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**Estimating Methane Content
of Bituminous Coalbeds
From Adsorption Data**



UNITED STATES DEPARTMENT OF THE INTERIOR

Report of Investigations 8245

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of Bituminous Coalbeds
From Adsorption Data**

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**UNITED STATES DEPARTMENT OF THE INTERIOR
Cecil D. Andrus, Secretary**

BUREAU OF MINES

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ESTIMATING METHANE CONTENT OF BITUMINOUS COALBEDS FROM ADSORPTION DATA

by

Ann G. Kim¹

ABSTRACT

The Bureau of Mines estimated the methane content of a coal, which depends primarily upon rank and pressure, from the adsorption equation $V = kP^n$, where k and n are constants related to rank. By incorporating corrections for moisture, ash, and temperature, and estimating pressure and temperature as a function of depth, the methane content of coal in place can be estimated from the following equation:

$$V = \frac{(100 - \% \text{ moisture} - \% \text{ ash})}{100} (0.75) [k_0 (0.096h)^{n_0} - 0.14(1.8h/100 + 11)].$$

Values calculated with this equation generally are in reasonable agreement with direct determinations. By assuming a standard moisture and ash content, and using the hydrostatic head to estimate pressure, a graph of rank and depth versus gas content was constructed. Although estimated values were consistently high for several high-volatile bituminous coals from an area where the pressure is known to be less than hydrostatic, the estimated methane content for most coals shows reasonable agreement with values determined by the direct method.

INTRODUCTION

Methane is always present in coal (3-4)² and constitutes a serious safety hazard in coal mining. It occurs admixed with other hydrocarbons, CO₂, N₂, O₂, H₂, and He. It is a normal byproduct of the coal-forming process. Although much of the gas formed during coalification migrates away from the coal, a significant portion is retained in the coal and adjacent rocks. Some free gas is present in cracks and fractures, but most is adsorbed on the internal surface of micropores within the coal. The amount of gas that the coal contains depends primarily upon pressure, temperature, adsorptive capacity, and moisture content of the coal. Permeability, porosity, degree of

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²Underlined numbers in parentheses refer to items in the list of references preceding the appendixes.

fracturing of the coal and adjacent rocks, and distance from the outcrop may also influence the gas content of a coalbed.

When coal is mined, 60 to 80 pct of the gas that it contains is emitted into the mine atmosphere, where gas accumulation creates an explosion hazard. The conventional method of dealing with this hazard is through ventilation, which dilutes the emitted methane with air to nonexplosive concentrations and carries it to the surface. The deeper, higher rank coalbeds that will be mined in the foreseeable future will contain more gas than the beds currently being worked, and it is possible that ventilation will not be adequate to control methane emission. It may be necessary to drain methane from the coal in advance of mining. If the drained gas is to be sold as a fuel, it will be necessary to estimate the amount of gas that can be recovered from the coal.

The methane content of a given coal can be estimated by measuring the amount of gas emitted by a core sample recovered during exploratory drilling (5-6). This direct method is simple and is considered accurate to ± 30 pct. However, it does require drilling a hole, and the data thus obtained apply only to a particular coal at a particular depth.

A more general estimate can be made using adsorption-isotherm data. An adsorption isotherm describes the variation in gas adsorption as a function of pressure at a constant temperature. If isotherms are run at several temperatures, the change in adsorptive capacity with temperature can be determined. Isotherms for dry and moist coals are run to determine the effect of moisture on the volume of adsorbed gas. The information from various isotherms can be combined into a general equation for adsorbed-gas volume as a function of temperature, pressure, and moisture content. By applying the adsorption equation to different coals, the effect of rank can be determined, and a graph of the gas content of high-rank coal can be constructed as a function of rank and depth.

ACKNOWLEDGMENTS

The adsorption isotherms upon which this report is based were obtained by the Energy Conversion Section, Pittsburgh Energy Research Center of the Energy Research and Development Administration (ERDA), under contract to the Pittsburgh Mining and Safety Research Center of the Bureau of Mines. Detailed reports of these studies have been published elsewhere (1-2, 8-9).

METHANE-ADSORPTION EQUATION

Most of the gas in coal is adsorbed on the internal surface of micropores. The amount of gas that a coal can adsorb varies directly with pressure and inversely with temperature. The relationship between the volume of gas adsorbed by the coal, and pressure and temperature can be described by the equation

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

where V = volume of gas adsorbed, in cubic centimeters per gram of moisture- and ash-free coal;

P = pressure, in atmospheres;

T = temperature, in degrees Centigrade;

k_0 = a constant, in cubic centimeters per gram per atmosphere;

n_0 = a constant;

and b = a constant, in cubic centimeters per gram per degree Centigrade.

Constants k_0 , n_0 , and b were determined for 18 coals and are listed in table 1.³ The temperature constant b averages $0.14 \text{ cm}^3/\text{g}^\circ \text{C}$ for coals studied, from

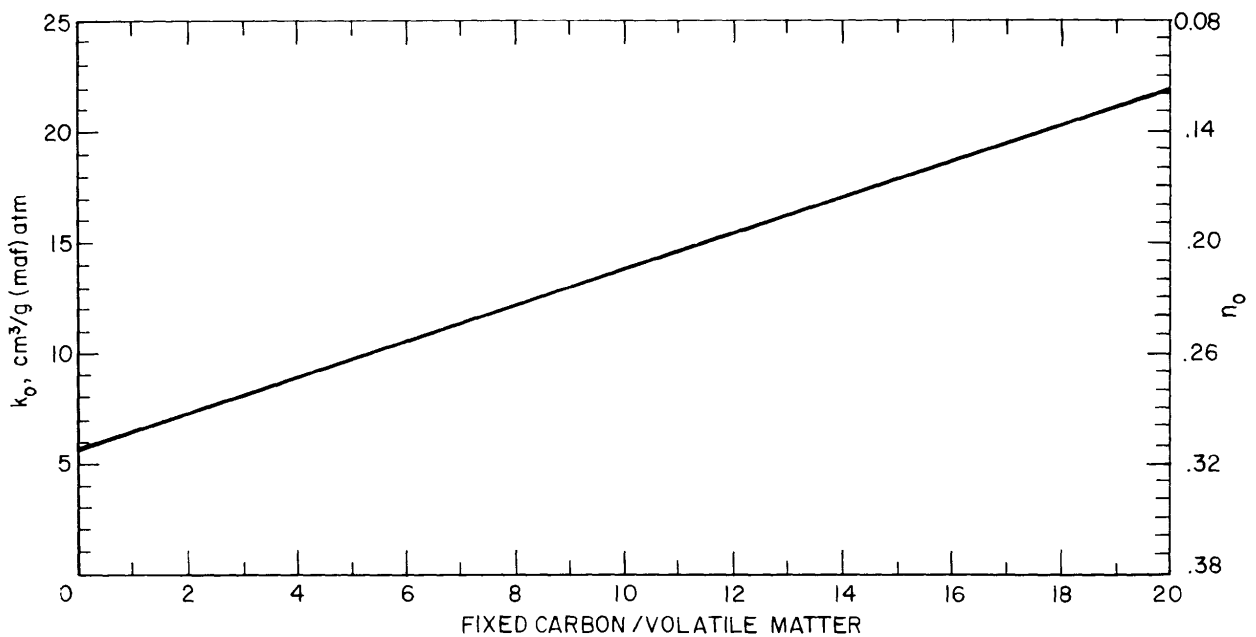


FIGURE 1. - Value of adsorption constants k_0 and n_0 versus the ratio of fixed carbon to volatile matter.

