

THE DIRECT METHANATION OF COAL

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The fact that coal is composed of various fractions with widely varying properties has long been realized. Recent attention to this fact has resulted in a number of proposed staged gasification schemes. In particular, research at BCR has led to the concept of a two-stage super-pressure gasifier to take specific advantage of the varied nature of coal in the production of a gas rich in methane and amenable to conversion to a high Btu pipeline gas. The two-stage super-pressure gasifier utilizes synthesis gas and heat generated in a high temperature stage to convert a portion of fresh coal in a lower temperature stage into a methane-rich gas.(5)

A study of the methane formation occurring at short gas-coal contact times in the low temperature stage is being carried out at Bituminous Coal Research, Inc., for the Office of Coal Research. This program has included batch tests in rocking autoclaves and continuous flow experiments in an externally-heated 5 lb/hr continuous flow reactor (CFR).(8) Tests in this unit have been carried out under a wide variety of conditions using North Dakota lignite, Elkol subbituminous "C" and Pittsburgh high volatile "A" bituminous coals. The program has produced considerable data on the methanation step and has led to the design and construction of an internally-fired 100 lb/hr process and equipment development unit now being placed in operation.(9)

This paper presents a method of analysis of the short contact time methanation step, based on the premise that rapid heating of coal in the presence of hydrogen produces, in addition to gaseous pyrolysis products, an active but transient species which undergoes rapid reaction with hydrogen to produce additional methane. A simplified rate expression is used to derive a relationship between methane yield and hydrogen partial pressure which fits the experimental data obtained by others.(8,13,16)

Background

Until recently, studies of the coal-hydrogen reaction were generally carried out with long gas-coal contact times, and the results are not directly applicable to short contact time methanation. Von Fredersdorf and Elliott (17) have provided an excellent review of the many such investigations through 1963. Although various methods of contacting were tried and a number of mechanisms for the reaction proposed, the general consensus based on these investigations was that the rate of methane production from coal or char is approximately proportional to hydrogen partial pressure, with the constant of proportionality dependent upon temperature, coal type, and percent carbon burnoff.

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Recent investigations have indicated that the rate of methane production varies with gas-coal reaction time. In experiments carried out at the U.S. Bureau of Mines, Hiteshue *et al.*, studied the hydrogasification of bituminous coals, lignite, anthracite, and char (10) and high volatile "A" bituminous coal. A packed bed of coal was used in these studies, but because of heating capacity limitations, two minutes were required to raise the system temperature to 800 C. Nevertheless, the Bureau of Mines group was able to demonstrate that the test coals reacted with hydrogen in the initial period at a rate much higher than that observed at longer contact times.

Further indication of the rapid gasification rates during the initial contact period was obtained by Feldkirchner and Linden in their study of high-pressure gasification with hydrogen and steam.(6)

In 1965, Moseley and Paterson (14,15) demonstrated this rapid initial rate more conclusively and reported the results of their experiments on the high-temperature hydrogenation of coal chars at hydrogen partial pressures up to 1000 atmospheres. By means of a specially constructed reactor heating device, Moseley and Paterson obtained rate data for methane production in 15-second intervals. With this resolution, they observed a rapid initial rate, which decreased with time until a final steady value was obtained. The steady-state methane production rate had many of the characteristics of rate data as reported earlier by others, i.e., it was roughly proportional to hydrogen partial pressure and depended on char type. However, the rapid initial rate necessitated a new explanation and prompted Moseley and Paterson to suggest a three-step mechanism for the solid phase hydrogenation of coal.

The first step is the devolatilization of coal by a process which is activated by hydrogen but whose rate is not affected by hydrogen. In addition to volatile products, a char is produced in this first step with exposed or labile carbon atoms, which is particularly susceptible to reaction with hydrogen. The second step in the proposed mechanism involves the reactions of the labile carbon atoms, either with hydrogen to form methane or with each other in a cross-linking polymerization to form an inactive char. The third step involves the slow reaction of hydrogen with the inactive char.

Blackwood and McCarthy (3) have discounted the three-step process, offering instead a two-step mechanism consisting of a rapid reaction of hydrogen with groupings in the coal which are associated with oxygen followed by a more sedate attack on the residual carbon structure. Blackwood and McCarthy cited their own data (2,3) as well as Hiteshue's data (10,11) to support their claim, but, in fact, the poor initial time resolution of these data makes it difficult to distinguish between a two- or three-step process.

On the basis of their three-step model, Moseley and Paterson (15) projected that contact times in excess of 0.5 second were unlikely to lead to significant gains in the extent of carbon conversion to methane, and

that complete conversion of the carbon in coal to methane should be possible at 1000 C and 500 atm hydrogen partial pressure. In 1967, they published results of rapid high-temperature hydrogenation of bituminous coal, virtually substantiating their claim.(16) The carbon in the coal was gasified to completion at 500 atm and 900 C.

In point of fact, for contact times of a few seconds, only the first two steps of the three-step model are significant, and a satisfactory accounting of the direct methanation of coal may be obtained on this basis. Moseley and Paterson have presented mathematical relationships between methane yield and gasifier parameters, derived on the assumptions that the decomposition of structures in coal to give the active intermediate is a first-order process, and that the intermediate is simultaneously removed by a first-order process. Methane formation is assumed to give no net consumption of the active species. In this paper, alternate rate expressions are proposed for the first two steps, which result in a simple methane yield expression that properly extrapolates to low and high conversion.

