technology*.http://dx.doi.o rg/10.27623/d.cnki.gzkyu.2020.001346. (in Chinese)

Jiao J-h,Wang Y-j,Li H. 2023. Application research on fixed-point sampling of negative pressure slag discharge for coal seam gas content determination. *Coal and Chemical Industry,* **46:** 95-100.http:// dx.doi.org/10.19286/j.cnki.cci.2023.08.024.

Jin Y. 2007. Research on Adaptive Single-Neuron Intelligent Control Strategy and Its Application in V ehicle Active Suspension Systems. *ph.D.*, *Hunan University*. (in Chinese)

Kang J,Elsworth D,Fu X,Liang S,Chen H. 2022. Contribution of thermal expansion on gas adsorption to coal sorption-induced swelling. *Chemical Engineering Journal,* **432:** 134427.http://dx.doi.org/1 0.1016/j.cej.2021.134427.

Kim D,Seo Y,Kim J,Han J,Lee Y. 2019. Experimental and Simulation Studies on Adsorption and Diffu sion Characteristics of Coalbed Methane. *Energies,* **12:** 3445.http://dx.doi.org/10.3390/en1218344 5.

Kołodziejek J,Główka E,Hyla K,Voelkel A,Lulek J,Milczewska K. 2013. Relationship between surface properties determined by inverse gas chromatography and ibuprofen release from hybrid materials based on fumed silica. *International Journal of Pharmaceutics,* **441:** 441-8.http://dx.doi.org/10.1016/j.ijpharm.2012.11.010.

Langmuir I. 1916. The constitution and fundamental properties of solids and liquids. Part I. Solids. *Journal of the American Chemical Society,* **38:** 2221-95.

Laxminarayana C,Crosdale PJ. 2002. Controls on Methane Sorption Capacity of Indian Coals. *AAPG Bulletin,* **86:** 201-12.http://dx.doi.org/10.1306/61eeda8a-173e-11d7-8645000102c1865d.

Levy JH,Day SJ,Killingley JS. 1997. Methane capacities of Bowen Basin coals related to coal properties. *Fuel,* **76:** 813-9.http://dx.doi.org/10.1016/s0016-2361(97)00078-1.

Li F,Jiang B,Song Y,Cheng G,Lu G. 2021. Multifractal Behavior of the Micro- and Mesopore Structures of Brittle Tectonically Deformed Coals and Its Influence on Methane Adsorption Capacity. *Energy & Fuels,* **35:** 3042-64.http://dx.doi.org/10.1021/acs.energyfuels.0c03526.

Li G,Hao D,Wang Z,Zheng C,Huang J,Sun D. 2024. Effects of drilling parameters on stress relief performance during mining. *Journal of Geophysics and Engineering,* **21:** 1392-400.http://dx.doi.org/10.1093/jge/gxae083.

Li M,Gu AZ,Ru XS,Wang RS. 2003. Study on methane adsorption above critical temperature by adsorption potential theory. *Natural Gas Chemical Industry,* **05:** 28-31. (in Chinese)

Li XC,Nie BS. 2006. Study of water adsorption properties of coal. *Journal of Taiyuan University of Technology*: 417-9.http://dx.doi.org/10.16355/j.cnki.issn1007-9432tyut.2006.04.011. (in Chinese)

Li Z-t,Yao Y-b,Zhou H-p,Bai X-h. 2012. Study on Coal and Rock Maceral Composition Affected to Methane Adsorption Capacity. *Coal Science and Technology,* **40:** 125-8.http://dx.doi.org/10.13199/j.c

st.2012.08.128.lizht.003. (in Chinese)

Li Z,Kang Y,Feng D,Wang X-M,Lv W,Chang J,Zheng WX. 2020. Semi-supervised learning for litholo gy identification using Laplacian support vector machine. *Journal of Petroleum Science and Engi neering,* **195:** 107510.http://dx.doi.org/10.1016/j.petrol.2020.107510.

Li Z,Ren T,Li X,Cheng Y,He X,Lin J,Qiao M,Yang X. 2023. Full-scale pore structure characterization of different rank coals and its impact on gas adsorption capacity: A theoretical model and experim ental study. *Energy,* **277:** 127621.http://dx.doi.org/10.1016/j.energy.2023.127621.