³ Derivation of the equation and calculation of constants are discussed in appendix A.

subbituminous to anthracite. The values of k_o and n_o depend on the rank of the coal, and can be expressed in terms of the ratio of fixed carbon (FC) to volatile matter (VM):

$$k_o = 0.8 \text{ FC/VM} + 5.6,$$

and
$$n_o = 0.315 - 0.01 \text{ FC/VM}$$

or
$$n_o = 0.39 - 0.013 k_o.$$

The relationship between the constants k_o , n_o , and the ratio FC/VM is shown in figure 1.

TABLE 1. - Adsorption constants for selected coals

Coalbed	k_o	n_o	b	V_w/V_d
Mammoth.....	21.1	0.15	0.18	0.80
Pocahontas No. 3.....	8.7	.27	.13	.76
Lower Kittanning.....	10.3	.26	.17	.76
Beckley.....	10.6	.27	.15	.77
Mary Lee.....	8.9	.26	.15	.63
Upper Freeport.....	6.8	.28	.12	.74
Lower Freeport.....	8.7	.26	.14	.69
Pittsburgh.....	5.7	.33	.12	.57
Sewell.....	6.6	.29	.13	.71
No. 5 Block.....	6.2	.30	.12	.55
Somerset B.....	6.8	.32	.15	.40
Castlegate.....	4.9	.37	.12	.42
Rosebud.....	7.5	.34	.15	.12
Elkhorn No. 3.....	6.8	.29	.13	ND
Hazard No. 4.....	6.1	.31	.12	ND
Pocahontas No. 4.....	10.1	.26	.16	ND
Stearns No. 2.....	4.6	.34	.11	ND
Hazard No. 7.....	7.0	.32	.14	ND

ND--Not determined.

Adsorption curves indicate that the amount of gas adsorbed by coal increases with increasing rank at a given temperature and pressure (figs. 2-3), and this has been verified by data on the gas content of the Mary Lee group of coalbeds (7). At a given temperature and pressure, higher rank coals contain larger volumes of methane than lower rank coals. The volume of adsorbed methane increases with increasing pressure, but decreases with increasing temperature.

Pressure and temperature are functions of depth. At a given depth, the pressure P is usually assumed to equal the hydrostatic head given by the equation--

$$P_{hyd} = 0.096h,$$

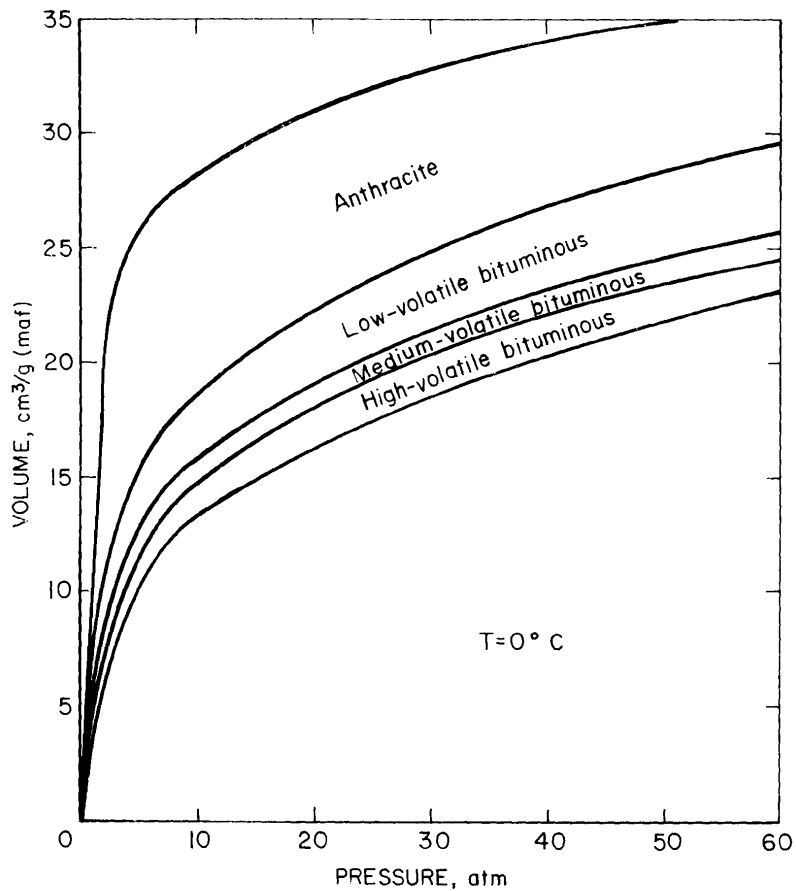


FIGURE 2. - Variation of adsorption isotherms with rank at 0° C.

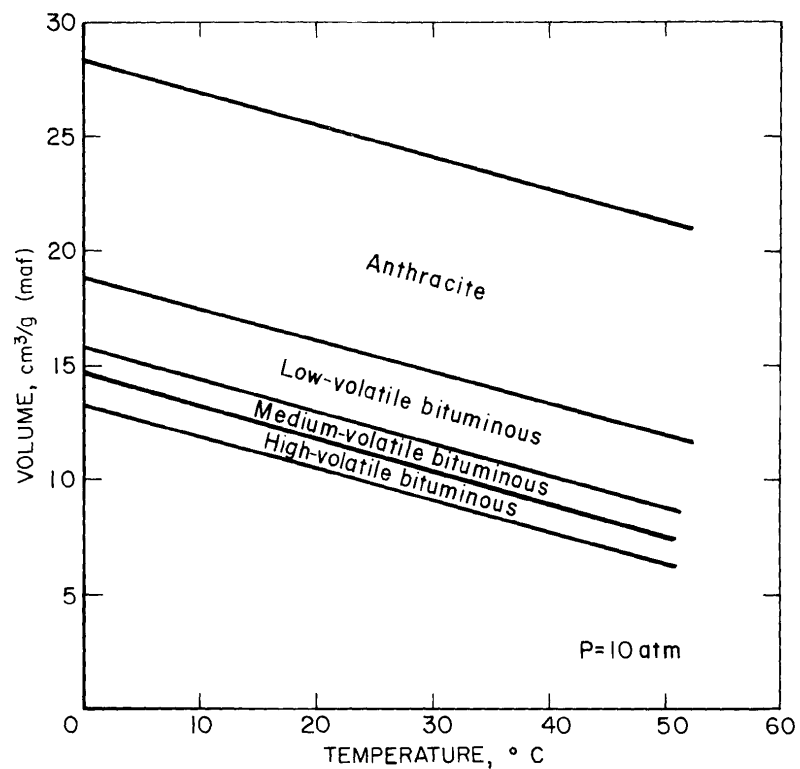


FIGURE 3. - Variation in adsorptive capacity with temperature and rank at 10 atm.

