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**Experimental Studies on the Origin
and Accumulation of Coalbed Gas**



UNITED STATES DEPARTMENT OF THE INTERIOR

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By Ann G. Kim



**UNITED STATES DEPARTMENT OF THE INTERIOR
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EXPERIMENTAL STUDIES ON THE ORIGIN AND ACCUMULATION OF COALBED GAS

by

Ann G. Kim¹

ABSTRACT

The Bureau of Mines investigated factors that influence the formation of methane and other hydrocarbon gases in coal, which is an integral part of the coalification process. Coalification begins with a biogenetic stage in which plant debris decomposes and peat is formed; methane and CO₂ are the predominant gases produced during this stage. During the diagenetic stage of coalification hydrogen and the hydrocarbon gases methane, ethane, ethylene, propane, propylene, butene, iso- and normal butane, and pentane are formed by dissociation of the organic material. Methane may also be produced by a secondary reaction of hydrogen with unsaturates or by the reduction of CO₂. The gas contained in coalbeds is a mixture of methane, C₂ through C₆ alkanes, CO₂, O₂, N₂, H₂, and He; its heating value is equivalent to that of natural gas. The gas content of coal depends on many variables, but an empirical relationship between adsorptive capacity, rank, and depth has been observed.

INTRODUCTION

Underground mining of coal has always been hazardous, owing partially to the release of explosive methane gas. Methane and other gases, natural byproducts of the coalification process, are held within the coalbed under pressure. When coal is mined, this gas is released and can form an explosive mixture with air. The traditional method of dealing with methane emission during mining is ventilation, pumping sufficient air through the mine to dilute emitted methane to concentrations below the explosive limit. This is a costly procedure, and even in moderately gassy mines it is not uncommon for methane emission to exceed the ventilation capacity. It is possible that conventional ventilation methods will be inadequate in handling the high methane emission rates expected when mines are sunk in deeper, gassier coalbeds.

Work by the Bureau of Mines on methane problems has also shown that conventional ventilation methods waste a valuable energy resource. Methane in coalbeds has a heating value of approximately 1,000 Btu/scf. U.S. coal mines

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vent more than 200 MMcf of this high-Btu gas to the atmosphere daily (3).² Methane cannot be recovered from the ventilation exhaust, where its concentration is less than 1 pct; but if it is drained from the coalbed in advance of mining, it can be used as a substitute natural gas (1).

The Bureau of Mines has conducted extensive research on methods of alleviating methane hazards in mining and on conserving a valuable, readily available energy resource. Part of this program has dealt with the origin and accumulation of methane in coal. The present report is a summary of experimental studies on the gases formed during the biogenetic phase of coal formation, the effect of low temperatures on the evolution of gas from coal, the determination of the composition of coalbed gas, and the effect of depth and rank on coal's gas adsorption capacity.

GAS FORMATION DURING BIOGENETIC COALIFICATION

The formation of coal is part of a cyclic process (fig. 1). Atmospheric CO_2 is incorporated into plants which decay to form peat. Temperature and time convert the buried peat to coal, methane, and other gaseous byproducts. Eventually the gases are released to the atmosphere, the carbon in the coal is converted to CO_2 by oxidation due to burning or weathering, thus completing the cycle.

The first important stage in the formation of coal is the biogenetic

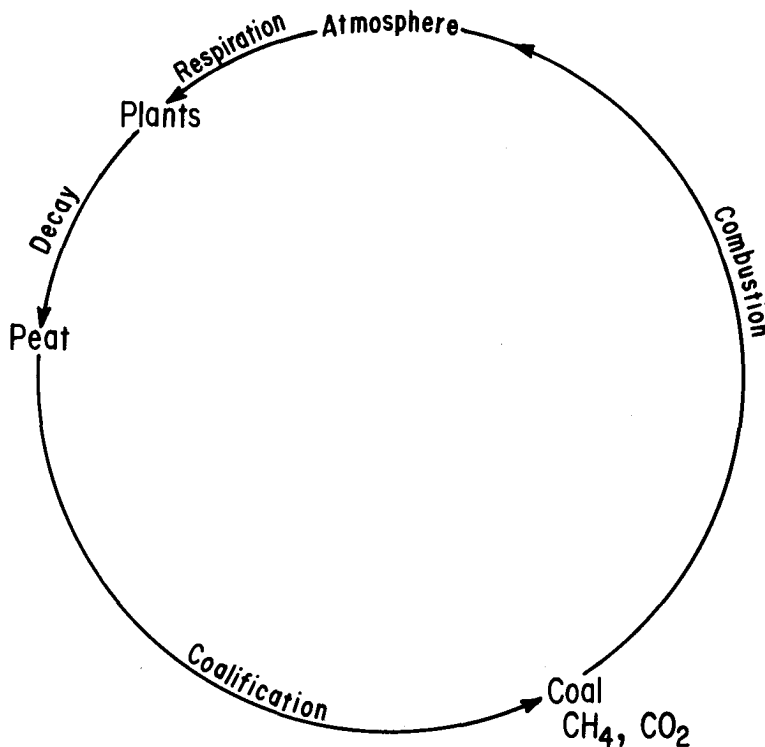
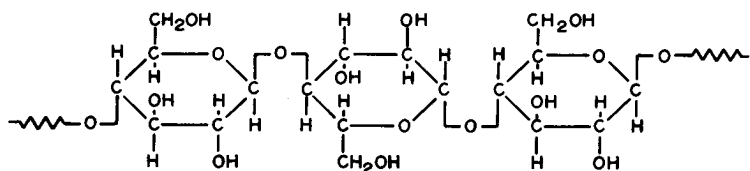


FIGURE 1. - Coal cycle.

² Underlined numbers in parentheses refer to items in the list of references at the end of this report.

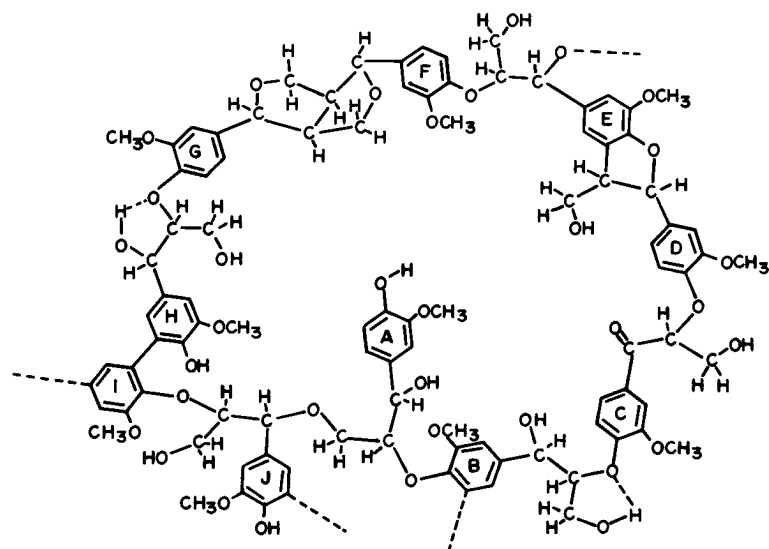
stage in which peat is formed. Most of the bituminous coals currently mined in the United States originated in Pennsylvanian age peat swamps between 275 and 300 million years ago. These swamps were broad coastal plains at or very near sea level. High humidity and heavy rainfall encouraged rapid and extensive plant growth, resulting in large volumes of plant debris. The plants of the Pennsylvanian age peat swamps were large, pithy land plants adapted to semi-aquatic or marshy conditions. Many plants grew to heights in excess of 100 feet and had diameters of over 4 feet.