Liu G. 2022. Influence of Pore Structure Characteristics of Primary Coal on Coalbed Methane Adsorpt ion. *Advances in Materials Science and Engineering,* **2022:** 3087252.http://dx.doi.org/10.1155/20 22/3087252.

Liu HH,Fan ZP,Xu HJ,Liu JL,Li NN. 2023. Recognition of adsorption phase density,adsorption model, and adsorption mechanism of CH4 in coal. *Journal of China Coal Society,* **48:** 3806-17.http://dx.d oi.org/10.13225/j.cnki.jccs.sq23.0466. (in Chinese)

Liu XY,Li PY. 2018. Soft measurement modeling of coal and gas outburst based on PCA and IFOA-B P. *Mining Research and Development,* **38:** 109-15.http://dx.doi.org/10.13827/j.cnki.kyyk.2018.04. 024.

Ma C-q,Xie W,Sun W-j. 2018. Research on Reinforcement Learning Technology: A Review. *Comman d Control & Simulation,* **40:** 68-72.http://dx.doi.org/10.3969/i.issn.1673-3819.2018.06.015.

Marcus R,Papaemmanouil O. 2019. Plan-structured deep neural network models for query performanc e prediction. *arXiv preprint arXiv:1902.00132,* **15**.http://dx.doi.org/10.48550/arXiv.1902.00132.

Mashhadimoslem H,Ghaemi A. 2023. Machine learning analysis and prediction of N2, N2O, and O2 a dsorption on activated carbon and carbon molecular sieve. *Environmental Science and Pollution R*

esearch, **30:** 4166-86.http://dx.doi.org/10.1007/s11356-022-22508-9.

Mastalerz M,Drobniak A,Rupp J. 2008. Meso- and Micropore Characteristics of Coal Lithotypes: Implications for CO2 Adsorption. *Energy & Fuels,* **22:** 4049-61.http://dx.doi.org/10.1021/ef800544g.

Meng M,Qiu Z,Zhong R,Liu Z,Liu Y,Chen P. 2019. Adsorption characteristics of supercritical CO2/CH4 on different types of coal and a machine learning approach. *Chemical Engineering Journal,* **368:** 847-64.http://dx.doi.org/10.1016/j.cej.2019.03.008.

Meng M,Zhong R,Wei Z. 2020. Prediction of methane adsorption in shale: Classical models and machine learning based models. *Fuel,* **278:** 118358.http://dx.doi.org/10.1016/j.fuel.2020.118358.

Miao ZK,Dong L,Wang Z. 2017. Study on Adsorption Behavior of Coalbed Methane at Different Depths under Variable Temperature and Pressure Conditions. *COAL QUALITY TECHNOLOGY,* **03:** 25-8. (in Chinese)

Mirzaei S,Ahmadpour A,Shahsavand A,Rashidi H,Arami-Niya A. 2020. Comparative Study between Regression and Soft Computing Models to Maximize the Methane Storage Capacity of Anthracite-Based Adsorbents. *Industrial & Engineering Chemistry Research,* **59:** 1875-87.http://dx.doi.org/10.1021/acs.iecr.9b04943.

Nie BS,Yang T,Li XC,Li L,Lu HQ. 2013. Research on diffusion of methane in coal particles. *Journal of China University of Mining & Technology,* **42:** 975-81.http://dx.doi.org/10.13247/j.cnki.jcumt.2013.06.015. (in Chinese)

Pajdak A,Kudasik M,Skoczylas N,Wierzbicki M,Teixeira Palla Braga L. 2019. Studies on the competitive sorption of CO2 and CH4 on hard coal. *International Journal of Greenhouse Gas Control,* **90:** 102789.http://dx.doi.org/10.1016/j.ijggc.2019.102789.

Palle K,Vunguturi S,Gayatri SN,Rao KS,Babu PR,Vijay R. 2022. The prediction of CO2 adsorption on

rice husk activated carbons via deep learning neural network. *MRS Communications,* **12:** 434-40. http://dx.doi.org/10.1557/s43579-022-00197-2.

Perera MSA,Ranjith P,Choi S,Airey D,Weniger P. 2012. Estimation of gas adsorption capacity in coal: a review and an analytical study. *International Journal of Coal Preparation and Utilization,* **32:** 25-55.http://dx.doi.org/10.1080/19392699.2011.614298.

Polanyi M. 1916. Adsorption von Gasen (Dampfen) durch ein festes nichtfluchtiges Adsorbens. *Verhandlungen der Deutschen Physekalischen Gesellschaft,* **18:** 55-80.