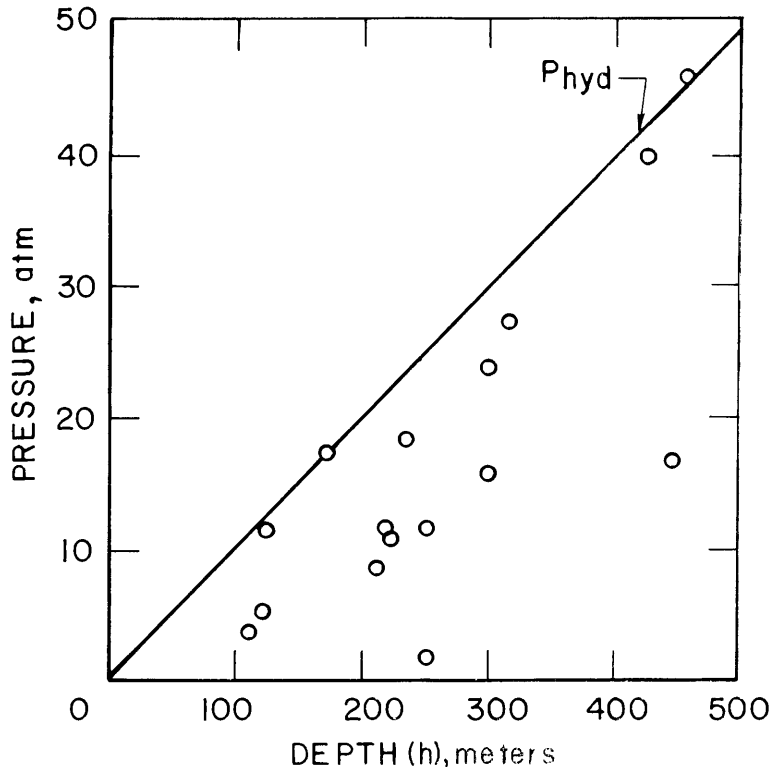


FIGURE 4. - Relationship of pressure to depth.

where P is expressed in atmospheres, and h is the depth, in meters. However, drill-stem tests have frequently shown that pressure within a coalbed is substantially less than hydrostatic (fig. 4). For these data (fig. 4), the average pressure gradient is 0.063 atm/m with a standard deviation of ± 0.027 atm/m. Since it is primarily dependent on pressure, the estimated adsorbed gas volume will be only as accurate as the pressure value. If the pressure at depth or pressure gradient for an area is known, this value should be used to estimate the adsorbed gas content of a coal. If hydrostatic head is used, it should be realized that this represents a limiting case, and actual gas content may be lower than the estimated value.

Temperature at a given depth h is estimated as the geothermal gradient multiplied by h and added to the ground temperature. Although the geothermal gradient varies in different areas, a commonly used value is $1.8^\circ \text{C}/100 \text{ m}$. Ground temperature--that temperature not affected by surface heating and cooling--is also variable. In this study, 11°C is used. Temperature at depth is estimated by the following relationship:

$$T = 1.8 \frac{h}{100} + 11.$$

At the relatively shallow depths considered in this report, it is unlikely that an error in estimating T will substantially affect the estimate of gas content.

To estimate the methane content of coal in place, its moisture content must also be considered. Moisture in coal reduces its capacity to adsorb methane. According to one study (1), below a critical value, the reduction in adsorption capacity of a coal is directly related to moisture content.⁴ Above this critical value, additional moisture causes no further reduction in gas adsorption. The ratio of volumes of gas adsorbed on wet and dry coal (V_w/V_d)

⁴The reduction in adsorption capacity related to moisture content is discussed in appendix B.

is given in table 1. For most high-rank coals, the minimum volume of methane adsorbed on wet coal is between 55 and 85 pct of the volume adsorbed on dry coal. In general, the reduction in gas-adsorption capacity is greater for lower rank coals. For coals for which experimental data is not available, moisture in coal can reasonably be assumed to reduce the volume of adsorbed methane by 25 pct. In a general gas-adsorption equation, 0.75 is used as the ratio of adsorbed gas in wet and dry coal (V_w/V_d).

In the preceding equations, adsorbed gas was estimated per gram of moisture- and ash-free (maf) coal. To estimate the gas content of coal in place, the calculated gas content is multiplied by the factor (100 minus the percentage of moisture minus the percentage of ash)/100. Incorporating the factors discussed above, a general equation for estimating adsorbed gas content of coal in place can be written as follows:

$$V, \text{cm}^3/\text{g} = \frac{(100 - \% \text{ moisture} - \% \text{ ash})}{100} \frac{V_w}{V_d} [k_o P^{n_o} - b (1.8h/100 + 11)]. \quad (1)$$

If P is estimated from the hydrostatic head, the equation is

$$V, \text{cm}^3/\text{g} = \frac{(100 - \% \text{ moisture} - \% \text{ ash})}{100} \frac{V_w}{V_d} [k_o (0.096h)^{n_o} - b (1.8h/100 + 11)], \quad (2)$$

where h is the depth, in meters.

ESTIMATING THE METHANE CONTENT OF COAL

Depending on the amount of information available, the gas content of a coal can be estimated in several ways. If the coal is listed in table 1 and if the pressure at depth is known, equation 1 can be used directly. For example, during drilling in the Castlegate coalbed in Utah, measured pressure was 24 atm at a depth of 310 m. From table 1, the constants for this coal are $k_o = 4.9$, $n_o = 0.37$, $b = 0.12$, and $V_w/V_d = 0.42$. Moisture and ash content totaled 8 pct. Using these values in equation 1, the estimated methane content of the Castlegate coal is $5.3 \text{ cm}^3/\text{g}$; the direct determination for this coal was $4.7 \text{ cm}^3/\text{g}$.

For coals that are not listed in table 1, adsorption constants can be estimated from proximate analysis. For a sample of the Lower Hartshorne coal from Oklahoma, the fixed carbon content was 80 pct maf, and volatile matter, 20 pct maf; moisture and ash content equaled 13 pct. Calculated values for the adsorption constants are $k_o = 8.7$ and $n_o = 0.28$. The average value of the temperature constant is $0.14 \text{ cm}^3/\text{g}^\circ \text{C}$, and V_w/V_d calculated according to equations in appendix B is 0.82. Measured pressure in the coalbed was 17 atm at a depth of 450 m. Using these data to calculate the methane content, a value of $11.8 \text{ cm}^3/\text{g}$ is obtained, compared with $11.1 \text{ cm}^3/\text{g}$ obtained by direct determination.