CELLULOSE

The poor drainage and the slow migration of fresh water contributed to an acidic, low-oxygen environment which favored anaerobic microbial activity. The slow rate of anaerobic decay, the lowered pH, and accumulation of toxic products inhibited decomposition and promoted the preservation of organic material and the accumulation of a carbonaceous sediment.

Plants are composed of several classes of chemical compounds, of which cellulose and lignin (fig. 2) are the most important from the standpoint of coal formation. Cellulose is a linear polymer readily decomposed by microorganisms to CO_2 , ethanol, and various acids. A secondary population of microorganisms produces methane from the acids and alcohol. Lignin is an aromatic polymer that anchors cellulose fibers and strengthens plant walls;



LIGNIN

FIGURE 2. - Structures of cellulose and lignin.

little is known about its microbial decomposition.

Since the microbial decomposition of cellulose and lignin initiates coal formation, gases formed during this process may be related to the gases in coal. To study gas formation during the biogenetic stage, sterile samples of wood, cellulose, and a lignin derivative were placed in an anaerobic environment at 34°C (7). Each sample was inoculated with soil microorganisms, and the gases produced were analyzed by gas chromatography. Methane and CO_2 were the predominant reaction products from all samples. Carbon dioxide was detected first; methane was detected several days later. Over a period of several months, the composition of the gas averaged 95 pct methane and 5 pct CO_2 . Hydrogen was detected in the gas produced initially from wood samples (fig. 3) but was not found after the production of methane began. The composition of the gas indicates that two mechanisms are involved in the production of methane from plant material--fermentation and reduction of CO_2 .

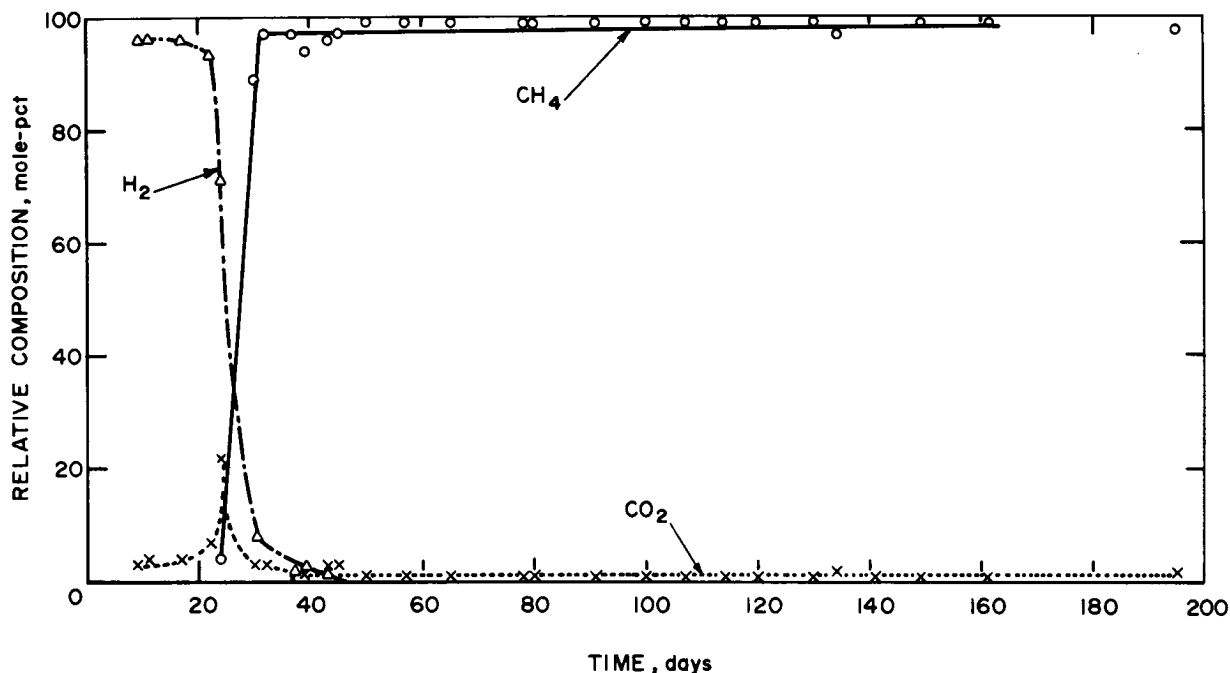


FIGURE 3. - Gas produced from wood.

The total amount of gas produced and the rate of production (table 1) are consistent with the structure and biodegradability of the source material. Both the amount and the rate of production were greater for cellulose, which is easily decomposed. Less gas was produced from lignin, a more complex substance that is not readily degraded. Gas production from wood, which contains both cellulose and lignin, was intermediate--less gas was produced from wood than from the lignin derivative, but it was produced at a faster rate.

TABLE 1. - Gas produced from plant material

Source.....	Cellulose	Lignin derivative	Wood
Total gas.....ml..	150	15	10
Total gas.....ml/g substrate..	100	10	6.6
Time.....mo..	3	20	8
Rate..... 10^{-6} mole/d..	9.9	2.5	4.4
CO ₂pct..	5.01	5.00	5.01
CH ₄pct..	94.94	94.98	94.99
Other hydrocarbons.....pct..	0.0496	0.0216	0.0005
CH ₄ /total hydrocarbons.....	0.999	0.999	0.999

Higher-molecular-weight hydrocarbons produced from plant material averaged less than 1 pct of the total gas. The ratio of methane to total hydrocarbons averaged 0.999, which is typical of microbially produced gases.

To compare the composition of the gas produced in this experiment with that produced by microbial action in swamps, the composition of the gas in

peat was determined. Samples from contemporary bogs in northeastern Pennsylvania were placed in a closed container, and the gases were desorbed by heating to 50° C, stirring the sample, and stripping the gas with helium. The hydrocarbons and CO₂ were collected on an activated carbon trap at -62° C. When the trap was heated, the freed gas was collected over water and analyzed by gas chromatography (9). The average amount of gas desorbed from the peat was 0.12 cm³/g; the average composition was 96.75 pct CO₂, 3.23 pct CH₄, and 0.02 pct other hydrocarbons (table 2). The average ratio of methane to total hydrocarbons was 0.987, a value consistent with microbial generation.

TABLE 2. - Gas desorbed from peat

Sample number.....	1	2	3	4	Average
Sample weight, as received.....g..	379	222	889	800	573
Sample weight, dry.....g..	57	48	191	72	92
Total gas, air free.....ml..	2.02	21.37	1.77	0.23	6.35
Total gas.....ml/g dry peat..	0.035	0.445	0.009	0.003	0.123
CO ₂pct..	97.0	99.9	98.8	91.3	96.75
CH ₄pct..	2.98	0.0097	1.18	8.59	3.23
Other hydrocarbons.....pct..	0.02	0.0003	0.02	0.01	0.019
CH ₄ /total hydrocarbons.....	0.992	0.970	0.987	0.999	0.987

The distribution of higher hydrocarbons in the total gas is similar for plant material and peat (table 3). However, on a CO₂-free basis the concentration of higher-molecular-weight hydrocarbons is greater in the gas from peat (table 4). The gas from plant materials and peat contains saturated and unsaturated C₂ and C₃ compounds. The gas from peat contains an unsaturated C₄ hydrocarbon and two unidentified compounds which were not detected in the gas from plant materials. The straight-chain C₄ isomer predominates in the hydrocarbons from plant material and peat. Although n-pentane (straight chain) is the predominant C₅ isomer derived from plant material, iso-pentane (branched) is the predominant C₅ isomer detected in the gas from peat. All three C₅ isomers were detected in the gas from cellulose and peat.