Prinz D,Littke R. 2005. Development of the micro-and ultramicroporous structure of coals with rank as deduced from the accessibility to water. *Fuel,* **84:** 1645-52.http://dx.doi.org/10.1016/j.fuel.2005.01.010.

Raj R,Kos A. 2025. An Extensive Study of Convolutional Neural Networks: Applications in Computer Vision for Improved Robotics Perceptions. *Sensors,* **25:** 1033.http://dx.doi.org/10.3390/s25041033.

Raschka S,Mirjalili V. 2019. *Python machine learning: Machine learning and deep learning with Python, scikit-learn, and TensorFlow 2*, Packt publishing ltd.

Sang SX, Huang FS, Y.S.Shan, X.Q.Zhou, S.Q.Liu, S.J.Han, S.J.Zheng, Liu T, et al. 2024. Technology processes of enhancement of broken soft and low permeability coal reservoir and surface development of coalbed methane. *Coal Science and Technology,* **52:** 196-210. (in Chinese)

Sang SX,Zhu YM,Zhang J,Zhang XD,Tang JX. 2005. Solid-gas interaction mechanism of coal-adsorbed gas (II)-physical process and theoretical model of coal-adsored gas. *Natural Gas Industry,* **01:** 16-18+21-205. (in Chinese)

Sarker IH. 2021. Machine learning: Algorithms, real-world applications and research directions. *SN co*

mputer science, **2:** 160.http://dx.doi.org/10.1007/s42979-021-00592-x.

Sheng M,Li G-s,Chen L-q,Shao S-q,Zhang R. 2014. Mechanisms analysis of shale-gas supercritical ad sorption and modeling of isorption adsorption. *Journal of China Coal Society,* **39:** 179-83.http://dx.doi.org/10.13225/j.cnki.jccs.2013.0474. (in Chinese)

Skrobek D,Krzywanski J,Sosnowski M,Kulakowska A,Zylka A,Grabowska K,Ciesielska K,Nowak W. 2020. Prediction of Sorption Processes Using the Deep Learning Methods (Long Short-Term Me mory). *Energies,* **13:** 6601.http://dx.doi.org/10.3390/en13246601.

Skrobek D,Krzywanski J,Sosnowski M,Kulakowska A,Zylka A,Grabowska K,Ciesielska K,Nowak W. 2022. Implementation of deep learning methods in prediction of adsorption processes. *Advances i n Engineering Software,* **173:** 103190.http://dx.doi.org/10.1016/j.advengsoft.2022.103190.

Song X,Lü X,Shen Y,Guo S,Guan Y. 2018. A modified supercritical Dubinin–Radushkevich model for the accurate estimation of high pressure methane adsorption on shales. *International Journal of C oal Geology,* **193:** 1-15.http://dx.doi.org/10.1016/j.coal.2018.04.008.

Sun J,Wei Q,Yan B,Xiao X-m. 2018. Full desorption process of coal bed adsorbed gas and changes of components and carbon isotopes:Results based on thermal simulation experiments. *Journal of Chi na Coal Society,* **43:** 2848-56.http://dx.doi.org/10.13225/j.cnki.jccs.2018.0198. (in Chinese)

Tagliabue M,Farrusseng D,Valencia S,Aguado S,Ravon U,Rizzo C,Corma A,Mirodatos C. 2009. Natu ral gas treating by selective adsorption: Material science and chemical engineering interplay. *Che mical Engineering Journal,* **155:** 553-66.http://dx.doi.org/10.1016/j.cej.2009.09.010.

Vigdorowitsch M,Pchelintsev A,Tsygankova L,Tanygina E. 2021. Freundlich Isotherm: An Adsorption Model Complete Framework. *Applied Sciences,* **11:** 8078.http://dx.doi.org/10.3390/app11178078.

Wang,Zhou D,X.J.Feng,M.L.Wang,Feng ZZ. 2023. Study of non-uniform potential well distribution o

f coal and its effect on methane adsorption/desorption. *Journal of China Coal Society* **48:** 3818-30. http://dx.doi.org/10.13225/j.cnki.jccs.2022.1499. (in Chinese)

Wang Y,Kang J,Zhou F,Yuan L,Pan Z. 2022. Evaluation of lost gas in the borehole drilling stage: Implication for the direct method of coalbed methane content determination. *Journal of Natural Gas Science and Engineering,* **105:** 104711.http://dx.doi.org/10.1016/j.jngse.2022.104711.