When pressure is estimated as a function of depth, the accuracy of the gas-content estimate depends on how closely the pressure gradient approaches

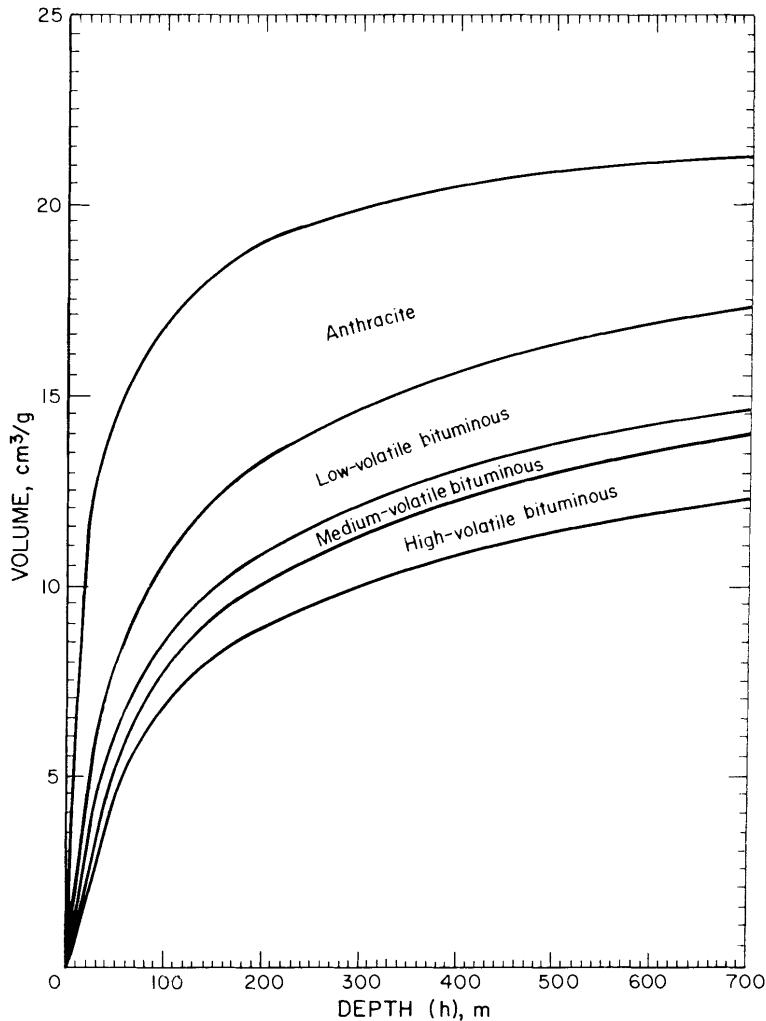


FIGURE 5: - Estimated methane content with depth and rank.

determination is considered accurate to ± 30 pct, and most of the values estimated from the adsorption graph are within ± 30 pct of the direct determinations.

the normal value of 0.096 atm/m. For example, for the Upper Freeport coal at a depth of 275 m, the gas content estimated with equation 2 is 9.5 cm³/g, but the direct determination is 3.9 cm³/g. The measured pressure gradient in this area of the Lower Freeport coal is 0.046 atm/m, approximately one-half of the normal value. The anomalously low pressure could account for the low gas content.

If it is assumed that the sum of the moisture and ash content is 10 pct, an estimated gas-content range can be calculated for various ranks of coal and depicted graphically (fig. 5). Although the range of gas content at a given depth becomes larger for higher rank coals, a reasonable estimate of the gas content of most coals can be obtained from the graph. When the estimated gas content is compared with the direct determination (table 2), the agreement is reasonably good. Direct

TABLE 2. - 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
Peach Mountain No. 18.	183	600	13	416	13-18	416-576	0
	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
Hartshorne.....	226	742	14	448	11-14	352-488	0
	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	488-544	0
	621	2,038	17	544	14-17	448-544	0
	529	1,736	11	352	14-17	488-544	-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	352-488	-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 direct determinations; usually such coals are low in rank and relatively shallow. For example, in table 2, 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. Using the pressure gradient 0.046 atm/m and the values of the constants listed for the Pittsburgh coal in table 1, gas contents were calculated for the coals in table 3 with the following equation:

$$V = 0.90 (0.55) [5.5 (0.046h)^{0.33} - 0.14 (1.8h/100 + 11)].$$

Values calculated with this equation are in better agreement with the direct-determination values (table 3).

TABLE 3. - 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
	259	850	7	224	5	160	+2

The direct determinations in table 3 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 must be considered in evaluating the accuracy of the estimate of a coal's 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. Rather than base the gas content estimates on insufficient data, estimates were limited to the higher rank coals. In view of the number of variables and assumptions, the gas content estimated from adsorption data

provides a general standard for determining the gassiness of most bituminous coals.

DISCUSSION

The estimated methane content of a coal can be used in mine planning and resource evaluation. In mining, the amount and rate of methane released depend on factors such as rib extent, age of the mine, production rate, gob area, and permeability of the coal. However, a simple measure of the gassiness of a mine is the methane content of the coal. When planning a mine, an estimate of the coal's gas content can be used to estimate methane production rates and ventilation requirements. The following example is based on data for the Lower Kittanning coalbed in Pennsylvania. All other factors being equal, a mine in which the methane content of a medium-volatile bituminous coal is $6.0 \text{ cm}^3/\text{g}$ at 50 m (163 ft) could produce $1.5 \text{ MMft}^3/\text{day}$ of methane; in a mine at 150 m (490 ft) with a methane content of $9.5 \text{ cm}^3/\text{g}$, the methane production rate would be $2.4 \text{ MMft}^3/\text{day}$. At 250 m (810 ft), the methane production rate could be $3.2 \text{ MMft}^3/\text{day}$ from coal with a methane content of $11.2 \text{ cm}^3/\text{g}$. Ventilation capacity for the deepest mine would have to be at least double that of the shallowest mine.

The estimated gas content can also be used to evaluate potential gas resources in coal. For example, assume that a high-volatile bituminous coal is known to underlie a 10- by 20-mile area; the average depth to the coal is 150 m (approximately 500 ft) and average coal thickness is 15 in. The 290 million tons of coal in this area is inaccessible to strip mining and too thin to be economically deep mined. The methane content of this coal (estimated from fig. 5) is $8.1 \text{ cm}^3/\text{g}$, or $260 \text{ ft}^3/\text{ton}$. Therefore, this relatively small, uneconomic coalbed contains 75 billion ft^3 of methane. Draining 50 pct of this would provide enough gas to heat 30,000 homes for 10 years. Of 727 billion tons of bituminous coal in the coterminous United States, only 60 pct is considered minable by current methods.⁵ To get the most of limited energy resources, the 290 billion tons of "uneconomic" coals could be considered as gas reservoirs, potentially containing over 70 trillion ft^3 of high-Btu gas.