The Initial Reaction

Studies of the thermal decomposition of coal have been carried out at BCURA, largely because of the importance of devolatilization in the ignition process of coal particles in pulverized fuel firing.(1,7) Although a large number of complex chemical reactions and physical changes are known to make up the devolatilization process, workers at BCURA were able to represent the grams of carbon lost as methane per gram of starting carbon, ΔW_I , for twelve coals tested as a function of absolute temperature, T, and time of residence at this temperature, t:

$$\Delta W_I = VM (1-C)Q \left\{ (1 - \exp - A [\exp - (B/T)] t) \right\} \quad (1)$$

where VM = volatile matter in coal on daf basis

Q = ratio of weight loss to change in volatile matter

ABC = empirical constants

Their results were obtained for 20 μ coal particles heated at rates of 2.5×10^4 to 5×10^4 C/sec. Since the mechanism for thermal decomposition depends upon the rate of heating of the coal particles, the quantitative results of this research may not apply directly to the initial reactions occurring in the direct methanation of coal. However, many of the aspects will undoubtedly remain the same--particularly the rapidity of the overall process.

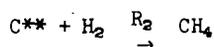
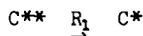
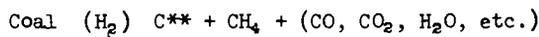
By using typical values reported for the constants in Equation 1, $A = 1 \times 10^6$ sec; $B = 8900$ K, a time constant for the devolatilization process of 14 milliseconds is obtained at a temperature of 1750 F.

The significance of this value is its indication that the initial reaction per se should be essentially complete as soon as hot hydrogen-containing gas contacts the coal feed.

The amount of carbon, ΔW_I , released as methane to the gas phase during this initial step may be dependent on temperature and coal type, but should be independent of other gasifier parameters such as residence time and gas composition.

As indicated by Moseley and Paterson, the presence of hydrogen does, without a doubt, activate the initial "breakdown" of the basic coal "molecule" during thermal depolymerization. Because of the rapidity of these reactions, little experimental evidence has been accumulated to indicate the degree to which the presence of hydrogen affects the rate of this initial "breakdown."

It is apparent, however, both from the work data of Moseley and Paterson and of Glenn and co-workers, that a highly active species or intermediate appears to be the principal primary product of this initial breakdown. This may be shown schematically as:



where,

C^{**} = active intermediate produced directly from coal when coal is thermally depolymerized; and

C^* = inactive char produced by reaction of the active intermediate with itself.

The Active Intermediate

The specific chemical processes involving the active intermediate are very complex; any attempt to model them must be viewed, as approximate. The approach taken by the present authors, as opposed to that proposed by Moseley and Paterson, is to consider explicitly the competition between the methanation reaction and the inactive char-forming reaction for the active intermediate.

To this end, consider that coal particles containing one gram of carbon are introduced into a reactor, maintained at a constant temperature, T , together with a gas whose hydrogen partial pressure is P_{H_2} . Consider that there is a sufficient supply of hydrogen so that P_{H_2} does not change as methanation proceeds and that the total gas-coal contact time in the reactor is τ . Assume that upon completion of the initial reaction W_0^* gram of active intermediate has been formed; W_0^* may in general be some fraction, f , of the ungasified carbon and that W_0^* may be represented by $f(1 - \Delta W_I)$.

The rate of reaction of hydrogen with carbon is generally taken as a linear function of hydrogen partial pressure and expressed per unit of surface area available for reaction.(4) If then, the rate at which the

active intermediate is removed by the char-forming mechanism is assumed to be a first-order process, a similar behavior may be postulated for the active intermediate, and the net rate of change of W^* , the grams of active intermediate per gram of carbon fed, will be given by the following:

$$\frac{dW^*}{dt} = k_1^1 (P_{H_2}) A^* - k_2 W^* \quad (2)$$

where A^* = area associated with active intermediate

k_1^1, k_2 = rate constants of methane formation and deactivation reactions respectively

There are ways in which A^* may be related to W^* ; however, at the temperatures and rates under which methanation proceeds, it is reasonable to assume that the methane formation reaction proceeds in a topochemical fashion at a shell-like reaction surface surrounding the active species. In this case A^* is proportional to $(W^*)^{2/3}$, so that Equation 2 may be written as follows:

$$\frac{dW^*}{dt} = -k_1 (P_{H_2}) (W^*)^{2/3} - k_2 W^* \quad (3)$$

where the rate constant k_1^1 and the proportionality constant relating A^* to $(W^*)^{2/3}$ have been confined together in the symbol k_1 .

