Supplementary file

Mechanisms of deep coalbed methane occurrence: Review and perspectives

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Appendix A: Methodology

This review employed a literature survey and analytical approach to evaluate the current state of research and recent developments regarding the occurrence mechanisms of deep CBM. The primary literature sources were the Web of Science and Google Scholar databases. The literature search was conducted between April 8, 2024, and June 1, 2026. Web of Science returned the largest number of records (n = 1,753), followed by Google Scholar (n = 670). The search terms included “deep coalbed methane”, “occurrence mechanisms”, and “critical depth”. A total of 1,010 publications were retrieved from the Web of Science database, of which 770 were published in the preceding five years. Among these publications, 78 were review articles, of which 56 were published during the same period. This search strategy ensured comprehensive coverage of the relevant literature.

Studies were initially screened based on their titles and abstracts, followed by a full-text evaluation of the selected articles. All eligible studies and additional relevant publications identified through citation tracking were included. The retrieved literature was classified and analyzed according to a predefined framework, including literature synthesis, thematic development, key areas of debate, and comparative analysis of consistent findings.

Appendix B: Detailed genetic mechanisms of deep coalbed methane

Mechanisms of biogenic methane generation

Microbial methane generation primarily proceeds through acetate fermentation and carbon dioxide reduction pathways. The corresponding reactions are as follows:

$$C_6H_{12}O_6 \rightarrow 2CH_3COOH + 2H_2 + 2CO_2 \quad \text{(S1)}$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad \text{(S2)}$$

$$CH_3COOH \rightarrow CH_4 + CO_2 \quad \text{(S3)}$$

In these reactions, the macromolecular structures of the original coalification products or low-rank coals cannot be directly degraded by microorganisms. Instead, complex organic matter first undergoes a series of transformation reactions, generating intermediates such as CH_3COOH, H_2, and CO_2. These intermediates are subsequently converted to CH_4 by methanogenic archaea (Welte, 2016; Chen et al., 2023). Compared with shallow coal seams, biogenic methane generation in deep coal seams is generally more constrained by elevated temperatures and pressures. However, it may still occur under favorable hydrogeochemical conditions, particularly through secondary microbial processes triggered by groundwater recharge or late-stage microbial colonization (Inagaki et al., 2015; Tamamura et al., 2020).

Mechanisms of thermogenic methane generation

Thermogenic methane is generated during coalification through the thermal degradation of oxygen-containing functional groups and subsequent cracking of residual organic structures. The corresponding reactions are as follows:

$$C_6H_{10}O_5 \rightarrow 3CH_4 + 3CO_2 + H_2O \tag{S4}$$

$$R\text{-}CH_3 \rightarrow R\text{-}H + CH_4 \tag{S5}$$

In these reactions, organic matter, including cellulose ($C_6H_{10}O_5$) and lignin derived from plant debris, undergoes thermal degradation under high-temperature and high-pressure conditions to generate CH_4, CO_2, and H_2O. During the coalification of high-rank coals, the molecular structure becomes increasingly aromatic. Methyl ($–CH_3$) and methylene ($–CH_2–$) side chains are cleaved via demethylation reactions, releasing CH_4. Here, *R* denotes the macromolecular backbone of the coal matrix (Moore, 2012; Lu and Gu, 2022). In deep coal seams, prolonged burial and elevated thermal stress intensify hydrocarbon cracking and increase gas yield. Consequently, methane-dominated gas compositions and high gas saturation, which are characteristic of deep CBM systems, are commonly observed.

Appendix C: Tables

The reported critical depths of deep CBM vary considerably among different basins because of differences in the geological setting, coal rank, and thermal evolution history. Representative datasets from major coal-bearing basins worldwide are summarized in Table S1.

Table S1. Reported critical depths of major coal-bearing basins worldwide.

No.	Country/region	Basin/coalfield	Tectonic type	Stratigraphic age	Coal rank	Critical depth (m)	CBM genesis Type	References
1	Colorado, USA	Piceance	Foreland	Cretaceous	Lignite	1,500	Biogenic	Colosimo et al. (2016)
2	Utah, USA	Uinta	Foreland	Cretaceous	Lignite	650–1,280	Biogenic, Thermogenic	Lamarre (2003)
3	Central USA	Appalachian	Foreland	Carboniferous	Bituminous-Anthracite	900–2,600	Biogenic, Thermogenic	Lyons (1998)
4	Wyoming, USA	Great Green River	Foreland	Upper Cretaceous-Paleogene	Lignite-Bituminous	1,830–2,280	Thermogenic	Tyler et al. (1994)
5	Jharkhand, India	Raniganj	Continental Rift	Lower Permian	Bituminous	1,050	Thermogenic	Kumar et al. (2018)
6	Dhanbad, India	Jharia	Continental Rift	Lower Permian	Coking Coal	800	Biogenic, Thermogenic	Adsul et al. (2023)
7	Queensland, Australia	Bowen	Craton	Permian-Triassic	Bituminous-Anthracite	800	Biogenic, Thermogenic	Hamilton et al. (2020)
8	Queensland, Australia	Surat	Craton	Triassic-Cretaceous	Lignite-Anthracite	600	Biogenic	Martin et al. (2013); Towler et al. (2016)
9	Southern Australia	Cooper	Craton	Upper Carboniferous-	Bituminous	1,500	Thermogenic	Salmachi et al. (2021)