The relationship between rank, depth, and gas content developed in this report can be extended to deeply buried coals. An estimated 378 billion tons of coal lie between 1,000 and 2,000 m below the surface of the coterminous United States.⁶ Using $15 \text{ cm}^3/\text{g}$ ($480 \text{ ft}^3/\text{ton}$) as a minimum gas content, these coals could contain 181 trillion cubic feet of gas. Using the data in this report as a basis for speculating on the gas content of thin coalbeds and deeply buried coals, these coals could contain over 250 trillion ft^3 of high-Btu gas, the equivalent of a 10-year supply of natural gas.

⁵Estimates of coal resources are from: Averitt, P. Coal Resources of the United States, January 1, 1974. Geol. Survey Bull. 1412, 1975, 131 pp.

⁶Work cited in footnote 5.

CONCLUSION

The gas-adsorption capacity of coal depends upon pressure, temperature, and rank. Since pressure and temperature are functions of depth, the gas content of most coals can be estimated from rank and depth or calculated from the general adsorption equation. In some cases, factors such as high moisture content, low pressure gradient, and anomalous temperatures should be considered in evaluating the accuracy of the gas-content estimate. The estimates of coalbed gas content derived from adsorption data provide reasonable preliminary figures and can be developed using readily available data.

BIBLIOGRAPHY

1. Joubert, J. I., C. T. Grein, and D. Bienstock. Sorption of Methane in Moist Coal. *Fuel*, v. 52, 1973, pp. 181-185.
 2. _____. Effect of Moisture on the Methane Capacity of American Coals. *Fuel*, v. 53, 1974, pp. 186-191.
 3. Kim, A. G. The Composition of Coalbed Gas. BuMines RI 7762, 1973, 9 pp.
 4. Kim, A. G., and L. J. Douglas. Gases Desorbed From Five Coals of Low Gas Content. BuMines RI 7768, 1973, 9 pp.
 5. Kissell, F. N., C. M. McCulloch, and C. H. Elder. The Direct Method of Determining Methane Content of Coalbeds for Ventilation Design. BuMines RI 7767, 1973, 17 pp.
 6. McCulloch, C. M., J. R. Levine, F. N. Kissell, and M. Deul. Measuring the Methane Content of Bituminous Coalbeds. BuMines RI 8043, 1975, 21 pp.
 7. McCulloch, C. M., and W. P. Diamond. Inexpensive Method Helps Predict Methane Content of Coalbeds. *Coal Age*, v. 81, No. 6, June 1976, pp. 102-106.
 8. Ruppel, T. C., C. T. Grein, and D. Bienstock. Adsorption of Methane/Ethane Mixtures on Dry Coal at Elevated Pressure. *Fuel*, v. 51, 1972, pp. 297-303.
 9. _____. Adsorption of Methane on Dry Coal at Elevated Pressure. *Fuel*, v. 53, 1974, pp. 152-162.
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APPENDIX A.--ESTIMATING METHANE CONTENT FROM ADSORPTION ISOTHERMS

Coal is a porous solid that can adsorb gas on the internal surface of its micropores. The amount of gas adsorbed depends upon pressure and temperature. The adsorptive capacity of a solid is determined by measuring the amount of gas adsorbed at various pressures and constant temperature. This procedure is repeated at several temperatures to obtain a series of adsorption isotherms (fig. A-1). Empirically, adsorption isotherms can be described by the equation

$$V = kP^n, \quad (\text{A-1})$$

where V = volume adsorbed, in cubic centimeters per gram of moisture- and ash-free coal;

P = pressure, in atmospheres;

k = a constant, in cubic centimeters per gram per atmosphere;

and n = a constant.

The constants k and n vary with temperature. Rather than determine these constants for all temperatures of interest, the effect of temperature can be estimated by using the following equation:

$$V = k_0 P^{n_0} - bT, \quad (\text{A-2})$$

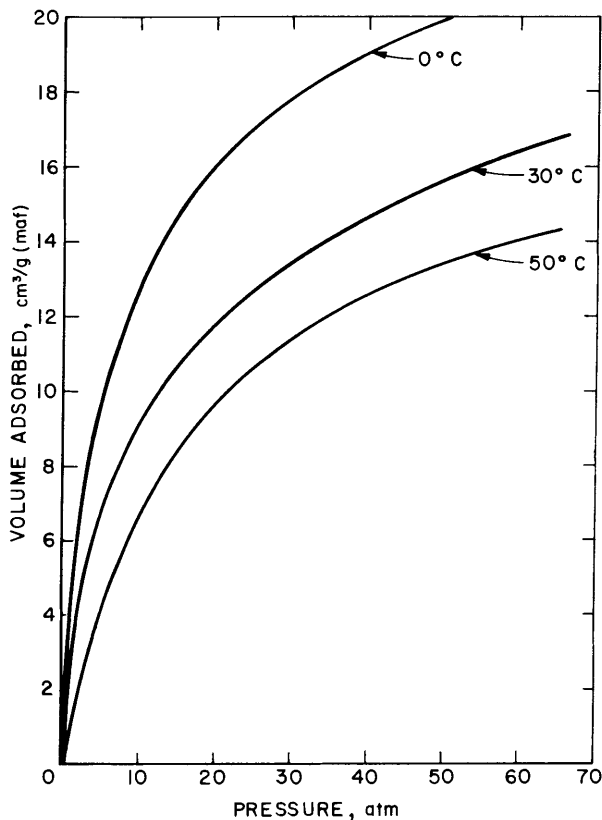


FIGURE A-1. - Adsorption isotherm.

where k and n are determined at a reference temperature (in this case 0°C); b is a constant, in cubic centimeters per gram per degree Centigrade; and T is the temperature, in degrees Centigrade.

To determine k_0 and n_0 , equation 1 is converted to logarithmic form:

$$\text{Log } V = \log k + n \log P. \quad (\text{A-3})$$

Plotting $\log V$ versus $\log P$ (with values of V and P taken from the 0°C isotherm) gives a straight line in which $\log k_0$ is the intercept and n_0 is the slope (fig. A-2). The temperature constant b is determined by plotting V versus T at constant pressure; b is the slope of the straight line (fig. A-3).

The constants k_0 , n_0 , and b were determined for the coals listed in table A-1. Experimental procedures used to determine the isotherms for dry coal are described in a previous report (1). Values of k_0 , n_0 , and b , determined from the isotherms for dry coal, are listed in table A-2. When k_0 and n_0 are plotted versus fixed carbon (fig. A-4), the straight lines obtained are described by the equations:

$$k_0 = 0.25 \text{ FC} - 9.41 \quad (r = 0.82), \quad (\text{A-4})$$

and
$$n_0 = 0.55 - 0.004 \text{ FC} \quad (r = 0.86). \quad (\text{A-5})$$

The regression coefficients for these lines, 0.82 and 0.86 for equations A-4 and A-5, respectively, show that the experimental data are in fair agreement with the linear equations. To minimize the deviation from the straight line at high and low values of fixed carbon, values of k_0 are plotted versus FC/VM (fig. A-5) to obtain the following equation:

$$k_0 = 0.79 \text{ FC}/\text{VM} + 5.62 \quad (r = 0.93), \quad (\text{A-6})$$

which has a regression coefficient of 0.93. The constant n_0 can be related to k_0 , since both are functions of rank, by the following equation:

$$n_0 = 0.39 - 0.013 k_0 \quad (r = 0.87). \quad (\text{A-7})$$

Values of k_0 and n_0 , calculated using equations A-6 and A-7, are listed in table A-2. Calculated values are generally within ± 20 pct of the experimentally determined value.