Wang ZF,Si SS,Cui YJ,Dai JH,Yue JW. 2023. Study on Adsorption Characteristics of Deep Coking Coal Based on Molecular Simulation and Experiments. *ACS omega,* **8:** 3129-47.http://dx.doi.org/10.1021/acsomega.2c06593.

Wei C,Liu S. 2023. Effect of non-isothermal adsorption model on gas diffusion in coal particle. *Chemical Engineering Journal,* **477:** 147171.http://dx.doi.org/10.1016/j.cej.2023.147171.

Weniger P,Kalkreuth W,Busch A,Krooss BM. 2010. High-pressure methane and carbon dioxide sorption on coal and shale samples from the Paraná Basin, Brazil. *International Journal of Coal Geology,* **84:** 190-205.http://dx.doi.org/10.1016/.coal.2010.08.003.

Wu Y,Wang W,Zhu G,Wang P. 2021. Application of seismic multiattribute machine learning to determine coal strata thickness. *Journal of Geophysics and Engineering,* **18:** 834-44.http://dx.doi.org/10.1093/jge/gxab054.

Wu YW,Pan JN. 2017. Isothermal adsorption model of coalbed methane. *Journal of China Coal Society,* **42:** 452-8.http://dx.doi.org/10.13225/j.cnki.jccs.2017.1267. (in Chinese)

Xie CY,Du SY,Wang JL,Lao JM,Song HQ. 2023. Intelligent modeling with physics-informed machine learning for petroleum engineering problems. *Advances in Geo-Energy Research,* **8:** 71-5.http://dx.doi.org/10.46690/ager.2023.05.01.

Xiouras C,Cameli F,Quilló GL,Kavousanakis ME,Vlachos DG,Stefanidis GD. 2022. Applications of A

rtificial Intelligence and Machine Learning Algorithms to Crystallization. *Chemical Reviews,* **122:** 13006-42.http://dx.doi.org/10.1021/acs.chemrev.2c00141.

Yao ML,Shao LY,Hou HH,Li Z,Zhao S,Tang Y. 2018. Pore Structure and Fractal Characteristics of Adsorption Pores in Coal Reservoirs of the Huainan and Huaibei Coalfields. *Coal Geology of China* **30:** 30-6+47. (in Chinese)

Yu C,Ma J,Xue J. 2024. Simulation and analysis of the transient electromagnetic method response in double-layer water-filled goaf in coal mines. *Journal of Geophysics and Engineering,* **21:** 782-95.http://dx.doi.org/10.1093/jge/gxae024.

Yu HN. 2020. Development of virtual simulation platform for coal seam gas content determination. *Master*, *Henan Polytechnic University*.http://dx.doi.org/10.27116/d.cnki.gjzgc.2020.000366. (in Chinese)

Yuan Y. 2021. Study on the characteristics of gas occurrence in middle and high rank coal and the technology of risk prediction. *Ph.D.*, *AnHui University of Science and Technology*.http://dx.doi.org/10.26918/d.cnki.ghngc.2021.000969. (in Chinese)

Zhang,Feng QH,Zhang XM,Hu QJ,Wen SM,Chen D,Zhai YY,Yan X. 2020. Multi-fractured horizontal well for improved coalbed methane production in eastern Ordos basin, China: Field observations and numerical simulations. *Journal of Petroleum Science and Engineering,* **194:** 107488.http://dx.doi.org/10.1016/j.petrol.2020.107488.

Zhang JY,Feng QH,Zhang XM,Hu QJ,Yang JS,Wang N. 2020. A Novel Data-Driven Method to Estimate Methane Adsorption Isotherm on Coals Using the Gradient Boosting Decision Tree: A Case Study in the Qinshui Basin, China. *Energies,* **13:** 5369.http://dx.doi.org/10.3390/en13205369.