TABLE 3. - Composition of gas from plant material and peat, pct

Source.....	Wood	Cellulose	Lignin derivative	Peat
Methane (CH ₄).....	94.99	94.94	94.98	3.23
Unidentified compound.....	ND	ND	ND	0.0088
Ethylene (C ₂ H ₄).....	0.0003	0.0036	0.0008	.0017
Ethane (C ₂ H ₆).....	.0001	.0062	.0010	.0026
Propylene and propane (C ₃ H ₄ , C ₃ H ₈)..	.0007	.0095	.0019	.0002
Unidentified compound.....	ND	ND	ND	.0137
Iso-butane (i-C ₄ H ₁₀).....	ND	.0003	.0033	.0056
1-Butene (1-C ₄ H ₈).....	ND	ND	ND	.0033
n-Butane (n-C ₄ H ₁₀).....	ND	.0085	.0076	.0140
Neo-pentane (neo-C ₅ H ₁₂).....	ND	.0066	ND	Trace
Iso-pentane (i-C ₅ H ₁₂).....	ND	.00001	.0003	.0006
n-Pentane (n-C ₅ H ₁₂).....	ND	.0149	.0064	.00007
Carbon dioxide (CO ₂).....	5.01	5.01	5.00	96.72

ND Not detected.

TABLE 4. - Hydrocarbon distribution: Gas from plant material and peat, pct

Source.....	Wood	Cellulose	Lignin derivative	Peat
CH ₄	99.99	99.94	99.98	98.44
Unidentified compound.....	ND	ND	ND	0.2700
C ₂ H ₄	0.0003	0.0038	0.0008	.0520
C ₂ H ₆0001	.0065	.0010	.0800
C ₃ H ₆ , C ₃ H ₈00007	.0100	.0020	.0063
Unidentified compound.....	ND	ND	ND	.4200
i-C ₄ H ₁₀	ND	.0003	.0035	.1800
l-C ₄ H ₈	ND	ND	ND	.1000
n-C ₄ H ₁₀	ND	.0090	.0080	.4300
Neo-C ₅ H ₁₂	ND	.0069	ND	Trace
i-C ₅ H ₁₂	ND	.00001	.0003	.0190
n-C ₅ H ₁₂	ND	.0157	.0067	.0023

ND Not detected.

A comparison of the air-free composition of gas from plant material, peat, and coal (table 5) shows an apparent concentration of CO₂ in peat. However, the peat was water saturated, and both sorbed gas and dissolved gas were analyzed. Only the gas phase was monitored in the plant material experiment. Carbon dioxide is approximately 20 times more soluble than methane in water, and the diffusion coefficient of methane is greater than that of CO₂. Because of its lower solubility and greater diffusion coefficient, methane is more likely to migrate out of the water-saturated peat deposit. During coalification, CO₂ formed during the peat stage could be removed with water or reduced to methane.

TABLE 5. - Composition of gas from plant material, peat, and coal, pct

Source.....	CO ₂	CH ₄	Other hydrocarbons
Plant material.....	5.0	94.99	0.01
Peat.....	96.75	3.23	.02
Coal.....	1.9	97.8	.3

HYDROCARBON GAS FORMATION DURING DIAGENETIC COALIFICATION

The diagenetic stage of coalification, which follows the biochemical stage, begins with inundation of the peat bog and deposition of inorganic sediments. Increased temperature and pressure and accumulation of toxic substances cause microbial activity to cease. Coalification comprises a complex series of chemical reactions that produce a sequence of coals: lignite, sub-bituminous, bituminous, and anthracite. During this process the fixed carbon content and heating value increase (fig. 4). Changes in chemical and physical properties reflect changes in the chemical structure of the coal "molecule." During coalification there is an increase in the aromatic character of the coal and a loss of alkyl moieties. There is a transition from simple randomly arranged molecules to complex clusters of ring compounds oriented parallel to the bedding plane (fig. 5). There are several possible mechanisms by which

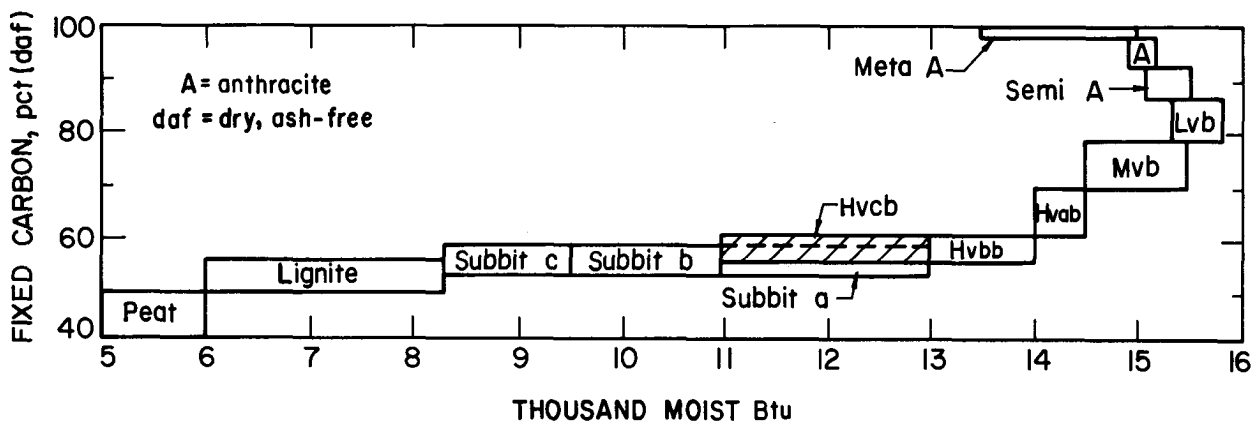


FIGURE 4. - Variation in fixed carbon and heating value of coal with rank.

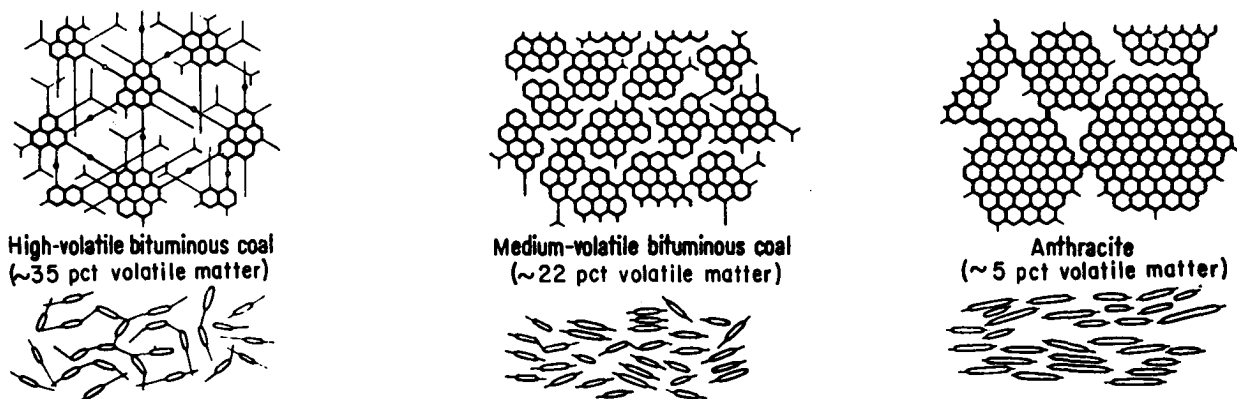


FIGURE 5. - Arrangement of micelles within the coal structure (12).

gases can be formed during this process. Methane, other hydrocarbons, and hydrogen can be produced by splitting off of alkyl side chains, by fragmentation of straight-chain compounds, or by condensation of straight chains to ring compounds. Methane can be formed by the reduction of CO_2 , the reduction of unsaturates, or the secondary decomposition of paraffins to lower-molecular-weight gases.