The temperature constant b (table A-2) does not vary with rank. It has a mean value of $0.14 \text{ cm}^3/\text{g}^\circ \text{C}$ with a standard deviation of ± 0.02 .

TABLE A-1. - Analyses of coal samples

Coal	Location (county and State)	Proximate analysis, pct			
		Moisture	Ash	Fixed carbon	Volatile matter
Mammoth.....	Schuylkill, Pa.....	1.4	7.9	86.5	4.2
Pocahontas No. 3.....	Wyoming, W. Va.....	0.3	5.4	75.0	19.3
Do.....	Buchanan, Va.....	.7	8.8	72.1	18.4
Lower Kittanning.....	Cambria, Pa.....	1.2	8.8	70.5	19.5
Do.....do.....	1.2	16.5	65.1	17.2
Beckley.....	Raleigh, W. Va.....	.7	22.9	61.0	15.4
Mary Lee.....	Jefferson, Ala.....	.7	9.3	70.1	19.9
Upper Freeport.....	Indiana, Pa.....	1.2	2.1	66.9	29.8
Lower Freeport.....do.....	.4	9.4	66.4	23.8
Upper Freeport.....do.....	1.0	7.6	63.6	27.8
Mary Lee.....	Jefferson, Ala.....	.6	15.9	62.4	21.1
Upper Freeport.....	Indiana, Pa.....	2.3	11.3	59.2	27.2
Pittsburgh.....	Washington, Pa.....	.9	4.0	63.4	31.7
Sewell.....	Randolph, W. Va.....	.6	2.9	62.2	34.3
No. 5 Block.....	Boone, W. Va.....	1.5	3.9	56.7	37.9
Pittsburgh.....	Greene, Pa.....	1.2	6.8	54.6	37.4
Mary Lee.....	Walker, Ala.....	1.4	15.2	52.5	30.9
Pittsburgh.....	Washington, Pa.....	1.3	9.3	52.0	37.4
Do.....	Marion, W. Va.....	.9	8.8	51.1	39.2
Somerset B.....	Gunnison, Colo.....	2.4	5.6	52.6	39.4
Castlegate.....	Carbon, Utah.....	2.0	6.4	45.4	46.2
Rosebud.....	Rosebud, Mont.....	18.7	10.2	40.6	30.5
Elkhorn No. 3.....	Floyd, Ky.....	NA	9.8	NA	NA
Hazard No. 4.....	Kentucky.....	NA	19.0	NA	NA
Pocahontas No. 4.....	McDowell, W. Va.....	NA	11.3	NA	NA
Do.....	Raleigh, W. Va.....	NA	8.3	NA	NA
Stearns No. 2.....	Kentucky.....	NA	14.4	NA	NA
Hazard No. 7.....do.....	NA	19.0	NA	NA
Pittsburgh.....	Allegheny, Pa.....	NA	¹ 4.8	¹ 56.4	¹ 38.8
Pocahontas No. 3.....	Buchanan, Va.....	NA	¹ 8.9	¹ 72.5	¹ 18.6

NA--Not available.

¹Moisture-free basis.

TABLE A-2. - Adsorption constants for methane on coal

Coalbed	$k_o, \text{cm}^3/\text{g atm}$		n_o		$b, \text{cm}^3/\text{g}^\circ \text{C}$
	Exper- imental	Calculated from equation A-6	Exper- imental	Calculated from equation A-7	
Mammoth.....	21.1	22.0	0.15	0.10	0.18
Pocahontas No. 3.....	8.2	8.7	.27	.28	.13
	8.9	8.7	.26	.28	.14
Lower Kittanning.....	9.6	8.5	.27	.28	.17
	11.1	8.6	.24	.28	.17
Beckley.....	10.6	8.7	.27	.28	.15
Mary Lee.....	9.7	8.4	.24	.28	.15
Upper Freeport.....	6.8	7.4	.29	.29	.12
Lower Freeport.....	8.7	7.8	.26	.29	.14
Upper Freeport.....	7.2	7.4	.27	.29	.12
Mary Lee.....	9.0	8.0	.27	.29	.15
Upper Freeport.....	6.3	7.3	.29	.30	.11
Pittsburgh.....	5.4	7.2	.35	.30	.13
Sewell.....	6.6	7.1	.29	.30	.13
No. 5 Block.....	6.2	6.8	.30	.30	.12
Pittsburgh.....	4.6	6.8	.38	.30	.12
Mary Lee.....	8.1	7.0	.28	.30	.15
Pittsburgh.....	6.2	6.7	.30	.30	.12
	5.8	6.7	.30	.30	.11
Somerset B.....	6.8	6.7	.32	.30	.15
Castlegate.....	4.9	6.4	.37	.31	.12
Rosebud.....	7.5	6.7	.34	.30	.15
Elkhorn No. 3.....	6.8	NA	.29	NA	.13
Hazard No. 4.....	6.1	NA	.31	NA	.12
Pocahontas No. 4.....	10.2	NA	.26	NA	.16
	10.0	NA	.26	NA	.15
Stearns No. 2.....	4.6	NA	.34	NA	.11
Hazard No. 7.....	7.0	NA	.32	NA	.14
Pittsburgh.....	6.5	6.8	.30	.38	.13
Pocahontas No. 3.....	8.9	8.7	.23	.27	.13

NA--Not available.

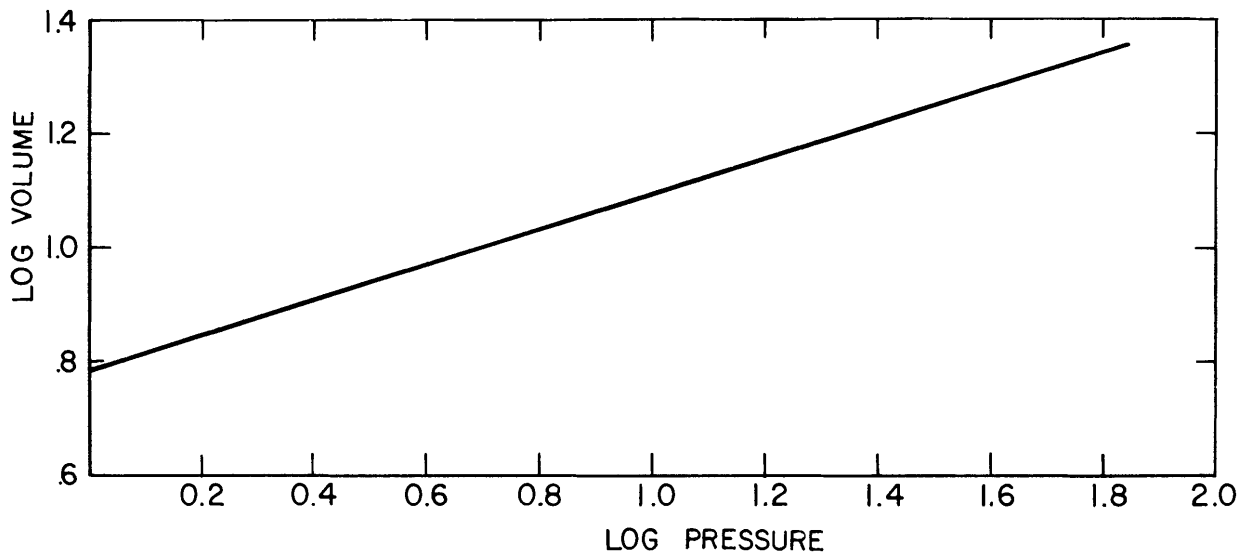


FIGURE A-2. - Log-log plot of volume adsorbed versus pressure.