Zhang K. 2022. Methane adsorption/desorption and diffusion behaviors in coals of different coal struc

tures and their controlling mechanisms. *Ph.D.*, *China University of Mining & Technology, Beijing*. http://dx.doi.org/10.27624/d.cnki.gzkbu.2022.000126. (in Chinese)

Zhang K,Tang D-z,Tao S,Liu Y-f,Chen S-d. 2017. Study on influence factors of adsorption capacity of different metamorphic degree coals. *Coal Science and Technology* **45:** 192-7.http://dx.doi.org/10.13199/j.cnki.cst.2017.05.032. (in Chinese)

Zhang Q,Cui YJ,Zhong LW,Zhang QL,Xiang WP,Li YH. 2008. Temperature-pressure comprehensive adsorption model for coal adsorption of methane. *Journal of China Coal Society,* **11:** 1272-8. (in Chinese)

Zhang X-d,Qin Y,Sang S-x. 2005. Status and Prospect of Studies on CBM Reservoir Adsorption Characteristics. *Coal Geology of China,* **01:** 19-24+32. (in Chinese)

Zhang XD,Zhang ZX. 2008. Recent research progress of the gas-adsorption mechanism in coal. *China Mining Magazine,* **06:** 70-2+6. (in Chinese)

Zhang Z,Liu Q,Wu D. 2022. Predicting stress–strain curves using transfer learning: Knowledge transfer across polymer composites. *Materials & Design,* **218:** 110700.http://dx.doi.org/10.1016/j.matdes.2022.110700.

Zhang Z,Schott JA,Liu M,Chen H,Lu X,Sumpter BG,Fu J,Dai S. 2019. Prediction of Carbon Dioxide Adsorption via Deep Learning. *Angewandte Chemie International Edition,* **58:** 259-63.http://dx.doi.org/10.1002/anie.201812363.

Zhang ZP. 2019. Study on adsorption/desorption characteristics of methane from 11-2 coal in Pansan Mine. *Master*, *AnHui University of Science and Technology*. (in Chinese)

Zhao P,Wang H,Wang L,Xu D,Ma H,Guo H. 2022. Prediction of methane adsorption capacity in different rank coal at low temperature by the Polanyi-based isotherm model. *Energy Science & Enginee*

ring, **10:** 1384-97.http://dx.doi.org/10.1002/ese3.1108.

Zhao W,Dong H,Ren J,Yuan Y,Wang K,Wang F. 2024. A software for calculating coal mine gas emissi on quantity based on the different-source forecast method. *International Journal of Coal Science & Technology,* **11:** 51.http://dx.doi.org/10.1007/s40789-024-00703-y.

Zhao W,Wan Y,Wang K,Zhao Z,Song Y,Guo X,Xiang G. 2025. Methods for constructing scenarios of coal and gas outburst accidents: Implications for the intelligent emergency response of secondary mine accidents. *Process Safety and Environmental Protection,* **199:** 107236.http://dx.doi.org/10.1 016/j.psep.2025.107236.

Zhao W, Wang K, Ju Y, Fan L, Cao H, Yang Y, Shu L, Feng Z, et al. 2023. Quantification of the async hronous gas diffusivity in macro-/micropores using a Nelder-Mead simplex algorithm and its appl ication on predicting desorption-based indexes. *Fuel,* **332:** 126149.http://dx.doi.org/https://doi.org /10.1016/j.fuel.2022.126149.

Zhao Z,Sui F,Yan J. 2020. Prediction of methane content of deep coal seams in the Sunan mining area in Anhui Province, China. *International Journal of Oil, Gas and Coal Technology,* **23:** 351-64.htt p://dx.doi.org/10.1504/ijogct.2020.105778.

Zhao ZG,Tang XY. 2002. Discussion about Langmuir equation concerning methane adsorption by coa l. *Journal of Henan Polytechnic University(Natural Science)* **01:** 1-4. (in Chinese)

Zhou,Li Q,Xue HQ,Guo W,Li XB,Lu B. 2017. Comparative study on the volumetric and gravimetric method for isothermal adsorption experiment of shale. *Chemical Industry and Engineering Progre ss*, **36:** 1690-7.http://dx.doi.org/10.16085/j.issn.1000-6613.2017.05.018.

Zhou FY,Jin LP,Dong J. 2017. A Review of Convolutional Neural Network Research. *Chinese Journal of Computers,* **40:** 1229-51. (in Chinese)

Zhou J,Liu M,Xian X,Jiang Y,Liu Q,Wang X. 2019. Measurements and modelling of CH4 and CO2 adsorption behaviors on shales: Implication for CO2 enhanced shale gas recovery. *Fuel,* **251:** 293-306.http://dx.doi.org/10.1016/j.fuel.2019.04.041.