Both time and temperature increase the rank of coal. Temperature determines the rate at which coalification proceeds, and the duration of heating influences the final rank of the coal (fig. 6). Very high temperature ($>300^\circ\text{C}$), associated with tectonic activity, can produce high-rank coals in relatively short periods (2, 12). At low temperatures ($<50^\circ\text{C}$) the rank of coal tends to remain low for very long periods. The majority of bituminous coals formed at temperatures below 200°C in periods of 50 to 100 million years.

To determine if variations in temperature affect the evolution of gas from coal, seven samples of coal--subbituminous and high-volatile bituminous--were crushed, placed in closed test tubes, and heated at 35° , 125° , and 150°C (5).

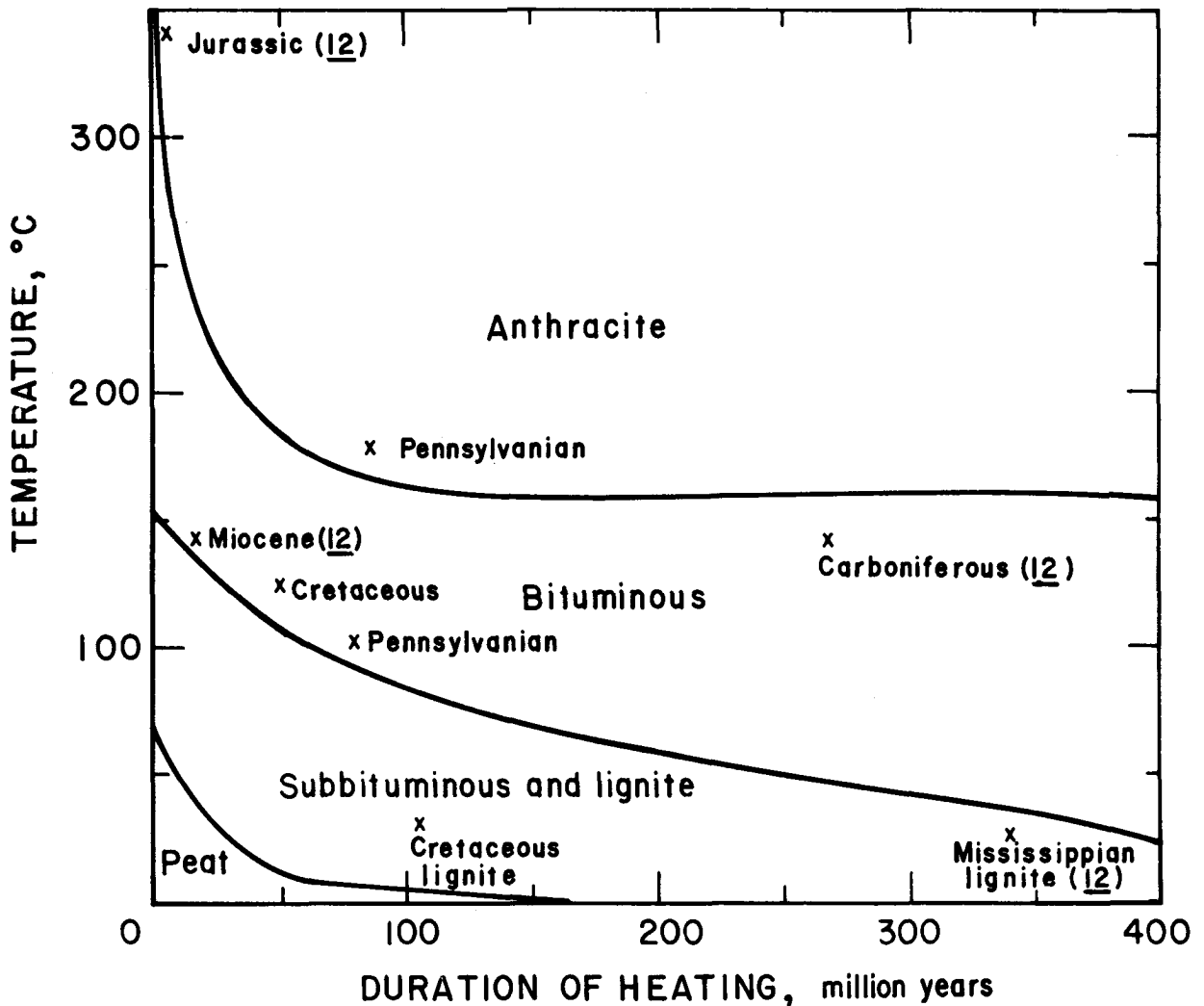


FIGURE 6. - Coal formation as a function of time and temperature.

The resulting gases were analyzed by gas chromatography. The coals were from mines with little detectable gas emission and were placed under vacuum at ambient temperature for 20 hours prior to the experiment to minimize contributions from adsorbed gases.

At all temperatures, total hydrocarbon emission per sample was related to the rank of the coal. Higher rank coals emitted less total hydrocarbons than lower rank coals (fig. 7). Total hydrocarbon emission, averaged over all samples, increased with temperature (fig. 8). Average hydrocarbon emission was 30×10^{-6} cm³/g at 35° C, 96×10^{-6} cm³/g at 125° C, and 172×10^{-6} cm³/g at 150° C. The average increase in total hydrocarbons per degree (table 6) over the entire temperature range was 1.2×10^{-6} cm³/g ° C, but the increase in hydrocarbon emission for each 1° C rise in temperature between 125° and 150° C was four times the increase between 35° and 125° C.

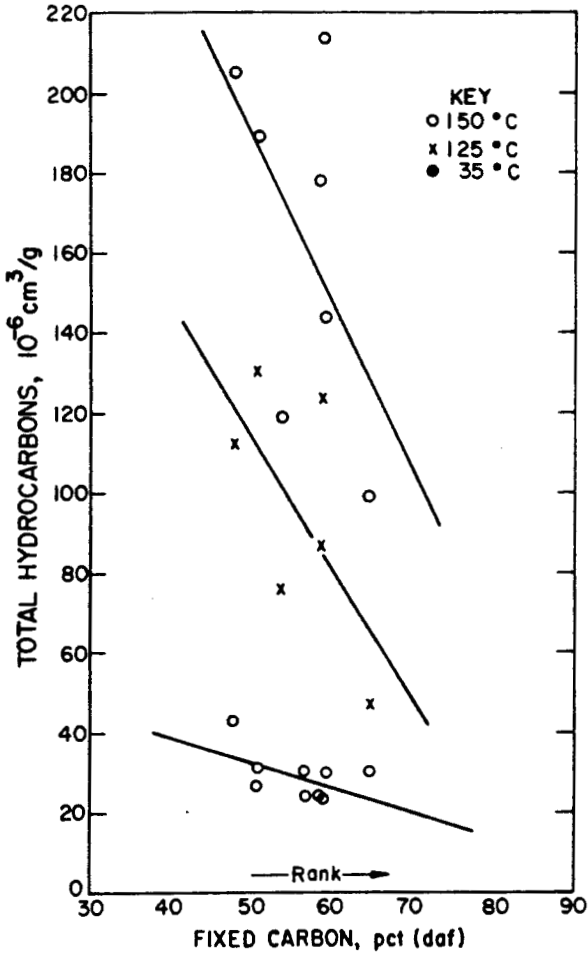


FIGURE 7. - Total hydrocarbon emission from coal versus rank of coal.