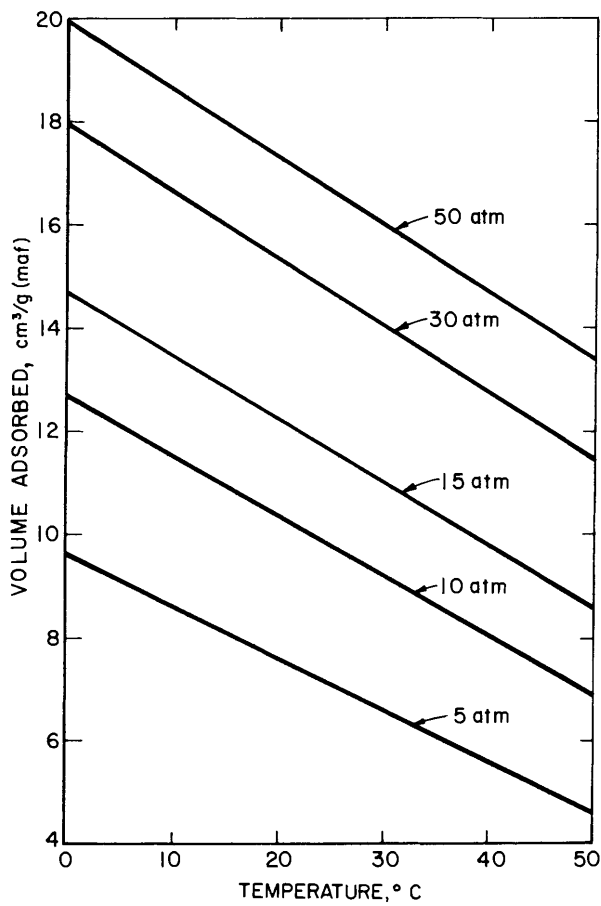
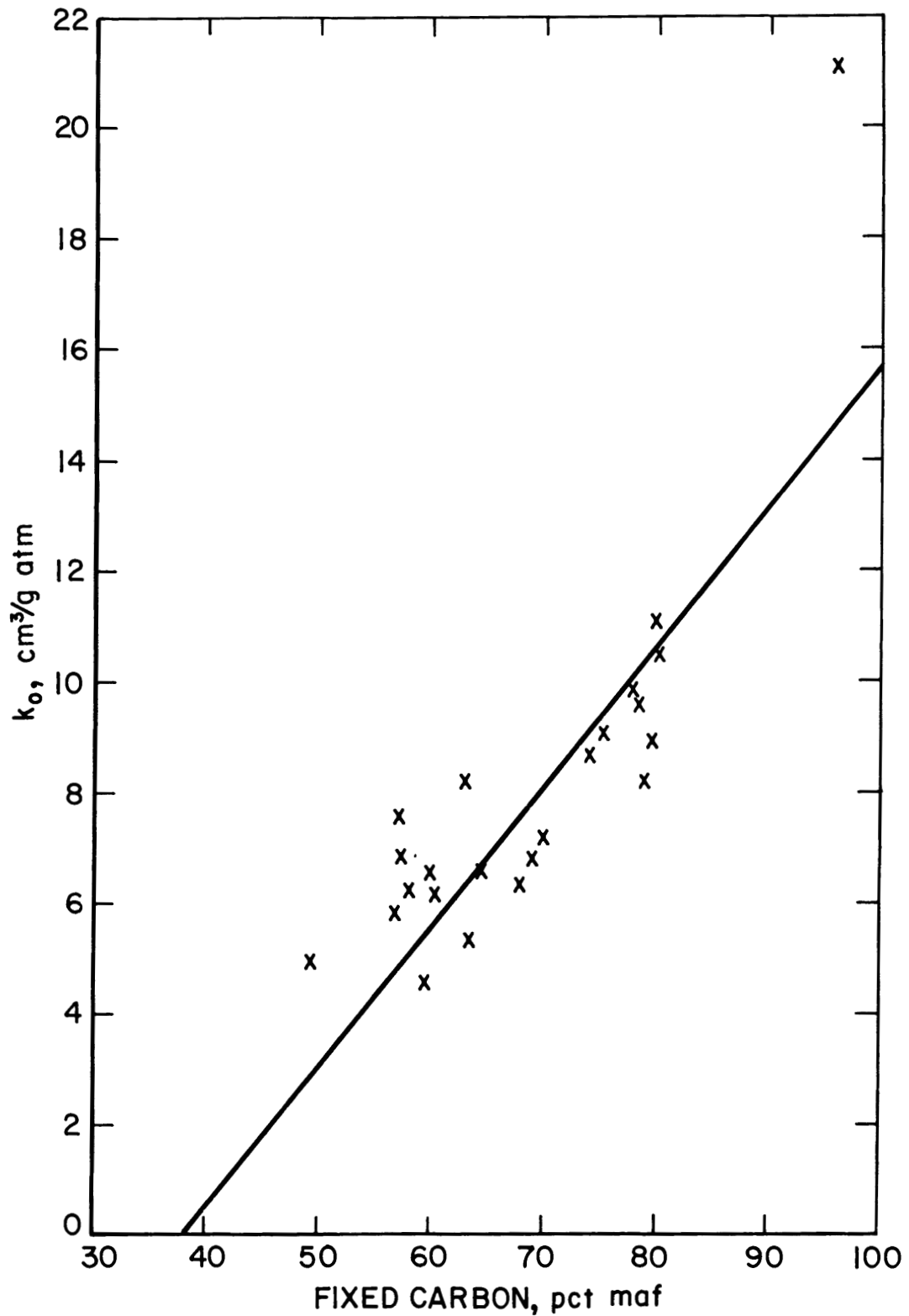


FIGURE A-3. - Volume adsorbed versus temperature at constant pressures.

FIGURE A-4. - Relationship of k_o to fixed carbon.