The boundary condition on Equation 3 is that of the completion of the initial reaction (essentially $t = 0$), $W^* = W_0^*$. Equation 3 may be integrated to find W^* at any time t .

$$\int_{W_0^*}^{W^*} \frac{dW^*}{k_1 (P_{H_2}) (W^*)^{2/3} + k_2 W^*} = - \int_0^t dt$$

or

$$\ln \left[\frac{k_1 (P_{H_2}) + k_2 (W^*)^{1/3}}{k_1 (P_{H_2}) + k_2 (W_0^*)^{1/3}} \right] = - \frac{k_2 t}{3} \quad (4)$$

Of particular interest is the time t^* when all of the active intermediate will have disappeared; i.e., at $t = t^*$, $W^* = 0$. From Equation 4

$$t^* = \frac{3}{k_2} \ln \left[1 + \frac{1}{S} \right] \quad (5)$$

where $S = \frac{k_1 (P_{H_2})}{k_2 (W_0^*)^{1/3}} = \frac{k_1 (P_{H_2}) (W_0^*)^{2/3}}{k_2 W_0^*} = \frac{\text{Initial rate of Methanation}}{\text{Initial rate of Deactivation}}$

Notice that S represents a selectivity for the reacting system.

If t^* is less than τ , the gas-coal contact time, then all of the available intermediate will be consumed in the reactor and methane yield will be independent of τ .

In order to compute the methane produced during this process, it is necessary to integrate the rate expression for the reaction of hydrogen with the active intermediate. If W_C denotes the weight fraction of carbon in coal which has appeared as methane, the rate expression for W_C is:

$$\frac{dW_C}{dt} = k_1 (P_{H_2}) (W^*)^{2/3} \quad (6)$$

where $t = 0$ corresponds to the end of the initial reaction and where $W_C = \Delta W_I$. Since the expression for W^* as a function of time is known from Equation 4, Equation 6 may be integrated to $t = t^*$, at which point the active intermediate has been completely consumed and $W_C = \Delta W_C$, the total yield of methane from the short time methanation process. Continued exposure of the inactive char to hydrogen will result in further methane production, but at a much reduced rate. The expression for ΔW_C is obtained from the integral

$$\int_{\Delta W_I}^{\Delta W_C} dW_C = 3W_0^* S \int_0^{t^*} [(1 + S) e^{-\frac{k_2 t}{3}} - S]^2 \frac{k_2}{3} dt$$

When the right hand side of this equation is integrated and the expression for t^* substituted from Equation 5, the resultant expression is:

$$\Delta W_C = \Delta W_I + 3W_0^* S^3 \left[\ln\left(1 + \frac{1}{S}\right) - \left(\frac{1}{S} - \frac{1}{2S^2}\right) \right] \quad (7)$$

If the series expansion for $\ln\left(1 + \frac{1}{S}\right)$ is invoked, the square bracketed term in Equation 7 becomes equal to

$$\frac{1}{3S^3} \left[1 - \frac{3}{4S} + \frac{3}{5S} - \dots \right]$$

which is closely approximated by the rational fraction

$$\frac{1}{3S^3} \left[\frac{1}{1 + \frac{3}{4S}} \right]$$

hence, Equation 7 becomes

$$\Delta W_c = \Delta W_I + \frac{\frac{4}{3} W_o^* S}{1 + \frac{4}{3} S}$$

Again, if W_o^* and S are replaced by their equivalent expressions, the final relationship between methane yield and gasifier parameters is

$$\Delta W_c = \Delta W_I + \frac{\frac{4 F (1 - \Delta W_I) k_1 (P_{H_2})}{3 k_2 (W_o^*)^{1/3}}}{1 + \frac{4 k_1 (P_{H_2})}{3 k_2 (W_o^*)^{1/3}}} \quad (8)$$

Equation 8 predicts that in the absence of hydrogen, methane yield is due only to the thermally induced decomposition. At small hydrogen partial pressures, the denominator is approximately one, and methane yield is proportional to hydrogen partial pressure. At high hydrogen partial pressures, methane yield again becomes constant, being given by the expression $\Delta W_c = \Delta W_I + f (1 - \Delta W_I)$. If $f = 1$, complete methanation of the carbon in coal is possible.

Correlation of Experimental Data

Equation 8 indicates that the methane yield resulting from the direct methanation of coal by gases containing large excesses of hydrogen should be correlated by an equation of the form

$$\Delta W_c = b_1 + \frac{b_2 (P_{H_2})}{1 + b_3 (P_{H_2})} \quad (9)$$

where b_1 , b_2 , and b_3 are correlation constants related to the kinetic parameters for the process.

The methane rate data for lignite and Elkol coal previously reported by Glenn and co-workers (8) were obtained in continuous flow experiments which did not employ large excesses of hydrogen. However, the presence of CO and H₂O in the feed gas permitted replacement of consumed hydrogen via the water-gas shift reaction. Comparison of inlet and outlet gas compositions for these continuous flow experiments shows only slight variations in hydrogen partial pressure values, so that the constancy of P_{H_2} is considered a reasonably valid assumption.

Equation 9 was fitted to the CFR data by a non-linear least squares curve fitting routine.(12) The results of the correlation were:

$$\text{Lignite: } \Delta W_c = 0.07 + \frac{0.0062 (P_{H_2})}{1 + 0.0067 (P_{H_2})} \quad (10)$$

$$\text{Elkol coal: } \Delta W_c = 0.08 + \frac{0.0054 (P_{H_2})}{1 + 0.006 (P_{H_2})} \quad (11)$$

Equation 10 explains 63 percent of the variance in the lignite data; equation 11 explains 52 percent of that in the Elkol coal data. The effect of changes in P_{H_2} on ΔW_c for the two coals is shown in Figure 1. In the operating region for the continuous flow reactor, the hydrogen partial pressures were low enough so that the predicted curve is approximately linear in hydrogen partial pressure.