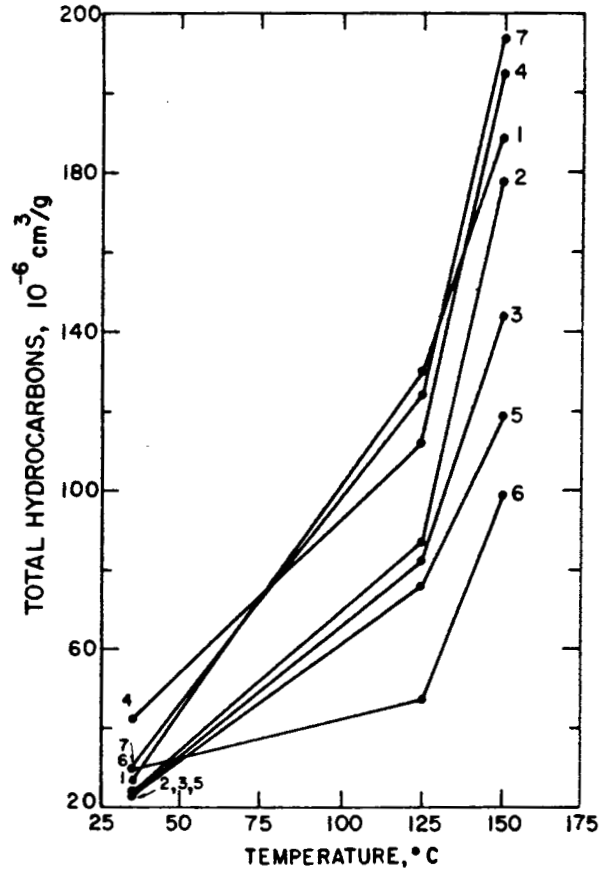


FIGURE 8. - Total hydrocarbon emission from coal versus temperature. Nos. 1-7 key to samples in table 6.

TABLE 6. - Changes in hydrocarbon and methane emission with increased temperature, $10^{-6} \text{ cm}^3/\text{g} \cdot \text{C}$

Sample No.	Coal	Total hydrocarbons			Methane		
		35° to 125° C	125° to 150° C	Average	35° to 125° C	125° to 150° C	Average
1.....	Rock Island.....	1.1	2.4	1.4	0.2	0.6	0.3
2.....	Laramie No. 3.....	.7	3.6	1.3	.2	.7	.3
3.....do.....	.7	2.5	1.1	.1	.5	.2
4.....	Mammoth, Iowa.....	.8	3.7	1.4	-.1	.9	.1
5.....	Uncorrelated bed--Iowa	.6	1.7	.8	.2	.5	.3
6.....	Upper Freeport.....	.2	2.1	.6	.01	1.0	.2
7.....	Pittsburgh.....	1.0	3.6	1.6	.1	1.2	.3

Methane emission also increased with temperature (fig. 9), but the percentage of methane in the emitted gas decreased at higher temperatures (fig. 10). At 35° C, the hydrocarbon gas contained more than 95 pct methane; at 125° C, methane content averaged 50 pct; and at 150° C, methane was about 30 pct of the hydrocarbon gas. At 125° and 150° C methane accounted for approximately 30 pct of the total increase in hydrocarbon emission (table 6). In other words, the composition of the gas is not constant with temperature. At higher temperatures the gas contained a larger proportion of higher-molecular-weight hydrocarbons.

The average composition of the hydrocarbon gas (table 7) shows that at 35° C only methane and ethane were emitted from the coal. At 125° C, the gas contained ethylene, propane, propylene, iso-butane, normal butane, 1-butene, and pentane, in addition to methane and ethane. The composition of the gas at 150° C was similar to that at 125° C, except that 1-butene was not detected; this may indicate a secondary reaction in which the unsaturated 1-butene is reduced to n-butane. The relative composition (fig. 11) shows that methane, iso-butane, and pentane predominate at higher temperatures. The concentration of iso-butane was 15 to 20 times that of n-butane, and only one of three pentane isomers was detected. The relative distribution of hydrocarbons does not correspond to their boiling points, molecular weights, or heats of formation. For the lower-molecular-weight compounds, there is a slight correlation to the heat of adsorption, but this does not account for the high concentrations of iso-butane and pentane or for the absence of two pentane isomers.

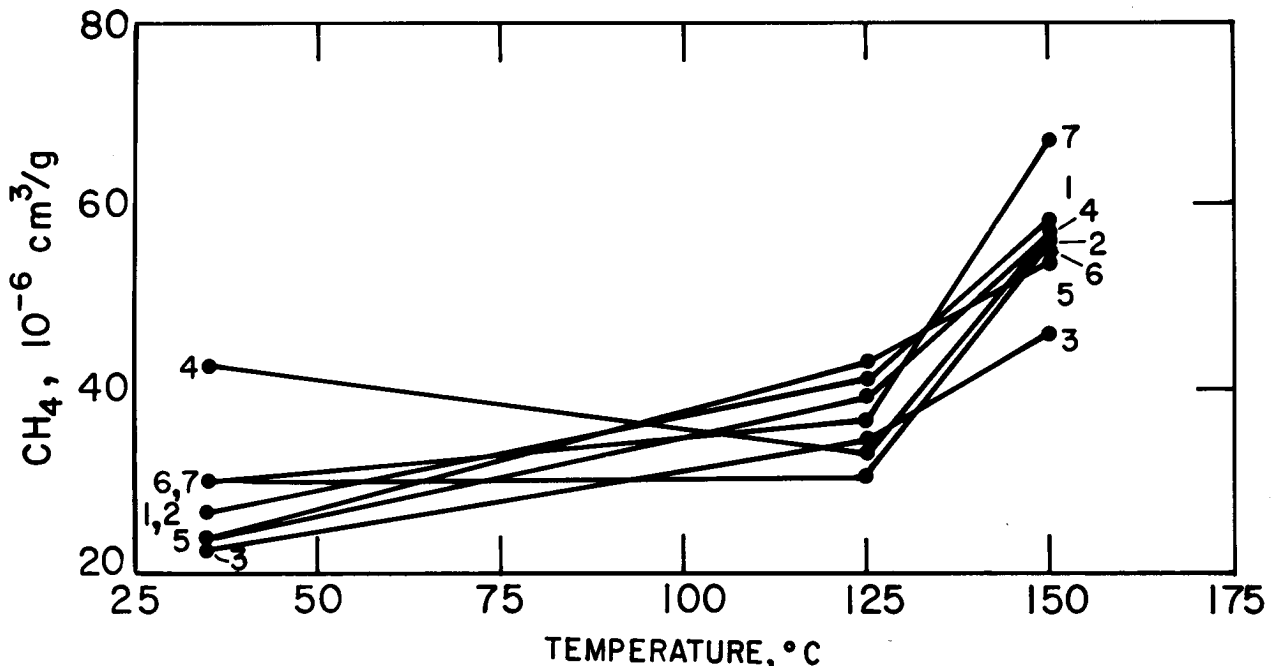


FIGURE 9. - Methane emission from coal versus temperature. Nos. 1-7 key to samples in table 6.