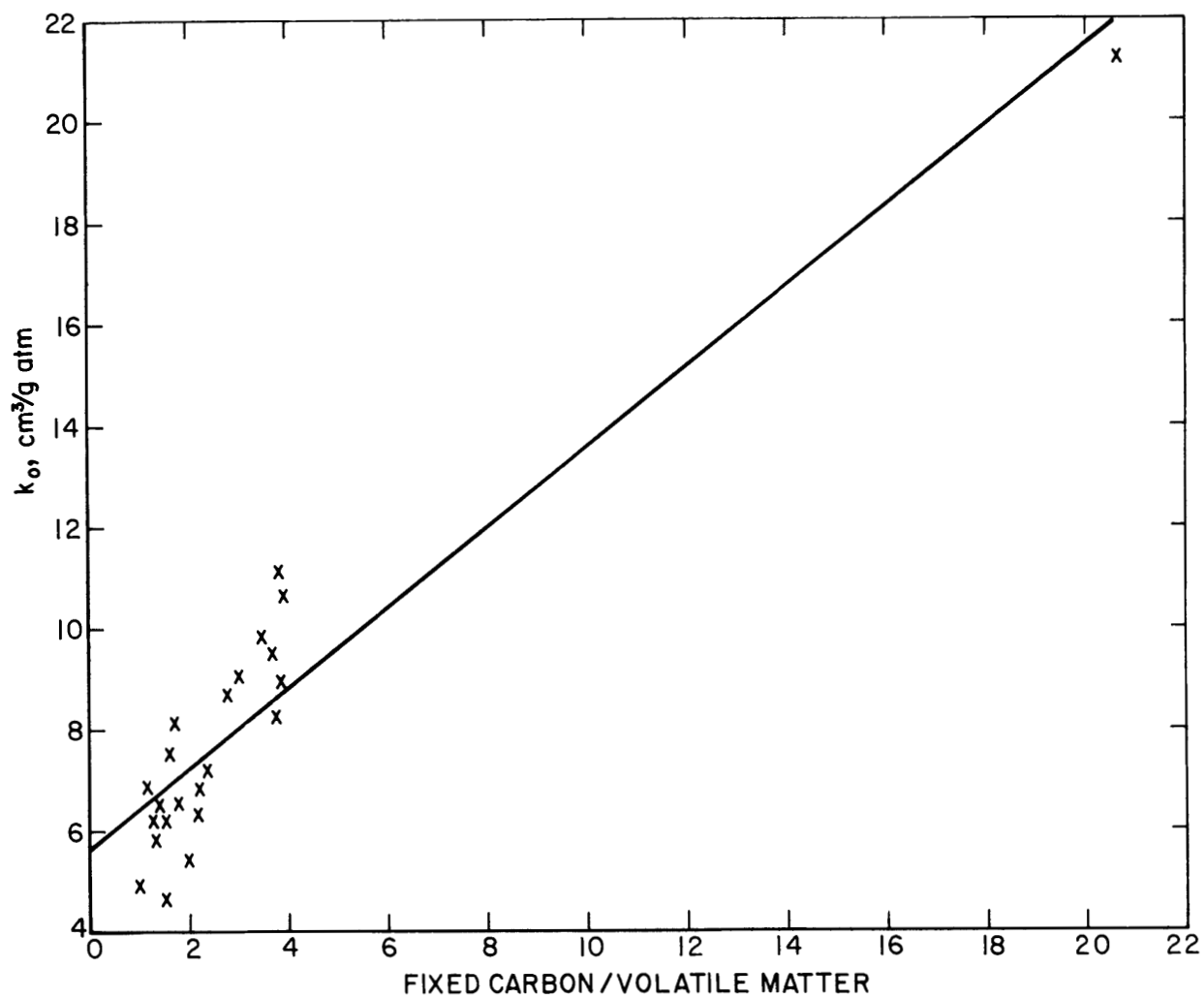


FIGURE A-5. - Relationship of k_o to the ratio of fixed carbon to volatile matter (FC/VM).

APPENDIX B. --ESTIMATING THE EFFECT OF MOISTURE
ON THE ADSORPTIVE CAPACITY OF COAL

The amount of gas that can be adsorbed by coal is inversely related to its moisture content, up to a critical moisture-content value (1-2). Above this value, which is apparently related to the oxygen content of the coal, additional moisture has no effect upon adsorptive capacity. Using the equation

$$m_c = (C_1 X_o + C_2) / C_o (1 - C_1 X_o - C_2), \quad (B-1)$$

where C_o , C_1 , and C_2 are constants,¹ and X_o is the percentage of oxygen, maf, the critical moisture was calculated for most of the coals listed in table A-1,² and compared with "as-received" moisture (table B-1). Generally, the calculated critical moisture is greater than the as-received moisture.

When ratios of adsorptive capacity in moist and dry coal (V_w/V_d) are calculated with the equation

$$V_w/V_d = 1 / (C_o m + 1) \quad (B-2)$$

(table B-1), the ratio is approximately the same for both critical and as-received moisture. With the exception of the subbituminous Rosebud coal, the ratio of gas adsorbed in wet and dry coal (V_w/V_d) has a mean value of 0.73 with a standard deviation of ± 0.13 . In the absence of other data, the amount of gas adsorbed in moist coal can be estimated as 75 pct of that adsorbed on dry coal.

¹The constants C_o and C_2 display some variation with pressure. However, the effect is small, and has been ignored in these calculations.

²Complete analyses were not available for all coal samples listed in table A-1.

TABLE B-1. - Critical moisture and reduction
in adsorptive capacity

Coalbed	Critical moisture, ¹ pct	As-received moisture, pct	V_w/V_d ²	V_w/V_d ³
Mammoth.....	1.0	1.4	0.80	0.74
Pocahontas No. 3.....	1.4	0.3	.74	.93
	1.2	.7	.77	.85
Lower Kittanning.....	1.4	1.2	.74	.77
	1.1	1.2	.78	.77
Beckley.....	1.2	.7	.77	.85
Mary Lee.....	1.4	.7	.74	.85
Upper Freeport.....	2.2	1.2	.65	.77
Lower Freeport.....	1.8	.4	.69	.91
Upper Freeport.....	1.0	1.0	.80	.80
Mary Lee.....	2.0	.6	.67	.87
Upper Freeport.....	1.2	2.3	.77	.63
Pittsburgh.....	4.1	.9	.49	.82
Sewell.....	1.6	.6	.71	.87
No. 5 Block.....	3.3	1.5	.55	.73
Pittsburgh.....	2.3	1.2	.63	.77
Mary Lee.....	4.1	1.4	.49	.74
Pittsburgh.....	3.3	1.3	.55	.75
	2.5	.9	.62	.82
Somerset B.....	6.1	2.4	.40	.63
Castlegate.....	5.6	2.0	.42	.67
Pittsburgh.....	3.2	NA	.55	NA
Pocahontas No. 3.....	1.2	NA	.77	NA
Rosebud.....	28.8	18.7	.12	.18

NA--Not available.

$$^1 m_c = \frac{(0.05X_o + 0.083)}{0.25 (1 - 0.05X_o - 0.083)}$$

² Calculated from critical moisture.

³ Calculated from as-received moisture.