				Triassic				
10	Central Siberia, Russia	Tunguska Basin	Craton	Carboniferous-Permian	Bituminous-Anthracite	900–1,000	Thermogenic	Svensen et al. (2018); Davydov (2021)
11	SW Siberia, Russia	Kuznetsk Basin	Continental Rift	Upper Carboniferous-Jurassic	Bituminous	1,100	Biogenic, Thermogenic	Davies et al. (2010); Trenchev et al. (2023)
12	Mongolia	South Gobi	Continental Rift	Permian	Bituminous	1,200	Thermogenic	Erdenetsogt et al. (2009)
13	Southern Poland	Upper Silesian Coal	Continental Rift	Carboniferous	Lignite-Bituminous	1,000	Biogenic, Thermogenic	Kotarba (2001); Kędzior and Teper (2024)
14	Wales, UK	South Wales	Foreland	Carboniferous	Bituminous-Anthracite	1,200	Biogenic, Thermogenic	Detheridge et al. (2019)
15	Shaanxi, China	Ordos	Craton	Carboniferous-Permian	Bituminous-Anthracite	900–1,600	Biogenic, Thermogenic	Li et al. (2018); Zhao et al. (2024)
16	Shanxi, China	Qinshui	Craton	Carboniferous-Permian	Bituminous-Anthracite	1,200–1,800	Thermogenic	Liu et al. (2022)
17	Xinjiang, China	Junggar	Foreland	Jurassic	Lignite-Bituminous	1,500–2,200	Biogenic, Thermogenic	Li et al. (2019)

Deep CBM productivity is jointly controlled by multiple factors during the exploration and development processes. The major influencing factors are listed in Table S2.

Table S2. Major factors affecting deep CBM productivity during exploration and development.

Stage	Item	Influencing factors	Analytical parameters	References
Preliminary exploration	Regional geology	Burial depth of coal seam	Sedimentary evolution; coal seam temperature; stability of coal seam and surrounding rock	Kang et al. (2023); Yan et al. (2023); Lu et al. (2025)
		Tectonic activity	Development of faults and folds; coal seam dip; cleat development	Johnson and Flores (1998); Cao et al. (2018); Ju et al. (2022)
		Stress variation	Principal stress direction; peak stress differential	Rajabi et al. (2024); Wen et al. (2025)
		Hydrological conditions	Hydrodynamic conditions; groundwater chemical composition	Underschultz et al. (2016); Hamilton et al. (2020)
	CBM reserves	Coal rank	Vitrinite content; ash content; vitrinite reflectance	Bannerjee et al. (2022); Glatz et al. (2022); Kędzior and Teper (2023)
		Coal seam thickness	Main seam thickness; interlayer and coal-rock thickness	Johnson and Flores (1998); Li et al. (2018)
		CH_4 content	Organic matter abundance; adsorption time	Mohanty and Pal (2017); Panwar et al. (2020)
		Adsorbed gas proportion	Langmuir pressure/volume	Langmuir (1918); Yang et al. (2019)
Later development	Production technology	Pore and permeability conditions	Porosity; permeability	Zou et al. (2022); Ji et al. (2026)
		Pressure variation	Coal reservoir pressure; fluid pressure; critical adsorption pressure	Wu et al. (2016); Liu et al. (2024); Govindarajan et

			al. (2025)
	Production forecast	Peak production; decline rate; inter-well spacing	Freij-Ayoub (2012); Hamilton et al. (2020); Everts et al. (2024)
	Drilling technology	Drilling fluid composition; cementing quality	Huang et al. (2023); Xu et al. (2023)
	Fracturing technology	Effective fracture length; fracturing fluid; proppant; conductivity	Sampath et al. (2017); Lu et al. (2023); Longinos et al. (2025)
	Production consistency	Stage-wise production analysis	Hamilton et al. (2020)
	Gas-liquid regulation	Desorption, diffusion, and seepage performance	Mostafa et al. (2023); Asif et al. (2024); He et al. (2025)
	Uncontrollable factors	Coal seam production analysis effect; equipment failures and duration of destructive tectonic movements underground	Yan et al. (2023); Rajabi et al. (2024)

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