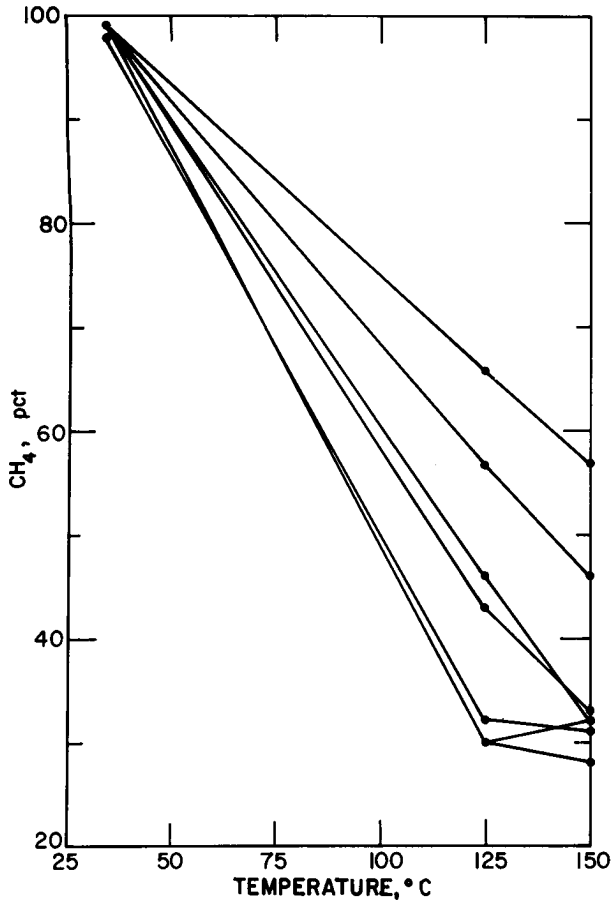


FIGURE 10. - Percentage of methane in emitted gas versus temperature.

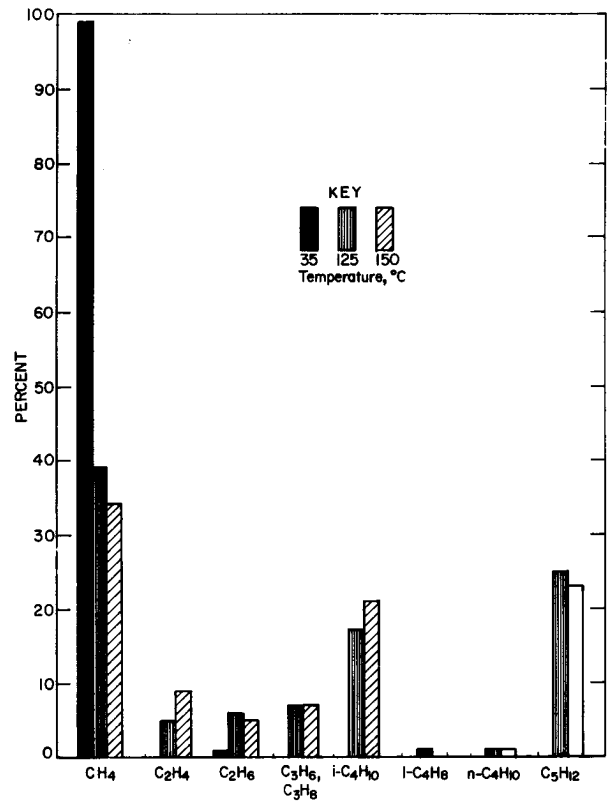


FIGURE 11. - Relative composition of hydrocarbon gas.

TABLE 7. - Hydrocarbon composition at various temperatures,
 $10^{-6} \text{ cm}^3/\text{g}$

	35° C	125° C	150° C
CH ₄	28.6	36.2	54.3
C ₂ H ₄1	5.0	13.7
C ₂ H ₆	ND	5.6	7.5
C ₃ H ₆ + C ₃ H ₈	ND	6.9	11.9
Unidentified compound.....	ND	.1	.6
i-C ₄ H ₁₀	ND	15.6	33.7
l-C ₄ H ₁₀	ND	.1	ND
n-C ₄ H ₁₀	ND	1.2	1.2
C ₅ H ₁₂	ND	23.1	36.2
Total.....	28.7	93.8	159.1

ND Not detected.

From the experiment it can be concluded that "demethanation" of the coal precursor is too simple a mechanism to explain the formation of hydrocarbon gases during coalification. Higher-molecular-weight gaseous hydrocarbons are

also formed during coalification, but simple fragmentation of a long-chain molecule does not account for the observed composition of hydrocarbon gas emitted from coal.

COMPOSITION OF COALBED GAS

Coalbed gas is frequently referred to as methane because methane is the major component (>80 pct). In many theories of coalification, methane was believed to be the only hydrocarbon gas formed. Ethane in coalbed gas was attributed to contamination from natural gas horizons below the coal (11). CO_2 , N_2 , O_2 , H_2 , and He are also present in gas drained from coalbeds. Carbon dioxide can be formed by decarboxylation of the coal precursor or by oxidation during early stages of coalification. Nitrogen and oxygen in coalbed gas may be occluded during deposition of the organic sediment or may be introduced by percolating ground water. Helium in coalbed gas is a product of radioactive decay.

In a previous study (4) gas chromatographic analyses of free-flowing gas from coalbeds demonstrated that coalbed gas contains methane and higher-molecular-weight hydrocarbons (table 8). The alkanes, ethane, propane, butane, and pentane were the only higher-molecular-weight hydrocarbons detected in gas samples taken directly from coalbeds. The unsaturated hydrocarbons emitted when coal was heated were not found in coalbed gas samples obtained at ambient temperature. The amounts of butane and pentane detected were insufficient to determine the ratios of isomeric forms. Carbon monoxide, sulfur compounds, and nitrogen oxides were not detected in gas from coalbeds.

TABLE 8. - Average composition of gas from coalbeds, pct

Coalbed...	Pocahontas No. 3 ¹	Pittsburgh ²	Upper Kittanning ³	B Seam ⁴	Lower Hartshorne ⁵	Mary Lee ⁵	Anthra- cite ³
CH_4	94.9	91.1	97.4	87.8	99.2	96.0	98.7
C_2H_6	1.3	.3	.01	.05	.01	.01	.1
C_3H_8004	ND	ND	.005	ND	ND	Trace
C_4H_{10}002	ND	ND	.001	ND	ND	ND
C_5H_{12}	Trace	ND	ND	ND	ND	ND	ND
CO_23	8.2	.1	12.0	.1	.1	.1
O_22	.2	.2	ND	.1	.1	ND
N_2	3.2	.5	2.3	.1	.6	3.5	1.0
H_202	ND	ND	ND	ND	Trace	ND
He.....	.04	ND	ND	ND	ND	.3	Trace
Btu/scf...	1,030	975	1,037	935	1,056	1,022	1,053

ND Not detected.

¹Virginia.

²Pennsylvania and West Virginia.

³Pennsylvania.

⁴Colorado.

⁵Oklahoma.

⁶Alabama.