If the proposed methane-hydrogen relationship is valid, Equations 10 and 11 should extrapolate correctly for methanation experiments carried out at similar temperatures and higher hydrogen partial pressures. In a study of the rapid high-temperature, high-pressure hydrogenation of bituminous coal, Moseley and Paterson gasified coal in pure hydrogen at temperatures of 950 C and pressures as high as 500 atm. (16) Figure 2 presents their experimental data together with typical data points from the CFR experiments of Glenn and co-workers. The curve through the data is Equation 11; the agreement is good over the entire pressure range.

Moseley and Paterson also reported data from a few experiments at 850 C. Since the parameters in the correlating equation depend upon temperature, Equation 11 cannot be applied directly to these lower temperature results. However, an equation of the form of Equation 9 does fit the data quite well, provided the constants are adjusted as indicated in the following equation:

$$\Delta W_c = 0.07 + \frac{0.0033(P_{H_2})}{1 + 0.0035(P_{H_2})} \quad (12)$$

The 850 C data points and Equation 12 are presented in Figure 3.

Lewis, Friedman, and Hiteshue (13) reported data on the direct conversion of untreated bituminous coal into high Btu gas in a dilute-phase concurrent flow apparatus similar to that used by Glenn and co-workers in the CFR experiments, and by Moseley and Paterson in their later work. The residence times used by Lewis *et al* were somewhat longer than those used by Glenn and co-workers and their operating temperature was lower, i.e., 725 C. The data of Lewis *et al* shown in Figure 4 may be correlated by the following equation:

$$\Delta W_c = 0.09 + \frac{0.0016(P_{H_2})}{1 + 0.0017(P_{H_2})} \quad (13)$$

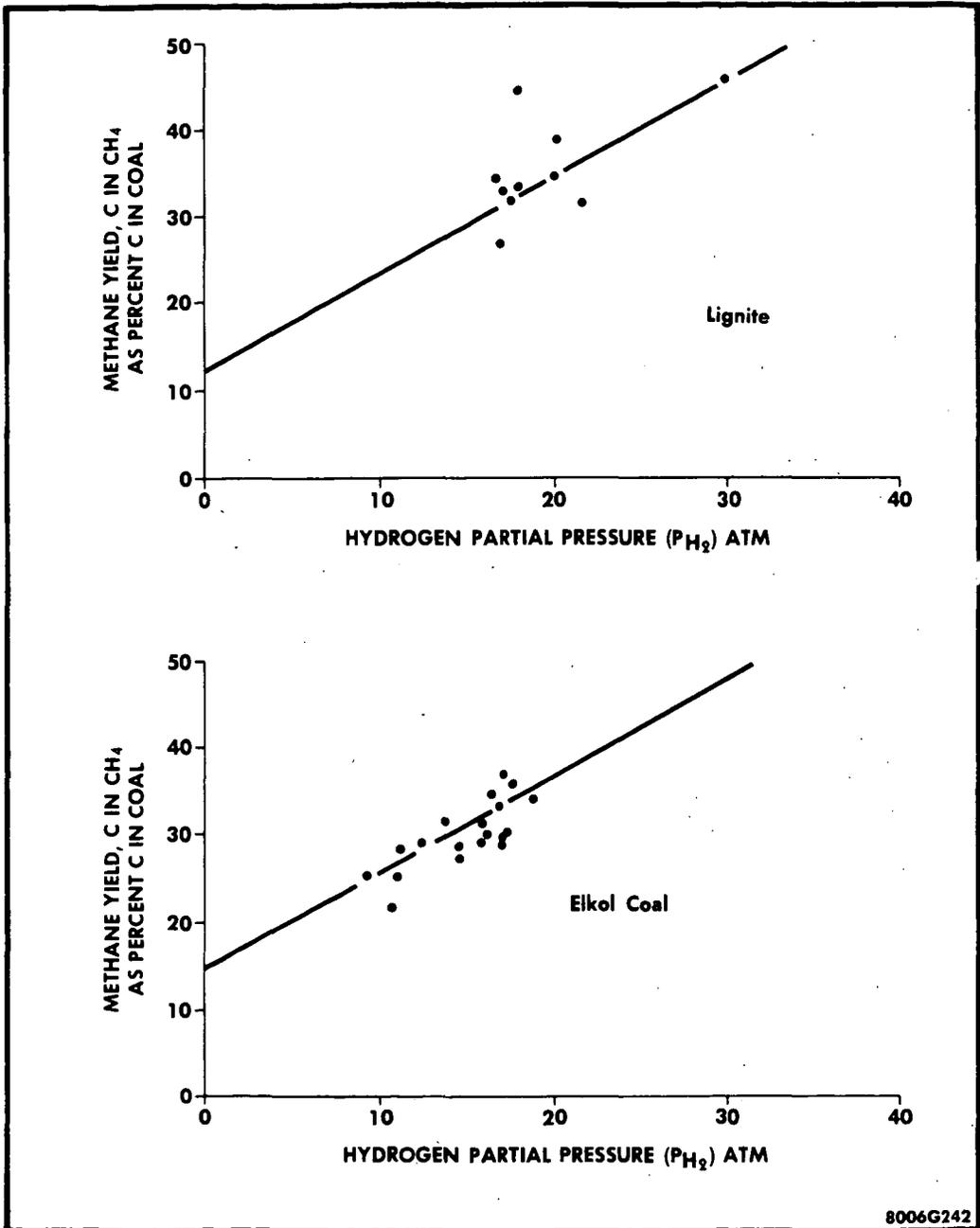


Figure 1. Correlation of Methane Yield with Hydrogen Partial Pressure

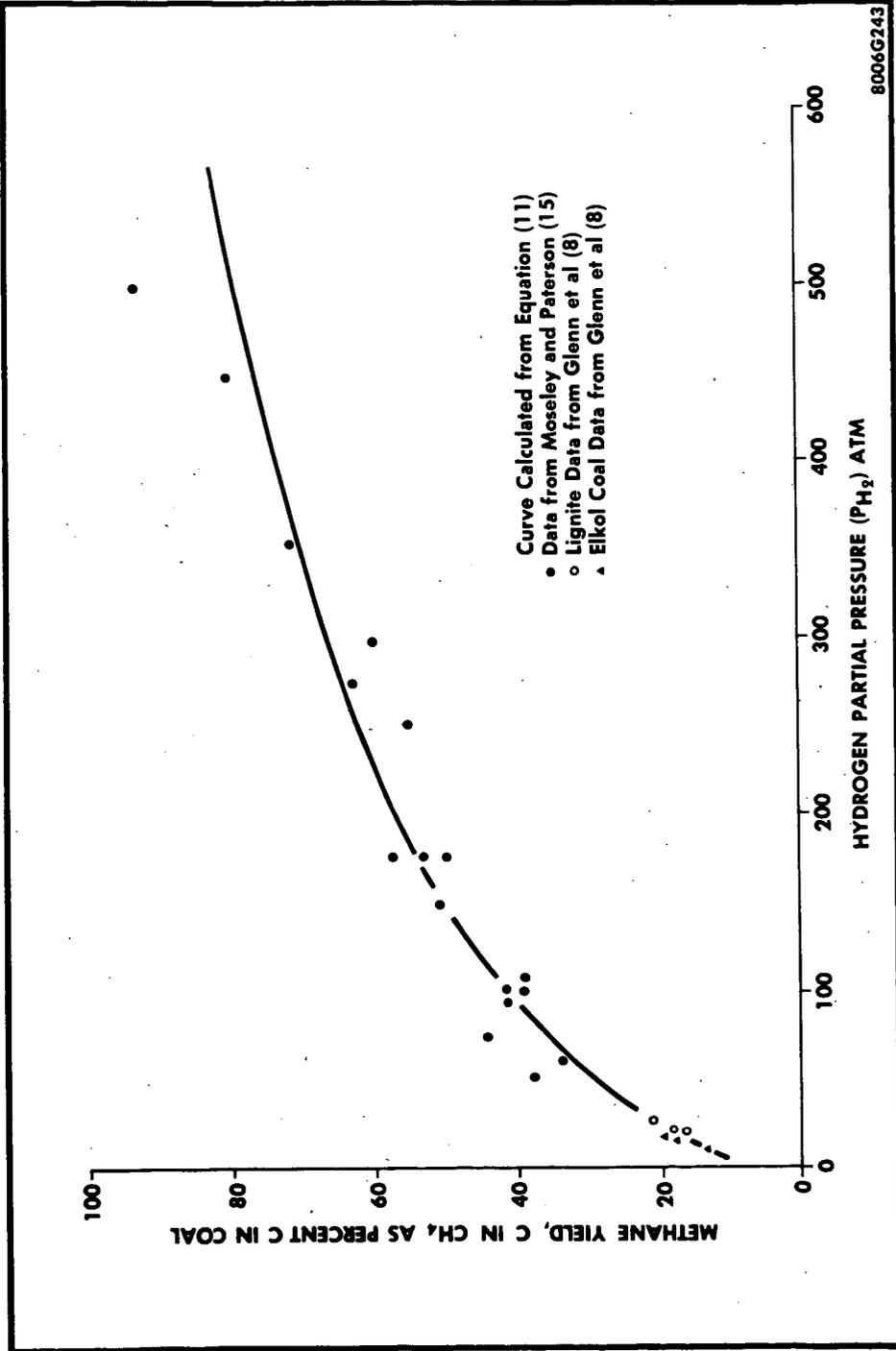


Figure 2. Correlation of Methane Yield with Hydrogen Partial Pressure at 950° C

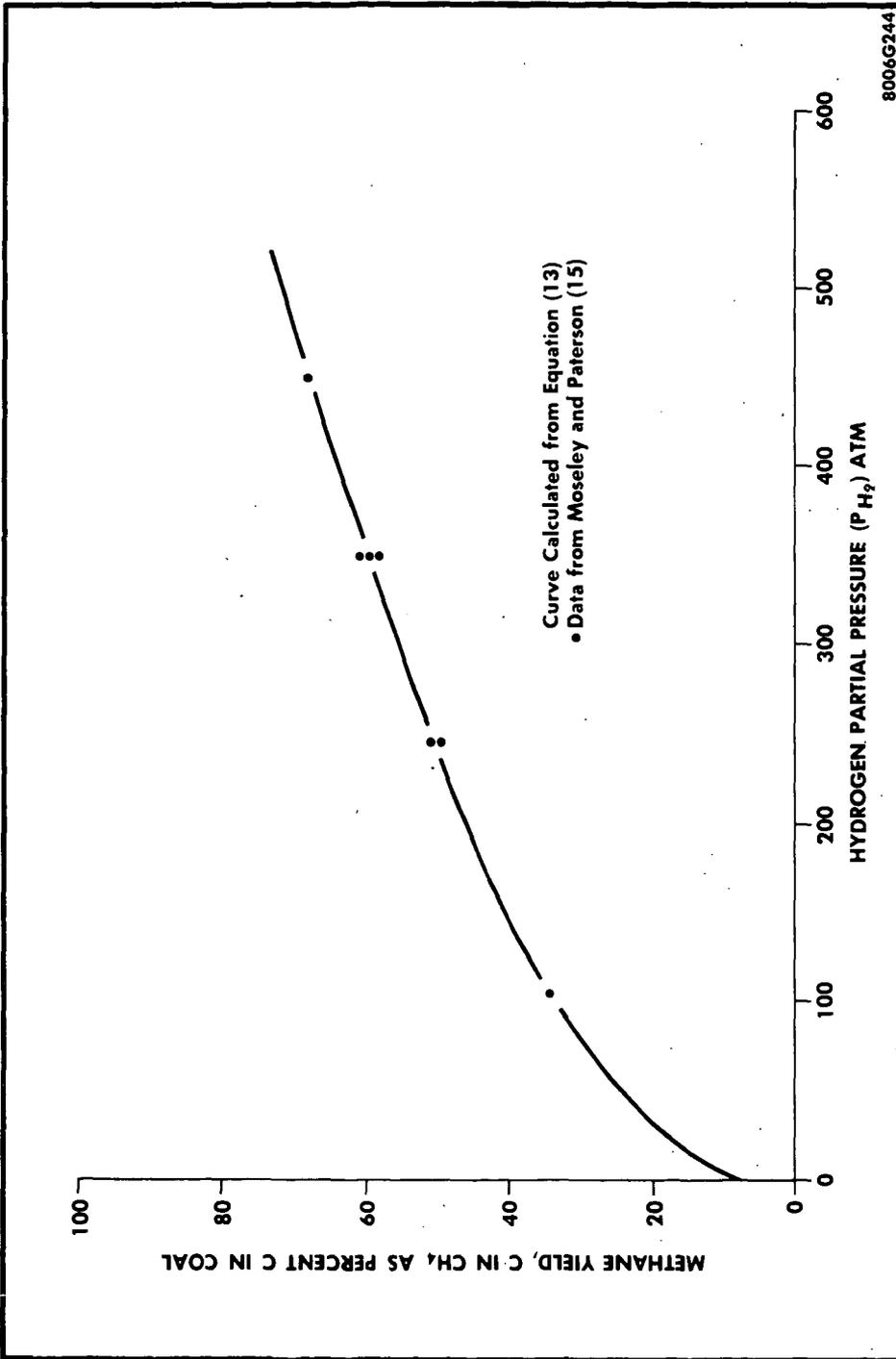


Figure 3. Correlation of Methane Yield with Hydrogen Partial Pressure at 850° C

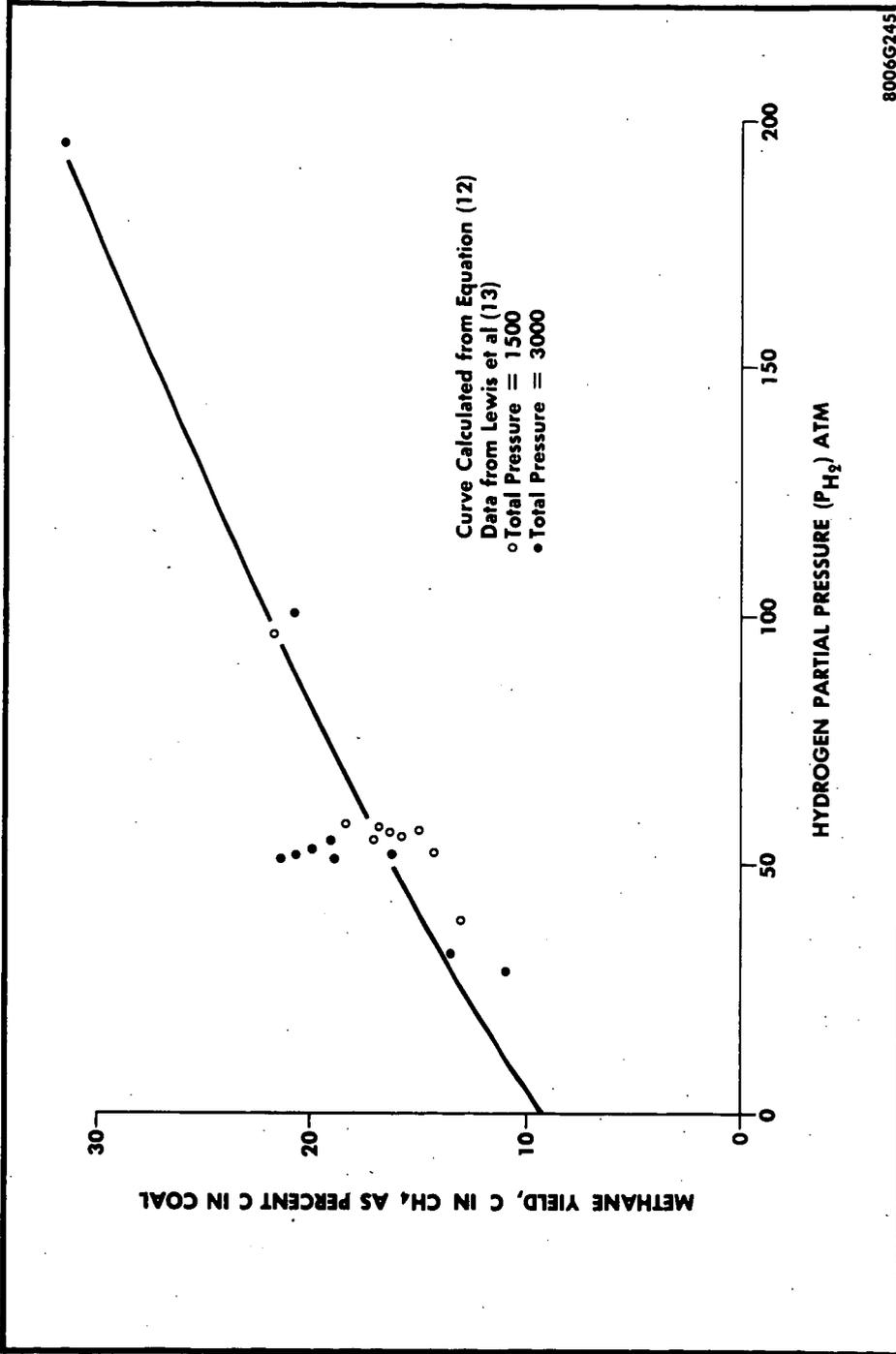


Figure 4. Correlation of Methane Yield with Hydrogen Partial Pressure at 725° C

All of these correlations indicate that methane yield values of one are possible if high enough hydrogen partial pressures are used. Furthermore, it is interesting that an Arrhenius plot of the parameter b_2 (or b_3) gives a reasonably straight line. (See Figure 5.) Since b_2 represents the ratio of k_1 to k_2 , one would expect such a fit, and the observed activation energy of 15 Kcal indicates the difference in activation energy between the methanation and the deactivation processes.