Since coal is formed in a reducing environment, the absence of sulfur dioxide and oxides of nitrogen is not unusual. However, hydrogen sulfide has not been detected in coalbed gas, even though coal contains sulfide sulfur, organically combined sulfur, and sulfates. Carbon monoxide is frequently detected in coal mine air, where it occurs as a product of low-temperature oxidation, but it is not found in gas drained from coal that has not been exposed to air. The heating value of gas drained from coalbeds is approximately 1,000 Btu/scf, which is comparable with that

of natural gas. Due to its high caloric value and absence of undesirable components (CO, sulfur compounds), coalbed gas is an excellent substitute for natural gas.

VARIATION IN GAS CONTENT OF COAL

The amount of gas a coalbed contains is highly variable. Measured values of gas in coal range from 0.001 to 16.5 cm³/g (1, 8). Even coals of the same rank may exhibit a 10,000-fold difference in gas content, an indication that present gas content of a coalbed is related not only to gas formation during coalification but also to the postdepositional history of the coalbed. The gas content of a coalbed depends primarily upon rank, pressure, and temperature, and to some extent upon the permeability and porosity of the coal, the degree of fracturing, the distance to the outcrop, and the permeability of adjacent strata.

Coal is a porous solid with two distinct pore systems. Gas can exist as free gas in cracks and fractures (macropores) or be adsorbed on the internal surface of the micropores. Most of the gas in coal is adsorbed, and an adsorption isotherm can be used to determine experimentally the adsorptive capacity of the coal as a function of pressure and temperature. Adsorption isotherms for coal can be described by the equation

$$V = k_0 P^{n_0} - bT,$$

where V is the volume adsorbed in cm³/g (maf), k_0 is a constant determined at 0° C in cm³/g atm, P is the pressure in atmospheres, n_0 is a constant determined at 0° C, b is a constant in cm³/g ° C, and T is the temperature in ° C (6). The constants k_0 and n_0 are functions of the rank of the coal and can be related to the ratio of fixed carbon to volatile matter (fig. 12). Since both

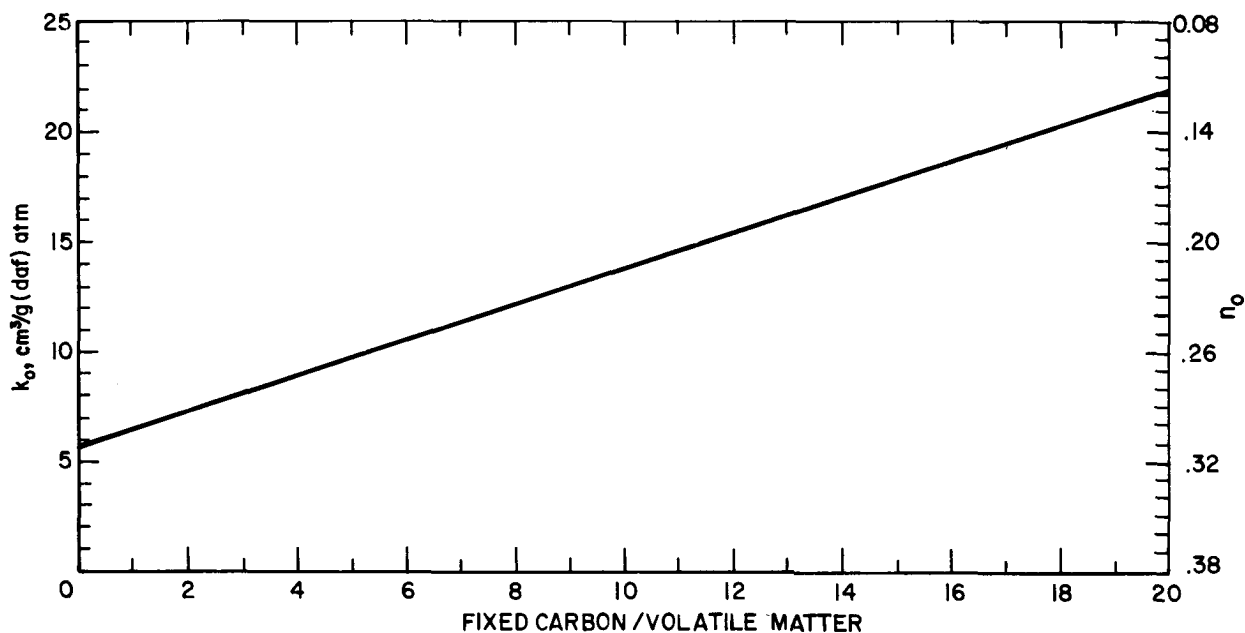


FIGURE 12. - Constants k_0 and n_0 as a function of fixed carbon-volatile matter ratio.

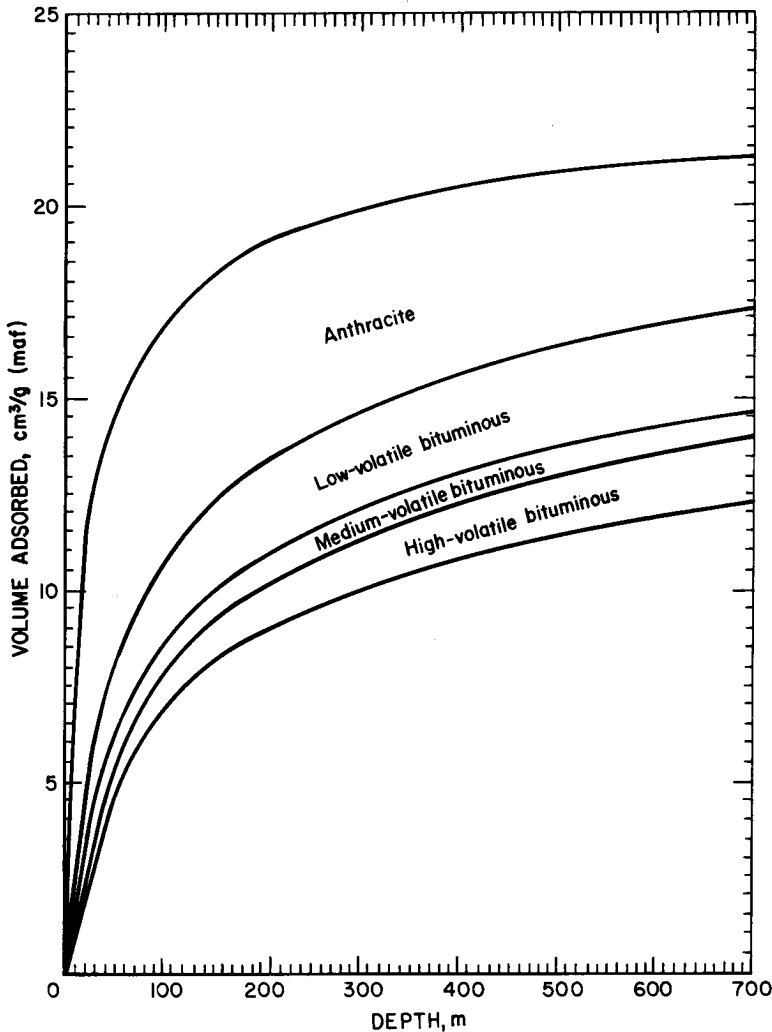


FIGURE 13. - Adsorptive capacity of coal as a function of rank and depth.

coal. To estimate the gas content of coal in place, it is necessary to correct for its moisture and mineral matter content. Incorporating corrections for moisture and mineral matter (MM) content and for the reduction of gas content in moist coal, the equation for adsorbed gas in place is written:

$$v = \frac{(100 - \text{moisture} - \text{MM})}{100} (0.75) [k_0 (0.096h)^{n_0} - b(1.8h/100 + 11)].$$

If it is assumed that moisture and mineral matter content is approximately 10 pct, the adsorbed gas content of various ranks of coal can be calculated and graphed as a function of depth (fig. 13). A reasonable estimate of the gas content can be obtained for most coals from the graph. Comparison of estimated values with values obtained by direct determination (10) (table 9) shows that most estimated values are within 30 pct of the measured value, which is the accuracy of the direct method.

temperature and pressure are functions of depth, the equation can be rewritten to give adsorptive capacity directly as a function of the depth of the coal:

$$V = k_0 (0.096h)^{n_0} - b(1.8h/100 + 11),$$

where h is the depth in meters.

The moisture content of a coal must also be considered in estimating its adsorptive capacity. Moisture in coal reduces its capacity to adsorb methane; the maximum reduction is related to the oxygen content of the coal. However, the experimentally determined ratio of gas adsorbed on wet and dry coal (V_w/V_d) is 0.75 with a variation of approximately 10 pct. For practical purposes, the amount of gas adsorbed on moist coal can be estimated as 25 pct less than that adsorbed on dry coal.

The preceding calculations estimated adsorbed gas per gram of dry, ash-free

TABLE 9. - Comparison of estimated and direct determination of methane content of coal

Coalbed	Depth		Direct determination		Estimated range		Difference between direct determination and estimated range, cm ³ /g
	Meters	Feet	Cm ³ /g	Ft ³ /ton	Cm ³ /g	Ft ³ /ton	
ANTHRACITE							
Tunnel No. 19.....	183	600	19	608	13-18	416-576	+1
	183	600	14	448	13-18	416-576	0
	183	600	13	416	13-18	416-576	0
Peach Mountain No. 18	213	699	22	704	14-19	448-608	+3
	213	699	19	608	14-19	448-608	0
LOW-VOLATILE BITUMINOUS							
Beckley.....	302	991	13	416	12-15	384-480	0
	267	876	14	448	12-14	384-448	0
	253	830	15	480	12-14	384-448	+1
	226	742	14	448	11-14	352-488	0
Hartshorne.....	451	1,480	16	512	13-16	416-512	0
	395	1,295	18	576	13-16	416-512	+2
	174	571	12	384	11-13	352-416	0
	169	553	13	416	11-13	352-416	0
	148	488	11	352	10-12	320-384	0
New Castle.....	77	252	5	160	8-10	256-320	-3
	651	2,137	17	544	15-17	480-544	0
Pocahontas No. 3....	643	2,110	14	448	14-17	448-544	0
	621	2,038	17	544	14-17	448-544	0
	529	1,736	11	352	14-17	448-544	-3
	494	1,621	12	384	13-16	416-512	-1
	484	1,588	16	512	14-16	448-512	0
	466	1,529	15	480	14-16	448-512	0
Pratt.....	232	761	9	288	11-14	352-448	-2
	416	1,365	15	480	14-16	448-512	0
MEDIUM-VOLATILE BITUMINOUS							
Mary Lee.....	666	2,185	16	512	13-15	416-480	+1
	520	1,706	12	384	13-14	416-448	-1
	519	1,703	14	448	13-14	416-448	0
	518	1,700	13	416	13-14	416-448	0
	335	1,099	14	448	12-13	384-416	+1
HIGH-VOLATILE BITUMINOUS							
Pittsburgh.....	259	850	7	224	10-11	320-352	-3
	235	771	6	192	9-11	288-352	-3
	206	676	5	160	9-10	288-320	-4
	130	427	3	96	8- 9	256-288	-5
	95	312	2	64	5- 6	160-192	-3
Redstone.....	225	747	4	128	9-11	288-352	-5
Sewell.....	207	679	9	288	9-10	288-320	0
Sewickley.....	205	675	5	160	9-10	288-320	-4
Waynesburg.....	122	402	3	96	8- 9	256-288	-5

For some coals, gas contents estimated from adsorption data may be substantially higher than those determined by the direct method; usually such coals are low in rank and relatively shallow. For example, in table 9, direct determinations for the Pittsburgh, Sewickley, Redstone, and Waynesburg coals are 30 to 65 pct lower than the range predicted from the graph, but the pressure gradient in the area from which these samples were obtained (Pennsylvania and West Virginia) is lower than average. Drill-stem tests have shown that pressure in the Pittsburgh coal in this area is approximately one-half the hydrostatic head. Gas contents calculated using the pressure gradient 0.046 atm/m are in better agreement with the direct-determination values (table 10)

TABLE 10. - Methane content of shallow, high-volatile bituminous coals

Coal	Depth		Direct determination		Calculated		Difference, cm ³ /g
	Meters	Feet	Cm ³ /g	Ft ³ /ton	Cm ³ /g	Ft ³ /ton	
Pittsburgh...	95	312	2	64	4	128	-2
Waynesburg...	122	400	3	96	4	128	-1
Pittsburgh...	130	427	3	96	4	128	-1
Sewickley....	205	673	5	160	5	160	0
Pittsburgh...	206	676	5	160	5	160	0
Redstone.....	225	738	4	128	5	160	+1
Pittsburgh...	235	771	6	192	5	160	-1
Do.....	259	850	7	224	5	160	+2

The direct determinations in table 10 can be described by a linear equation ($V = 0.025h - 0.5$; correlation coefficient = 0.90), but whether this relationship is generally accurate for shallow, low-rank coals cannot be determined from the limited data available. The relationship between gas content and depth for shallow, high-volatile coals in the southwestern Pennsylvania-northern West Virginia area illustrates the point that local geology, anomalous pressure-depth relationships, and characteristics of individual coals affect the gas content.

Lack of data precluded extending the estimate to lower rank coals. Of 22 coal samples studied, only 4 were not bituminous. The adsorption isotherm for anthracite fitted the pattern observed for other coals, but the results for subbituminous coals were ambiguous. Such coals are known to be high in moisture, and theoretically their gas-adsorption capacity is minimal. However, subbituminous coals and lignites have been known to liberate substantial quantities of gas. Because of limited data, gas content estimates are considered most accurate for bituminous coals.

SUMMARY

Coalification is a complex process, and the attendant formation of gaseous byproducts cannot be explained by a single, simple mechanism. During the biogenetic stage of coal formation, methane is the predominant gas produced, accompanied by CO₂ and small amounts of higher hydrocarbons. The gas retained in peat is predominantly CO₂ with some methane and C₂ through C₆ hydrocarbons. The concentrations of higher hydrocarbons are approximately equal in the gas generated from plant material and the gas desorbed from peat.

During the diagenetic stage of coalification, methane and other hydrocarbons are produced. In experiments on the effect of temperature on gas evolution from coal, methane, iso-butane, and pentane were the predominant hydrocarbons detected. As the temperature rose, the amount of hydrocarbons emitted increased, but the percentage of methane decreased. Therefore, the mechanism of gas formation during coalification cannot be limited to a simple demethanation reaction but may involve several reactions such as the fragmentation of long-chain molecules, the splitting of alkyl side chains, and the reduction of unsaturates and CO_2 .

Free-flowing gas from coalbeds is usually more than 90 pct methane with other hydrocarbons, CO_2 , N_2 , O_2 , H_2 , and He. To date, carbon monoxide, sulfur compounds, and oxides of nitrogen have not been detected in gas from coalbeds. Gas drained directly from coalbeds has an average heating value of approximately 1,000 Btu/scf. The gas content of coalbeds is highly variable, but an empirical relationship has been observed between adsorptive capacity, rank, and depth.

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