The expression for methane yield, as represented by Equation 8, provides a framework for unifying and correlating data on the direct methanation of coal with hydrogen. The fact that the behavior of a variety of coals is consistent with this expression lends support to the hypothesis of the formation of an active intermediate. The fact that the postulated ratio of rate constants for the reactions involving this active intermediate exhibits an Arrhenius behavior further supports this claim and indicates the general validity of the derivation.

It should be pointed out, however, that the rate expressions used to obtain Equation 8 are by no means unique. The unique concept in the analysis is the treatment of the methanation and deactivation steps as being competitive reactions which essentially consume the entire supply of active intermediate in a finite time. For example, if both reactions are assumed to be zero-order with respect to the active intermediate, or if the intermediate concentration at the reaction sites is assumed to be a constant, the equation for the rate of change of W^* would be as follows:

$$\frac{dW^*}{dt} = -\hat{k}_1(P_{H_2}) - \hat{k}_2 \quad (14)$$

where \hat{k}_1 and \hat{k}_2 are the rate constants associated with the methane formation and deactivation reactions, now considered zero-order with respect to intermediate concentration.

Integration of Equation 9 in the same manner as before, defines the time to consume the intermediate entirely, t^* , to be in this case

$$t^* = \frac{1}{\hat{k}_2} \frac{W_0^*}{1 + \hat{S}}$$

where $\hat{S} = \frac{\hat{k}_1(P_{H_2})}{\hat{k}_2}$ = selectivity for zero-order assumption.

The methane yield under this condition, ΔW_C , is given as follows

$$\Delta W_C = \Delta W_I + \hat{k}_1 P_{H_2} t^* = \Delta W_I + \frac{f(1 - \Delta W_I) \frac{\hat{k}_1(P_{H_2})}{\hat{k}_2}}{1 + \frac{\hat{k}_1(P_{H_2})}{\hat{k}_2}} \quad (15)$$

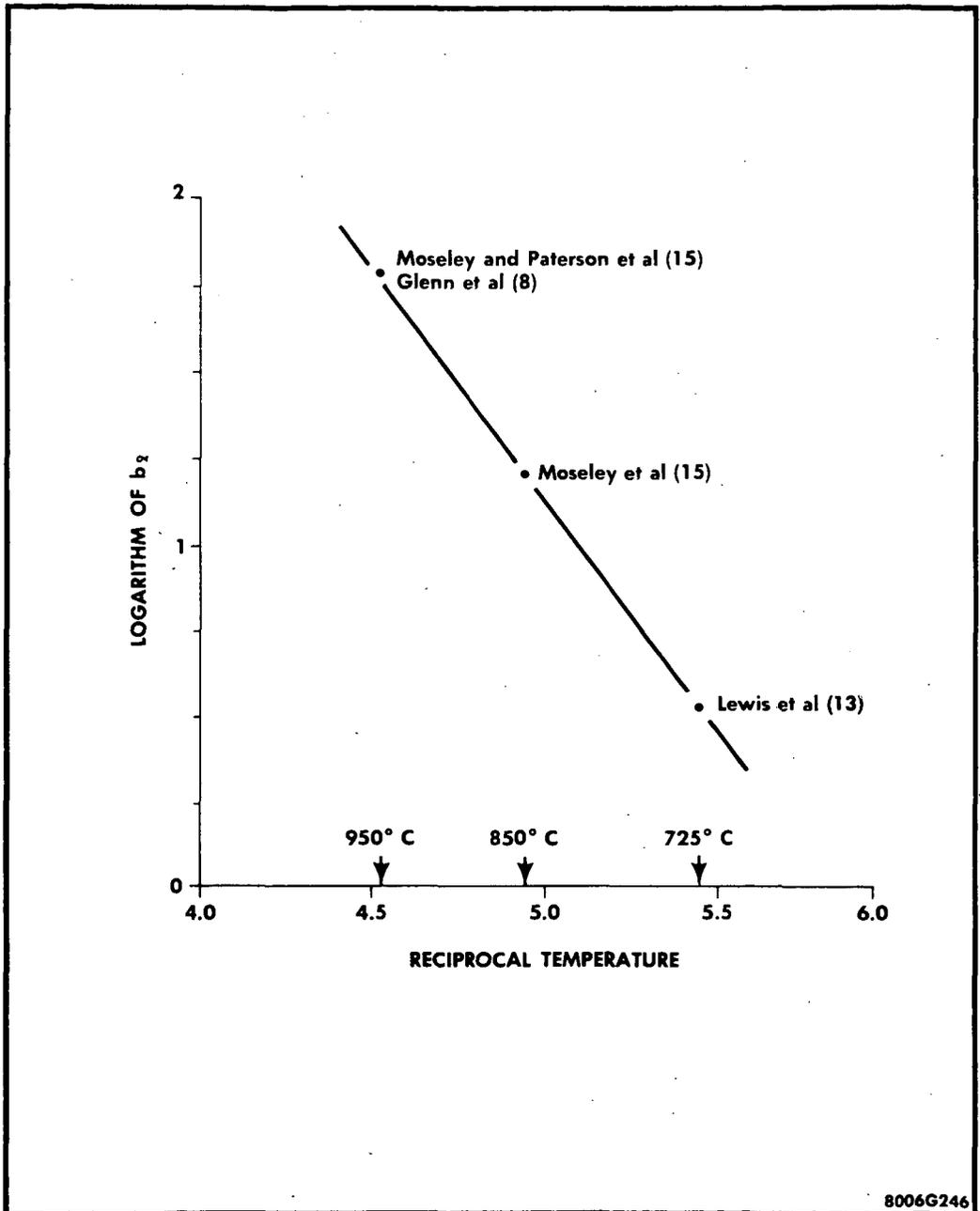


Figure 5. Arrhenius Plot of Parameter b_2

Equation 15 is identical in form to Equation 8 and indicates that there are a number of ways of obtaining the expression which correlates methane yield with hydrogen partial pressure. Thus, even though Equation 8 successfully fits the available data, the nature of the exact mechanism of the reactions involving the active intermediate is still unresolved.

This does not detract from the utility or significance of the yield expression, however. The important point is that the rapid rate of methanation of coal, observed by Moseley and Paterson (16) at high hydrogen partial pressures, has also been shown to be achieved at lower hydrogen partial pressures and in the presence of other gaseous species. Moreover, both conditions are explained by a single equation. The implication, then, is that synthesis gas and steam can be effectively used in a short-contact-time reactor to take advantage of the high activity imparted to coal by rapid heating in the presence of hydrogen. This feature, of course, is the essence of the BCR two-stage super-pressure gasifier.

The specific equations for methane yield, because of their simplicity and independence of most gasifier parameters, can be utilized in the design and engineering evaluation of integrated, multistage gasifiers. This is being done for the BCR two-stage gasifier in order to make better predictions of its ultimate capability as well as to assess effects of process variables and novel operating practices.

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NOMENCLATURE

A*	area associated with active intermediate, cm^2
A, B, C	empirical constants in devolatilization yield equation
b_1, b_2, b_3	empirical constants in methane yield correlation equation
C**	active intermediate
C*	inactive char
k_1^1, k_1, k_2	kinetic parameters in methanation reactions
P_{H_2}	partial pressure of hydrogen, atm
Q	constant in devolatilization equation representing the ratio of unit change in coal weight per unit change in volatile matter content
S	reaction selectivity
T	reactor temperature, $^{\circ}\text{K}$
t	time of reaction, sec
t*	time required to deplete active intermediate, sec
τ	residence time of coal particles in reactor, sec
VM	volatile matter in coal, daf basis, percent
W*	weight of active intermediate per gram of carbon fed at any time
W_0^*	weight of active intermediate per gram of carbon fed at time zero
ΔW_I	weight of carbon lost by initial devolatilization per gram of carbon fed
W_C	total weight of carbon appearing as methane at any time per gram of carbon fed